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Quantum Gravity corrections to Quantum Field Theory: Born-Oppenheimer approach to the canonical formalism

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Giulia Maniccia
ID number 1680009

Advisor
Prof. Giovanni Montani

Scientific Board Advisor
Prof. Paolo Pani

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Prof. Salvatore Capozziello (chairman)
Prof. Alfredo Urbano (Internal Examiner)
Prof. Flavio Mercati (External Referee)

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Author's email: giulia.maniccia@uniroma1.it
manicciagiulia@gmail.com

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Abstract

The role of time is intrinsically different between Quantum Mechanics and General Relativity: while the former associates time with an external observer, the latter unifies time and space, making them indistinguishable in a covariant framework. The absence of a clear time variable in GR stems from its symmetry and parametrized nature, resulting in the so-called frozen formalism. For this reason, the search for a theory of Quantum Gravity must face the challenge of time absence in the Wheeler-de Witt equation. Efforts to quantize gravity have led to various approaches to define time, categorized into pre-quantization, post-quantization, and timeless proposals. This thesis focuses on post-quantization time constructions, particularly within the Wentzel-Kramers-Brillouin approach, which perturbatively expands the wave function to derive dynamical equations. Previous attempts have shown that the introduction of an internal clock from gravitational variables yields non-unitary dynamical effects on the matter sector at the next order.

This thesis implements a Born-Oppenheimer-like scheme that separates the matter and gravitational sectors, leveraging their distinct energy scales: the matter's faster evolution is contrasted with the slower gravitational field, both properly quantum. Two novel time constructions are proposed, making use of a fast component derived from introducing the kinematical action or (reparametrized) Gaussian frame fixing respectively; the discussion of their geometrical and physical meaning proves that both are essentially tied to the concept of a reference system. These clocks for the matter subsystem overcome previous non-unitarity concerns, resulting in an Hermitian dynamics at the first order where quantum-gravitational corrections emerge. A direct equivalence between the two implementations is proved in the homogeneous minisuperspace setting.

The present investigation also faces the challenge posed by the dependence of the matter wave functional on intrinsically quantum gravitational components, particularly evident in the cosmological context. To address this, a more rigorous Born-Oppenheimer separation of dynamics is proposed, distinguishing the classical gravitational background from its small quantum fluctuations (i.e. gravitons) and then proper quantum matter contributions. By introducing an appropriate gauge choice for the gravitons' sector, the zero-th order of this model allows to recover the standard Quantum Field Theory dynamics. We show how this refined scheme can be combined with the concept of a reference fluid time (or equivalently the kinematical action one), offering a unitary evolution for the quantum matter subsystem with quantum gravity corrections, free of previously mentioned concerns. Such unified approach clarifies the quantum nature of gravitational components and shows how gauge requirements address the emergence of quantum gravity effects in subsequent orders of the expansion.

The central achievement of the present thesis is the development of a suitable Born-Oppenheimer scheme for the quantum gravity-matter system, in which the matter's evolution modified by quantum gravitational effects has a unitary character. This framework offers insights into how quantum gravity influences our understanding of the universe and contributes to a deeper comprehension of gravitational phenomena.

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Introduction

The following PhD thesis faces the frozen formalism in Quantum Gravity and Cosmology, discussing and developing different techniques to recover a dynamical description at the Quantum Field Theory (QFT) level and compute small corrections due to the quantum nature of the gravitational interaction, which could play a role in early cosmological settings. This “Chapter 0” serves as an introduction to the context necessary for understanding the development of Quantum Physics and the search for a quantum gravitational theory. Here, we present the core concepts that will thread through the following chapters, inviting the reader to reflect on some posed questions, which are at the basis of our investigation.

The most immediate contrast between Quantum Mechanics (QM) and General Relativity (GR) is the role of the time parameter, which results to be intrinsically different. For QM, time is associated to an external (essentially classical) observer which describes the changes inside a certain system and assigns labels to each snapshot. On the other hand, in GR time and the physical space are deeply tied together in a unified formalism, and one cannot in principle distinguish between moving in a certain direction (such as up or down) and forward/backwards in time. The “lack of time” in GR is essentially just a consequence of its symmetry: it is a parametrized theory, whose action is invariant under coordinate transformations (including time). This is the key property at the base of the Principle of General Covariance. Therefore, one of the biggest ambitions of today’s physics is the development of a theory that combines GR and QM into Quantum Gravity (QG) and how this theory would reconnect with classical aspects.

When attempting a quantization of the gravitational interaction, one faces many technical and interpretative challenges.

At the quantum level, the classical Einstein equations are replaced by the Wheeler-de Witt (WdW) equation. In this formulation the Hamiltonian of gravity is a combination of constraints known as superHamiltonian and supermomentum ones. In this view, the quantum wave function of the Universe depends on a “3-geometry” reflecting the equivalence class of metrics under 3-diffeomorphisms, regardless of the specific metric tensor coordinates. Thus the WDW equation stands out for its absence of a time variable. This peculiarity mirrors the classical Hamilton-Jacobi formulation of GR, which has no clock for the observable Universe, therefore inviting a quantum interpretation of cosmic evolution. Indeed, it has been shown in literature that the WDW equation can be recast as a quantum Schrödinger-like one with suitable time constructions.

The approaches developed to define a clock can be cast into three main categories: i) times introduced *before the quantization scheme*, usually recovering the reduced phase space picture, ii) times *after quantization* based on approximate methods, or iii) *timeless proposals* describing the system evolution via the evolving relation between observables. The present thesis focuses on the second path, implementing the Wentzel-Kramers-Brillouin (WKB) approach: a perturbative expansion of the system's wave function in a chosen parameter that allows, by looking at increasing orders, to obtain dynamical (approximate) equations starting from the initial constraint. Such path is particularly promising for the study of quantum-gravity-induced effects on the standard QFT dynamics, since it is naturally valid in a perturbative low-energy setting of the matter content and allows for phenomenological investigations.

The first proposal to overcome the frozen formalism via a WKB scheme identified a small quantum subsystem from the quasi-classical (gravitational) background; a relational clock was there introduced from the gravitational variables themselves, recovering both a meaningful dynamics at the QFT order and the probabilistic interpretation for the Universe wave function. However, an interesting question is to delve deeper and explore whether such expansion can infer quantum gravitational corrections to the matter dynamics that are not described by QFT. This point was addressed through a WKB expansion in a different (Planckian) parameter developed to the next order, where such QG effects have to arise. The main shortcoming was the emergence of a non-unitary modified evolution (i.e. non-Hermitian operators enter the dynamics), leaving its physical interpretation not consistent. In this respect, possible solutions to the problem of time in QG represent a crucial tool of investigation in the cosmological framework: indeed, limiting our attention to the first two orders of WKB approximation, the procedure gives meaningful insights on the primordial Universe evolution.

A later Born-Oppenheimer (B-O)-like WKB reformulation of the problem juxtaposed the "fast" matter contribution with the slower gravitational sector, the latter experiencing an averaged backreaction. However, this scheme was unable to provide a consistent definition of the Hilbert space for the system dynamics, not fully solving in this sense the non-unitarity problem. Actually, it was shown that a specific condition must be identified to recover the standard QFT dynamics and at the same time preserve the desired algebraic structure.

A variation of the problem adopts the de Broglie-Bohm (dBB) interpretation, eliminating the need for an external observer. Here classical trajectories are adjusted for quantum corrections via a "quantum potential" derived from the system's wave functional in the Hamilton-Jacobi equation. This paradigm offers insights into the emergence of bounces in the universe evolution and addresses fundamental questions on the ontology and measurement process.

It is important to remark that in the mentioned WKB approaches the time parameter was always defined via the dependence of the matter subsystem on the "slow" gravitational variables. Such feature suggests to look for a possible implementation based on a different, "fast" matter time.

The present thesis focuses on a WKB perturbative treatment of the WDW equation for gravity and matter, defining a time after the total constraint is fully quantized. We develop a B-O-like scheme based on the observation that the typical energy scale of the gravitational sector (of Planckian size) is clearly separated from the corresponding values of matter fields. This situation is analogous to the dynamics in molecular physics, where the (light) electrons orbit around the slow heavy nuclei. In the same way, we consider the matter content to develop at a faster scale than the gravitational field, having quantized all degrees of freedom. Differently from previous approaches, we make use of the difference in scales to derive "adiabatic" conditions on the wave functionals: they quantify the fast matter evolution through its small dependence on the gravitational variables (which are almost fixed, as the heavy atoms).

In this scheme, we propose two novel constructions of a time coordinate from the fast matter component. The first one is based on the so-called kinematical action, which can be formulated as an additional constraint recovering the geometrical meaning of the space-time foliation; in the second one, the reparametrized choice of a Gaussian reference frame "materializes" as a fluid in the theory, so giving a candidate for the time parameter.

These two formulations allow to define suitable clocks for the matter subsystem. Indeed, when the kinematical action or Gaussian fluid terms are regarded as fast contributions at the same level of the matter content, they emerge in the Hamiltonian formalism via terms that are parabolic in their conjugate momenta. Thus, these additional terms to the system's constraints provide an escape from the frozen formalism, effectively acting as a clock for the matter component living on a quantized gravitational background. The main outcome of such proposals, when WKB expanded, is that a unitary Schrödinger functional equation emerges also at the next order, where one finds QG-induced effects on the matter dynamics. Thus, the kinematical action or reference fluid are both related to the core concept of a reference frame and provide a physical clock for the matter subsystem, overcoming the unitarity concerns of previous proposals. Actually, we prove a direct correspondence between the two procedures in homogeneous minisuperspace settings. We examine a cosmological implementation of such analysis, de facto valid for both time constructions, showing the consistency of the procedure.

A delicate question can be outlined from this investigation, that is the dependence of the matter wave functional on an intrinsically quantum gravitational component, which corresponds in the application to the cosmic scale factor of the isotropic Universe. This feature, absent in previous cosmological applications of WKB schemes, must indeed be addressed for phenomenological studies if one wishes to take into account the quantum nature of the gravitational sector. We therefore illustrate a model based on an extended B-O separation of the dynamics: we consider a classical gravitational background, small "slow" gravitational fluctuations, and a "fast" quantum matter contribution. By other words, we characterize the quantum gravitational sector made up of additional (independent) degrees of freedom, corresponding to tensor fluctuations. Clearly, such an approach requires an averaging procedure to remove the dependence of the matter field on the arbitrary fluctuations, in the spirit of an effective field theory. We first show that, if one wishes to preserve the WKB time as the dependence on the (now completely classical) gravitational background, an appropriate gauge choice allows to recover the standard QFT dynamics at the zero-th order. Such requirement consists of a specific rescaling of both the gravitational and matter wave functionals, by a phase dependent on the background quantities (that is exactly the geometric phase of the B-O separation). However the next-order predictions of such model would give, with this time definition, the same non-unitarity contributions of the previous WKB proposals.

For this reason, we later merge this refined B-O scheme with the proposal of the reference fluid clock (analogous to the kinematical action one in the minisuperspace). The model is still WKB expanded in a single Planckian parameter, but we develop the analysis up to the first order of QG effects. The unitary modified dynamics exactly matches, after the averaging procedure, the one obtained using only the Gaussian fluid time without considering the gravitons degrees of freedom. The only requirement for this result is to modify the gauge-fixing condition of the arbitrary graviton fluctuations, which is no more the WDW gravitational constraint. Therefore the treatment of the gravity-matter quantized system in an extended B-O picture is consistent with the physical Gaussian fluid clock which describes a unitary evolution.

The overall result of this thesis is to provide a clearer physical picture of the reconstruction of QFT in the presence of graviton corrections in the B-O approximation: at the next order of WKB expansion, the time evolution of the matter sector is amended for quantum-gravitational effects, but still regains a unitary formulation with a suitable reference clock. More so, the gravitational component is fully characterized in its quantum nature by assigning different variables and properties to the classical part and the small fluctuations. The two procedures are unified in a clear formulation, showing that the gauge freedom allows to recover, at the next order, the same QG effects that one would find without such B-O extension.

The resulting unitary dynamics emerging from this expanded model represents the starting point to investigate how QG can affect (in the appropriate WKB limit) the evolution of the matter content in our Universe. Through the investigation of such small corrections, we are able to expand our knowledge closer to a fuller understanding of QG.

The thesis is structured as follows. In Chapter 1, we review the Hamiltonian formalism of gravity through its covariant ADM formulation, showing that it is a constrained theory. In Chapter 2, we introduce its canonical quantization and discuss the frozen formalism, together with previous proposals to overcome it via the WKB expansion and their main concerns. From the third Chapter onward, the original content of the thesis begins. In Chapter 3, we first unify the previous WKB approaches which draw non-unitarity; then we construct a B-O-like model that predicts a unitary evolution with QG corrections using the kinematical action as a time. In Chapter 4, we develop an analogous model constructing the physical clock via the (reparametrized) Gaussian reference frame fixing in the B-O picture, still describing a unitary evolution amended for QG effects. Chapter 5 is dedicated to the predictions of such model in cosmology: we compute how these QG corrections modify the early evolution of our Universe, with particular focus on the inflationary spectrum of primordial perturbations. In Chapter 6, we develop the B-O-extended procedure to take into account the quantum nature of the gravitational sector, making use of the related gauge symmetry to properly recover the QFT limit. We first apply this reformulation to previous WKB time constructions at the zero-th order and then unify the B-O extension with the Gaussian fluid time proposal, demonstrating in the latter case that the next-order dynamics with QG corrections is obtained after an average procedure and is indeed unitary. We apply this extended formulation to calculate the deviation from the standard scale-invariant primordial power spectrum in the exact de Sitter phase. Finally, in Chapter 7 we propose an alternative view of the quantum gravity-matter evolution in the Bohmian picture, finding that the modified trajectory causes a mode-dependent deformation of the primordial power spectrum associated to inflaton perturbations in a de Sitter phase of the universe.

The core results of this thesis are contained in the following papers, published or in preparation, which will also be referenced during the text:

- F. Di Gioia, G. Maniccia, G. Montani, and J. Niedda (2021). *Nonunitarity problem in quantum gravity corrections to quantum field theory with Born-Oppenheimer approximation.* Phys. Rev. D 103, p. 103 511. DOI: `10.1103/PhysRevD.103.103511`.

- G. Maniccia and G. Montani (2022). *Quantum gravity corrections to the matter dynamics in the presence of a reference fluid.* Phys. Rev. D 105, p. 086 014. DOI: `10.1103/PhysRevD.105.086014`.

- G. Maniccia, M. De Angelis, and G. Montani (2022). *WKB approaches to restore time in quantum cosmology: Predictions and shortcomings.* Universe 8, 11, p. 556. DOI: `10.3390/universe8110556`.

- G. Maniccia and G. Montani (2023) *WKB approach to the gravity-matter dynamics: A cosmological implementation.* In The Sixteenth Marcel Grossmann Meeting, World Scientific. DOI: `10.1142/9789811269776_0345`.

- G. Maniccia, G. Montani, and L. Torcellini (2023). *Study of the inflationary spectrum in the presence of quantum gravity corrections.* Universe 9, 4, p. 169. DOI: `10.3390/universe9040169`.

- G. Maniccia, G. Montani, and S. Antonini (2023). *QFT in curved spacetime from quantum gravity: Proper WKB decomposition of the gravitational component.* Phys. Rev. D 107, L061901. DOI: `10.1103/PhysRevD.107.l061901`.

- G. Maniccia, G, Montani, M. Tosoni (2024). *Modified minisuperspace dynamics from a Kuchař-Torre clock with graviton fluctuations.* To be submitted to Physical Review D.

- G. Maniccia, G. Montani (2024). *Quantum Gravity Corrections to the inflationary spectrum in a Bohmian approach.* To be submitted to Symmetry.

- G. Maniccia, P. Peter (2024). *Trajectory approach in cosmology with a Kuchař-Torre fluid.* In preparation.

Notations, conventions and acronyms

In this thesis we will use the following notation (unless differently specified n specific points):

Spacetime metric signature	$(- + + +)$
Four-dimensional indices	$\mu, \nu, \rho, \sigma \ldots = 0, 1, 2, 3$
Three-dimensional (spatial) indices	$i, j, k, l \ldots = 1, 2, 3$
Partial derivatives	$\frac{\partial}{\partial x^\mu} f \equiv \partial_\mu f$
Covariant derivatives	$\nabla_{\partial/\partial x^\mu} f \equiv \nabla_\mu f$
Functional derivatives	$\frac{\delta}{\delta A(x)} f \equiv \delta_{A(x)} f$
Vectors	$\mathbf{V}$ with components V^i or V^μ
Tensors	$A^{\nu_1 \nu_2 \ldots \nu_n}_{\mu_1 \mu_2 \ldots \mu_m}$
Poisson brackets (N-dimensional system $k = 1, 2, \ldots N$)	$\{f, g\}_{q,p} = \frac{\partial f}{\partial q^k} \frac{\partial g}{\partial p_k} - \frac{\partial f}{\partial p_k} \frac{\partial g}{\partial q^k}$
Commutator brackets	$[A, B] = A\,B - B\,A$
Lagrangian, Hamiltonian density	$\mathcal{L}, \mathcal{H}$
Lagrangian, Hamiltonian function	L, H
ADM Super-Hamiltonian	$H(h^{ij}, \Pi_{ij}, \phi_n)$
ADM Super-momentum	$H_i(h^{ij}, \Pi_{ij}, \phi_n)$

Table 0.1. Notation and conventions used in the thesis.

We will follow the Einstein convention for summation over repeated indices, and use in many calculations natural units $c = 1$. A number of short-hand acronyms will be used, listed below:

Acronym	Meaning
GR	General Relativity
QFT	Quantum Field Theory
QG	Quantum Gravity
CQG	Canonical Quantum Gravity
QC	Quantum Cosmology
ΛCDM	Λ-Cold-Dark-Matter
BO	Born-Oppenheimer
ADM	Arnowitt-Deser-Misner
WKB	Wentzel-Kramers-Brillouin
FLRW	Friedmann-Lemaitre-Robertson-Walker
dBB	de Broglie-Bohm

Table 0.2. List of acronyms used in the text.

Chapter 1

Hamiltonian formulation of gravity

This chapter is devoted to the description of geometrodynamics, i.e. the dynamical representation of the gravitational theory. As in Classical Field Theory, this requires to provide two elements both the set of equations governing the dynamics and an initial configuration for the system. The Hamiltonian formulation of gravity, which is based on the Arnowitt-Deser-Misner (ADM) decomposition, provides a suitable framework for this purpose. A remarkable advantage of such formalism, based on a spacetime foliation into hypersurfaces, is its ability to still preserve covariance, despite its apparent departure from the standard tensorial approach of GR. It will also be the fundamental building block for the quantization process, as we will see in the next chapter. We here introduce the basic concepts for the ADM and Hamiltonian formulation of gravity.

1.1 The historical success of General Relativity

Albert Einstein's General Theory of Relativity (GR), formulated in 1915, has stood the test of time and continues to be one of the most successful and influential theories in the history of physics. The core of the theory stands in the Einstein's equations:

$$\mathscr{G}_{\mu\nu} + \Lambda g_{\mu\nu} = \frac{8\pi G}{c^4} T_{\mu\nu} \,, \tag{1.1}$$

which are a set of ten tensorial equations (due to symmetry properties) involving two main objects. $\mathscr{G}_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R$ is the Einstein tensor describing the spacetime curvature, while $T_{\mu\nu}$ is the stress-energy tensor of the matter content within that same spacetime. We also take into account the presence of a cosmological constant, acting as a "dark energy" source (this aspect will be cleared in Chapter 5) in the gravitational sector; on the right-hand side, $G \simeq 6.674 \cdot 10^{-11}\,\mathrm{N\,m^2\,kg^{-2}}$ is Newton's gravitational constant and $c \simeq 2.998 \cdot 10^{8}\,\mathrm{m\,s^{-1}}$ is the speed of light. The curvature terms in $\mathscr{G}_{\mu\nu}$, and so all the left-hand side of (1.1), depend on the tensor field $g_{\mu\nu}$, which is the spacetime metric of a manifold $\mathcal{M}$ describing its geometry i.e. how such manifold "curves". Essentially, the law (1.1) relates (locally) the geometry of spacetime to the distribution of matter within it.

The most basic principle on which GR is based is the Principle of General Covariance:

> Physical laws must be invariant in form under an arbitrary differential transformation of coordinates., i.e. they must be the same in any frame (inertial or accelerating).

While there are many restatements of this principle, the core idea can be summarized in the following: we tend to describe and label events using coordinates, however coordinates themselves do not exist *a priori* in nature, hence they should play no role in the formulation of fundamental physical laws. Those laws must keep the same form under any (differentiable) change of coordinates. The answer to this puzzle stands in the tensor formulation (1.1) of GR, which allows for a coordinate-independent formulation of physical laws. Indeed, if we are able to write tensorial equations of motion, then the transformation laws of such elements will assure the form of those equations to be preserved: this is the case of (1.1), where both the right-hand and left-hand sides transform as tensors.

By this principle, an equation holds in a general gravitational field if both following conditions are satisfied [1]:

1) it holds in the absence of gravitation, that is the Special Relativity case (the metric tensor $g_{\mu\nu}$ is nothing else than the Minkowski tensor $(-1, +1, +1, +1)$;

2) it is covariant under a general coordinate transformation $x \to x'$.

We remark that the term "covariance" generally indicates that the physical laws maintain the same form under a specified group of transformations. Specifying such group gives different level of the covariance (or equivalence) requirement. Indeed, the group of Galilean coordinate transformations identifies laws of Classical Mechanics, while Lorentz coordinate transformations correspond to the Special Relativity case. General Covariance takes its name from the group of arbitrary differentiable coordinate transformations, and it is in this sense the most general formulation of the Equivalence Principle.

The successes of GR extend across a wide range of astronomical, astrophysical, and cosmological phenomena, yielding insights and predictions that have been consistently verified through empirical observation. Noteworthy examples include the confirmation of gravitational lensing (with Sir Arthur Eddington's landmark experiment during the 1919 solar eclipse, where the deflection of starlight near the sun was measured), the time dilation effect (with the precision tests involving atomic clocks on orbiting satellites), the emission and detection of Gravitational Waves (with the groundbreaking achievement of LIGO and VIRGO in 2015 [2]), the synchronization of satellite clocks for the GPS systems, and the measure of gravitational redshift via observations of light from distant astronomical objects.

The original formulation of GR, based on the field equations (1.1), emerged as a generalization of Poisson's equation for Newtonian gravity; the relation between geometry and matter is expressed via tensor equations, but no other fundamental objects are defined. Following from its successes, many years of scientific production were dedicated to a recast of GR into more abstract frameworks, i.e. those used in Classical and Quantum Field Theory. The Lagrangian formulation was developed by David Hilbert and others in 1915-1916 and came as an alternative representation of the theory in the Lagrangian language; it describes the dynamics via the action principle in terms of the spacetime metric and its derivatives, therefore it is particularly useful in the context of variational principles and quantum field theory. The Hamiltonian formulation, which is closely related to the Lagrangian one, also emerged later from the works of Arnowitt, Deser and Misner [3] as another way to express the theory in a canonical context; it is based on the metric and its conjugate momenta and addresses in a clearer way the constraints arising from diffeomorphism invariance. Indeed, gravity is a constrained theory, a property following from the requirement of General Covariance. This feature has important repercussions at the dynamical level, most of all leading to the so-called *frozen formalism*, as we will discuss in the next chapter.

Before delving into the Lagrangian and Hamiltonian formulation of gravity, it is useful to remark some aspects of the general theory of constrained systems. We will also introduce some concepts on geometry, curvature and foliations on manifolds, which are contained in the following sections.

1.2 Preliminaries on Lagrangian and Hamiltonian formulations

In Classical Mechanics, one can identify trajectories solving the motion by the variational principle, or principle of least action, stating that the path followed by a physical system is the one which minimizes the action functional. More specifically, in Maupertuis's version [4], one should minimize the action integral

$$\tilde{\mathrm{S}}[\mathbf{q}(t)] := \int \mathbf{p} \cdot d\mathbf{q} \tag{1.2}$$

over the generalized coordinates $\mathbf{q} = (q_1, q_2, \dots q_N)$, requiring conservation of energy ; equivalently, in Hamilton's version the action

$$\mathrm{S}[\mathbf{q}(t)] = \int_{t_1}^{t_2} \mathrm{L}(q^k, \dot{q}^k, t)\, dt \tag{1.3}$$

is the time integral of the Lagrangian $\mathrm{L}(q^k, \dot{q}^k, t)$ of the system (being q^k generalized configuration coordinates) and it is varied between two fixed endtimes t_1, t_2 and endpoints q_1, q_2 such that $\delta q^k(t_1) = \delta q^k(t_2) = 0$. In both cases, the action is a functional S : function space $\rightarrow \mathbb{R}$, i.e. it returns a value when a function is given as an input. We here focus on Hamilton's formulation of the variational principle for clarity.

It is well known that the stationarity condition $\delta S = 0$ of $S[\mathbf{q}(t)]$ is a necessary and sufficient condition to obtain the equations of motion for an N-dimensional physical system (with coordinates q^i, $i = 1, 2, \dots N$), i.e. the Euler-Lagrange equations

$$\frac{\partial \mathrm{L}}{\partial q^k} - \frac{d}{dt}\frac{\partial \mathrm{L}}{\partial \dot{q}^k} = 0\,. \tag{1.4}$$

One can here understand why the Lagrangian is defined up to boundary terms: such terms can arise when one derives (1.4) from (1.3) from integration by parts, but they will not affect the dynamics at all. Eqs. (1.4) represent a set of N second-order differential equations, therefore the associated Cauchy problem requires to give initial values for the coordinates and velocities. While equations of the second order present more difficulties to reach an analytical exact solution, this approach has two important features. Firstly, only the q^k are varied, i.e. the velocities $\dot{q}^k$ are not treated as independent degrees of freedom. Secondly, the Lagrangian formalism is already covariant by definition under coordinate transformations, therefore the stationarity condition of the action determines the *physical* trajectories irrespective of the coordinate system. In other words, different parametrizations in the configuration space give the same physical content of the theory, that is dictated by the Euler-Lagrange equations.

Whenever the Lagrangian does not depend explicitly on a configuration coordinate, labeled cyclical variable, one of the eqs. (1.4) turns out to be

$$\frac{d}{dt}\frac{\partial \mathrm{L}}{\partial \dot{q}^i}(q^k, \dot{q}^k, t) = 0 \to f(q^k, \dot{q}^k, t) = \text{const.} \tag{1.5}$$

The conserved quantity f is a *first integral* of motion. Such conservation can be written as a condition of the form $\mathcal{C}(q^k, \dot{q}^k, t) = 0$, which identifies a constrained system. The relation between constraints and symmetries in gauge theories will be discussed in Sec. 1.3.

The Hamiltonian formulation proposes an alternative to the Lagrangian one, which replaces the N second-order eqs. (1.4) with $2N$ differential equations of the first order. This formulation is obtained by defining the conjugate momenta (we restrict here to time-independent Lagrangians for simplicity):

$$p_i(q^k, \dot{q}^k) = \frac{\partial \mathrm{L}}{\partial \dot{q}^i}(q^k, \dot{q}^k) \tag{1.6}$$

which are N new variables to be used instead of the velocities $\dot{q}^k$. This is possible if the relation (1.6) is invertible, i.e.

$$det\left(\frac{\partial^2 \mathrm{L}}{\partial \dot{q}^i \partial \dot{q}^l}\right) = det\left(\frac{\partial p_i}{\partial \dot{q}^l}\right) \neq 0 \tag{1.7}$$

One then performs the Legendre transformation from the configuration space $(q^k, \dot{q}^k)$ to the phase space (q^k, p_k), where each pair satisfies the canonical commutation relations $\{q^i, p_j\}_{q,p} = \delta^i_j$ and $\{q^i, q_j\}_{q,p} = \{p_i, p_j\}_{q,p} = 0$ by definition[1]. In this way, one obtains the Hamiltonian as

$$\mathrm{H}(q^k, p_k) = p_k\, \dot{q}^k(q^i, p_i) - \mathrm{L}(q^k, \dot{q}^k(q^i, p_i)) \tag{1.8}$$

and the action functional (1.3) can be equivalently written as

$$\mathrm{S}[q^i, p_i] = \int_{t_1}^{t_2} dt\left(p_k\, \dot{q}^k(q^i, p_i) - \mathrm{H}(q^i, p_i)\right) . \tag{1.9}$$

[1]The symbol $\{\cdot,\cdot\}_{q,p}$ denotes the Poisson brackets of two quantities with respect to the phase-space variables q^k, p_k as defined in Table 0.1. They are proportional to the commutator brackets by the coefficient $1/i\hbar$.

The equations of motion are simply obtained via the variations $\delta_q S = 0, \delta_p S = 0$ and are referred as Hamilton's equations:

$$\dot{q}^k = \frac{\partial \mathrm{H}}{\partial p_k}\,, \quad \dot{p}_k = -\frac{\partial \mathrm{H}}{\partial q^k}\,. \tag{1.10}$$

It is useful to note that in this framework one does not have automatic covariance under coordinates changes; indeed, those would modify the evolution of the system expressed by (1.10) unless also the conjugate momenta are transformed at the same time in a compatible way. The group of time-independent transformations that preserve the Hamilton's equations (1.10) are the so-called canonical transformations $(\mathbf{q}, \mathbf{p}) \to (\mathbf{Q}, \mathbf{P})$, i.e. they transform an Hamiltonian system $\mathrm{H}(q^k, p_k)$ to a new Hamiltonian system with $\mathrm{H}'(Q^k, P_k)$. More specifically, the map describing the transformation must be such that the form $\mathbf{p}d\mathbf{q} - \mathbf{P}d\mathbf{Q}$ is an exact differential dF, which allows to write a generating function F for the transformation. An extension to time-dependent canonical transformations (and therefore time-dependent generating functions) is possible; in any case, the new Hamiltonian is related to the old one by

$$\mathrm{H}'(Q^k, P_k, t) = \mathrm{H}\left(q^k(Q^i, P^i, t), p_k(Q^i, P^i, t)\right) + \frac{\partial F}{\partial t} \tag{1.11}$$

To stress the departure from the Lagrangian case, we can consider the example of a generating function of the first type $F_1(q^k, Q^k)$[2], which express a change from the old coordinates $\mathbf{q}$ to new ones $\mathbf{Q}$, satisfying the condition $det\left(\frac{\partial^2 F_1}{\partial q^i \partial Q^j}\right) \neq 0$. This change is a canonical transformation if and only if the old and new momenta are defined as the following

$$p_k = \frac{\partial F_1}{\partial q^k}\,, \quad P_k = -\frac{\partial F_1}{\partial Q^k}\,. \tag{1.12}$$

Therefore in Hamiltonian formalism, which is not automatically covariant, we cannot perform arbitrary coordinate changes without changing the Hamiltonian structure and so dynamics of the system. Actually this is an advantage, since we are allowed to perform a more general class of transformations: indeed, the coordinate changes of the Lagrangian level are recovered in the limit $Q^k = f^k(q^i)$ i.e. requiring the new variables Q^k to be functions of the old coordinates only. The class of canonical transformation is more general and allows for "mixed" transformations which combine together coordinates and momenta. This feature is particularly useful when solving physical systems via the Hamilton-Jacobi method: by finding a suitable generating function, one obtains a new Hamiltonian system in which all new phase-space variables are constants of motion ($\mathrm{H}' = 0$) [5] or all the new coordinates are cyclic ($\mathrm{H}'(P^k)$) [6], and then traces back the solutions for the starting system.

The nature of (1.5) is clearer in the Hamiltonian formulation, since the conserved quantities correspond exactly to momenta of the system by the definition (1.6): if the Hamiltonian is independent of a variable q^k then its associated momentum p_k is conserved. We remark that the presence of a symmetry related to a first integral actually reduces by two the dimensionality of the system (1.10) from $\mathbb{R}^{2N}$ to $\mathbb{R}^{2N-2}$

[2]We do not list here the other three types of generating functions, however they can be obtained from F_1 via Legendre transformations.

(since we have both the independence from q^k and one p_k which can be trivially integrated) therefore they represent a powerful tool in this formalism. Another way to find first integrals is to look at the evolution of observables, which can be expressed via the Poisson brackets as

$$\frac{d}{dt}f(q^i, p_i, t) = \frac{\partial f(q^i, p_i, t)}{\partial t} + \{f, \mathrm{H}\}_{q,p}\,. \tag{1.13}$$

We here referred to the Lagrangian and Hamiltonian functions, however one can also work with their (spatial) density equivalents $\mathcal{L}(q, \dot{q})$ and $\mathcal{H}(q, p)$, as will be done in Sec. 1.5.

1.3 Theory of constrained systems

Gauge theories, i.e. those that present a gauge symmetry, frequently emerge in the understanding of fundamental forces and particle interactions. Gauge symmetry groups are associated to transformations caused by a change of the arbitrary reference frame which leave the system's physical variables (or *observables*) unchanged; in other words, they cause physically irrelevant ambiguities. The quantities which are not modified by these transformations are labeled as gauge-invariant. Due to the arbitrariness in the choice of reference frame, not all canonical variables of a gauge theory will be independent; when possible, it is more convenient to work with gauge-invariant quantities directly (we will see an application of this method in Chap. 5).

As elucidated by Noether's theorem [7], each invariance under a transformation group corresponds to the conservation of a physical quantity associated to the generator of that symmetry group. A simple example is a system invariant under the Lie group of 3d rotations $SO(3)$: in that case, angles will be cyclical coordinates and the three components of the angular momentum L_x, L_y, L_z (which correspond to the generators of the Lie algebra in the coordinate representation) will be associated to the Casimir invariant L^2 [8]. In other words, a system invariant under 3d rotations will conserve its angular momentum.

A direct consequence of symmetry is that gauge theories are represented by constrained Hamiltonian systems [5], of which we discuss the main points. The first observation is that condition (1.7) is not satisfied in presence of constraints, therefore we cannot invert all the velocities $\dot{q}^k$ in terms of the conjugate momenta p_k. Then, some canonical variables will be constrained by relations of the form

$$\phi_m(q^k, p_k) = 0\,, \qquad m = 1, 2, \ldots M \tag{1.14}$$

being M the number of constraints. The conditions (1.14) are referred to as *primary constraints*, since they emerge first without applying the equations of motion. Let us assume for simplicity that all Eqs. (1.14) are independent and that they define a smoothly embedded submanifold of phase space, which has dimension $2N - M$. The system will evolve on this manifold, i.e. the primary constraint hypersurface.

From the variational point of view, the constraints are guaranteed by the stationarity condition of the action if one adds M new independent variables λ^m as the following:

$$S[q^i, p_i, \lambda^m] = \int_{t_1}^{t_2} dt \left(p_k \, \dot{q}^k(q^i, p_i) - \mathrm{H}(q^i, p_i) + \lambda^m \phi_m(q^i, p_i) \right) . \tag{1.15}$$

Here the λ^m clearly act as Lagrange multipliers, enforcing the conditions (1.14). It follows from (1.15) that the equations of motion are modified as

$$\begin{aligned} \dot{q}^k &= \frac{\partial \mathrm{H}}{\partial p_k} + \lambda^m \{q^k, \phi_m\}_{q,p} \, , \\ \dot{p}_k &= -\frac{\partial \mathrm{H}}{\partial q^k} + \lambda^m \{p_k, \phi_m\}_{q,p} \, . \end{aligned} \tag{1.16}$$

The definition of the Hamiltonian itself is possible, even if some p_k cannot be written as functions of the $\dot{q}^k$, by using Lagrange multipliers to replace each non-invertible $\dot{q}^k$; this procedure gives an action functional with a well-defined Hamiltonian, i.e. function of all invertible p_k. We remark that the Hamiltonian is well-defined only on the constraints surface, i.e. up to a linear combination of such constraints:

$$\mathrm{H} \to \mathrm{H} + c^m(q^k, p_k) \, \phi_m(q^k, p_k) \tag{1.17}$$

being c^m arbitrary coefficients. The natural requirement that primary constraints are preserved by the system's evolution leads to the following conditions

$$\dot{\phi}_m = \{\phi_m, \mathrm{H}\}_{q,p} + \lambda^n \{\phi_m, \phi_n\}_{q,p} = 0 \tag{1.18}$$

being $m, n = 1, 2, \ldots M$. If the Eqs. (1.18) turn out to be independent of the λ^m, they cannot be expressed as linear combinations of the primary constraints; therefore, we have new restrictions on the system, which are labeled as *secondary constraints*: $X_m(q^k, p_k) = 0$ [3].

The classification into primary and secondary constraints is very insightful at the dynamical level and will appear in the discussion of the ADM formalism in the next section. However, an alternative formulation is possible, more linked to the gauge transformations causing the constraints in gauge theories: this the classification into first-class and second-class.

A function the phase-space variables is said to be first-class if and only if its Poisson brackets with the entire set of constraints weakly vanish:

$$\{f(q^k, p_k), \phi_m\}_{q,p} \approx 0 \quad \forall \, m = 1, 2, \ldots M \, . \tag{1.19}$$

If instead there is at least one constraint for which (1.19) does not hold, the function f is said to be second-class. It is possible to define a Hamiltonian which is first-class only, when Eqs. (1.18) act as a restriction on the Lagrange multipliers, see for example [9].

First-class constraints are postulated to generate gauge transformations, according to the so-called Dirac's conjecture [10, 5]. At the geometrical level, transformations generated by first-class constraints are tangential to the constraints

[3] Analogously, requiring the conservation of secondary constraints might also give *tertiary constraints*, and so on until no new constraints arise; we will not discuss those types in this thesis.

hypersurface, while this is not true for second-class ones. With this classification, one can count the number of true degrees of freedom of a physical system with the formula

$$N_{phys} = \frac{1}{2}\left(N_t - N_s - 2N_f\right) \tag{1.20}$$

where N_t is the total number of phase-space coordinates and N_f and N_s count the number of first- and second-class constraints respectively. We remark that first-class constraints "strike twice" since they reduce by one the number of degrees of freedom and also require observables to be gauge-invariant.

1.4 Manifolds and geometry

GR is based on a covariant formalism, with physical properties described by four-dimensional tensor objects that satisfy precise transformation laws, as we will clarify below. One describes spacetime as a four-dimensional pseudo-Riemannian manifold $\mathcal{M}_4$, whose metric $g_{\mu\nu}$ embodies the gravitational field's information: it dictates the measurement of distances between events and establishes gravity's influence on the trajectories of all objects.

We recall that a pseudo-Riemannian manifold $(\mathcal{M}_n, g)$ is a smooth manifold $\mathcal{M}_n$ of dimension n equipped with a Riemannian metric g, which is a smooth tensor field that defines a symmetric non-degenerate inner product on the tangent space $T_p(\mathcal{M}_n)$ at each point p. More specifically, given any two vectors $\mathbf{v}, \mathbf{u} \in T_p(\mathcal{M}_n)$ we can compute $g(\mathbf{v}, \mathbf{u})$ that satisfies the properties of symmetry and linearity [11]. This quantity allows us to compute distances, angles, and volumes on the manifold. It is therefore a generalization of our experience of the flat 3d Euclidean metric $diag(+1, +1, +1)$ and of the Minkowski metric of special relativity $\eta_{\mu\nu} = diag(-1, +1, +1, +1)$ the latter one casting space and time together but with zero curvature.

The spacetime metric tensor $g_{\mu\nu}$ is the fundamental field, as can be seen from the Einstein equations (1.1). As will be shown in the next section, the 3+1 formulation of gravity developed by Arnowitt, Deser and Misner [3] allows to obtain its Hamiltonian formulation in a covariant way. This formulation makes use of a foliation procedure to identify a "reduced" metric, containing a limited amount of information. In order to better understand this picture, we here remind the basics of the embedding procedure, i.e. the process of representing a lower-dimensional manifold or space within a higher-dimensional space.

Embedding From the mathematical point of view, the embedding procedure is a technique employed to study the properties of manifolds embedded in higher-dimensional ones by a map $F : \mathcal{M} \hookrightarrow \mathbb{M}$. If $\mathbb{M}$ is a Riemannian manifold, this procedure induces a new Riemannian metric on $\mathcal{M}$ [12]; it is actually a way to construct interesting Riemannian metrics starting from some other Riemannian manifold [11].

For example, it is possible to embed a 4d manifold (representing spacetime) into a a 5d flat space $\mathbb{M}_5$, see Figure 1.1. We stress that this does not apply for space-times that are solution of Einstein's vacuum equations, in which case one needs a higher dimensional space [13], but it is a useful example to illustrate how the metric and affine properties naturally emerge in such procedure. Given a differentiable 4d manifold $\mathcal{M}_4$ embedded in a Minkowskian 5d space $\mathbb{M}_5$ endowed with the natural scalar product and with signature $(-,+,+,+,+)$, one can define an adapted basis $\mathbf{b}_\mu(u)$ for $\mathcal{M}_4$, where u_μ are generic coordinates (we refer for the details to [9]).

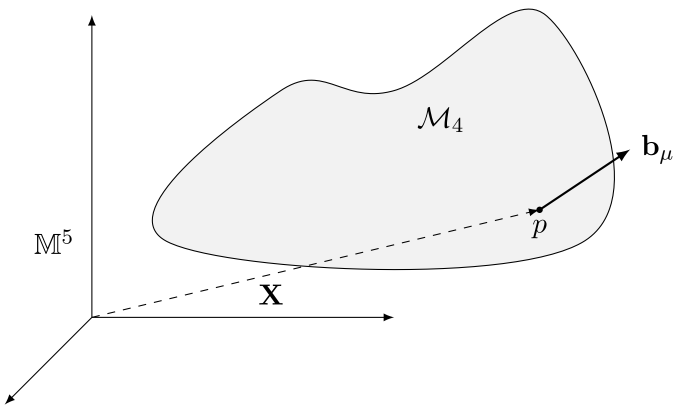

Figure 1.1. Parametric representation of the embedding of $\mathcal{M}_4$ in 5d Minkowskian space via a 5d vector $\mathbf{X}$. The vectors $\mathbf{b}_\mu$ act as a basis on the space tangent to $\mathcal{M}_4$ in the point p.

Now a vector $\mathbf{V} \in \mathcal{M}_4$ can be expressed as $\mathbf{V} = V^\mu(u)\ \mathbf{b}_\mu(u)$. Applying an invertible coordinate transformation $u^\mu \to z^\mu = z^\mu(u)$, the basis transforms as:

$$\mathbf{b}_{\mu'}(z) = \mathbf{b}_\alpha(u)\,\frac{\partial u^\alpha}{\partial z^{\mu'}} \tag{1.21}$$

that is the transformation law of *covariant* objects on $\mathcal{M}_4$, i.e. with the Jacobian matrix $\Lambda^\alpha_{\mu'}$ of the inverse transformation. The law for *contravariant* objects immediately follows by

$$\mathbf{V} = V^\alpha(u)\cdot\mathbf{b}_\alpha(u) = V^\alpha(u)\frac{\partial z^{\mu'}}{\partial u^\alpha}\ \mathbf{b}_{\mu'}(z) = V^{\mu'}(z(u))\ \mathbf{b}_{\mu'}(z(u)) \tag{1.22}$$

i.e. with the Jacobian matrix of the direct transformation.

It is a fundamental property of tensor formalism that all covariant and contravariant quantities, and so all tensor components, must transform following one of the two rules (1.21), (1.22). Scalar quantities are independent of coordinate transformations. This enforces the principle of General Covariance (Sec. 1.1): once a physical law is written in tensorial form (with all covariant and contravariant indices contracted), the respective components will balance out and its form will be preserved under coordinate transformations.

The action of the ordinary derivative on a vector

$$\frac{\partial V_\alpha(u)}{\partial u^\rho} = \frac{\partial z^{\mu'}}{\partial u^\rho}\frac{\partial}{\partial z^{\mu'}}\Big(V_{\nu'}(z)\frac{\partial z^{\nu'}}{\partial u^\alpha}\Big) = \frac{\partial z^{\mu'}}{\partial u^\rho}\frac{\partial z^{\nu'}}{\partial u^\alpha}\frac{\partial V_{\nu'}(z)}{\partial z^{\mu'}} + V_{\nu'}(z)\frac{\partial^2 z^{\nu'}}{\partial u^\alpha \partial u^\rho} \tag{1.23}$$

clearly behaves as a *pseudo-tensor*, i.e. it acts as a tensor under linear coordinate transformations only. This ill behavior stems from the local definition of $T_p(\mathcal{M}_4)$:

in curved space, given two close tangent vectors it is not clear how to compute the distance between the two, since they belong to different tangent spaces $T_p(\mathcal{M}_4)$ and $T_{p'}(\mathcal{M}_4)$ and the corresponding bases are different[4]. The derivative of the basis vectors $\mathbf{b}_\mu$ can be expanded on a basis of the environment manifold $\mathbb{M}_5$ via

$$\frac{\partial \mathbf{b}_\mu(u)}{\partial u^\nu} = \Gamma^\rho_{\mu\nu}(u)\, \mathbf{b}_\rho(u) + \Pi_{\mu\nu}(u)\, \mathbf{n}(u)\,, \tag{1.24}$$

where $\mathbf{n} \perp \mathbf{b}_\mu$ belongs to $\mathbb{M}_5$. Here we have two new objects: $\Gamma^\rho_{\mu\nu}(u)$ is the *affine connection*, describing the variation of the basis onto $\mathcal{M}_4$, and $\Pi_{\mu\nu}(u)$ is a tensor called *extrinsic curvature*, representing the curvature of the tangent hypersurface as seen from the environment manifold $\mathbb{M}_5$. The latter only exists since we are considering a manifold embedded into another space, and carries the "extra" information of the embedding in such space.

In the following Section, we will see how the embedding procedure gives rise to the 3+1 formalism of the Arnowitt-Deser-Misner formulation of gravity. Let us briefly recall how the spacetime curvature appearing in the Einstein's equations (1.1) emerges in this formalism. Given a space-time metric $g_{\mu\nu}$, the affine connection is

$$\Gamma^\rho_{\mu\nu} = \frac{1}{2} g^{\rho\gamma} (\partial_\mu g_{\gamma\nu} + \partial_\nu g_{\mu\gamma} - \partial_\gamma g_{\mu\nu}) \tag{1.25}$$

and is symmetric under the exchange of its lower indices. One then introduces the notion of *parallel transport*, that is the transport conserving the angle between the vector itself and the curved surface along which the coordinates vary, and then the *covariant derivative*

$$\nabla_\mu V^\rho(u) = \frac{\partial V^\rho}{\partial u^\mu} + \Gamma^\rho_{\mu\nu} V^\nu(u)\,, \tag{1.26}$$

$$\nabla_\mu V_\nu(u) = \frac{\partial V_\nu}{\partial u^\mu} - \Gamma^\rho_{\mu\nu} V^\rho(u) \tag{1.27}$$

for contravariant and covariant vectors respectively.

From the commutator of the covariant derivatives one can obtain the Riemann tensor $R_{\mu\nu\rho\sigma} = g_{\mu\epsilon} R^\epsilon{}_{\nu\rho\sigma}$ via

$$\left(\nabla_\rho \nabla_\sigma - \nabla_\sigma \nabla_\rho\right) V^\mu = R^\mu{}_{\nu\rho\sigma} V^\nu\,, \tag{1.28}$$

satisfying the following properties

$$R_{\mu\nu\rho\sigma} = -R_{\nu\mu\rho\sigma}\,, \quad R_{\mu\nu\rho\sigma} = -R_{\mu\nu\sigma\rho}\,, \quad R_{\mu\nu\rho\sigma} = R_{\rho\sigma\mu\nu} \tag{1.29}$$

and the Bianchi identity

$$R_{\mu\nu\rho\sigma} + R_{\mu\sigma\nu\rho} + R_{\mu\rho\sigma\nu} = 0\,. \tag{1.30}$$

Since (1.29) and (1.30) are tensor equations, they are true in all coordinate systems. From a geometrical point of view, the commutator in (1.28) expresses the parallel

[4] An immediate example of this problem is the sphere $\mathbb{S}_n$, where there is no automatic way to define a derivative for tangent vectors that behaves the same way in all directions. Indeed the parallel transport of a tangent vector along a closed curve on $\mathbb{S}_n$ does not return the vector pointing in the original direction, but it rotates it.

transport of the vector V^μ along an infinitesimal closed path. If the vector results to be changed when computed back in the same starting point, this is an effect effect of the spacetime curvature and we have a non-vanishing Riemann tensor; in the Minkowskian flat space-time, the covariant derivatives reduce to ordinary ones and we have that the commutator identically vanishes so $R_{\mu\nu\rho\sigma}$ is zero.

The (symmetric) Ricci tensor and curvature scalar

$$R_{\mu\nu} = g^{\rho\sigma} R_{\rho\mu\sigma\nu} \,, \tag{1.31}$$

$$R = g^{\mu\nu} R_{\mu\nu} \,, \tag{1.32}$$

are the objects entering in the Einstein tensor $\mathscr{G}_{\mu\nu}$ (1.1):

$$\mathscr{G}_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R \tag{1.33}$$

which conveys how the spacetime geometry influences (and is influenced by) the matter content of the universe.

1.5 The ADM formulation

We now apply the concepts contained in the previous sections to present the Lagrangian and Hamiltonian formulations of gravity. A peculiar feature of GR is that many different Lagrangian formulations are possible, corresponding to different boundary conditions of the integration domain (as we have seen in Sec. 1.2, any Lagrangian density is defined up to a boundary term). In defining the corresponding action functional as a gauge-invariant object, the integration volume element depends on the metric itself. When the variation of such gravitational action with respect to $g^{\mu\nu}$ is required to vanish, one must obtain the field equations (1.1); in doing so, standard boundary conditions are not enough since the first derivatives of $g^{\mu\nu}$ must also be fixed on the boundary:

$$\delta g^{\mu\nu}|_{\partial\mathcal{M}} = 0 \,, \qquad \delta(\partial_\rho g^{\mu\nu})|_{\partial\mathcal{M}} = 0 \,. \tag{1.34}$$

This is a stark difference from QFT, in which the field dynamics is derived by variation of the corresponding action with boundary conditions applied on the field alone. A number of different Lagrangian densities exist to solve this issue by requiring only $g^{\mu\nu}$ to be fixed on the boundary [9]; however, not all of them present the desired symmetries. For example, one might construct a Lagrangian without second-order derivatives of the metric, so that only the first condition in (1.34) is needed: this is the case of the $\Gamma\Gamma$ formulation, which is however not scalar nor covariant. We will here refer to the Einstein-Hilbert Lagrangian (and action), which is indeed scalar and covariant.

We start from the Einstein-Hilbert action functional

$$\mathrm{S}_{EH}[g_{\mu\nu}] = \frac{c^4}{16\pi G} \int_{\mathcal{M}} d^4x \sqrt{-g}\, (R - 2\Lambda) \tag{1.35}$$

corresponding to the following Lagrangian density for GR

$$\mathcal{L}_{EH} = \frac{c^4}{16\pi G} \sqrt{-g}\, (R - 2\Lambda) \,, \tag{1.36}$$

where a cosmological constant contribution is taken into account for generality (its role will be discussed in Chap. 5). By considering (1.35) along with the inclusion of matter sources through a Lagrangian density $\mathcal{L}_m$, one can verify that the Einstein equations (1.1) involving the matter stress-energy tensor

$$T_{\mu\nu} = \frac{2}{\sqrt{-g}} \left(\frac{\delta(\sqrt{-g}\mathcal{L}_m)}{\delta g^{\mu\nu}} - \frac{\partial}{\partial x^\rho} \frac{\delta(\sqrt{-g}\mathcal{L}_m)}{\delta(\partial_\rho g^{\mu\nu})} \right) \tag{1.37}$$

arise from the stationarity condition $\delta S = 0$ upon varying the metric tensor. This variation encompasses contributions from $\delta\sqrt{-g}$, $\delta g^{\mu\nu}$, and $\delta R_{\mu\nu}$.[5]. Also, since $\mathcal{L}_{EH}$ does not depend on the matter fields, varying the total action with respect to them will give the same equations as the variation of the matter action only.

To obtain the Hamiltonian formulation via the Legendre transformation, one needs to identify a time variable or at least a time "direction", apparently breaking the General Covariance of GR. However, Arnowitt, Deser and Misner developed a diffeomorphism-invariant Hamiltonian description of gravity, achieved with the so-called ADM splitting (or foliation) of spacetime [3].

In the general picture, a foliation consists of decomposing a manifold into a collection of submanifolds (or *leaves* of the foliation) which are required to be smooth and non-overlapping [6]. In GR, the ADM formalism illustrates how to slice the 4d manifold $\mathcal{M}_4$ into a family of 3d space-like hypersurfaces of equal time, each one representing a "snapshot" of space at a specific instant. Being these hypersurfaces space-like, events within each one are connected by spatial distances i.e. with no time-like separation. This is why the parameterization of time across these hypersurfaces provides a convenient way to describe the evolution of the gravitational field in terms of spatial geometry. We stress that this is possible only with globally hyperbolic spacetimes [14], for which it is possible a decomposition of the form $\Sigma_{x^0} \otimes \mathbb{R}$ (necessary to have a well-posed initial-value formulation for the metric).

Let us introduce a time-like vector field $\mathbf{n}$ on $\mathcal{M}_4$ and identify the hypersurfaces Σ_{x^0} as those normal to the time-like direction. Following the formalism of Sec. 1.4, these 3d hypersurfaces are embedded in $\mathcal{M}_4$ [15].

We describe the one-parameter family of hypersurfaces $\Sigma_{x^0} \equiv T_{x^0}(\mathcal{M}_4)$ via parametric equations:

$$y^\mu = y^\mu(x^i; x^0)\,. \tag{1.38}$$

Such hypersurfaces are in the general case curved, hence we will have an induced metric associated to an intrinsic curvature, and a non-zero extrinsic curvature, i.e. the information of the metric tensor $g_{\mu\nu}$ will be split into these two objects. Given the basis vectors $\mathbf{e}_\mu$ of $\mathcal{M}_4$, we define a new basis on Σ_{x^0} via

$$\mathbf{b}_i = \frac{\partial y^\mu}{\partial x^i}\mathbf{e}_\mu\,. \tag{1.39}$$

Together with the time-like vector $\mathbf{n} = n^\mu \mathbf{e}_\mu$, they form a basis $\{\mathbf{b}_i, \mathbf{n}\}$ for the environment (space-time) manifold.

[5] This term gives a boundary contribution, containing the first derivatives of the variation of $g_{\mu\nu}$ so it does not vanish when $\delta g_{\mu\nu}|_{\partial\mathcal{M}} = 0$. It is however possible to choose a class of manifolds where this contribution vanishes, such as asymptotically Minkowskian manifolds.

[6] An introductory description of foliation for generic manifolds can be found in the textbook [12], however we here restrict ourselves to the spacetime foliation.

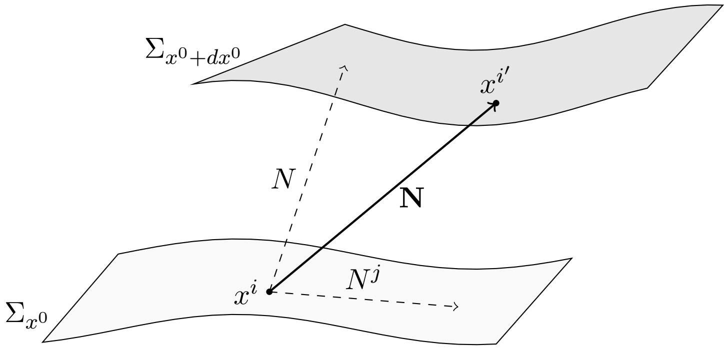

Figure 1.2. Foliation of space-time into space-like hypersurfaces. The deformation vector $\mathbf{N}$ connects two points with the same spatial coordinates $x^i \equiv x^{i'}$ on hypersurfaces separated by dx^0. We also show its projections on the time-like direction N and on the hypersurface basis N^i.

We now introduce a vector connecting points of identical coordinates x^i (dictated by the basis (1.39)) on two infinitesimally close hypersurfaces Σ_{x^0} and $\Sigma_{x^0+dx^0}$, see Fig. 1.2, labeled as *deformation vector* $\mathbf{N}$. We remind that the two hypersurfaces are both intrinsically and extrinsically curved (since they are embedded in $\mathcal{M}_4$), therefore $\mathbf{N}$ has non-vanishing projections both on $\mathbf{n}$ and on the vectors (1.39):

$$N^\mu = \dot{y}^\mu = N n^\mu + N^i b_i^\mu \,. \tag{1.40}$$

where $\dot{y}$ represent the time derivative (time is identified by the coordinate x^0 dictated by the time-like vector $\mathbf{n}$). The component N expresses displacements along the x^0 direction, while N^i measures displacement along the tangent vectors within the hypersurface; they are called *lapse function* and *shift vector* respectively. Given the basis (1.39), it possible to compute the three-dimensional metric h_{ij} induced on the hypersurfaces Σ_{x^0} linked to the coordinates x^i; this tensor shall be used for lowering or raising indices of 3d objects on Σ_{x^0}. However, we remind that we started from $\mathcal{M}_4$ with a given four-dimensional metric tensor $g_{\mu\nu}$, from which it is easier to compute h_{ij}: indeed one can write the spacetime interval as

$$ds^2 = (-N^2 + N^m N^n h_{mn}) dx^0 dx^0 + 2N^k h_{ki} dx^0 dx^i + h_{ij} dx^i dx^j \,. \tag{1.41}$$

Here we are using N, N^i and h_{ij} as set of variables, called ADM variables. Their relation with $g_{\mu\nu}$ is easily found:

$$N = \frac{1}{\sqrt{-g^{00}}} \,, \qquad N^i = -\frac{g^{0i}}{g^{00}} \,, \qquad h_{ij} = g_{ij} \,. \tag{1.42}$$

We note that the change of variables (1.42) is invertible only for $g^{00} < 0$. The determinant of the metric tensor is given by $\sqrt{-g} = N\sqrt{h}$.

A 3d covariant derivative on the hypersurfaces Σ_{x^0} can be defined by inspecting the partial derivative of a vector $\mathbf{A} = A^k \mathbf{b}_k \in \Sigma_{x^0}$:

$$\partial_i \mathbf{A} = (\partial_i A^k + \bar{\Gamma}^k_{il} A^l)\mathbf{b}_k + \Pi_{il}\mathbf{n} \,. \tag{1.43}$$

Here the extrinsic curvature causes a contribution on the time-like direction. The 3d Christoffel symbols $\bar{\Gamma}^k_{il}$, analogously defined from h_{ij} as

$$\bar{\Gamma}^k_{il} = \frac{1}{2} h^{kl} (\partial_i h_{jl} + \partial_j h_{li} - \partial_l h_{ij}) \tag{1.44}$$

allow to construct the 3d covariant derivative D_i as the projection of (1.43) on the hypersurface Σ_{x^0}:

$$D_i A^k = \partial_i A^k + \bar{\Gamma}^k_{il} A^l \,, \tag{1.45}$$

$$D_i A_k = \partial_i A_k - \bar{\Gamma}^l_{ik} A_l \,. \tag{1.46}$$

The 3d Riemann tensor $\tilde{R}^\sigma_{\rho\mu\nu}$ follows from the commutator of covariant derivatives:

$$[D_\mu, D_\nu] A_\rho = -\tilde{R}^\sigma_{\rho\mu\nu} A_\sigma \,, \tag{1.47}$$

however the relation between the scalar curvature R (1.32) and its 3d counterpart $\tilde{R}$ is not trivial. In this passage, the extrinsic curvature plays a significant role: it is defined as the symmetric tensor

$$K_{\mu\nu} = b^i_\mu b^\rho_i \, b^i_\sigma b^\nu_i \, \nabla_\rho n_\sigma = K_{\nu\mu} \,, \tag{1.48}$$

with a 3d counterpart

$$K_{ij} = \mathbf{b}_i \cdot \partial_j \mathbf{n} = \frac{1}{2N} (\partial_0 h_{ij} - D_i N_j - D_j N_i) \,. \tag{1.49}$$

It is possible to write R in terms of the 3d scalar curvature $\tilde{R}$ and (1.48), (1.49) with the so-called Gauss-Codazzi equation (we refer for example to [9]):

$$R = \tilde{R} - \epsilon (K_{\mu\nu} K^{\mu\nu} - K^2) + 2\epsilon \nabla_\mu (n^\nu \nabla_\nu n^\mu - n^\mu K) \tag{1.50}$$

where $K = K^i_i$ and $\epsilon = n^\mu n_\mu = -1$. Since $b^\mu_i b^j_\mu = \delta^i_j$ by definition, $K_{\mu\nu} K^{\mu\nu} = K_{ij} K^{ij}$ and the expression for (1.36) further simplifies:

$$\sqrt{-g}\; R = N\sqrt{h} (\tilde{R} + K_{ij} K^{ij} - K^2) + 2N\sqrt{h} \nabla_\mu (n^\nu \nabla_\nu n^\mu - n^\mu K) \,. \tag{1.51}$$

Here we are suppressing the cosmological constant contribution Λ in (1.36) in order to properly show the relation between the 4d and 3d metric functions; the same would apply in the presence of Λ, see for example Chap. 5. We observe that the second parenthesis in (1.51) is a boundary term, which can be discarded with appropriate boundary conditions [9]; in this case, using the induced metric to rewrite the first parenthesis, we have a well-posed variation principle for the action functional

$$\begin{aligned} \mathrm{S}_{ADM}[h_{ij}, N, N^i] &= \frac{c^3}{16\pi G} \int_{\mathcal{M}} d^4x \; \mathcal{L}_{ADM} \\ &\equiv \frac{c^3}{16\pi G} \int dx^0 d^3x N \sqrt{h} \left(\tilde{R} + (h^{ir} h^{js} - h^{ij} h^{rs}) K_{ij} K_{rs} \right) \,. \end{aligned} \tag{1.52}$$

It is now straightforward to perform the Legendre transform and achieve the Hamiltonian formulation of GR. Here the constrained nature of gravity emerges:

since $\dot{N}$ and $\dot{N}^i$ are cyclical, we immediately find from (1.52) the following first integrals

$$\Pi = \frac{\partial \mathcal{L}_{ADM}}{\partial \dot{N}} = 0\,, \qquad \Pi_k = \frac{\partial \mathcal{L}_{ADM}}{\partial \dot{N}^k} = 0 \tag{1.53}$$

which are the primary constraints of GR and are by definition the momenta conjugate to N, N^i. Together with the momentum conjugate to the three-dimensional metric h_{ij}

$$\Pi^{ij} = \frac{\partial \mathcal{L}_{ADM}}{\partial \partial_0 h_{ij}} = \frac{c^3}{16\pi G}\sqrt{h}(h^{ri}h^{sj} - h^{ij}h^{rs})K_{rs}\,, \tag{1.54}$$

we now have all the elements to compute H_{ADM}. First we shall invert the velocities of the ADM variables as functions of the momenta Π, Π_k, Π^{ij}. By combining (1.49) and (1.54) and inverting the 3d tensor $h^{ri}h^{sj} - h^{ij}h^{rs}$ with

$$\mathcal{G}_{ijrs} = \mathcal{G}_{rsij} = \frac{1}{\sqrt{h}}\Big(h_{ir}h_{js} - \frac{1}{2}h_{ij}h_{rs}\Big)\,, \tag{1.55}$$

whose properties will be specified later, one finds $K_{rs} = \frac{16\pi G}{c^3}\mathcal{G}_{ijrs}\Pi^{ij}$ and the metric velocity

$$\dot{h}_{rs} = \partial_0 h_{rs} = \frac{16\pi G}{c^3} 2N\mathcal{G}_{ijrs}\Pi^{ij} + D_r N_s + D_s N_r\,. \tag{1.56}$$

Now expressing the Lagrangian density (1.52) with the conjugate momenta

$$\mathcal{L}_{ADM} = \frac{c^3}{16\pi G}N\sqrt{h}\tilde{R} + \frac{16\pi G}{c^3}N\mathcal{G}_{ijrs}\Pi^{ij}\Pi^{rs} \tag{1.57}$$

one can finalize the Legendre transform:

$$\begin{aligned}\mathcal{H}_{ADM} &= \Pi^{ij}\,\partial_0 h_{ij} + \lambda\,\Pi + \lambda^i\,\Pi_i - \mathcal{L}_{ADM}(\Pi, \Pi_k, \Pi_{ij}) \\ &= \lambda\,\Pi + \lambda^i\,\Pi_i + N^k H_k + NH + 2D_i(\Pi_{ij}N^k h_{kj})\,.\end{aligned} \tag{1.58}$$

Here, the coefficients λ and λ_i stemming from the terms $\Pi\,\partial_0 N$, $\Pi_i\,\partial_0 N^i$ act as Lagrange multipliers enforcing the primary constraints (1.53), thus they are arbitrary; in other words, Π and Π_i are not dynamical variables (this will be more clear when applying the canonical quantization procedure in the next Chapter). Suitable boundary conditions can be chosen such that the last term in (1.58) vanishes, so we will discard it in the following. The objects H and H_i are introduced as the *super-Hamiltonian* function and *super-momentum* vector respectively:

$$H = \frac{16\pi G}{c^3}\mathcal{G}_{ijrs}\Pi^{ij}\Pi^{rs} - \frac{c^3}{16\pi G}\sqrt{h}\tilde{R}\,, \tag{1.59}$$

$$H_k = -2h_{kj}D_i\Pi^{ij}\,. \tag{1.60}$$

Let us now briefly discuss the object $\mathcal{G}_{ijrs}$. Since it is contracted with symmetric tensors in (1.59), it is useful to switch to its symmetric restriction

$$\mathcal{G}^{(sym)}_{ijrs} = \frac{1}{2\sqrt{h}}(h_{ir}h_{js} + h_{is}h_{jr} - h_{ij}h_{rs}) \tag{1.61}$$

that is the *supermetric tensor*, and we relabel $\mathcal{G}^{(sym)}_{ijrs} \rightarrow \mathcal{G}_{ijrs}$ for simplicity. Being a symmetric 6x6 matrix at each space point, it can be diagonalized, finding a signature $(-,+,+,+,+,+)$. Due to the presence of a negative eigenvalue, the kinetic term of the gravitational field is said to be *indefinite* [16] and the Hamiltonian constraint turns out to be a hyperbolic partial differential equation, see Sec. 2.1.

Following the discussion of Sec. 1.3, Eqs. (1.53) provide secondary constraints through the equations of motion:

$$\{\Pi, \mathcal{H}_{ADM}\} = -H = 0\,, \tag{1.62}$$

$$\{\Pi_k, \mathcal{H}_{ADM}\} = -H_k = 0\,. \tag{1.63}$$

Eqs. (1.62) and (1.63) are the super-Hamiltonian (or *scalar*) and super-momentum (or *vector*) constraints of gravity, and they are related to Einstein's equations in vacuum $G_{0\mu} = 0$ via

$$G_{\mu\nu} n^\mu n^\nu = -\frac{H}{2\sqrt{h}}\,, \tag{1.64}$$

$$G_{\mu\nu} b^\mu_i b^\nu_i = \frac{H_i}{2\sqrt{h}}\,. \tag{1.65}$$

To understand this, we remark that the physical relevance of the Einstein's equations (1.1) is not to simply solve the spacetime geometry based on the distribution of mass-energy, but it takes into account the initial data, as in classical Field Theory. A full solution can be found only for the associated Cauchy problem, i.e. we have to provide initial values for the variables and their "velocities" both for the metric field and mass-energy contribution. In absence of matter, gravity requires four degrees of freedom for the initial data, so that only six of the starting 10 equations (1.1) are dynamical and $G_{0\mu} = 0$ acts as a requirement on initial values.

Let us remark a fundamental property of such formulation. The action (1.52) can be rewritten in terms of the superHamiltonian and supermomentum functions as

$$\mathrm{S}_{ADM}[h_{ij}, N, N^i] = \frac{c^3}{16\pi G} \int_{\mathcal{M}} dx^0 d^3x \left(\Pi_{ij} \partial_0 h_{ij} - NH - N^i H_i \right)\,. \tag{1.66}$$

We first observe that the supermomentum constraint generates coordinate transformations on Σ_{x^0}, i.e. diffeomorphisms of $\mathcal{M}$ that preserve Σ_{x^0}. To show this, let us consider an infinitesimal spatial diffeomorphism $x^i = x^i + \xi^i$; at first order, the supermetric and wave functional transform as [16]

$$\delta_\xi h_{ij} = h'_{ij}(x) - h_{ij}(x) \simeq -2 D_{(i}\xi_{j)}\,, \tag{1.67}$$

$$\delta_\xi \Psi = -2 \int d^3x \frac{\delta \Psi}{\delta h_{ij}(x)} D_i \xi^j \tag{1.68}$$

and we recall that D_i is the covariant derivative on Σ_{x^0}. Performing a partial integration and assuming that ξ_j vanishes at infinity, since ξ_j is arbitrary it must hold that

$$D_i \frac{\delta \Psi}{\delta h_{ij}(x)} = 0\,. \tag{1.69}$$

As a consequence Ψ depends only on the 3-geometry, irrespective of the coordinate choice on Σ_{x^0}. This corresponds to the quantum version of the supermomentum constraint (1.63), as will be elucidated in the next Chapter.

On the other hand, it can be shown that the superHamiltonian H generates infinitesimal diffeomorphisms of $\mathcal{M}$ parallel to the time-like vector $\mathbf{n}$ i.e. orthogonal to Σ_{x^0} (we refer for the calculation to [17]). It follows that the ADM formulation based on the superHamiltonian and supermomentum identification is covariant with respect to arbitrary coordinate transformations, which was the main motivation behind its introduction. Clearly, the cost of this symmetry is the emergence of the secondary constraints.

The theory here presented, providing a dynamical Hamiltonian description of GR, is usually referred to as (classical) *geometrodynamics*; its quantization will be dealt with in the next chapter. It is important to stress that the constraints (1.53) and (1.62)-(1.63) represent a closed set, i.e. they are preserved by the evolution, so no tertiary constraints emerge (see discussion in Sec. 1.3); clearly, they also greatly reduce the space of admissible initial conditions and the phase-space spanned through the evolution. These constraints will bring fundamental repercussions when the canonical quantization is applied, see Chapter 2. This is expected, since as we mentioned before GR is a heavily constrained theory: of the ten degrees of freedom of $g_{\mu\nu}$, only two are truly independent (commonly associated to the polarization of gravitational waves propagating in spacetime); the others are gauge variables and just express the principle of General Covariance.

1.6 Minisuperspace models

Before proceeding with the quantized Hamiltonian formulation presented in the next Chapter, an important remark is needed. The configuration space of the theory, i.e. the *superspace*, includes both geometric and matter variables when we consider a gravitational system with matter content. Focusing on the gravitational sector, for each spacetime point there is a finite number of degrees of freedom. However, considering all possible points, the result is an infinite-dimensional theory. Then some renormalization procedure is needed to obtain finite predictions from the functional (since the variables are are fields defined over a curved spacetime) theory.

Highly symmetric spacetimes are relevant cases of study: the symmetries reduce the number of degrees of freedom (the others are essentially “frozen out”), yielding a finite-dimensional scheme, called *minisuperspace*. This is the case in Quantum Cosmology, where spatially homogeneous (or also isotropic) space-times are considered, as we will discuss in Chapter 5.

Let us consider a diffeomorphism-invariant system of gravity and one scalar field: this symmetry greatly reduces the number of degrees of freedom and gives a more manageable framework. Indeed, we can write the gravitational superHamiltonian (1.62) in terms of some minisuperspace variables h_a and the supermomentum (1.63) can be discarded, since it enforces the diffeomorphism-invariance of the theory thus it is automatically satisfied, as we will show in Sec. 2.1. The corresponding metric, which we leave unspecified, is therefore homogeneous; examples are provided by the Bianchi models in Sec. 1.6.1 and the special case of the Friedmann-Lemaitre-

Robertson-Walker metric, implemented in Chapter 5.

The minisuperspace is thus $\{h_a, \phi\}$. The superHamiltonian explicitly reads

$$H^{(tot)} = H_{MSS}(h_a) + \frac{1}{2\sqrt{h}} p_\phi^2 + \sqrt{h}\, U(h_a, \phi) \,, \tag{1.70}$$

where $H_{MSS}(h_a)$ is the minisuperspace reduction of (1.62) and the following terms come from the introduction of matter: p_ϕ is conjugate to ϕ and $U(\phi)$ is the self-interaction scalar potential. Let us stress that, by varying the action (1.52) with respect to N, one still finds the vanishing of (1.70) and this fact reflects the time diffeomorphism invariance of the theory. The wave function $\Psi(h_a, \phi)$ is intrinsically taken over 3-geometries, reflecting the symmetry of the system: indeed, it is not a function on $\mathrm{Riem}(\Sigma_{x^0})$ but on the minisuperspace.

The specific form of $H_{MSS}(h_a)$ depends on the "degree of symmetry" of the system. We recall that a homogeneous system exhibits the same properties at every point, while isotropy refers to the same behaviour in different directions. For homogeneous anisotropic spacetimes, all possible cases can be divided into categories by the so-called Bianchi classification, which is briefly illustrated in the next Section.

1.6.1 The Bianchi classification of homogenenous spacetimes

The classification developed by Bianchi consists of nine different classes of spacetimes numbered I, II, III, ..., IX, each representing a distinct type of spatial symmetry. Indeed, it is based on the Lie algebra structure associated with the isometry group of each spacetime, which encodes information about the local symmetries.

To describe such classification, we first note that the line element for a homogeneous (anisotropic) Universe admits the general form

$$ds^2 = -N(t)^2 dt^2 + \eta_{ab}(t) \ell^a_i(x^k) \ell^b_j(x^k) dx^i dx^j \,, \tag{1.71}$$

where the matrix η_{ab} contains dynamical degrees of freedom and ℓ^a_i are spatial vectors ($a = 1, 2, 3$) determining the specific shape of the 3-geometry. In the vacuum case one can always diagonalize the matrix $\eta_{ab} = diag\{a^2,\, b^2,\, c^2\}$, such that the 3-metric becomes

$$h_{ij}(t, x^k) = a^2 \ell^1_i \ell^1_j + b^2 \ell^2_i \ell^2_j + c^2 \ell^3_i \ell^3_j \,. \tag{1.72}$$

Clearly, the vectors $\boldsymbol{\ell}^a$ define three different (linearly independent) space directions which scale in time according to the corresponding scale factors a, b, c, sourcing the anisotropy. These vectors must satisfy suitable conditions for homogeneity: a group of symmetry must exist which maps a given space point x^i into another $G^i(x^i)$ such that h_{ij} is preserved, i.e. $\ell^a_{i'}(G^{l'}) dG^{i'} = \ell^a_i(x^l) dx^l$ must hold. This condition, together with Schwarz theorem for the commutativity of ordinary partial derivatives, leads to the following Lie algebra for partial derivatives

$$[\partial_a \,,\, \partial_b] = C^c_{ab} \partial_c \,, \tag{1.73}$$

where the quantities C^c_{ab} are the structure constants identifying the specific groups of symmetry and therefore the different Bianchi models. Indeed, one can write them as two-indices tensors as $C^{ab} \equiv \varepsilon_{abd} C^{dc}$ and then diagonalize them. The most trivial case with all eigenvalues equal to zero is the Bianchi I type, which corresponds to a spatial geometry equal to a vacuum 3d Euclidean space. The other types are increasingly more sophisticated, up to the Bianchi type IX which is the most general and admits spacetimes with a positive cosmological constant.

The matrix in the line element (1.71) can be recast in a simpler form using the so-called Misner variables α, β_+, β_-:

$$ds^2 = -N^2 dt^2 + e^{2\alpha}(e^{2\beta})_{ab}\, \sigma^a_i \sigma^b_j dx^i dx^j \, . \tag{1.74}$$

In cosmological settings, α can be interpreted as the logarithmic volume of the universe (i.e. $\alpha = ln(v)/3$), while the two degrees of freedom $\beta_\pm$ encoded in the matrix $\beta_{ab} = diag(\beta_+ + \sqrt{3}\beta_-, \beta_+ - \sqrt{3}\beta_-, -2\beta_-)$ represent the anisotropies (we reserve a better cosmological description for Chapter 5). Here N, α and $\beta_\pm$ are all functions of time only due to homogeneity.

The Hamiltonian formulation of Bianchi types is expressed by

$$\mathrm{S}_B = \int dt \left(P_\alpha \dot{\alpha} + P_+ \dot{\beta}_+ + P_- \dot{\beta}_- - N H_B \right) \tag{1.75}$$

where the supermomentum term is identically vanishing due to the homogeneity symmetry, and the superHamiltonian is (up to a fiducial volume set to one)

$$H_B = \frac{e^{-3\alpha}}{3(8\pi)^2} \left(-P_\alpha^2 + P_+^2 + P_-^2 + e^{4\alpha} U_B(\beta_\pm) \right) \, . \tag{1.76}$$

Here the potential U_B depends on the spatial curvature of the specific model. The Bianchi I case has $U_B = 0$ and it is the simplest and most symmetric model to account for inhomogeneities, which could play a relevant role in the early evolution of our Universe. The implementation of such models will be discussed in depth in Chapter 5, dedicated to Quantum Cosmology.

1.6.2 FLRW spacetime with a homogeneous field

When the anisotropy effects are switched off (i.e. $\beta_\pm$ are set to vanish) one recovers from the Bianchi line element (1.74) a homogeneous isotropic spacetime, that is the (spatially flat) Friedmann-Lemaitre-Robertson-Walker (FLRW) metric:

$$ds^2 = -N^2(t)\, dt^2 + a^2(t) \left(dx^2 + dy^2 + dz^2 \right) \tag{1.77}$$

with only one scale factor $a(t)$ associated to the three space directions. This metric leads to a non-vanishing Einstein tensor, and therefore describes the solution for a Universe filled with a matter source. A possibility is to consider a scalar matter field source ϕ, characterized by

$$\mathcal{L}_m = -\frac{1}{2}\sqrt{-g}(g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - m^2\phi^2) \, , \tag{1.78}$$

$$T_{\mu\nu} = \partial_\mu\phi\partial_\nu\phi - \frac{1}{2}g_{\mu\nu}(g^{\alpha\beta}\partial_\alpha\phi\partial_\beta\phi - m^2\phi^2) \, ; \tag{1.79}$$

we remark that actually both expressions are simplified by the requirement that $\phi = \phi(t)$, in accordance with the homogeneity of the model.

Let us briefly recall the classical properties of the FLRW model filled a massless scalar source $m = 0$; this case is of cosmological interest, as will be discussed in Chapter 5. Although the degrees of freedom are $N(t)$, $a(t)$ and $\phi(t)$, N is related to the choice of the time parameter and in this sense it is not dynamical (i.e. it behaves as a Lagrangian multiplier). Here we select the so-called synchronous gauge $N = 1$, i.e. we use the label time. Then, one finds the coupled evolution of $a(t)$ and $\phi(t)$ governed by the non-zero components of the Einstein equations:

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{6}\dot{\phi}^2\,, \tag{1.80}$$

$$\frac{\ddot{a}}{a} = -\frac{8\pi G}{3}\dot{\phi}^2\,, \tag{1.81}$$

and the scalar field's equation of motion

$$\ddot{\phi} + 3\frac{\dot{a}}{a}\dot{\phi} = 0\,. \tag{1.82}$$

We note that Eq. (1.80),that is the 00 component of the Einstein field equations, connects the geometry of the Universe to the matter content filling the space: this is the Friedmann equation. Its general form for a FLRW model with spatial curvature k and matter source with energy density ρ is (in $c = 1$)

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G\,\rho}{3} - \frac{k}{a^2}\,. \tag{1.83}$$

For example, when one considers as the only content a cosmological constant term, coming from an approximately constant potential $V(\phi)$ of a scalar field, it is easy to recover that the classical behaviour of $a(t)$ is an exponentially growing solution; this toy model suitably describes the slow-rolling phase of inflation, see Chapter 5.

Let us go back to Eqs. (1.80)-(1.82), that describe a free field (in a spatially flat metric). The associated solutions are easily found:

$$a(t) = a_0\,t^{1/3}\,, \tag{1.84}$$

$$\phi(t) = \phi_0 + \delta_0\,log(t)\,. \tag{1.85}$$

The parameter t can be eliminated from these equations to give the relation

$$a(\phi) = a_0\,e^{\frac{c_0}{3}(\phi-\phi_0)} \tag{1.86}$$

where the sign of the constant c_0 identifies the expansion or contraction phases [18]. Therefore, one can describe the intrinsic dynamics of the system via the correlation between these two quantities, independently from the chosen time; this is a simple example of the relational time program that we will discuss in Sec. 2.2.

Finally, we note that in the limit $t \to 0$ the scale factor a also goes to 0, causing the FLRW metric to be degenerate and the quantity $\dot{a}/a$ to diverge. It can be shown from the divergence of the energy density of the scalar field (which in this case is simply $\rho = \dot{\phi}^2/2$) and the behavior of the curvature invariants that $a = 0$ corresponds to a physical divergence, i.e. a *singularity* of the model [4]. This is a characteristic property of the Big Bang formulation of the history of the Universe [19], that we will overview in Chapter 5.

Chapter 2

Time in the Wheeler-deWitt picture

The quantization of a gravitational field is a necessary step towards the unification of all types of interactions, and it is expected that in the cosmological case the quantization approach will remove the initial singularity of our Universe, replacing it with a regular regime [20]. However, a complete theory of QG is still object of investigation at the present day.

In this chapter we explore quantum geometrodynamics in the canonical picture, i.e. the theory of Canonical Quantum Gravity (CQG), and discuss the emerging problems which must be faced in this framework, most notably the frozen formalism. We then review the approaches based on the WKB expansion of a system of gravity and matter, focusing on their different time implementations and the next-order effects, where the quantum nature of gravity is expected to modify the matter dynamics.

2.1 Quantum geometrodynamics and standing problems in CQG

For now we consider the superspace treatment and quantize the gravitational sector alone; the minisuperspace reduction in presence of matter will be discussed in the following sections.

We start by identifying the space of the states with functionals of the ADM variables, which are required to be differentiable. A generic wave function of the gravitational system will be:

$$\Psi = \Psi[N, N^i, h_{ij}] \tag{2.1}$$

We now implement the canonical quantization *à la* Dirac [10]. The ADM configuration variables and conjugate momenta are promoted to operators:

$$\begin{aligned} h_{ij}(x) &\to \hat{h}_{ij}(x)\,, \qquad & \Pi^{ij}(x) &\to \hat{\Pi}^{ij}(x)\,, \\ N(x) &\to \hat{N}(x)\,, \qquad & \Pi(x) &\to \hat{\Pi}(x)\,, \\ N^i(x) &\to \hat{N}^i(x)\,, \qquad & \Pi_i(x) &\to \hat{\Pi}_i(x)\,, \end{aligned} \tag{2.2}$$

which are required satisfy the canonical commutation relations

$$[\hat{h}_{ij}(x), \hat{\Pi}^{kl}(y)] = i\hbar\delta_i^{(k}\delta_j^{l)}\,\delta^{(3)}(x-y)\,, \tag{2.3}$$

$$[\hat{N}(x), \hat{\Pi}(y)] = i\hbar\,\delta^{(3)}(x-y)\,, \tag{2.4}$$

$$[\hat{N}^i(x), \hat{\Pi}_j(y)] = i\hbar\delta_j^i\,\delta^{(3)}(x-y)\,. \tag{2.5}$$

This is possible by introducing a representation of such algebra, in which the variable and momenta act on the wave functional Ψ as multiplicative or derivative operators respectively. This corresponds to an infinite-dimensional functional Schrödinger picture, as a generalization of the QFT case. We recall that in QFT the Schrödinger representation for finite-dimensional systems (e.g. the harmonic oscillator) describes quantum states as wave functions $\psi(q^i)$, as an alternative to the Fock representation identifying states via the basis of eigenkets of the Hamiltonian [21]. Let us remark that, at this level, the representation space on which the operators (2.2) act is only auxiliary and (2.1) is not yet a Hilbert space[1]. We will discuss the latter point in a dedicated paragraph below.

From the primary constraints (1.53) we have the vanishing of Π and Π_i, so their quantum version corresponds to

$$-i\hbar\frac{\delta}{\delta N}\Psi[N, N^i, h_{ij}] = 0 \tag{2.6}$$

$$-i\hbar\frac{\delta}{\delta N^i}\Psi[N, N^i, h_{ij}] = 0 \tag{2.7}$$

This means that the wave function (2.1) is actually independent of the variables N, N^i that constitute the deformation vector; the physical meaning of such condition will be cleared in the following.

Now we focus on the secondary constraints. It is useful to start from the supermomentum one (1.63), that gives

$$\hat{H}_i\Psi \equiv D_j\Big[\frac{\delta\Psi}{\delta h_{ij}(x)}\Big] = 0 \tag{2.8}$$

where the operator ordering is chosen such that the momenta are positioned on the right of the covariant derivative (other choices are possible, as elucidated in the super-Hamiltonian discussion). This condition expresses the invariance under 3d-diffeomorphisms: Ψ can depend only on the different 3-geometries $\{h_{ij}\}$ and not on the specific representations (i.e. the choice of hypersurface 3d-coordinates). In other words, the configuration space of the theory corresponds to the quotient space in which all metrics corresponding to the same 3-geometry are identified:

$$\{h_{ij}\} = \frac{\text{Riem}(\Sigma_{x^0})}{\text{Diff}(\Sigma_{x^0})}\,, \tag{2.9}$$

[1]In quantum mechanics the Hilbert space is a complex vector space, on which states of a physical system live as vectors, equipped with an inner product such that the product of a vector with itself is positive-definite. While the term was originally intended for infinite-dimensional spaces satisfying the completeness or closedness property, it is now widely used for finite-dimensional spaces too, which are automatically complete.

being Riem(Σ_{x^0}) the set of all 3-metrics on Σ_{x^0}, and Diff(Σ_{x^0}) identifies the group of diffeomorphisms of Σ_{x^0}.

It follows from (2.6)-(2.8) that physical states are independent of the particular choice of variables for the ADM splitting, and take into account only the (induced) 3-geometry. This is a direct consequence of the principle of General Covariance.

The most meaningful constraint for the system's dynamics is the superHamiltonian (1.62) constraint, also called the Wheeler-DeWitt (WDW) equation:

$$\frac{16\pi G}{c^3}\hat{H}\Psi = -(16\pi\ell_{Pl}^2)^2 \text{“}\mathcal{G}_{ijkl}(x)[h_{mn}]\frac{\delta^2\Psi}{\delta h_{ij}(x)\delta h_{kl}(x)}\text{”} - \sqrt{h}\tilde{R}(x)\Psi = 0 \tag{2.10}$$

where the supermetric $\mathcal{G}_{ijkl}$ has been defined in (1.61) and we have introduced a fundamental scale

$$\ell_{Pl} = \sqrt{\frac{G\hbar}{c^3}} \simeq 1,616\cdot 10^{-35}\,\mathrm{m} \tag{2.11}$$

that is the Planck length, signaling the start of the QG regime. Also in (2.10), the choice of operator ordering is ambiguous in the sense that it is not prescribed *a priori* by the theory. For this reason we use symbols "(...)" to denote some choice of factor ordering, for example requiring that the commutation relations (2.3)-(2.5) are preserved (for further details we refer to [9, 16]).

We remark that, in general, a quantum theory of GR is known to be perturbatively non-renormalisable, and in this sense the Wheeler-deWitt description might not be the most suitable one, suggesting to switch to different more fundamental quantum theories that include GR (such as String Theory or Loop Quantum Gravity). However, the discussion involving the Wheeler-DeWitt equation is here considered as a meaningful physical study, which could be relevant in low-energy and minisuperspace settings [22].

The problem of time Eq. (2.10) is a functional differential equation of the hyperbolic type, due to the signature of its Hessian matrix (it has non-zero eigenvalues with different signs, recalling the properties of (1.61)). A direct comparison with the evolutionary Schrödinger equation in QFT

$$i\hbar\frac{\partial}{\partial t}\psi = \hat{\mathcal{H}}\psi\,, \tag{2.12}$$

which is parabolic, lads to the immediate observation that the WDW equation is timeless, i.e. there is no time evolution operator applied on Ψ in (2.10). Indeed the Hamiltonian operator $\hat{\mathcal{H}}$, linear combination of the superHamiltonian and supermomentum functions (see Eq. (1.58)), annihilates the wave function. In the Schrödinger formulation of QFT, this would be analogous to an energy spectrum composed of a single possible state, that the wave function is in at all times. This is the essence of the so-called *problem of time*: the gravitational system alone appears to be frozen. We remark that this property is a direct and necessary consequence of the symmetries of GR, since is stems from the quantized constraints. Indeed in GR we cannot distinguish a specific time coordinate, since it has to take the same role as the other variables. However, in QM, one indeed expects that the identification of an "external" time parameter measured by an external observer is possible, according to the Copenhagen interpretation [23]. This contradiction is a core difficulty in the reconciliation of GR and QM.

It is possible to cast a dynamical description from (2.10), i.e. in a Schrödinger-like form, by defining some sort of time parameter, as we will describe in the next section.

The Hilbert space The time absence in (2.10) is not the only point of concern in the canonical quantization of gravity. In the general prescription of QM, the set of eigenstates of a system should span and live in a Hilbert space. For gravity, constructing such a Hilbert space is challenging due to the algebra of the constraints (2.8), (2.10) [16]: the identification of a basis is troublesome, and the same applies for defining a scalar product on such space.

To better understand this point, we observe that (2.10) is equivalent to a Klein-Gordon equation with variable mass. In analogy with the Klein-Gordon case (see for example [24]), one might propose a superspace current as [25, 26]

$$J_{12ij}(x)[\Psi_1, \Psi_2] = \frac{1}{2} G_{ijkl}(x) \Psi_1 \frac{\overleftrightarrow{\delta}}{\delta h_{kl}(x)} \Psi_2 \tag{2.13}$$

between any two states, where the double arrow means that the derivative acts first on the left and then on the right:

$$\Psi_1 \frac{\overleftrightarrow{\delta}}{\delta h_{kl}(x)} \Psi_2 = \Psi_1 \frac{\delta \Psi_2}{\delta h_{kl}} - \frac{\delta \Psi_1}{\delta h_{kl}} \Psi_2 \tag{2.14}$$

Indeed, it can be shown from (2.10) that such current is conserved: $\delta J_{12ij}/\delta h_{ij} = 0$. Then, one can try to implement the associated inner product

$$\Omega[\Psi_1, \Psi_2] = \prod_x \int d\Sigma^{ij}(x)\; J_{12ij}(x)[\Psi_1, \Psi_2] \tag{2.15}$$

where the integration is over a surface in $\text{Riem}(\Sigma_{x^0})$, in order to remove the dependence on the hypersurface choice, and $d\Sigma^{ij}$ denotes the corresponding surface element. However the scalar product (2.15) is not positive-definite. For the standard Klein–Gordon equation of QFT (i.e. in Minkowski space), one can separate between "positive" and "negative" frequencies, corresponding to particles and anti-particles respectively; within the one-particle picture, it is consistent to restrict to the positive-frequency sector and then (2.15) is positive, therefore the probabilistic interpretation is recovered [27]. Here however, one cannot even proceed to the frequency separation, since the superspace itself is singular in $\mathbf{n} = 0$ (being $\mathbf{n}$ the time-like vector of the ADM foliation), let alone restrict to positive ones [28]. This feature can be avoided in some cases with *ad-hoc* conditions [29], but it remains standing in general; therefore (2.15) cannot be implemented as an inner product. In QFT, when the single-particle description is not possible, one implements the second quantization approach. Here however, we already have a field-theoretic description achieved by the Wheeler-deWitt equation (2.10)[2]. Therefore the problem of defining the proper

[2]We mention that one could instead proceed with a *third quantization* procedure, see Sec. 3.5, which we will not adopt in the present thesis.

Hilbert space stands and it influences the probabilistic interpretation of the wave functional itself.

We also stress that (2.10) should also be regularized for the product of operators on the same point: indeed, to construct a Hilbert space of the quantum states one should identify a complete set of observables that are commuting at a fixed time. In other words, the concept of events happening at the same time is needed. We also recall the microcausality requirement in relativistic QFT

$$\left[\hat{\phi}(x), \hat{\phi}(x')\right] = 0 \qquad \text{for } |x - x'| \text{ spacelike}\,, \tag{2.16}$$

which essentially states that only the events A being inside the light-cone of B can be causally related to B. However, it is not clear how to translate these concepts within a quantum theory of gravity. In this regard, we mention the discrete approach of Regge calculus [30] and the theory of Causal Dynamical Triangulations [31], which address the causal structure of the theory.

While the question of the Hilbert space can also be addressed within the illustrated schemes, in the present thesis we will focus our attention on the frozen formalism to recover an evolution in time.

2.2 Paths for recovering time

The previously discussed points can be overcome by recasting the equations for the quantized system in a different way with appropriate assumptions. More specifically, the procedures by which a time parameter can be extracted from (2.10) can be divided into three main categories, following Kuchař and Isham's classification [22, 28].

Time before quantization In these schemes, an internal time is defined as a function of the canonical variables, and the canonical constraints are resolved before quantization. The quantization is then carried out for the reduced system, reconstructing a typical Schrödinger equation with this chosen time parameter. It can be considered the most conservative approach among the three, since it presupposes a concept of time very similar to the classical, external one of standard QM.

Between the many examples, we mention matter clocks (identifying a matter field with time) [32], volume variables [33], and the Unimodular gravity proposal [34]. In the latter, GR is modified by considering Λ as a dynamical variable and using its conjugate as a time parameter [35, 36]; this scheme presents some similarities with the reparametrized procedure described in Sec. 2.5, which will be then applied in Chapter 4.

Time after quantization One could instead follow the inverse of the process described earlier, i.e. the constraints are imposed at the quantum level as limitations on possible state vectors and time is identified only afterwards. Therefore, the starting point is the quantized version of the Wheeler-DeWitt equation (2.10) and states are functionals $\Psi[h]$ of the three-geometry $\{h_{ij}\}(x)$. The concept of time is somehow derived from the solutions to (2.10), after which one can recover the probabilistic interpretation. This poses a challenge if one wants to identify the Hilbert space structure of the original quantum theory *a priori*. Relevant discussions of this approach can be found in [37, 29, 38, 39, 40], while the implementations [41, 42, 43, 44] will be reviewed in more detail in the following Sections.

This path is the one that will be implemented in this thesis, more specifically we will make use of the WKB approximation to recover the time parameter. Through such expansion, the constraint (2.10) is found to approximate a conventional Schrödinger equation, deriving a time variable from the state $\Psi[h_{ij}]$. This interpretation suggests that the (recovered) time holds significance within a semi-classical limit of QG, as opposed to the full quantum picture.

Timeless approaches In this third class one includes various methods that aspire to maintain the timeless nature of GR by avoiding to specify the concept of time in the quantum theory. They all aim to construct a technically coherent and conceptually complete quantum theory (including the probabilistic interpretation) without direct references to a clock. Here, differently from other approaches, time takes a purely phenomenological status. We mention here Rovelli's proposal [45, 46] and the conditional probabilities research line, see for example [47].

2.3 WKB expansion for quantum subsystems

In this section we follow the path proposed by Vilenkin [41], i.e. we partition the system into two sets: one identifying a "small" but fully quantum subsystem, and the other corresponding to the "large" semiclassical environment system. Starting from the formalism developed in Sec. 2.1, we now take into account the presence of matter in the system. Therefore, the constraints (1.62)-(1.63) and their quantized versions (2.10), (2.8) are modified by additional contributions. A meaningful example is the presence of a self-interacting scalar field ϕ, which can be interpreted as the inflaton field driving the inflationary phase of the Universe (as will be clarified in Chap. 5).

Following the original proposal, we here consider the minisuperspace reduction of such a system with gravity and matter (see Sec. 1.6). Implementing the Dirac quantization prescription (2.2), the superHamiltonian constraint is expressed by the following WDW equation

$$\left[-\hbar^2\mathcal{G}^{ab}(h_a)\frac{\partial^2}{\partial h_a\partial h_b}-\frac{\hbar^2}{2\sqrt{h}}\frac{\partial^2}{\partial\phi^2}+V(h_a)+\sqrt{h}\,U(h_a,\phi)\right]\Psi=0\,, \tag{2.17}$$

where we have labeled the variables h_a as minisuperspace ones. We have also redefined the minisupermetric by a factor $\sqrt{h}$ for convenience and used a natural operator ordering, with the minisupermetric on the left of derivatives operators. Since the ordering choice must ensure general covariance in the minisuperspace for a consistent formulation (see discussion in Sec. 1.5), the second-order derivative operator will be be understood as the Laplace-Beltrami one in the following applications. The analogous "metric tensor" for the matter component is assumed to be the trivial one δ_{ab} (the generalization immediately follow by reinstating such tensor in front of ∂_ϕ terms). Here we have no functional derivatives in the strict sense due to the minisuperspace symmetry reduction.

We remark that here no specific value for the lapse function is set, in order to obtain a covariantly-performed quantization. It is then clear that the frozen formalism arises again, since the total wavefunction is annihilated by the Hamiltonian, and one needs a procedure to extract a time parameter in (2.17) after the quantization.

In the spirit of [41], one identifies a "small" subsystem behaving in a fully quantum way, as opposite to the remaining "environment" system which behaves semiclassically. We remark that this separation does not clearly distinguish the gravitational and matter contributions, but in principle a mixing is possible. In order to characterize the two components, we label

$$s = s_a : \quad \text{semiclassical variables } (a = 1, 2, \dots n_s)\,, \tag{2.18}$$

$$q = q_m : \quad \text{quantum variables } (b = 1, 2, \dots n_q)\,, \tag{2.19}$$

where n_s and n_q are the number of degrees of freedom necessary to completely describe the two sectors, finite thanks to the minisuperspace reduction. Subsequently, (2.17) can be expressed in a compact way as

$$\hat{H}\Psi = \left(-\hbar^2 \mathcal{G}^{ab}(s_a)\partial_a\partial_b + U_s(s_a) + \hat{H}_q(s_a, q_m)\right)\Psi(s_a, q_m) = 0, \tag{2.20}$$

where $H_s(s_a) \equiv -\hbar^2 \mathcal{G}^{ab}\partial_a\partial_b + U_s$ is the superHamiltonian obtained neglecting all quantum variables, and we have introduced the compact notation $\partial_a = \partial/\partial s_a$. The quantum superHamiltonian H_q instead depends on both the semiclassical and quantum degrees of freedom (this is evident by noting the presence of the metric in the scalar field contributions of (2.17)).

WKB approximation The Wentzel-Kramers-Brillouin (WKB) approach aims to establish a framework for defining a time label when certain variables are treated classically or semiclassically. These variables establish, in some limit, a classical fixed background, crucial for ensuring the positive semidefiniteness of the Klein-Gordon-like scalar product induced by the WDW equation. The motivation is conceptually grounded in the role of classical devices in the interpretation of quantum measurements.

The core idea of the WKB approach involves solving Eq. (2.20) perturbatively in some quantum parameter. The expansion is carried out by considering the following ansatz:

$$\psi(s_a, q_m) = e^{\frac{i}{\hbar}\mathcal{S}} = e^{\frac{i}{\hbar}\sum_n \kappa^n S_n} \tag{2.21}$$

where κ is the expansion parameter and $\mathcal{S}$ is a complex function (yielding both amplitude and phase contributions) expanded into the nth-order functions S_n. We stress here that $\mathcal{S}$ is not the (classical) action of the theory, which instead is recovered from the above expansion only in the limit in κ corresponding to the classical dynamics (i.e. for $\kappa \equiv \hbar$ it will be $\kappa \to 0$).

Once the form (2.21) is plugged into (2.20), one obtains order-by-order differential equations in κ which can be explicitly solved, finding approximate solution for the total wave function Ψ and so solving the dynamics with a certain accuracy. When one considers the Planck constant $\kappa \equiv \hbar$ the WKB approach is also called semiclassical expansion [21]. Here we will use this choice and also a modified form of (2.21) with real functions, following Vilenkin's work[3]; a different choice will be discussed in the next section.

In order to properly decompose the dynamics (2.20), [41] presented the following assumptions:

1. The typical (average) values of the quantum Hamiltonian are considered small compared to the semiclassical one:
$$\frac{\langle \hat{H}_q \rangle}{\langle \hat{H}_s \rangle} = \mathcal{O}(\hbar)\,. \tag{2.22}$$
Such hypothesis is driven by the observation that (2.20) is perfect symmetric between geometric and matter terms concerning $\hbar$.

2. The classical and quantum subspaces are assumed to be orthogonal at the lowest order, such that terms $\mathcal{G}_{am} = \mathcal{O}(\hbar)$ are moved to the next one; also the semiclassical minisupermetric is considered independent of the quantum variables at the lowest order $\mathcal{G}_{ab} = \mathcal{G}_{ab}(s_a) + \mathcal{O}(\hbar)$.

3. Following from point 1, the semiclassical system is supposed to satisfy its own constraint, i.e. it is possible to write in some way $H_s \Psi(s_a) = 0$. This means that no backreaction is present due to the "smallness" condition of the quantum subsystem.

Following these hypotheses, the wave function can be separated in
$$\Psi(s_a, q_m) = \psi(s_a)\chi(q_m, s_a) = A(s_a) e^{\frac{i}{\hbar} S(s_a)}\, e^{\frac{i}{\hbar}\hbar Q(s_a, q_m)}\,. \tag{2.23}$$
We recognize that ψ is considered of the WKB form (2.21), but rewritten with a real phase $S(s_a)$, while the imaginary part is reabsorbed into the amplitude $A(s_a)$, describing the non-classical behaviour [21]. Both A and S are considered to be of order $\hbar^0$, while χ starts at the next order following the assumption 1 and we will use for convenience χ directly instead of its exponential form. The separation of a purely semiclassical sector and the quantum one shares many similarities with the Born-Oppenheimer one, see Chapters 3 and 4, and in this sense Vilenkin's proposal can be considered a special implementation of it.

Due to point 3, ψ must satisfy
$$\left(-\hbar^2 \mathcal{G}^{ab}\partial_a\partial_b + U_s\right)\psi = 0\,, \tag{2.24}$$
while the total wave function $\psi\,\chi$ follows the total constraint (2.20), which gives the following equation for χ (using the gravitational constraint and dividing by ψ):
$$-\hbar^2 \mathcal{G}^{ab}\partial_a\partial_b\chi - 2\hbar^2 A^{-1}\mathcal{G}^{ab}\partial_a A\,\partial_b\chi - 2i\hbar\,\partial_a S\,\partial_b\chi + \hat{H}_q\chi = 0\,. \tag{2.25}$$
We are now ready to expand (2.24) and (2.25) in powers of $\hbar$ using (2.23).

[3] Actually, Vilenkin implemented a parameter κ proportional to $\hbar$ and (2.23) was written absorbing $\hbar$ is S; here we use directly $\hbar$ for convenience and collect it in front to better show the expansion orders.

At $\mathcal{O}(\hbar^0)$, only (2.24) gives contribution:

$$(\partial_a S)^2 + U_s = 0\,, \tag{2.26}$$

where the square implies the use of the minisupermetric $\mathcal{G}^{ab}$ to contract indices. This is the Hamilton-Jacobi (HJ) equation for the function S, ensuring the classical limit of the model. The next order $\mathcal{O}(\hbar)$ gives from (2.24) and (2.20) respectively:

$$2\mathcal{G}^{ab}\partial_a A\, \partial_b S + A\,\mathcal{G}^{ab}\partial_a\partial_b S = 0\,, \tag{2.27}$$

$$\hat{H}_q\chi = 2i\hbar\,\mathcal{G}^{ab}\partial_a S\, \partial_b\chi\,, \tag{2.28}$$

since all terms except the last two in (2.25) are of higher order in the expansion parameter ($H_q = \mathcal{O}(\hbar)$ due to assumption 1).

We first comment on the probabilistic interpretation following from the ψ sector. Eq. (2.27) is equivalent to the covariant conservation (with respect to the minisupermetric) of the current

$$j_s^a = |A|^2\,\mathcal{G}^{ab}\partial_b S\,, \tag{2.29}$$

associated to a semiclassical probability distribution ρ_s. Indeed, the real function S defines a congruence of classical trajectories, see (2.26), and each point in a classically allowed region of minisuperspace belongs to a trajectory with momentum $p_b = \partial_b S$ and velocity

$$\dot{s}_a = 2N\,\partial_a S \tag{2.30}$$

that depends on the choice of $N(t)$ from the foliation. This presupposes a time derivative of the form

$$\frac{\partial}{\partial\tau} = 2N\mathcal{G}^{ab}\partial_a S\,\partial_b\,, \tag{2.31}$$

which is indeed compatible with (2.30) since $\partial_b s_a = \delta_{ab}$. We note that (2.31) is close to the notion of a composite derivative $\partial_\tau s^a\,\partial_a$: indeed $\partial_a S \equiv p_a$ provides the classical momentum (we recall from (2.26) that S corresponds to the classical action), hence it is enough to write down the first Hamilton equation (varying with respect to p_a) to recover the desired definition. By other words, this time definition expresses the evolution in terms of the dependence that the semiclassical variables s^a acquire, at the leading order, on the label time of the space-time slicing. Clearly, as a simple example we could choose one of the h^a themselves as time coordinate, by suitably choosing the lapse function $N(t)$.

By requiring that each hypersurface in the classically allowed region of minisuperspace is crossed only once by the congruence of trajectories

$$\dot{s}^a\,d\Omega_a > 0\,, \tag{2.32}$$

where $d\Omega_a$ is the hypersurface element, then the probability density $dP = j_s^a\,d\Omega_a$ is positive semi-definite, thus the Universe wave function can be properly normalized. The same can be implemented for a superposition of wave functions $\sum_k \psi_k$ of the form (2.23), requiring the condition (2.32) for each component, such that the total probability is conserved.

Now we can focus on the quantum subsystem. It is possible to use the notion of time (2.31) derived from the classical trajectory also for the wave function χ: indeed, multiplying (2.28) by $N(t)$ one finds

$$i\hbar\frac{\partial}{\partial\tau}\chi = N\hat{H}^{(q)}\chi\,, \tag{2.33}$$

namely a functional Schrödinger equation for the subsystem wave function. In this sense, the dynamical interpretation is recovered for the quantum subsystem defining a time parameter analogous to a composite derivative with respect to the semiclassical variables. A clearer discussion of the consequences of such choice is provided in Sec. 3.3.

The analysis [41] actually started from the observation that, for the general quantum system, the probabilistic interpretation is lost since one should integrate $|\Psi(h_a)|^2$ over all the minisuperspace variables h_a (both semiclassical and quantum ones, including the label time), which would be divergent. Therefore it is interesting to discuss how such analysis was able to recover a probabilistic interpretation for the quantum subsystem too. Considering a Klein-Gordon-like current (2.13), its leading-order expansion would give for the semiclassical and quantum sectors respectively

$$j^a = |\chi|^2|A|^2\mathcal{G}^{ab}\partial_b S \equiv j_s^a\,\rho_\chi\,, \tag{2.34}$$

$$j^m = -\frac{i}{2}|A|^2\Big(\chi^*\partial^m\chi - \chi\partial^m\chi^*\Big) = \frac{1}{2}|A|^2 j_\chi^m\,. \tag{2.35}$$

In (2.34), j_s^a is the same as (2.29) and $\rho_\chi = |\chi|^2$ is the probability distribution of the quantum variables computed on the semiclassical trajectories, while in (2.35) j_χ^ν is a Klein–Gordon-like current for χ only ($\partial^m \equiv \partial/\partial q_m$). From the conservation of both the total current j^ν given by the full WDW constraint (2.25) and the semiclassical one from assumption (2.24), it can be shown that at leading order

$$\frac{\partial\rho_\chi}{\partial\tau} + N\partial_m j_\chi^m = 0\,, \tag{2.36}$$

which is a continuity equation for the probability current associated quantum variables. Moreover, both ρ_c and ρ_χ can be normalized on their respective subspaces, so that the standard probabilistic interpretation is recovered for Ψ.

However, there is still one case to discuss, that is when in such a framework one (or more) quantum variables become semiclassical at later time. This means that the two subsets (2.18)-(2.19) change: we now have s'_a and q'_m with $n'_s = n_s + 1$, $n'_q = n_q - 1$ respectively. For a initial wave function of the form (2.23) we now have $\psi\chi \to \psi'\chi' = \sum_l \psi(s')\chi_l(s', q')$, where the sum is explained by the transition during which each semiclassical trajectory branches into many paths, each one for a different initial condition of the "new semiclassical" variable. For this reason, one has to impose a unitarity (normalization) condition on the semiclassical current

$$\int d\Omega_a j_s^a = \sum_l \int d\Omega_{al}\,(j_s)_l^a, \tag{2.37}$$

that is satisfied only at an approximate level, i.e., when cross terms between the new and old sets can be neglected. Since the division itself between the two subspaces is arbitrary in a certain sense, this concept of unitarity is approximate.

Finally we mention the related point concerning how to impose boundary conditions on the wave function (2.23). Vilenkin's proposal was to construct the wave function describing an ensemble of Universes that tunnel from "nothing" to a de Sitter space (by choosing the purely expanding solution), i.e. the so-called *tunneling proposal* [48]. Such conjecture can also be reformulated in a path integral approach [49] to quantum gravity, more specifically with the Lorentzian path integral [50]. A different implementation is the *no-boundary* proposal by Hartle–Hawking [51], where the wave function for a closed Universe is constructed within the Euclidean path integral with different hypotheses.

Here we presented Vilenkin's proposal discussing also the probabilistic interpretation, up to the order where a Schödinger-like dynamic emerges, in this sense the analysis up to the order $\hbar$ was enough. Such result can be considered as the recovery of the QFT limit (see also Chapter 6) from a quantized system of gravity and matter. Since the focus of the present thesis is the emerging dynamics when one applies a Born-Oppenheimer-like separation to the gravity and matter sectors, rather than between semiclassical and quantum degrees of freedom, we wish to investigate the next orders of expansion. It is then useful to discuss Kiefer and Singh's proposal [42] where the next order is discussed, as we will see in the next section.

2.4 WKB expansion for gravity and matter

Kiefer and Singh's work [42], which we here review, was the first to consider a WKB regime in which the "classical limit" is the absence of matter, i.e., vacuum solutions. This is possible by choosing the expansion parameter to be of Planckian size:

$$M \equiv \frac{c^2}{32\pi G} = \frac{c m_{\mathrm{P}}^2}{4\hbar}\,, \tag{2.38}$$

being $m_P = \sqrt{\hbar c/8\pi G}$ the reduced Planck mass. Such a choice implies that the WKB expansion will hold for particles with small mass over Compton length ratio, or equivalently with mass $m \ll m_P$. It is clear from the definition that M identifies the Planckian scale, and so the reference values of the gravitational interaction. Indeed, differently from Vilenkin's approach, the parameter (2.38) here always separates the system into a gravitational and a matter sector, both of them properly quantized. As we will see, this property will have key consequences in the following derivation. We identify the two sets by

$$h_a = \text{gravitational semiclassical variables}\,, \tag{2.39}$$

$$\phi = \text{quantum matter variable}\,. \tag{2.40}$$

Here again, the use of a single scalar matter component is more convenient for the cosmological picture, but a generalization to more scalar components is straightforward. We start by rewriting the WDW equation (2.17) as

$$\begin{aligned}\Bigg(-\frac{\hbar^2}{2M}\left(\mathcal{G}_{ab}\frac{\delta^2}{\delta h_a \delta h_b} + f_a\frac{\delta}{\delta h_a}\right) + MV(h_a) - \frac{\hbar^2}{2\sqrt{h}}\frac{\partial^2}{\partial\phi^2} \\ + \sqrt{h}\,U(h_a,\phi)\Bigg)\,\Psi(h_a,\phi) = 0\,,\end{aligned} \tag{2.41}$$

where the term $f \cdot \delta_{h_a}$ is inserted to overcome issues stemming from a specific operator ordering choice (a suitable f_a will allow to recover other possible orderings). We stress here the use of functional derivatives, since no minisuperspace reduction is considered. Actually, a general formulation would require to consider the supermomentum constraint (1.63) too; we will consider this contribution in the next chapter.

In the ansatz (2.21) $\mathcal{S}$ is expanded in powers of M, at the same time separating each order as $S_n(h_a) + Q_n(h_a, \phi)$[4]. This is because, instead of the small quantum subsystem of the previous section, here a purely gravitational component is isolated via the choice (2.38). The aim is to obtain not only a dynamics for the matter sector (which will emerge at $\mathcal{O}\left(M^0\right)$) but also the next-order modifications induced by the quantum nature of gravity ($\mathcal{O}\left(M^{-1}\right)$); therefore the following expansion

$$\Psi(h_a, \phi) = \psi(h_a)\chi(h_a, \phi) = e^{\frac{i}{\hbar}(MS_0 + S_1 + M^{-1}S_2)} e^{\frac{i}{\hbar}(Q_1 + M^{-1}Q_2)} \tag{2.42}$$

will prove to be sufficient for the task. An immediate comparison with (2.23) emphasizes that here the highest-order function (i.e. the one at $\mathcal{O}\left(M\right)$) S_0 depends on gravitational variables only; this is a necessary condition for the consistency of the approach since at the Planck scale only gravity survives. One could also consider $S_0(h_a, \phi)$, in that case the independence from the matter variables would naturally emerge from the perturbative expansion. The matter enters only at the next order, such that the gravitational background is naturally recovered without further assumptions. This feature represents a striking difference from Vilenkin's proposal, where the gravitational constraint was taken as an additional hypothesis (point 3 of Sec. 2.3). Indeed here a classical matter contribution can only emerge with some suitable rescaling of the matter fields themselves (see [52]).

Substituting (2.42) into (2.41), at $\mathcal{O}\left(M\right)$ one immediately finds

$$\frac{1}{2}\mathcal{G}_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta S_0}{\delta h_b} + V(h_a) = 0, \tag{2.43}$$

that is the HJ equation for gravity; this equation corresponds to the classical limit, namely Einstein's equations in vacuum. The only difference with (2.26) is a coefficient 1/2, which appears in the starting WDW Equation (2.41) due to the definition (2.38) and it is not related to any physical properties. We remark that it is precisely the choice (2.38) for expansion parameter that separates the gravitational and matter subsets in the limit $M \to \infty$ (or $G \to 0$).

The next order M^0 brings

$$\begin{aligned} \mathcal{G}_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta S_1}{\delta h_b} + \mathcal{G}_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta Q_1}{\delta h_b} - \frac{i\hbar}{2}\left(\mathcal{G}_{ab}\frac{\delta^2 S_0}{\delta h_a \delta h_b} + f_a\frac{\delta S_0}{\delta h_a}\right) \\ + \frac{1}{2\sqrt{\hbar}}\left(\frac{\delta Q_1}{\delta \phi}\right)^2 - \frac{i\hbar}{2\sqrt{\hbar}}\frac{\delta^2 Q_1}{\delta \phi^2} + U(h_a, \phi) = 0\,. \end{aligned} \tag{2.44}$$

Here, the following condition for $S_1(h_a)$ is required, being S_0 known from the previous order:

$$\mathcal{G}_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta S_1}{\delta h_b} - \frac{i\hbar}{2}\left(\mathcal{G}_{ab}\frac{\delta^2 S_0}{\delta h_a \delta h_b} + f_a\frac{\delta S_0}{\delta h_a}\right) = 0\,. \tag{2.45}$$

[4]In the original work [42], each WKB order of the wave function was separated in these two components; here we perform the two actions immediately for the sake of clarity

This can be considered a continuity equation for S_1, although differently from (2.36) no probability current has been defined; it represents in this sense a gauge choice for the gravitational component. Indeed, while in Vilenkin's case an additional constraint was hypothesized from the beginning, here the condition (2.45) is obtained from the perturbative procedure (see also the unified reformulation in Sec. 3.1 and the proposal of Chapter 6). This passage is crucial to recover the functional QFT dynamics for the matter sector: (2.44) now turns into an equation for the matter function $\chi_0 = e^{\frac{i}{\hbar}Q_1}$

$$i\hbar\frac{\delta}{\delta\tau}\chi_0 \equiv i\hbar N\,\mathcal{G}_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta}{\delta h_b}\chi_0 = N\hat{H}_m\,\chi_0\,. \tag{2.46}$$

We recognize that (2.46) is a (functional) Schrödinger dynamics for the matter component, with a time parameter defined analogously to Vilenkin's case (2.31) i.e. via the dependence from the other sector's variables (here the gravitational ones). To maintain the parallelism with (2.31), we have reinserted the lapse function that was removed in the original work via a temporal gauge choice.

The most innovative result in [42] comes from developing the analysis to the next order M^{-1}, where one finds

$$\begin{aligned}
&\mathcal{G}_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta S_2}{\delta h_b} + \mathcal{G}_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta Q_2}{\delta h_b} + \frac{1}{2}\left(\mathcal{G}_{ab}\frac{\delta S_1}{\delta h_a}\frac{\delta S_1}{\delta h_b} + \mathcal{G}_{ab}\frac{\delta Q_1}{\delta h_a}\frac{\delta Q_1}{\delta h_b}\right)\\
&\quad + \mathcal{G}_{ab}\frac{\delta S_1}{\delta h_a}\frac{\delta Q_1}{\delta h_b} - \frac{i\hbar}{2}\left(\mathcal{G}_{ab}\frac{\delta^2 S_1}{\delta h_a\delta h_b} + \mathcal{G}_{ab}\frac{\delta^2 Q_1}{\delta h_a\delta h_b} + f_a\frac{\delta S_1}{\delta h_a} + f_a\frac{\delta Q_1}{\delta h_a}\right)\\
&\quad + \frac{1}{\sqrt{h}}\frac{\delta Q_1}{\delta\phi}\frac{\delta Q_2}{\delta\phi} - \frac{i\hbar}{2\sqrt{h}}\frac{\delta^2 Q_2}{\delta\phi^2} = 0\,,
\end{aligned} \tag{2.47}$$

Again this equation can be cast in a clearer form once a continuity condition is required on S_2

$$\mathcal{G}_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta S_2}{\delta h_b} + \frac{1}{2}\mathcal{G}_{ab}\frac{\delta S_1}{\delta h_a}\frac{\delta S_1}{\delta h_b} - \frac{i\hbar}{2}\left(\mathcal{G}_{ab}\frac{\delta^2 S_1}{\delta h_a\delta h_b} + f_a\frac{\delta S_1}{\delta h_a}\right) = 0\,, \tag{2.48}$$

thus leaving only

$$\begin{aligned}
&\mathcal{G}_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta Q_2}{\delta h_b} + \frac{1}{2}\mathcal{G}_{ab}\frac{\delta Q_1}{\delta h_a}\frac{\delta Q_1}{\delta h_b} + \mathcal{G}_{ab}\frac{\delta S_1}{\delta h_a}\frac{\delta Q_1}{\delta h_b} - \frac{i\hbar}{2}\left(\mathcal{G}_{ab}\frac{\delta^2 Q_1}{\delta h_a\delta h_b} + f_a\frac{\delta Q_1}{\delta h_a}\right)\\
&\quad + \frac{1}{\sqrt{h}}\frac{\delta Q_1}{\delta\phi}\frac{\delta Q_2}{\delta\phi} - \frac{i\hbar}{2\sqrt{h}}\frac{\delta^2 Q_2}{\delta\phi^2} = 0\,.
\end{aligned} \tag{2.49}$$

We can now decompose the derivatives δ_{h_a} in tangent and normal components to the hypersurfaces $S_0 = const$ and neglect the former by assuming an adiabatic (i.e. small) dependence of H_m on the induced metric. Summing (2.49) with the previous order and choosing now $N = 1$ (for correspondence with the original work), the resulting equation for $\chi = e^{\frac{i}{\hbar}\left(Q_1 + \frac{1}{M}Q_2\right)}$ is

$$i\hbar\frac{\delta}{\delta\tau}\chi = \hat{H}_m\chi + \frac{1}{8M\sqrt{h}\bar{R}}\left[\hat{H}_m^2 + i\hbar\left(\frac{\delta}{\delta\tau}\hat{H}_m - \frac{1}{\sqrt{h}\bar{R}}\frac{\delta(\sqrt{h}\bar{R})}{\delta\tau}\hat{H}_m\right)\right]\chi\,. \tag{2.50}$$

Here the terms after $\hat{H}_m$ modify the standard quantum matter dynamics and thus can be interpreted as quantum gravity corrections, since the gravitational sector is inherently quasi-classical. An inspection of these terms (one quadratic in H_m and the other imaginary) reveals that they violate unitarity in the evolution, although it was stated that they can be neglected in most cases [42]. We will discuss this feature more specifically in Sec. 3.3, and we will also present within Chapter 3 an original formulation of the problem able to overcome non-unitary corrections.

2.4.1 The Born–Oppenheimer-like averaged approach

We here describe a further implementation of the WKB approach for gravity and matter presented in [43], later applied in the context of quantum cosmology in [53, 54, 55]. There, in analogy with the Born-Oppenheimer approximation for molecules, the matter sector (which is characterized by a lower mass scale with respect to the Planckian one) is regarded as the "fast" component, while gravity is the "slow" one in (2.42). The fast wave function χ is taken to be properly normalized over the gravitational space

$$\langle\chi|\chi\rangle = \int \chi^*(h_a,\phi)\chi(h_a,\phi)\, dh_a = 1 \tag{2.51}$$

from the beginning. The analysis, which is set in the minisuperspace by considering only one gravitational variable a and a single scalar matter field ϕ, examines two equations for the total system, although they are obtain in a novel way. Differently from Sec. 2.3 and 2.4, the second constraint does not come from an additional hypothesis or gauge choice; instead, the average of the WDW equation over $\chi(a,\phi)$ is subtracted from the initial equation, obtaining an equation for the gravitational background ψ and another one for the matter sector χ, namely

$$\left[-\frac{\hbar^2}{2M}\left(D^2 + \langle\bar{D}^2\rangle\right) + MV + \langle\hat{H}_q\rangle\right]\psi = 0\,, \tag{2.52}$$

$$\left[-\frac{\hbar^2}{2M}\left(D^2 - \langle\bar{D}^2\rangle + 2D\ln\psi\bar{D}\right) + \hat{H}_q - \langle\hat{H}_q\rangle\right]\chi = 0\,, \tag{2.53}$$

where $\langle f\rangle = \langle\chi|f|\chi\rangle$ and $D = \partial_a + i(-i\hbar\langle\partial_a\rangle)$, $\bar{D} = \partial_a - i(-i\hbar\langle\partial_a\rangle)$ are "covariant" derivatives constructed with the connection $-i\hbar\langle\partial_a\rangle$ (being $\partial_a = \partial/\partial a$). Clearly Eq. (2.52) does not represent the quantized gravitational constraint, since a quantum matter backreaction is emerging from the average procedure.

A core feature of this implementation is the rescaling of both ψ and χ through a phase depending on the gravitational variables only:

$$\psi = e^{-\frac{i}{\hbar}\int -i\hbar\langle\partial_a\rangle\, da}\,\widetilde{\psi}, \quad \chi = e^{\frac{i}{\hbar}\int -i\hbar\langle\partial_a\rangle\, da}\,\widetilde{\chi}\,, \tag{2.54}$$

where $-i\hbar\langle\partial_a\rangle$ takes the role of an adiabatic phase. This transformation makes use of the gauge invariance of the system related to the separation $\Psi = \psi\chi$. Then, scaling again χ via the average value $\langle\hat{H}_m\rangle$ and applying the WKB expansion for ψ, it was shown that the HJ equation is modified by the presence of the matter backreaction:

$$\frac{1}{2}(\partial_a S_0)^2 + V + \langle\hat{H}_m\rangle = 0\,. \tag{2.55}$$

Implementing the time definition as in (2.46), the matter dynamics is given by

$$\begin{aligned}&\left(\hat{H}_m - i\hbar\frac{\partial}{\partial\tau}\right) e^{-\frac{i}{\hbar}\int\langle H_q\rangle\,d\tau - \frac{i}{\hbar}\int -i\hbar\langle\partial_a\rangle\,da}\,\chi \\ &= \frac{\hbar^2}{2M} e^{-\frac{i}{\hbar}\int\langle H_m\rangle\,d\tau - \frac{i}{\hbar}\int -i\hbar\langle\partial_a\rangle\,da}\left[\bar{D}^2 - \langle\bar{D}^2\rangle + 2\left(D\ln|\psi|^{-1}\right)\bar{D}\right]\chi\,.\end{aligned} \tag{2.56}$$

Again in the semiclassical limit $M \to \infty$ the second line vanishes and Eq. (2.56) describes a Schrödinger-like dynamics. Furthermore, labeling in (2.56)

$$\chi_s \equiv e^{-\frac{i}{\hbar}\int\langle H_q\rangle\,d\tau - \frac{i}{\hbar}\int -i\hbar\langle\partial_a\rangle\,da}\,\chi \tag{2.57}$$

the authors suggest that the obtaining dynamics is unitary due to the vanishing of

$$i\hbar\frac{\partial}{\partial\tau}\langle\chi_s|\chi_s\rangle = 0\,. \tag{2.58}$$

However, this approach does not completely solve the non-unitarity problem. Indeed, while the norm of a quantum matter state satisfies (2.58), that same condition might be violated when considering different matter states: $i\hbar\partial_\tau\langle\chi_r|\chi_s\rangle \neq 0$ for $r \neq s$. The construction of the Hilbert space associated to the matter sector is thus troublesome. It has been shown that the decomposition of the total Hilbert space can be addressed by imposing further specific conditions in order to recover the QFT limit, see [56].

We will provide an extensive discussion of both the matter backreaction presence (2.55) and the unitarity condition (2.58) in the reformulation of Chapter 3.

2.5 Reparametrization and reference fluids

Another way to develop a quantum formulation of geometrodynamics from the WDW constraint is the one discussed in [57]. The core idea of the proposal is the notion of a *reference fluid*: a fluid "emerging" as a matter source in the system as a consequence of fixing a certain reference frame, in order to identify the dynamically relevant components of the metric describing the evolution. This passage is nontrivial and demands careful consideration: indeed, if the coordinate choice is imposed before the quantized constraints, the resulting theory will be valid only in that specific frame. By construction the reference fluid would break the diffeomorphism invariance of the theory. To avoid so, a reparametrization procedure is implemented to formalize the reference fluid in a covariant and consistent way.

In the original paper [57], the reference frame chosen is the Gaussian one. One could, in general, try to construct an analogous procedure for a different system of coordinates, which turns out to be quite a troublesome task (see [58]). Choosing the Gaussian coordinates $X^\mu = (T, X^i)$, the corresponding metric $\gamma^{\alpha\beta}$ must satisfy

$$\gamma^{00} = -1, \quad \gamma^{0i} = 0\,. \tag{2.59}$$

Since we are imposing such conditions before the variation of the action, the metric now assumes an ambiguous role as it can no longer be freely varied. To solve this, one can either express the metric in terms of new freely variable quantities so that the (2.59) are identically satisfied, or adjoin the conditions (2.59) to the action by

Lagrange multipliers and vary these as well as the metric freely. Following the second path, the conditions (2.59) can be ensured by inserting Lagrangian multipliers $\mathcal{F}, \mathcal{F}_i$ into the total action of the system. For the gravity case, $S^{tot} = S^g + S^f$ with S^g is the usual Einstein-Hilbert action and S^f is the novel contribution

$$S^f = \int d^4x \left[-\frac{\sqrt{-\gamma}}{2} \mathcal{F} \left(\gamma^{00} + 1 \right) + \sqrt{-\gamma}\, \mathcal{F}_i \, \gamma^{0i} \right] \tag{2.60}$$

containing the Gaussian conditions. As we will see, these additional terms emerge in the Einstein's equations as a source for gravity, thus breaking the diffeomorphism invariance.

A *reparametrization* of the action is then needed in order to work in new arbitrary coordinates, other than the starting ones; this is clearly linked to the first proposed path. This procedure reflects the fact that the Gaussian fluid is here the "privileged" system of coordinates, but one could, in principle, choose another arbitrary set. For this reason, new freely varying coordinates x^α are introduced, with associated metric $g_{\alpha\beta}$, so that one can rewrite the Gaussian coordinates in terms of those:

$$\begin{aligned} S^f_{par} = \int d^4x \Big[& -\frac{\sqrt{-g}}{2} \mathcal{F} \left(g^{\alpha\beta} \partial_\alpha T(x) \, \partial_\beta T(x) + 1 \right) \\ & + \sqrt{-g}\, \mathcal{F}_i \left(g^{\alpha\beta} \partial_\alpha T(x) \, \partial_\beta X^i(x) \right) \Big] \, . \end{aligned} \tag{2.61}$$

The variation of this action will give equations of motion invariant under coordinate transformations of the x^α: in other words, the reparametrization procedure has restores covariance of the theory, although in the new set of coordinates. To be compatible with the Gaussian choice, one must require that (2.61) coincides with (2.60) when the arbitrary coordinates are chosen as the Gaussian ones: $x^\alpha \equiv \delta^\alpha_\mu X^\mu$. For compactness of notation, we avoid writing the dependence on the x^α, which will be implicitly understood.

The name of the reference fluid comes from the study of the Einstein's equations associated to the action (2.61). Due to these novel terms, the Hamiltonian content of the theory and so the Hamilton-Jacobi equation (from which the Einstein's equations are recovered) are modified with respect to the pure gravity (i.e. vacuum) case. Defining

$$U^\alpha = g^{\alpha\beta} \partial_\beta T \, , \tag{2.62}$$

$$\mathcal{F}_\alpha = \mathcal{F}_i \partial_\alpha X^i \, , \tag{2.63}$$

it can be shown that the following source term appears in the corresponding Einstein's equations (1.1):

$$T^{\alpha\beta} = \mathcal{F} U^\alpha U^\beta + \frac{1}{2} \left(\mathcal{F}^\alpha U^\beta + \mathcal{F}^\beta U^\alpha \right) \, . \tag{2.64}$$

Thus a source emerges purely from the addition of (2.61), which takes the form of a fluid with four-velocity U^α, mass density $\mathcal{F}$, and heat flow $\mathcal{F}_\alpha$. Actually, since the above tensor has no stress term, it corresponds to a heat-conducting dust. This case presents analogies with the anisotropic hydrodynamics theory, in which one studies sources that are far from isotropic thermal equilibrium (for example quark-gluon plasmas), see [59]. Here we will refer to (2.64) as a fluid to avoid ambiguity with the reduced formalism of the Brown-Kuchař proposal [32], where a homogeneous dust is added and its proper time assumed as a clock before the quantization procedure; being the superHamiltonian constraint solved with respect to the momentum conjugate to the dust time, that work represents a reduced phase-space quantization of the system, which is intrinsically different from the approach followed in this thesis.

It is also possible to implement only the Gaussian time condition in (2.59), but not the spatial one by adjoining the corresponding constraints to the action: in that case the fluid reduces to an incoherent dust, with only the quadratic term in U^α appearing in (2.64), since the heat transport (containing the Gaussian spatial coordinates) is switched off.

The Hamiltonian description of the fluid is then computed starting from (2.61), implementing the ADM foliation, finding the following superHamiltonian and supermomentum contributions:

$$H^f = W^{-1}P + WW^kP_k\,, \tag{2.65}$$

$$H^f_i = P\,\partial_i T + P_k\,\partial_i X^k\,, \tag{2.66}$$

where P, P_k are the momenta canonically conjugate to T, X^k and the coefficients

$$W \equiv (1 - h^{jl}\partial_j T\,\partial_l T)^{-1/2}\,, \tag{2.67}$$

$$W^k \equiv h^{jl}\partial_j T\,\partial_l X^k \tag{2.68}$$

correspond to three-dimensional sector of the Gaussian restrictions in (2.61). The system of gravity and reference fluid is then subjected to the new constraints:

$$H^g + H^f = 0\,, \tag{2.69}$$

$$H^g_i + H^f_i = 0\,. \tag{2.70}$$

A core feature of the fluid superHamiltonian (2.65) (and supermomentum (2.66)) is its linearity in P, P^k, which after canonical quantization correspond to the operators $\delta/\delta T(x)$ and $\delta/\delta X^k(x)$ respectively. Since the fluid momenta emerge linearly in the constraints, clearly separated from the other variables (from which they are independent), they can play the role of a clock after the quantization procedure. Indeed, the quantum version of (2.69) and (2.70) can be recast as a Schrödinger equation of the form

$$i\hbar\,\partial_t\Psi \equiv i\hbar\int_\Sigma d^3x\,\frac{\delta\Psi\left(T(x),X^k(x),h^{jl}(x)\right)}{\delta T(x)}\Bigg|_{T=t}\Psi = \hat{\mathcal{H}}\Psi = \int_\Sigma d^3x\,H^g\Psi \tag{2.71}$$

when the Gaussian time condition $t = T$ is implemented in the ADM formalism. We remark that in (2.71) the wave function Ψ is still a functional of $X^k(x)$, $h^{jl}(x)$, but it is now an ordinary function of the Gaussian time. In other words, the time for the ADM splitting is precisely identified with the time-like direction of the fluid worldlines. At this level, the Gaussian time choice has provided a meaningful clock for the system evolution, whose state is now a functional of the remaining variables. One could also choose to implement the spatial Gaussian condition only, or both (2.59) together; these possibilities still give a functional Schrödinger evolution, although with different time definitions [57].

Eq. (2.71) is equipped with the standard positive-definite conserved norm

$$\langle\psi|\phi\rangle = \int Dh_{ij}\; \psi^*(T, X^k, h_{ij})\; \phi(T, X^k, h_{ij})\,, \tag{2.72}$$

with the functional integral taken over the three-geometries h_{ij}, so one would be tempted to construct the Hilbert space of states with it. However, such construction is physically sensible only if the fluid itself is physical, since the integrand of such norm (i.e. the probability density) contains the fluid variables. In other words, the reference fluid as a time and the construction (2.72) can be used only if the fluid satisfies its own *energy conditions*, ensuring that its energy density and energy current measured by an arbitrarily moving local observer have reasonable physical properties. To investigate this, one checks if the associated stress-energy tensor satisfies the weak, dominant and strong energy conditions: calling v^α the four-velocity of the observer ($v^\alpha v_\alpha = -1$), they translate to the requirements that the energy density shall not be negative $T_{\alpha\beta}v^\alpha v^\beta \geq 0$, that the energy flow cannot be spacelike $(-T_{\alpha\beta}v^\beta)(-T^{\alpha\gamma}v^\gamma) \leq 0$ and that $T_{\alpha\beta}v^\alpha v^\beta \geq -T^\beta_\beta/2$ (a discussion on the general form of these conditions can be found in [60]).

The incoherent dust case (with only $\mathcal{F}$ in (2.61), $\mathcal{F}_i$=0) is the most straightforward, since they all result in the same condition

$$\mathcal{F} \geq 0\,. \tag{2.73}$$

Actually, (2.73) is preserved by the evolution due to the algebra of the constraints with the multiplier $\mathcal{F}$ itself: this means that, if one defines the fluid such that (2.73) is satisfied at the beginning, the fluid will remain "physical" at all times.

However, a different situation arises in the general case. Indeed, for the heat-conducting fluid, the energy conditions require the following inequality

$$\mathcal{F} \geq 2\sqrt{\gamma^{\alpha\beta}\mathcal{F}_\alpha\mathcal{F}_\beta}\,. \tag{2.74}$$

to be satisfied. Since (2.74) involves the multipliers $\mathcal{F}, \mathcal{F}_i$, which are in principle all independent i.e. they can take arbitrary values, and we have no proper equation of state for the Gaussian fluid, the the energy conditions are not satisfied and moreover they can be violated during the dynamical evolution.

Another way to understand this point is to look at the Hamiltonian formalism directly. The energy conditions require $H^f \geq 0$, which using the constraint (2.69) becomes $H^g \leq 0$. This condition can be written as an equality using the Heaviside function Θ, as discussed in [57]; thus, it can be considered an additional constraint for the system. However, the authors show that its Poisson brackets with the super-Hamiltonian constraints do not always vanish, so they are not first class for the general heat-conducting Gaussian fluid. This property reflects the fact that(2.74) are not preserved in the evolution. Thus, the system must be now closed with additional constraints $P_k = 0$, which turn off the heat conduction (i.e. $\mathcal{F}_k = 0$). It follows that, in this implementation, the quantum version of the energy conditions can be imposed in a consistent way only for the incoherent dust.

These aspects prevent a full implementation of the Gaussian fluid as a quantum clock. A different approach making use of the Gaussian reference fluid, able to provide a clock and thus a Schrödinger equation for the Universe wave function overcoming the previous points, will be proposed in Chapter 4.

Chapter 3

Time via kinematical action

Having reviewed the state of the art regarding the frozen formalism in quantum geometrodynamics and the WKB picture, we now turn to the original content of this thesis. The main content of this Chapter is based on [61] and it is divided in two parts. In the first one, we expand on the previous WKB approaches, whose clock is based on the dependence of the quantum subsystem on the gravitational (semiclassical) variables; in particular, we show the equivalence of the expansions in $\hbar$ and M up to the first order of QG corrections and how both result in non-unitary effects. The second part is devoted to the original proposal of defining a clock through the kinematical action, so obtaining a unitary dynamics with QG corrections at the first leading order i.e. $1/M$.

3.1 Equivalence of the WKB expansions in $\hbar$ and M

Let us recall the main features of the two WKB approaches review in Sec. 2.3 and 2.4. In both cases, the wave function of the system is decomposed into a semiclassical (i.e. gravitational) component representing the background and another one characterizing the quantum subsystem, in an adiabatic approximation akin to a Born-Oppenheimer (B-O) separation, though realized differently from the mathematical point of view. Despite some structural differences, both proposals portray a functional description of the system and recover a Schrödinger dynamics via the analogous time definitions (2.31) and (2.46), describing the evolution of the subsystem via the dependence on the background degrees of freedom. They also do not consider the backreaction of the quantum subsystem on the background, a factor that could play a role in incorporating quantum effects on the semiclassical sector. The second approach [42] however investigated the next order of expansion, to examine the first-order corrections imputed to quantum gravity effects.

A critical difference between the two approaches stands in the corresponding assumptions. The $\hbar$ expansion actually considered a separate constraint to hold for the semiclassical component of the total wave functional (2.24), based on the idea that in such regime any effects coming from the quantum subset would be negligible (3). The M expansion did not implement such an *a priori* constraint, working with a gauge choice procedure for the semiclassical part of Ψ at each order of expansion. This significant divergence actually has a very simple origin: Eq. (2.20) has a perfect symmetry between geometric and matter terms with respect to the parameter $\hbar$, while in powers of M there is a one-order gap between them. In other words, the $\hbar$ expansion allows for backgrounds generated by both matter and gravitational sources, since it identifies a quantum subsystem of whichever nature; the gap in (2.20) is precisely recovered with the additional hypothesis of smallness (1).

It is then interesting to ask whether the formalism of [41] can be expanded up to arbitrary orders, and if the non-unitarity of [42] emerges also in that case, hinting at a criticality in the time definitions (2.31), (2.46). Actually, we here derive such result with a more general statement, showing that the two approaches are equivalent up to the order of quantum gravity corrections and can be reunited n a single formulation.

We first note that the ansatz (2.21) corresponds to the $\hbar$ expansion via $\kappa^n = \hbar^n$ and the M one with $\kappa^n = M^{1-n}$. Both (2.23) and (2.42) are factorized wave functions of the B-O-like form $\Psi(s_a, q_m) = \psi(s_a)\chi(s_a, q_m)$, where we are using the same labels as (2.18)-(2.19) for convenience (although the s_a represent in the M expansion the gravitational variables, and q_m the matter ones). More specifically, the respective WKB ansatzs are given separating each S_n as $S_n = \sigma_n(s_a) + \eta_n(s_a, q_m)$ for $n \geq 1$, with the exception of the zero-th order where one has a function pertaining to the semiclassical sector only $S_0(s_a)$. This gives

$$\Psi = \psi(s_a)\chi(s_a, q_m) = e^{\frac{i}{\hbar}(\kappa^0 S_0 + P + Q)}\,, \tag{3.1}$$

where

$$P(s_a) = \sum_{n=1}^{\infty} \kappa^n \sigma_n\,, \tag{3.2}$$

$$Q(s_a, q_m) = \sum_{n=1}^{\infty} \kappa^n \eta_n \tag{3.3}$$

In other words, the lowest order is represented by S_0 alone in the $\hbar$ expansion, while in the M one it takes the form MS_0. Following Vilenkin's formulation, the background component ψ is assumed to satisfy its corresponding constraint

$$\left(-\hbar^2 \mathcal{G}^{ab}\partial_a\partial_b + U_s\right)\psi(s_a) = 0\,. \tag{3.4}$$

In the prospect of uniting the two formulations, the above constraint is imposed also in the M expansion: that means that

$$\left(-\frac{\hbar^2}{2M}\mathcal{G}^{ab}\partial_a\partial_b + MV_s\right)\psi(s_a) = 0\,, \tag{3.5}$$

i.e. the gravitational part only of of Eq. (2.41), must also hold. As we will see, such additional equations will replace the gauge conditions imposed in [42] at each order, allowing to write that proposal in the same way as [41].

The "semiclassical" constraint (3.4) or (3.5) yields, by substitution of ψ with (3.1) and expansion order by order, the Hamilton-Jacobi equation for the classical action S_0 (which must be a real function in order to give the correct classical limit, as discussed in [42]) and then the equations for each σ_n. For the $\hbar$ expansion, up to $\mathcal{O}(\hbar)^2$ we get

$$(\partial_a S_0)^2 + U_s = 0\,, \tag{3.6a}$$

$$2\mathcal{G}^{ab}\partial_a S_0\,\partial_b\sigma_1 - i\mathcal{G}^{ab}\partial_a\partial_b S_0 = 0\,, \tag{3.6b}$$

$$2\mathcal{G}^{ab}\partial_a S_0\,\partial_b\sigma_2 + (\partial_a\sigma_1)^2 - i\mathcal{G}^{ab}\partial_a\partial_b\sigma_1 = 0\,. \tag{3.6c}$$

Here the first two equations (which emerge at $\mathcal{O}(\hbar^0)$ and $\mathcal{O}(\hbar)$, having dropped the factors $\hbar^n$ in front) coincide with (2.26) and (2.27) respectively; the minisupermetric $\mathcal{G}_{ab}$ is implied in the squared terms. On the other hand, Eq. (3.6c)is a novel contribution with respect to [41], coming from the extension of such formulation up to the order $\hbar^2$. Analogously, the expansion of (3.5) in M gives at $\mathcal{O}(M)$, $\mathcal{O}(M^0)$ and $\mathcal{O}(M^{-1})$ respectively (again dropping the factors M^n in front)

$$\frac{1}{2}(\partial_a S_0)^2 + V_s = 0\,, \tag{3.7a}$$

$$\mathcal{G}^{ab}\partial_a S_0\,\partial_b\sigma_1 - \frac{i\hbar}{2}\mathcal{G}^{ab}\partial_a\partial_b S_0 = 0\,, \tag{3.7b}$$

$$\mathcal{G}^{ab}\partial_a S_0\,\partial_b\sigma_2 + \frac{1}{2}(\partial_a\sigma_1)^2 - \frac{i\hbar}{2}\mathcal{G}^{ab}\partial_a\partial_b\sigma_1 = 0\,. \tag{3.7c}$$

As evident from the comparison of (3.4) and (3.5), the two expansions give the same applied operators on the gravitational component $\psi_2 = e^{\frac{i}{\hbar}(\kappa^0 S_0+\kappa\sigma_1+\kappa^2\sigma_2)}$, apart from numerical factors attributed to the form of the semiclassical constraint and the choice of expansion parameter.

Turning our attention to the quantum subsystem's description, we plug the B-O-like ansatz (3.1) into the total WDW constraint (2.25) or (2.41), labeling H_q the subsystem's superHamiltonian and focusing on the first three orders and use the sets of Eqs. (3.6a)-(3.6c) or (3.7a)-(3.7c) to remove the semiclassical dynamics. Terms acting on the semiclassical functions only disappear, leaving just mixed derivative terms of the form $\partial_a S_0 \partial_b\chi$ or $\partial_a\sigma_n\partial_b\chi$. Dividing by ψ_2, we obtain for both cases

$$2\hbar^2 c_1\,\mathcal{G}^{ab}\partial_a(\ln\psi)\,\partial_b\chi = H_q\chi - \hbar^2 c_1\,\mathcal{G}^{ab}\partial_a\partial_b\chi \tag{3.8}$$

where we are able to write a single equation by introducing the parameter

$$c_1 = \begin{cases} 1 & \text{for the } \hbar \text{ expansion}\,, \\ \frac{1}{2M} & \text{for the } M \text{ expansion}\,, \end{cases} \tag{3.9}$$

which is imputable to the $1/2M$ factor in (3.5) with respect to (3.4), and not to any physical reason. Now we implement the time definition

$$\frac{\partial}{\partial\tau} \equiv 2c_2\,\mathcal{G}^{ab}\partial_a S_0\,\partial_b\,, \tag{3.10}$$

$$c_2 = \begin{cases} 1 & \text{for the } \hbar \text{ expansion}\,, \\ \frac{1}{2} & \text{for the } M \text{ expansion}\,. \end{cases} \tag{3.11}$$

as done in (2.31), (2.46), having chosen $N = 1$ for convenience as in Sec. 2.4[1]; we remark that the absence of M in c_2 is due to the lowest order of ψ, which is MS_0 in

[1]The result we will obtain is valid also for generic N, as can be seen by defining (3.10) with N inside and multiplying each order equation by N.

the M expansion and S_0 only in the $\hbar$ one by hypothesis. Eq. (3.8) then yields the corrected Schrödinger equation

$$i\hbar\frac{\partial\chi}{\partial\tau} = H_q\chi - \hbar^2 c_1 \mathcal{G}^{ab}\partial_a\partial_b\chi - 2i\hbar c_1\mathcal{G}^{ab}\partial_a P\,\partial_b\chi. \tag{3.12}$$

The semiclassical function S_0 is absent since it exhausted its role in the time definition (3.10), so that only the $P(s_a)$ part (3.2) remains.

It is important to notice that at orders $\mathcal{O}(\hbar)$ and $\mathcal{O}(M^0)$, Eq. (3.12) reduces to the exact Schrödinger equation for the quantum wave functional $\chi_1 = e^{\frac{i}{\hbar}Q_1}$:

$$i\hbar\frac{\partial\chi_1}{\partial\tau} = H_q\chi_1. \tag{3.13}$$

Then at the next orders $\mathcal{O}(\hbar^2)$ and $\mathcal{O}(1/M)$ the corrections to the standard dynamics emerge for χ_2: it is immediate to reconstruct with the previous order the following equation

$$i\hbar\frac{\partial\chi_2}{\partial\tau} = H_q\chi_2 - \left(2i\hbar c_1\mathcal{G}^{ab}\partial_a\sigma_1\,\partial_b + \hbar^2 c_1\mathcal{G}^{ab}\partial_a\partial_b\right)\chi_2\,. \tag{3.14}$$

Since the corrective terms here have the same form as (2.50), they are not unitary for the same reason. This result shows that, if we restrict the semiclassical subspace to the geometrical variables only in Vilenkin's formulation [41], the $\hbar$ expansion yields precisely the same results of the M expansion, also at the quantum gravity order.

It is possible to rewrite Eq. (3.12) in a nicer form with the procedure described in [44]. We assume the existence of a total "Hamiltonian" operator $\bar{H}$ (choosing $N = 1$ as in Sec. 2.4), in general not Hermitian, such that

$$i\hbar\frac{\partial\chi}{\partial\tau} = \bar{H}\chi, \tag{3.15}$$

and we also assume that

$$\partial_a\chi = \alpha(s_a)\partial_a S_0, \tag{3.16}$$

which is some sort of adiabatic approximation. The HJ equations (3.6a) and (3.7a) give

$$\alpha = -\frac{1}{2c_1 U_s}\frac{\partial\chi}{\partial\tau} = \frac{i}{2\hbar c_1 U_s}\bar{H}\chi, \tag{3.17}$$

where in the M expansion $U_s = MV_s$ such that $2c_1U_s = V_s$. Using eqs. (3.6b) and (3.7b), the corrected Schrödinger equation (3.12) becomes

$$i\hbar\frac{\partial\chi}{\partial\tau} \equiv \bar{H}\chi = H_q\chi - \frac{1}{4k_1U_s}\left(\bar{H}^2 + i\hbar\frac{\partial\bar{H}}{\partial\tau} - i\hbar K\bar{H}\right)\chi\,, \tag{3.18a}$$

$$K = \frac{1}{U_s}\frac{\partial U_s}{\partial\tau} - \frac{ik_2}{\hbar}\sum_{n=2}^{\infty}k_3^n\frac{\partial\sigma_n}{\partial\tau}, \tag{3.18b}$$

where in the $\hbar$ expansion $k_1 = k_2 = 1$ and $k_3 = \hbar$, while in the M expansion $k_1 = 2$, $k_2 = 2M$ and $k_3 = 1/M$. We remark that $\bar{H}$ is an abstract Hamiltonian operator containing H_q and all the corrections at every order. This procedure is just the generalization of that used in [42] to decompose the contributions tangential and orthogonal to the hypersurfaces $S_0 = \text{const}$. The use of eqs. (3.6b) and (3.7b) causes the sum in the expression of K here to begin from $n = 2$. At the quantum gravity order $\mathcal{O}(\hbar^2)$ and $\mathcal{O}(1/M)$, Eq. (3.18a) reconstructs exactly (2.50) that was derived in Sec. 2.4. However at higher orders, quantum gravity corrections arise not only from the $\mathcal{G}^{ab}\partial_a\partial_b$ operator in Eq. (3.12), but also from the one containing $\partial_a P$. As noted in [44], this result can equivalently be obtained if one considers σ_n, the potential U_s and χas functions of τ only from the beginning and leaves only the $\mathcal{G}_{\tau\tau}$ term of the (mini)supermetric, dropping all the other geometric components.

Let us now summarize the situation. Both the $\hbar$ and the M expansions recover GR through a HJ equation, that fixes a background, and a Schrödinger equation in curved space-time for QM (actually the $\hbar$ expansion is more general, since it admits backgrounds generated by matter sources and quantum geometry). The backreaction of the quantum subsystem on the background is not present in both approaches; including such a nonadiabatic effect would allow for quantum gravitational effects on the semiclassical sector itself, thus modifying the HJ equation as in Sec. 2.4.1. At the next order, both expansions yield non-Hermitian corrections due to quantum gravity effects that break the unitarity of the theory.

We now turn to a more in-depth discussion of such result, taking into account also the formulations [43, 44].

3.2 Phase rescaling and quantum backreaction

In the context of WKB formulations of quantum gravity and matter systems, exploring the concept of a quantum backreaction onto the semiclassical sector proves to be intriguing. Considering Vilenkin's work, this contribution is absent from the HJ due to the background assumption (2.24), while in [42] it is forbidden by the choice of expansion parameter, as mentioned above. In quantum cosmology, when perturbations are present, such backreaction would describe how small scale inhomogeneities influence the large-scale structure of the universe. We mention here the review [62] and the Space-Adiabatic Perturbation Theory (SAPT) proposal [63], a generalization of the Born–Oppenheimer procedure to study the adiabatic evolution of quantum states with spatially varying Hamiltonians.

We recall that the proposal [43] of Sec. 2.4.1 actually dealt with the backreaction effects, applying a rescaling to the two components of the wave function in a Born-Oppenheimer-like way. We remind that there the wavefunction is $\Psi(h_a, \phi) = \psi(h_a)\chi(h_a, \phi)$ taken with χ satisfying (2.51); so, if one considers a normalized total wave function Ψ, such condition will follow also for the background component ψ. The only freedom in such decomposition stands in the choice of the phase factor (2.54), which leaves Eqs. (2.52)-(2.53) invariant due to presence of the covariant derivatives D, $\bar{D}$.

Actually, since the matter component χ was rescaled using the average value of H_m (see (2.57)), the background wave functional should also be transformed as

$$\widetilde{\psi} = \mathrm{e}^{-\frac{i}{\hbar}\int \langle H_q \rangle d\tau} \psi_s \,, \tag{3.19}$$

in order to preserve the total wave function $\Psi = \psi\chi = \widetilde{\psi}\widetilde{\chi} = \psi_s\chi_s$. AS we will show, this transformation leads to drastic consequences which were not accounted in the original proposal. We here use again the WKB expansion in M for a clearer comparison with [42, 44] and decompose the quantity P in the ansatz (3.1) into its real and imaginary parts

$$\psi_s = e^{\frac{i}{\hbar}(MS_0+P)} = e^{\frac{M\rho}{\hbar}} e^{\frac{i}{\hbar}M(S_0+\zeta)}, \tag{3.20}$$

having labeled

$$\mathrm{Re}(P) \equiv \zeta = \frac{1}{M}\zeta_1 + \frac{1}{M^2}\zeta_2 + \dots\,, \tag{3.21a}$$

$$-\mathrm{Re}(P) \equiv \rho = \frac{1}{M}\rho_1 + \frac{1}{M^2}\rho_2 + \dots\,. \tag{3.21b}$$

The procedure of defining the WKB time as (3.10) still yields at order $\mathcal{O}\left(M^0\right)$ the Schrödinger equation (3.13). In contrast with [43], the rescaling (3.20) now corresponds to a different classical limit: at $\mathcal{O}\left(M\right)$ the usual HJ equation (3.7a) emerges, and at the next order one has

$$\begin{aligned} -\frac{i\hbar}{2}\mathcal{G}^{ab}\partial_a\partial_b S_0 + \mathcal{G}^{ab}\partial_a S_0\,\partial_b\zeta_1 - i\mathcal{G}^{ab}\partial_a S_0\,\partial_b\rho_1 \\ - \mathcal{G}^{ab}\partial_a S_0\,\partial_b \int \langle H_q\rangle d\tau + \langle H_q\rangle = 0\,. \end{aligned} \tag{3.22}$$

Thus, the backreaction has shifted from the HJ equation to the continuity equation; also, since the last two terms of (3.22) cancel because of (3.10), the rescaling (3.20) actually made the backreaction disappear. The same result would stand in the $\hbar$ expansion, because of the hypothesis of smallness of the quantum subsystem.

We note that the real and imaginary parts of (3.22) are

$$\mathcal{G}^{ab}\partial_a\partial_b S_0 + \mathcal{G}^{ab}\partial_a S_0\,\partial_b\rho_1 = 0\,, \tag{3.23}$$

$$\mathcal{G}^{ab}\partial_a S_0\,\partial_b\zeta_1 = 0. \tag{3.24}$$

The first corresponds to Eq. (3.7b), while the second points out that ζ_1 has no dynamical relevance: through (3.10), Eq. (3.24) reads

$$\partial_\tau\zeta_1 = 0. \tag{3.25}$$

Until now, we recovered precisely the results of [42] (and equivalently [41]), but with the adoption of the more advanced formalism of [43]. To investigate the quantum gravity corrections in such formulation, we again consider a simple cosmological model with the single gravitational degree of freedom a. This will keep us from dealing with the separation of the derivatives ∂_a, ∂_b into normal and tangential components (with respect to the $S_0 =$ const hypersurfaces) as in Sec. 2.4. We highlight that the present procedure is valid only if $\bar{R} \neq 0$, otherwise $\partial_\tau S_0 \propto V$ would vanish, giving trouble in the next steps (being V the geometric superpotential). The corrected Schrödinger equation up to $\mathcal{O}\left(M^{-1}\right)$ is

$$\begin{aligned} i\hbar\partial_\tau\chi_s =& \hat{H}_m\chi_s - \frac{1}{4MV}\bigg[\left(H_m^2 - \langle H_m^2\rangle\right) + i\hbar(\dot{H}_m - \langle\dot{H}_m\rangle) \\ & -i\hbar\frac{\dot{V}}{V}(H_m - \langle H_m\rangle)\bigg]\chi_s \end{aligned} \tag{3.26}$$

equivalent to Eq. (3.18a) of the approach [42]. An analogous equation for the background component ψ can be obtained, giving

$$\begin{aligned} -\frac{\hbar^2}{2}\mathcal{G}_{aa}\frac{\partial_a^2\widetilde{\psi}}{\widetilde{\psi}} =& \hbar^2\partial_\tau\zeta_2 - i\hbar^2\partial_\tau\rho_2 - \frac{1}{4V}\langle H_q\rangle^2 + \frac{i\hbar\dot{V}}{4V^2}\langle H_q\rangle - \frac{i\hbar}{4V}\langle\dot{H}_q\rangle \\ & - \frac{\hbar^2}{4V}(\partial_\tau\rho_1)^2 - \frac{\hbar^2\dot{V}}{4V^2}\partial_\tau\rho_1 + \frac{\hbar^2}{4V}\partial_\tau^2\rho_1\,, \end{aligned} \tag{3.27}$$

which can be further separated into real and imaginary parts, givings equations in which the backreaction is now present (we refer for the detailed calculation to the Appendix B of [61]). We note that, in (3.26), the non-Hermiticity of the quantum gravity Hamiltonian is still a problem, unless one takes the norm of a state, in which case Eq. (2.58) holds and all quantum gravity corrections vanish, presenting a stark difference from [42].

The concept of phase rescaling for the quantum subsystem was implemented also in [44], although in a different way. In that case, the procedure aimed to remove the non-unitary contribution and make the quantum gravity Hamiltonian a Hermitian operator. We here discuss such proposal within a toy model consisting of only one geometric variable, that we identify with the time τ from the beginning. With the ansatz (3.1), the dynamics of the quantum component (3.8) reads

$$\frac{\hbar^2}{M}\mathcal{G}_{\tau\tau}\partial_\tau\ln\psi\,\partial_\tau\chi = H_m\chi - \frac{\hbar^2}{2M}\mathcal{G}_{\tau\tau}\partial_\tau^2\chi + \rho_\psi\chi, \tag{3.28}$$

where the background term

$$\rho_\psi = \frac{1}{\psi}\left[-\frac{\hbar^2}{2M}\mathcal{G}_{\tau\tau}\partial_\tau^2 + MV_s\right]\psi \tag{3.29}$$

corresponds to the quantity set to zero in Eq. (3.5). Let us assume, differently from the previous proposal [42], that the background term ρ_{ψ_0} (where $\psi_0 = \exp\left(iMS_0/\hbar\right)$) is of order $\mathcal{O}\left(M^0\right)$: this means that the HJ equation

$$\frac{1}{2}\mathcal{G}_{\tau\tau}(\partial_\tau S_0)^2 + V = 0 \tag{3.30}$$

has to be itself of $\mathcal{O}\left(M\right)$, while in [42] it was the HJ equation (3.7a) multiplied by M that emerged at that order. Hence

$$\rho_{\psi_0} = -i\hbar\frac{\partial_\tau V_s}{2V_s} \tag{3.31}$$

and assuming the existence of an abstract Hamiltonian operator $\bar{H}$ as the one defined in (3.18a), we find

$$i\hbar\partial_\tau\chi_0 \equiv \bar{H}\chi_0 = \hat{H}_m\chi_0 - \frac{i\hbar}{2}\frac{\partial_\tau V}{V}\chi_0 - \frac{1}{4MV}\left[\bar{H}^2 + i\hbar\partial_\tau\bar{H}\right]\chi_0, \tag{3.32}$$

being χ_0 is the quantum wave function in $\Psi = \psi_0\chi_0$. Since this equation still exhibits non-Hermitian corrections, the authors then assume that two eigenvalue functions exist, $E(\tau)$ (complex) and $\epsilon(\tau)$ (real) such that

$$\bar{H}\chi_0 = E(\tau)\chi_0\,, \qquad \hat{H}_m\chi_0 = \epsilon(\tau)\chi_0, \tag{3.33}$$

which are then expanded in powers of $1/M$. Focusing on the eigenvalue $E(\tau)$ of the abstract Hamiltonian operator $\bar{H}$, Eq. (3.32) yields at orders M^0 and M^{-1}

$$E^{(0)} = \epsilon^{(0)} - \frac{i\hbar}{2}\frac{\partial_\tau V}{V}\,, \tag{3.34}$$

$$E^{(1)} = \epsilon^{(1)} - \frac{1}{4V}\left[\left(\epsilon^{(0)}\right)^2 + \hbar^2\frac{\partial_\tau^2 V}{2V} - \frac{3\hbar^2}{4}\left(\frac{\partial_\tau V}{V}\right)^2\right] - \frac{i\hbar}{4}\partial_\tau\left(\frac{\epsilon^{(0)}}{V}\right). \tag{3.35}$$

If one rescales the quantum wavefunction by

$$\chi_1 = e^{-\frac{1}{\hbar}\int \mathrm{Im}(E^{(0)})\,d\tau}\chi_0 = e^{\int \frac{\partial_\tau V}{2V}}\chi_0, \tag{3.36}$$

then Eq. (3.32) takes the simple form

$$i\hbar\partial_\tau\chi_1 = \hat{H}_m\chi_1\,, \tag{3.37}$$

i.e. the time derivative of the rescaled quantum state exactly compensates the non-Hermitian corrections on the right-hand side of Eq. (3.32) thanks to (3.31), leaving only the standard Schrödinger evolution. The background component ψ_1 must also be rescaled in such a way that $\Psi = \psi_1\chi_1$, i.e.

$$\psi_1 = e^{-\int \frac{\partial_\tau V}{2V}}\psi_0 = e^{\frac{i}{\hbar}MS_0 - \frac{1}{2}\ln V}\,. \tag{3.38}$$

We remark that, due to the rescalings (3.36),(3.38) of ψ and χ, their respective equations of motion are modified, while the total wave function Ψ remains invariant. By doing so, we find that ρ_{ψ_1} vanishes at order $\mathcal{O}\left(M^0\right)$, yielding the continuity equation

$$\partial_\tau^2 S_0 - \frac{1}{2}\partial_\tau S_0\partial_\tau\left(\ln V\right) = 0 \tag{3.39}$$

which naturally vanishes from (3.30). As a consequence ρ_{ψ_1} is of order M^{-1} and corresponds to

$$\rho_{\psi_1} = \frac{\hbar^2}{4MV}\left[\frac{3}{4}\left(\frac{\partial_\tau V}{V}\right)^2 - \frac{\partial_\tau^2 V}{2V}\right]. \tag{3.40}$$

The same steps can be followed at order $\mathcal{O}\left(M^{-1}\right)$, including Eq. (3.40) into (3.32) and redefining the quantum state as

$$\chi_2 = \mathrm{e}^{-\frac{1}{M\hbar}\int \mathrm{Im}(E^{(1)})\,d\tau}\chi_1\,, \tag{3.41}$$

so that the corrected Schrödinger equation for χ_2 will have only the Hermitian part of the Hamiltonian operator $\bar{H}$, therefore a unitary evolution. Actually at this order the background term calculated for ψ_2 such that $\Psi = \psi_2\chi_2$ will not vanish naturally, as an effect of the backreaction of the quantum subsystem.

This approach is founded on the concept that the non-Hermitian component of $\bar{H}$ can be eliminated from the dynamics governing the quantum subsystem by an appropriately redefinition of the composite wave functions within $\Psi = \psi\chi$. However, it is essential to acknowledge that the operator $\bar{H}$ is generally unknown and can only be systematically constructed in a perturbative manner. Additionally, to perform the rescaling of ψ and χ through phase factors, one must rely on the eigenvalues of

$\bar{H}$. The expressions (3.33) are based on the assumption that H_m and $\bar{H}$ commute at every order, allowing for simultaneous diagonalization; here a significant challenge arises, since such property is not valid in the general case. Indeed, as evident from (3.35), $E^{(1)}$ contains $\epsilon^{(0)}$ and its time derivative $\partial_\tau \epsilon^{(0)}$, therefore at $\mathcal{O}\left(M^{-1}\right)$ $\bar{H}$ contains both H_m and its time derivative, coherently with Eq. (3.18a). But H_m and $\dot{H}_m$ do not commute unless some specific conditions are met: this follows from observing that $\dot{H}_m$ will contain coordinate and conjugate momenta operators not commuting with H_m itself.

A simple example is a Friedmann-Lemaitre-Robertson-Walker (FLRW) model with cosmological constant and a free massless scalar field as matter component, with super-Hamiltonian and potential respectively

$$H_{\text{FRW}} = -\frac{G}{32c^3\pi a}p_a^2 + \frac{c}{4\pi^2 a^3}p_\phi^2 - V\,, \tag{3.42}$$

$$V(a;\Lambda) = \frac{3\pi c^3}{4G}\left(a - \frac{\Lambda}{3}a^3\right)\,. \tag{3.43}$$

Clearly, the momentum conjugate the scale factor a is proportional to the time derivative of a:

$$p_a \sim \frac{a}{N}\frac{da}{dt} = a\partial_\tau a. \tag{3.44}$$

The matter Hamiltonian in this simple model is just

$$H_m = \frac{c}{4\pi^2}a^{-3}p_\phi^2\,, \tag{3.45}$$

and its time derivative

$$\partial_\tau H_m = -\frac{3c}{4\pi^2}a^{-4}\partial_\tau a p_\phi^2 \sim a^{-5}p_a p_\phi\,, \tag{3.46}$$

contains the scale factor a, whose presence clearly leads to $[H_m, \partial_\tau H_m] \neq 0$. Therefore the proposal of [44] can be applied only in specific (cosmological) settings in which the matter Hamiltonian does not possess this property.

3.3 Discussion and origin of non-unitarity

In the literature, there has been extensive discussion regarding the issues of non-unitarity [64, 65, 44, 61, 40] and the establishment of a Hilbert space, e.g. [66, 67], within these types of approaches. A cosmological investigation of the proposal [42] with time definition (3.10) was outlined in [68, 52], despite the non-unitary features, to compute quantum-gravitational corrections to the power spectra of gauge-invariant scalar and tensor perturbations during the inflationary phase of the Universe (see discussion in Chapter 5). One could also request additional conditions such that the resulting dynamics is unitary: this is the case of [40], where implementing a scalar field clock the request of unitarity leads to a quantum recollapse of the model. In [69], a different inner product is discussed in relation to a Faddeev–Popov gauge-fixing procedure, which can reabsorb some troubling non-unitary terms.

It is important to stress that the non-unitarity here discussed is not an exclusive of the WKB approach to canonical quantum gravity. Indeed, it can also emerge in the context of modified theories of gravity when one adds renormalizability requirements to the corresponding quantum theory, see one of the earliest discussions in [70]. We mention the case of massive gravity, a theory in which the graviton particle acquires a non-zero mass, first introduced by Pauli and Fierz [71] and later reformulated via higher-derivative curvature terms or with the "gravitational Higgs mechanism" [72] i.e. via a spontaneously broken symmetry associated to coordinate reparametrization invariance. Massive gravity is in general plagued by the emergence of ghost fields, which are unphysical states associated to non-dynamical variables; their presence induces negative probabilities in the theory and so a violation of unitarity [73, 74]. A proposed solution to this issue is the so-called dRGT model [75], with predicted deviations from GR discussed in [76].

Resuming the discussion on the WKB approaches [41, 42, 43], one now faces the question if the non-unitary corrections here discussed are due to some common feature. A main point is that, in all of them, the clock for quantum matter (3.10) is constructed with the use of the semiclassical variables, i.e. using the dependence of the matter wave function χ from those. As it appears from the previous analyses, the most relevant term in the dynamics of χ which brings non-unitary effects is the semiclassical Laplacian $\mathcal{G}^{ab}\partial_a\partial_b$. Be it through some adiabatic assumption on χ, some projection parallel and orthogonal to the hypersurfaces $S_0 = \text{const}$, or simply by having time as the classical variable from the beginning, at some point that Laplacian generates terms of the form $\partial_\tau^2\chi$. We argue that this is the crucial point generating non-unitarity, since

$$-\hbar^2\partial_\tau^2\chi = i\hbar\partial_\tau(H_m\chi) = i\hbar\dot{H}_m\chi + H_m^2\chi\,. \tag{3.47}$$

This observation hints that, until time is defined through such Laplacian, the model is probably doomed to find non-Hermitian corrections at the quantum gravity level.

3.4 Unitarity via the kinematical action and Born-Oppenheimer separation

Here we present the proposal of [61] to solve the non-unitarity features previously found. This construction is based on a WKB expansion in the M parameter as in [42] but using different assumptions and, most importantly, a different construction of time: the physical clock for the gravity-matter system will not be given via the dependence of the subsystem on the semiclassical variables (3.10), but introducing a kinematical sector linked to the reference frame itself.

The kinematical action The introduction of the so-called kinematical action was first discussed in [77] as a tool to maintain the constraint equations of a quantum system by adding variables in the Lagrangian (and Hamiltonian) formalisms. Let us consider the case of scalar fields in a curved background. The kinematical action in the ADM representation reads:

$$\mathrm{S}^{kin} = \int d^4x(p_\mu\partial_t y^\mu - N^\mu p_\mu), \tag{3.48}$$

where the coordinates y^μ are those defining the parametric equations of the hypersurfaces in the ADM splitting, as in $y^\mu = y^\mu(x^i; x^0)$, see Sec. 1.5, and p^μ are the associated momenta. The additional equations of motion, obtained by variations of y^μ, p_μ and N^μ, show that the momenta p_μ are trivial (equal to 0) and recover the definition of the deformation vector (1.40). Additional contributions to the total super-Hamiltonian and supermomentum constraints clearly arise:

$$H^{kin} = n^\mu p_\mu \,, \tag{3.49}$$

$$H_i^{kin} = b_i^\mu p_\mu \,. \tag{3.50}$$

The form of the above expressions is the key to define a meaningful time variable for the matter field dynamics, in a different way than the works analyzed above. Indeed, let us consider a massive scalar field immersed in a given gravitational background (i.e. an assigned metric tensor). In the ADM variables, the corresponding action reads:

$$\mathrm{S}^\phi = \int dx^0 d^3x \left(\pi\dot{\phi} - NH^\phi - N^i H_i^\phi\right) \,, \tag{3.51}$$

$$\pi = \left(-\frac{1}{N^2}\dot{\phi} + 2\frac{N^i}{N^2}\partial_i\phi\right) N\sqrt{h} \,, \tag{3.52}$$

with corresponding super-Hamiltonian and supermomentum

$$H^\phi = \frac{1}{2\sqrt{h}}\pi^2 + \frac{1}{2}\sqrt{h}h^{ij}\partial_i\phi\partial_j\phi + \frac{1}{2}\sqrt{h}m^2\phi^2 \,, \tag{3.53}$$

$$H_i^\phi = (\partial_i\phi)\pi. \tag{3.54}$$

At this level, the lapse function and shift vector N and N^i are assigned functions up to a restriction given by the initial Cauchy problem. This means that N and N^i are not to be varied; thus, the physical definition of the ADM foliation on the background is lost.

However, one can add the term (3.48) which is independent from the metric and matter field variables. Then the total action reads

$$\mathrm{S}^{tot} = \int dx^0 d^3x \left[p_\mu \dot{y}^\mu + \pi\dot{\phi} - N\left(H^\phi + H^{kin}\right) - N^i\left(H_i^\phi + H_i^{kin}\right)\right] \,, \tag{3.55}$$

which leaves unchanged the dynamics of the scalar field but also reintegrates the definition (1.40) and so the structure of the space-time foliation, which would otherwise be lost. As a matter of fact, S^{kin} now allows to perform $\delta\mathrm{S}$ with respect to th kinematical action variables and restores the geometrical meaning of N, N^i. The super-Hamiltonian and supermomentum constraints

$$H^\phi = -H^{kin} = -p_\mu n^\mu \,, \tag{3.56}$$

$$H_i^\phi = -H_i^{kin} = -p_\mu b_i^\mu \tag{3.57}$$

are now nontrivial: the dynamics of the quantum field ϕ is characterized by parabolic constraints, linear in the momenta p_μ canonically conjugate to the four-dimensional variables y^μ, thought as fields depending on the slicing space-time variables. In the canonical quantization procedure, p^μ take the role of derivative operators, and so they can be crucial in the construction of the time derivative.

We now depart from the early analysis [77] and show how the kinematical action can be implemented in a Born-Oppenheimer-like approach as a clock for the matter dynamics, describing a unitary matter dynamics with quantum gravity corrections.

We closely follow the content of [61], considering a single scalar matter field ϕ with potential U_m, immersed in a given background; the generalization to the case of n matter fields is straightforward by replacing ϕ with $\sum_a \phi_a$ and inserting the cross-interaction terms into U_m. We also consider for the sake of generality the total superspace, without assuming specific symmetries of the problem, differently from Sec. 2.3 and 2.4. For this reason we implement the supermomentum constraints (which would be automatically satisfied in the homogeneous minisuperspace). Since we will implement the WKB expansion in a Planckian parameter as in Sec. 2.4, the notation here is analogous to (2.39)-(2.40) for a clearer comparison; we however do not change the variables h_{ij} representing the 3d metric with the labels h_a (which are essentially minisuperspace variables in Sec. 2.4 where no supermomentum constraint is implemented), but we leave the couples of spatial indices as in the ADM formulation (Sec. 1.5). We start from

$$\begin{aligned}\mathrm{S}^{\mathrm{tot}} &= \mathrm{S}^g + \mathrm{S}^m + \mathrm{S}^{kin} \\ &= \int dx^0 d^3x \Big[\Pi_a \dot{h}^a + p_\mu \dot{y}^\mu + \pi\dot{\phi} - N\left(H^g + H^m + H^{kin}\right) \\ &\qquad\qquad -N^i\left(H^g_i + H^m_i + H^{kin}_i\right)\Big]\,,\end{aligned} \tag{3.58}$$

where

$$H_i^g = -2h_{ij}D_k\Pi^{kj}\,, \tag{3.59}$$

$$H_i^m = (\partial_i\phi)\pi\,, \tag{3.60}$$

D_k is the (3-dimensional) induced covariant derivative associated to h_{ij} (see (1.60)), and the contributions of the kinematical action are (3.49)-(3.50). We now apply the canonical quantization to the whole system of gravity, matter and kinematical variables. Since the momenta p_μ in (3.56) act as functional derivative operators, now the total super-Hamiltonian and supermomentum constraints become:

$$(\hat{H}^g + \hat{H}^m)\Psi = -\hat{H}^k\Psi \;\to\; i\hbar n^\mu \frac{\delta}{\delta y^\mu}\Psi, \tag{3.61}$$

$$(\hat{H}^g_i + \hat{H}^m_i)\Psi = -\hat{H}^k_i\Psi \;\to\; i\hbar b_i^\mu \frac{\delta}{\delta y^\mu}\Psi\,, \tag{3.62}$$

clearly showing the advantage of such choice. It is now necessary to investigate if the added degrees of freedom of S^{kin} modify the classical content of the theory. Indeed, the kinematical action would emerge in the classical limit as a physical fluid [78], representing in a sense the "materialization" of the reference frame. This is analogous to the reference frame fixing procedure [57] of Sec. 2.5, where a Gaussian fluid emerges (although with some unphysical properties). We reserve a deeper discussion on this emergence of the reference frame for Chapter 4.

We here highlight a core aspect of this proposal: while we add the kinematical action to the full quantum system of gravity and matter, we regard it as a fast quantum component on the same footing of the quantum matter field ϕ. This means that the fluid associated to S^{kin} does not appear at the classical level in the HJ equation thanks to the WKB expansion, as we will see below.

We consider the following B-O-like separation

$$\Psi(h_{ij}, \phi, y^\mu) = \psi(h_{ij})\chi(\phi, y^\mu; h_{ij}) \tag{3.63}$$

which closely resembles the exact factorization program of molecular physics [79, 80]. Here, in analogy with (3.1) the slow-varying semiclassical part depends only on the induced 3d metric, while the "fast" quantum part depends on the matter and kinematical variables and parametrically (i.e. slowly) on the others. This separation is justified by considering the different energy scales of the two components, in a case where the scalar fields act as test fields giving negligible contribution to the background; then, their fast dynamics can be computed at nearly (but not truly) fixed values of the semiclassical variables. This observation is analogous to the original Born-Oppenheimer formulation in molecules, where the electrons play the part of the fast quantum component interacting with the slow atoms. The main difference here is that the slow sector, i.e. gravity, can be regarded as an environment interaction for the subsystem (in the sense that it influences the subsystem without being modified by it in the limit of negligible backreaction, see the following assumptions).

We now perform the WKB expansion of the system with respect to the parameter M (2.38) linked to the Planck mass, as in Sec. 2.4, although with some different assumptions. We recall that the choice of such expansion parameter allows to consistently separate the gravitational and matter sectors, which is the relevant case here. Our ansatz is constructed up to $\mathcal{O}(1/M)$, which is the one sufficient to investigate the corrections arising from the quantum-gravitational background (as in Sec. 2.4):

$$\Psi(h_{ij}, \phi, y^\mu) = \mathrm{e}^{\frac{i}{\hbar}\left(MS_0 + P_1 + \frac{1}{M}P_2\right)} \cdot \mathrm{e}^{\frac{i}{\hbar}\left(Q_1 + \frac{1}{M}Q_2\right)}. \tag{3.64}$$

Due to the separation (3.63), S_0 and P_n are functions of h_{ij} only, while the functions Q_n representing the fast component depend also on the matter and kinematical variables.

In order to follow more closely the original reasonings of the B-O molecular approximation, we assume the following:

I) Since typical matter scales are of the order $\simeq 100\,\mathrm{GeV}$ (for example, the most massive elementary particle in the Standard Model has $m_t \simeq 173\,\mathrm{GeV/c^2}$) thus very far from the Planckian one $m_{Pl} \simeq 10^{19}\,\mathrm{GeV/c^2}$, it is reasonable to assume that

$$\frac{\langle \hat{H}^m \chi \rangle}{\langle \hat{H}^g \Psi \rangle} = \mathcal{O}\left(\frac{1}{M}\right) \tag{3.65}$$

i.e. that the average values of the matter sectors are always one order smaller with respect to the gravitational (semiclassical) ones. This is analogous to Vilenkin's first hypothesis 1.

II) Reflecting Vilenkin's third one 3, we consider that a separate WDW constraint holds (actually two, one super-Hamiltonian and one super-momentum) for the background wave function ψ, as in (3.4):

$$\hat{H}^g \psi(h_{ij}) = 0\,, \qquad \hat{H}^g_i \psi(h_{ij}) = 0\,. \tag{3.66}$$

This fact is linked to our first hypothesis 3.65, since we are considering the backreaction of the quantum component to be not only small, but also negligible for the gravitational dynamics.

III) We also consider that the fast χ component has a small variation with respect to the slow variables, i.e.

$$\frac{\delta}{\delta h_{ij}} Q_n(\phi, y^\mu; h_{ij}) = \mathcal{O}\left(\frac{1}{M}\right)\,. \tag{3.67}$$

The equations to solve are the constraints of the total system and the constraints satisfied by the background wave function $\psi(h_{ij})$, which can be written in the form:

$$\left[-\frac{\hbar^2}{2M}\left(\mathcal{G}_{ijkl}\frac{\delta}{\delta h_{ij}}\frac{\delta}{\delta h_{kl}} + f_{ij}\frac{\delta}{\delta h_{ij}}\right) + MV_g\right]\psi = 0\,, \tag{3.68}$$

$$2i\hbar\, h_{ij} D_k \frac{\delta}{\delta h_{kj}}\psi = 0\,, \tag{3.69}$$

$$\begin{aligned}\Bigg[-\frac{\hbar^2}{2M}\left(\mathcal{G}_{ijkl}\frac{\delta}{\delta h_{ij}}\frac{\delta}{\delta h_{kl}} + f_{ij}\frac{\delta}{\delta h_{ij}}\right) + MV_g - \frac{\hbar^2}{2\sqrt{h}}\frac{\delta^2}{\delta\phi^2} + U_m \\ -i\hbar\, n^\mu \frac{\delta}{\delta y^\mu}\Bigg]\Psi = 0\,,\end{aligned} \tag{3.70}$$

$$\left(2i\hbar\, h_{ij} D_k \frac{\delta}{\delta h_{kj}} + i\hbar(\partial_i\phi)\frac{\delta}{\delta\phi} - i\hbar\, b^\mu_i \frac{\delta}{\delta y^\mu}\right)\Psi = 0\,, \tag{3.71}$$

where $V_g = V(h_{ij})$ and the matter potential U_m has been redefined incorporating the factor $\sqrt{h}$ present in (2.20). The present formulation, developed with a single matter field for which $H_m = -\hbar^2/2\sqrt{h}\,\delta^2_\phi + U_m$, can be easily generalized for more scalar fields ϕ_n by considering an appropriate sum over all constituents in (3.70)-(3.71) and replacing the single potential U_m with the the total matter interaction potential. The additional term $f_{ij}\delta_{h_{ij}}$ takes care of generic factor orderings for the derivative operators, as in Sec. 2.4. All derivative operators are to be considered as functional ones for the general case.

Plugging (3.63) into the above constraints, the first order of expansion is clearly the order M, giving:

$$\frac{1}{2}\mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\frac{\delta S_0}{\delta h_{kl}} + V_g = 0\,, \tag{3.72}$$

$$-2h_{ij}D_k\frac{\delta S_0}{\delta h_{kj}} = 0\,. \tag{3.73}$$

Here the first equation recovers the HJ for the purely gravitational part of the wave function; hence, the classical limit of gravity is ensured. Indeed, the (real) classical action S_0 can be computed from (3.72). Eq. (3.73) instead expresses its invariance under 3d diffeomorphisms, due to the hypothesis which holds even though we are working in the general superspace due to the hypothesis 3.66.

We now move to the next order $\mathcal{O}\left(M^0\right)$:

$$-\frac{i\hbar}{2}\mathcal{G}_{ijkl}\frac{\delta^2 S_0}{\delta h_{ij}\delta kl}+\mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\frac{\delta P_1}{\delta h_{kl}}-\frac{i\hbar}{2}f_{ij}\frac{\delta S_0}{\delta h_{ij}}=0\,, \tag{3.74}$$

$$-2h_{ij}D_k\frac{\delta P_1}{\delta h_{kj}}=0\,, \tag{3.75}$$

$$\begin{aligned}&-\frac{i\hbar}{2}\mathcal{G}_{ijkl}\frac{\delta^2 S_0}{\delta h_{ij}\delta kl}+\mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\frac{\delta P_1}{\delta h_{kl}}-\frac{i\hbar}{2}f_{ij}\frac{\delta S_0}{\delta h_{ij}}+U_m-\frac{i\hbar}{2\sqrt{h}}\frac{\delta^2 Q_1}{\delta\phi^2}\\&+\frac{1}{2\sqrt{h}}\left(\frac{\delta Q_1}{\delta\phi}\right)^2+n^\mu\frac{\delta Q_1}{\delta y^\mu}=0\,,\end{aligned} \tag{3.76}$$

$$-2h_{ij}D_k\frac{\delta P_1}{\delta h_{kj}}-(\partial_i\phi)\frac{\delta Q_1}{\delta\phi}+b_i^\mu\frac{\delta Q_1}{\delta y^\mu}=0\,. \tag{3.77}$$

We remark that all terms of the form $\delta Q_1/\delta h_{ij}$ are inherently of order M^{-1} due to the adiabatic assumption (4.12), therefore they do not appear at this level[2]. The Eq. (3.74) allows to compute the gravitational function P_1, which is also invariant under 3d diffeomorphisms due to (3.75).

The wave function at this order can be rewritten as:

$$\Psi_0=e^{\frac{i}{\hbar}(MS_0+P_1+Q_1)}=e^{\frac{i}{\hbar}MS_0}\psi_1\chi_1 \tag{3.78}$$

By plugging (3.74) into (3.76), and using Eq. (3.78), it is possible to rewrite the total super-Hamiltonian constraint in an interesting form:

$$\left(-\frac{\hbar^2}{2\sqrt{h}}\frac{\delta^2}{\delta\phi^2}+U_m\right)\chi_1=\hat{H}^m\chi_1=i\hbar\, n^\mu\frac{\delta}{\delta y^\mu}\chi_1 \tag{3.79}$$

where H^m is the matter super-Hamiltonian. This equation can be combined with the analogous one obtained by plugging (3.75) into (3.77), that gives:

$$i\hbar(\partial_i\phi)\frac{\delta}{\delta\phi}\chi_1=\hat{H}_i^m\chi_1=i\hbar\, b_i^\mu\frac{\delta}{\delta y^\mu}\chi_1\,. \tag{3.80}$$

It is now possible to assemble (3.79) and (3.80) with the coefficients N and N^i, in order to obtain the definition of the deformation vector (1.40) and the matter Hamiltonian density. Then, by integrating over the ADM hypersurfaces, those derivative operators become independent from the spatial coordinates and one can define:

$$\begin{aligned}i\hbar\frac{\delta}{\delta\tau}\chi_1&\equiv i\hbar\int_\Sigma d^3x\left(Nn^\mu+N^ib_i^\mu\right)\frac{\delta}{\delta y^\mu}\chi_1=i\hbar\int_\Sigma d^3xN^\mu\frac{\delta}{\delta y^\mu}\chi_1\\&=\hat{\mathcal{H}}^m\chi_1=\int_\Sigma d^3x\left(N\hat{H}^m+N^i\hat{H}_i^m\right)\chi_1\end{aligned} \tag{3.81}$$

[2]Even the combination $M\frac{\delta S_0}{\delta h_{ij}}\frac{\delta Q_1}{\delta h_{ij}}$ scales to the next order due to the factor $1/M$ which is in front of the whole gravitational superHamiltonian.

In other words, through the Dirac implementation and using the definition of the deformation vector, we have recast the total WDW constraint at this order as a functional Schrödinger equation for χ, overlapping with standard quantum field theory. We have not set specific choice of the lapse function N and shift vector N^i, n order for the result to be valid for a generic foliation i.e. not restricted to any gauge. This equation expresses the quantum dynamics of the matter field immersed in the (given) gravitational background, with a time parameter τ that clearly describes a nontrivial evolution.

We stress here the difference in the choice of the time coordinate from the proposals [41] and [42], since the time is not recovered from the dependence from the "slow" variables, shown to be source of concerns in Sec.3.3, but from the kinematical action variables y^μ. These variables are present in the definition of the deformation vector, that here has a geometrical connotation, since its values correspond to choices of ADM foliation on the background. The use of its definition (1.40) allows to combine and rewrite the momenta p_μ as a single derivative operator, thus constructing the time parameter for the matter subsystem from the kinematical action itself. Nonetheless, the results are formally the same as in [41] and [42], since the Schrödinger equation is recovered in all cases. The main difference and consequences of this approach is visible in the next order of expansion.

Let us write the corresponding equations of the WKB expansion at the order M^{-1}:

$$-\frac{i\hbar}{2}\mathcal{G}_{ijkl}\frac{\delta^2 P_1}{\delta h_{ij}\delta h_{kl}}+\frac{1}{2}\mathcal{G}_{ijkl}\frac{\delta P_1}{\delta h_{ij}}\frac{\delta P_1}{\delta h_{kl}}+\mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\frac{\delta P_2}{\delta h_{kl}}-\frac{i\hbar}{2}f_{ij}\frac{\delta P_1}{\delta h_{ij}}=0\,, \tag{3.82}$$

$$-2h_{ij}D_k\frac{\delta P_2}{\delta h_{kj}}=0 \tag{3.83}$$

$$\begin{aligned}-&\frac{i\hbar}{2}\mathcal{G}_{ijkl}\frac{\delta^2 P_1}{\delta h_{ij}\delta h_{kl}}+\frac{1}{2}\mathcal{G}_{ijkl}\frac{\delta P_1}{\delta h_{ij}}\frac{\delta P_1}{\delta h_{kl}}+\mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\frac{\delta P_2}{\delta h_{kl}}+M\mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\frac{\delta Q_1}{\delta h_{kl}}\\&-\frac{i\hbar}{2}f_{ij}\frac{\delta P_1}{\delta h_{ij}}-\frac{i\hbar}{2\sqrt{h}}\frac{\delta^2 Q_2}{\delta\phi^2}+\frac{1}{\sqrt{h}}\frac{\delta Q_1}{\delta\phi}\frac{\delta Q_2}{\delta\phi}=-n^\mu\frac{\delta Q_2}{\delta y^\mu}\end{aligned} \tag{3.84}$$

$$-2h_{ij}D_k\frac{\delta P_2}{\delta h_{kj}}-2h_{ij}D_k\frac{\delta Q_1}{\delta h_{kj}}-(\partial_i\phi)\frac{\delta Q_2}{\delta\phi}=-b_i^\mu\frac{\delta Q_2}{\delta y^\mu} \tag{3.85}$$

Here the contribution $\delta Q_1/\delta h_{ij}$ appears together with $\delta S_0/\delta h_{ij}$ for the assumption (4.12), since this term is of zeroth order in M and there is a factor $1/M$ in front. Eq. (3.82) allows to compute the function P_2, which is invariant under 3d diffeomorphisms by Eq. (3.83). We remark that all the gravitational functions of the ansatz (3.64) can thus be identified, thanks to the hypothesis (3.66). Now in the total wave function (3.64) we label

$$\Psi=e^{\frac{i}{\hbar}MS_0}\psi_1\,\chi_1\,\psi_2\,\chi_2\,, \tag{3.86}$$

$$\psi_2=e^{\frac{i}{\hbar}\frac{1}{M}P_2}\,,\quad \chi_2=e^{\frac{i}{\hbar}\frac{1}{M}Q_2}\,, \tag{3.87}$$

where χ_1 satisfies the Schrödinger equation (3.81). Now using Eq. (3.82) together with the results at the previous orders, after some manipulation Eq. (3.84) becomes:

$$i\hbar n^\mu\frac{\delta}{\delta y^\mu}\Psi=\hat{H}^m\Psi+\left(\mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\frac{\delta Q_1}{\delta h_{kl}}\right)\Psi \tag{3.88}$$

where we have omitted the term:

$$\hbar^2 \left(\frac{1}{\Psi} \frac{\delta}{\delta \phi} \Psi - \frac{1}{\psi_1} \frac{\delta}{\delta \phi} \psi_1 \right)^2 \Psi = - \frac{1}{M^2} \left(\frac{\delta Q_1}{\delta \phi} \right)^2 \Psi \tag{3.89}$$

since it is naturally of order $1/M^2$.

It is now evident that the corrections to the Schrödinger equation are emerging at this order, as in Sec. 3.1. To recover the total matter Hamiltonian and investigate the evolution, the supermomentum constraint must be used; plugging (3.83) into (3.85) gives:

$$i\hbar b_i^\mu \frac{\delta \Psi}{\delta y^\mu} = \hat{H}_i^m \Psi - 2 h_{ij} D_k \frac{\delta Q_1}{\delta h_{kj}} \Psi \tag{3.90}$$

and with the linear combination and integration over the hypersurfaces, that reconstruct the total Hamiltonian of the matter field $\mathcal{H}_m$, we obtain:

$$i\hbar \frac{\delta}{\delta \tau} \Psi = \hat{\mathcal{H}}^m \Psi + \int_\Sigma d^3x \left(N \mathcal{G}_{ijkl} \frac{\delta S_0}{\delta h_{ij}} \frac{\delta Q_1}{\delta h_{kl}} - 2 N^k h_{ij} D_k \frac{\delta Q_1}{\delta h_{kj}} \right) \Psi \tag{3.91}$$

where we remark that Ψ is the total wave function of the system up to order $1/M$, as defined in (3.87).

We can now further modify this expression to describe the matter field dynamics only. In fact, even though the WKB approach allows to solve the equations of the constraints order by order, and so the functions S_0 and Q_1 present here are already defined by the constraints at the previous orders, it is useful to rewrite the equation (3.91) such that only the wave function relative to the matter field $\chi(\phi, y^\mu; h_{ij})$ and the purely geometrical functions S_0, P_n appear. This because the explicit forms of S_0, P_1 and P_2 are defined by the purely gravitational constraints which can be solved separately, obtaining the expressions to substitute in the equation.

However, some attention is required to replace the total wave function Ψ with the matter wave function χ. Since by assumption the functions S_0, P_n do not depend on the variables y^μ nor ϕ, they can pass through the derivative operators $\delta/\delta\phi$ and $\delta/\delta y^\mu$ without changing the result. They can also be taken outside the integral $\int_\Sigma d^3x$, present in the definition of $\mathcal{H}$ and of the time derivative: indeed, the whole ψ is a functional of the geometries h_{ij} (and not all the induced metrics, since the supermomentum constraint for the gravitational part at each order assures that these functions are invariant under 3d diffeomorphisms).

To rewrite the corrections in the desired form, we can make use of assumption (3.67). Then, summing the orders M^0 and M^{-1}, the dynamics of the matter field including quantum gravity corrections becomes:

$$\begin{aligned} i\hbar \frac{\delta}{\delta \tau} \chi = \hat{\mathcal{H}}^m \chi + \int_\Sigma d^3x \Bigg[& N \mathcal{G}_{ijkl} \frac{\delta S_0}{\delta h_{ij}} \left(-i\hbar \frac{\delta}{\delta h_{kl}} \chi \right) \\ & - 2 N^k h_{ij} D_k \left(-i\hbar \frac{\delta}{\delta h_{kj}} \chi \right) \Bigg] \end{aligned} \tag{3.92}$$

Thus, at order $1/M$, we have arrived to write down a functional Schrödinger equation containing corrections from the quantum nature of the gravitational field.

We stress that the corrections here computed are of order $1/M$, where M is the appointed parameter of expansion, thanks to the adiabatic assumption (3.67) so they are of low magnitude and become relevant near the Planckian scale. Further discussion on this result is reserved for the following section.

3.5 On the kinematical action as a time

At this level, we present some remarks on the implementation [61], which hopefully help clarify some assumptions and put the analysis into a broader perspective:

- The decomposition into slow quantum system and fast quantum component is not carried out at the fundamental level of the Hilbert space. That is instead the case of the Page-Wootters mechanism, where the Hilbert space takes the form of a tensor product between a clock subsystem and the rest, the two components being non-interacting but entangled [81]. Here instead we are identifying different behaviors of the two parts, but allowing for an interaction between them; it is precisely this interaction (more specifically, the gravitational momenta acting on the fast wave function) that describes quantum-gravity-induced effects.

- One could construct a time starting from the observation that (2.17) has a Klein–Gordon-like structure[25, 26, 82] due to the pseudo-Riemmannian nature of $\mathcal{G}^{ab}$. By rescaling the minisupermetric by a factor $\sqrt{h}$ and taking $h^{1/4}$ as a generalized coordinate (with $h \neq 0$), which clearly has a different signature with respect to the remaining ones, one could use it as internal time. The system will then resemble the quantum description a relativistic particle. However the construction of the Hilbert space is still problematic, see next point.

- It is also possible to use the scalar field itself as a clock, even though it has the same signature of the "space-like" variables in $\mathcal{G}^{ab}$. Also here, one obtains a quantum dynamics analogous to that of a relativistic particle. However the system is affected by a subtle question concerning the construction of a Hilbert space [27]: the frequency separation is generally prevented by the presence of the two potential terms, one of matter and one gravitational, as in Eq. (1.62). Only under specific assumptions or in suitable asymptotic limits such separation can be achieved.

- Actually, the choices of $h^{1/4}$ or of ϕ as internal time coordinates could also be performed before the quantization procedure. Indeed, one could choose a classical time parameter by fixing the temporal gauge first, and then quantizing the system: this naturally leads to a reduction of the classical variational principle [3] and the quantum dynamics takes a Schrödinger-like form. However this approach has some ambiguities concerning the background independence of the theory, due to the gauge fixing. We refer the reader to the review [83] and meaningful cosmological examples in [84, 85].

- Lastly, we stress that the WDW equation is here considered in analogy to a single particle dynamics (see also [29]), without applying the so-called "third quantization approach" [86, 87]. Such formulation was originally introduced as a possible solution to the cosmological constant problem and postulated the production of "baby Universes", by considering an operator which could destroy or create universe wave functionals, in the same way one has operators of creation and destruction of particles in QFT [88, 89, 90].

In view of these considerations, the use of the kinematical action as a quantum clock for matter takes a new role: it is not an external field that defines time, since we have seen that its degrees of freedom are exactly the variables y^μ linked to the ADM foliation (1.5). Actually, it is the set of momenta conjugate to those variables that help us define the time evolution. Therefore, while this proposal does not constitute a relational approach in the strict sense, it shares the view of describing the evolution of the system as seen from such "fluid". We briefly mentioned that at the classical level the kinematical action would emerge as a fluid, in analogy with Kuchař and Torre's Gaussian fluid of Sec. 2.5, if one considered it as a "slow" gravitational component instead of a purely quantum nature. This aspect, which has not been further investigated here due to the assumption of the kinematical variables to belong to the "fast" sector, will be cleared in the next Chapter where we will implement the Kuchař-Torre fluid time in a B-O-like fashion.

The additional terms of (3.92), which now have a clear dependence on the gravitational sector (as opposed to (2.49)), are attributed to quantum gravity corrections. More specifically, they account for the fact that the "slow" sector is not completely classical, i.e. not completely fixed in the B-O analogy.

As a final remark, we motivate why the modified dynamics expressed by Eq. (3.92) is unitary, in contrast with those in Sec. 3.1, 3.3. To motivate this point, we first observe that these contributions are linear in the canonical gravitational momenta, acting as derivative operators in the Dirac quantization; by construction, these cannot lead to non-Hermitian terms. The factors N, N^i, $\mathcal{G}_{ijkl}$, h_{ij}, D^k, namely the ADM variables and superspace functions, also provide Hermitian contributions. Then only term left to investigate is $\delta_{h_{ij}}S_0$, being S_0 the lowest order function of the WKB expression (3.64). We have proved that S_0 belongs to the gravitational sector only, since it emerges at the $\mathcal{O}(M)$ as the function satisfying the HJ equation (3.72) corresponding to the classical vacuum limit (in the M expansion, matter does not enter this limit). One could argue that a matter contribution might emerge at the HJ level, so that the general expression of S_0 would not coincide with the one here chosen (or equivalently to the one in Sec. 2.4). However, by considering a more general $S_0(h_{ij},\phi)$ in (3.64), one would find an additional order in the WKB expansion i.e. $\mathcal{O}(M^2)$ giving

$$\left(\frac{\delta S_0}{\delta\phi}\right)^2 = 0\,. \tag{3.93}$$

This term would emerge from the action of $\hat{H}_m$ on Ψ in the total constraint, forcing S_0 to be independent of the matter field(s). Also, an $S_0(h_{ij},\phi)$ belonging to the fast sector would bring an inconsistency with the HJ equation (3.72), in which only the classical limit appears. In short, the choice of a gravitational-only function $S_0(h_{ij})$ in (3.64) is the only one coherent with the present B-O implementation. We recall that, in Sec. 3.2, we illustrated how the inclusion of classical matter sources in [43, 44] (by considering the average contribution $\langle H_q \rangle$ or setting (3.72) to not vanish, respectively) can lead to some inconsistencies; further considerations on the backreaction problem will be reserved for Sec. 5.3.1 and 6.2.

Having cleared the nature of S_0, it is now straightforward to demonstrate that (3.92) describes a unitary evolution at the $\mathcal{O}\left(1/M\right)$ level. Since S_0 is precisely the HJ function in the classical limit, it must be a real function and more precisely its derivative must coincide with the classical momentum, as reasoned in Vilenkin's original proposal itself (see the expression (2.28) in Sec. 2.3). Therefore $\delta_{h_{ij}} S_0$ is an Hermitian factor, which together with the canonical momenta acting on χ result in a unitary evolution with first-order quantum gravitational effects.

We stress the striking difference with the resulting dynamics of the approaches of Sec. 2.3-2.4 and 3.2: there, the terms $\delta_{h_{ij}} S_0 \delta_{h_{kl}}$ were used for the clock construction, leading to violations of unitarity ad the next order; here instead, with the motivated adiabatic hypothesis (4.12), they actually represent corrections emerging from the quantum gravitational character, while the kinematical action has taken the role of time.

Chapter 4

Time via the Gaussian reference fluid

The present Chapter is devoted to a formulation of the B-O model with WKB expansion in which the time parameter is derived in a different way. We start here from Kuchař and Torre's original proposal of fixing the Gaussian reference frame in a reparametrized way, but we implement the corresponding "reference fluid" in the gravity-matter system as a fast component. In analogy with the kinematical action, we show that the momenta associated to the fluid variables provide a physical time such that next-order dynamics of the matter component (i.e. with QG-induced corrections) is still unitary. We show that the two time constructions are completely equivalent in the homogeneous minisuperspace setting. Finally, we examine the effects of this modified dynamics in a FLRW toy model.

The content of this Chapter is based on Refs. [91, 92].

4.1 Motivation for a quantum-level fluid

In the previous Chapter we presented a dynamical description of the quantum gravity-matter system implementing the kinematical action as a fast sector to construct the time parameter. While by construction S^{kin} allowed to reinstate the geometric meaning (1.40) of the deformation vector for the ADM foliation, there is no manifest link between the variables y^μ, p_μ of S^{kin} and the reference system. In this sense, the original Kuchar and Torre's proposal (see Sec. 2.5) implemented the reference system in a clearer way, manifested as a fluid component through the action S^f_{par}.

Thus, we aim to reformulate the Kuchar-Torre fluid in light of a Born-Oppenheimer separation, as in Sec. 3.4, between gravity and matter. The system is again WKB expanded, taking into account also the supermomentum contributions. We work under the assumption that the slow-varying gravitational component obeys separately a corresponding (vacuum) Wheeler-DeWitt equation, as in [41] and in analogy with the previous Chapter. This is conceptually more coherent with a standard Born-Oppenheimer decomposition of the dynamics, at the same time it allows a result similar to [42] which instead uses gauge conditions order by order.

The use of the reference fluid is intrinsically very different from the proposals in [41, 42, 44] in the way a time coordinate emerges for the functional Schrödinger equation describing the quantum matter evolution. As stressed in Sec. 3.1, in those proposals the time is constructed via the dependence of the matter wave functional on the gravitational degrees of freedom, which at $\mathcal{O}(M)$ are purely classical functions of the label time. In other words, the time derivative of the functional χ is constructed by the sum:

$$\partial_t h \cdot \frac{\delta \chi}{\delta h}\,; \tag{4.1}$$

the morphology of such time coordinate is at the ground of nonunitary effects emerging at $\mathcal{O}\left(M^{-1}\right)$, as discussed in Sec. 3.3.

Through the reparametrized reference frame fixing, however, the time variable is provided by the reference fluid, emerging when the procedure of [57] is implemented via the WKB algorithm. We stress an important difference with respect to Kuchar and Torre's original proposal: we here formalize (as in Chapter 3) a Born-Oppenheimer separation of the system, in which the reference fluid is treated as fast matter-like component. The reason under this assumption is that the reference fluid variables (as the kinematical action ones) do not carry an intrinsic dynamics and only serve us to reinstate a notion of the starting geometry; therefore, the classical evolution of the gravitational sector in vacuum is self-contained in its respective equations, without adding S^{f}_{par} (or S^{kin}), as discussed in Sec. 3.4 and Sec. 2.5,so the most natural choice for the slow semiclassical sector is to contain only the gravitational degrees of freedom. This treatment permits us to reduce the presence of the fluid to an additional contribution for the quantum matter dynamics only, and no additional terms affect the gravitational HJ equation in this approximation scheme. More specifically, we aim to describe the time derivative as in [57], but with the absence of a reference fluid contribution in the classical limit.

We remark that in the proposed picture the reference fluid plays a role very similar to the kinematical action of Sec. 3.4 and actually, the results presented in this Chapter here overlap those of Chapter (3).

This very different methodology in constructing a clock for the quantum dynamics of matter has two advantages: (i) it allows us to avoid the dilemma of nonunitarity of the theory discussed in [42, 44], and (ii) we can clarify how some difficulties of the original analysis in [57] are overcome when the B-O separation takes place. Clearly, when considering the full quantum gravity problem as in [57] i.e. with gravity, matter, and the reference fluid are all on the same footing, the presence of a physical reference system (see also [45]) becomes nontrivial. We stress that the presence formulation relies on the B-O separation and on the WKB expansion in the Planckian parameter for the full dynamics, as in the previous Chapter; therefore, investigating the classical contribution of the reference fluid has a limited sense and is actually in contrast with such view. The reason is straightforward: with respect to the expansion in M, the gravitational degrees of freedom approach the quasi-classical limit at the highest order of expansion, while the matter and the reference fluid remain still in a quantum picture, i.e., the concept of classical matter must be limited as applied only to macroscopic phenomenological sources.

4.2 B-O model of gravity, matter, and the fluid

Let us consider the gravitational field together with the reference fluid and a self-interacting scalar field ϕ with potential $U_m(\phi)$. This field schematically represents the matter sector, which can be generalized for more scalar fields, and it assumes a key role in cosmological applications (see Chapter 5). The action of such a model corresponds to

$$\mathrm{S} = \int dt \int_\Sigma d^3x \left(\Pi^{ij}\dot{h}_{ij} + p_\phi\dot{\phi} - N(H^g + H^m) - N^i(H_i^g + H_i^m) \right) + \mathrm{S}^f_{par}, \quad (4.2)$$

where we have performed the ADM foliation, and the added term S^f_{par} represents the parametrized fluid of Kuchar and Torre's formulation of Sec. 2.5. This term can be written explicitly in ADM coordinates by observing that the Gaussian reference frame conditions give the following requirements on the components of the deformation vector $\mathbf{N}$:

$$N = \pm 1, \quad N^i = 0 \quad (4.3)$$

corresponding to the fluid action

$$\mathrm{S}^f = \int dt \int_\Sigma d^3x\sqrt{h} \left[-\frac{\mathcal{F}}{2}\left(N - \frac{1}{N} \right) + \mathcal{F}_i N N^i \right]. \quad (4.4)$$

As done in Sec. 2.5, the fluid terms can be rewritten by using the momenta associated with the Gaussian coordinates and introducing the coefficients (2.67) and (2.68), so that the fluid super-Hamiltonian and supermomentum are (2.65) and (2.66).

The Hamiltonian content of the theory is straightforward from Eq. (4.2). Wit the presence of the additional fields, the total super-Hamiltonian and supermomentum must still vanish:

$$H = H^f + H^g + H^m = 0\,, \quad (4.5)$$

$$H_i = H_i^f + H_i^g + H_i^m = 0\,, \quad (4.6)$$

being H^f and H_i^f those specified in (2.65) and (2.66). We use for the matter and gravitational superspace functions the same notation of the previous Chapter, i.e. the expressions (3.68)-(3.71) apart from the kinematical action contribution which is now absent.

Following from the previous Chapter (see Sec. 3.4), we implement a B-O-like separation in analogy with the the molecular problem [93]. The main idea is to postulate that the system can be separated into a slow quantum gravitational sector and a fast quantum component, now including both the reference fluid and the matter field. The corresponding energy scales are clearly separated by the Planckian parameter M, thus allowing a clearer treatment of the two sectors order by order. The inclusion of the Gaussian reference fluid in the fast sector draws is analogous to the kinematical action, whose role was to construct the time parameter in the WDW constraint. A graphical representation of this scheme is provided in Fig. 4.1.

Our ansatz is

$$\Psi\left(h_{ij}, \phi, X^\mu\right) = \psi\left(h_{ij}\right)\chi\left(\phi, X^\mu; h_{ij}\right), \quad (4.7)$$

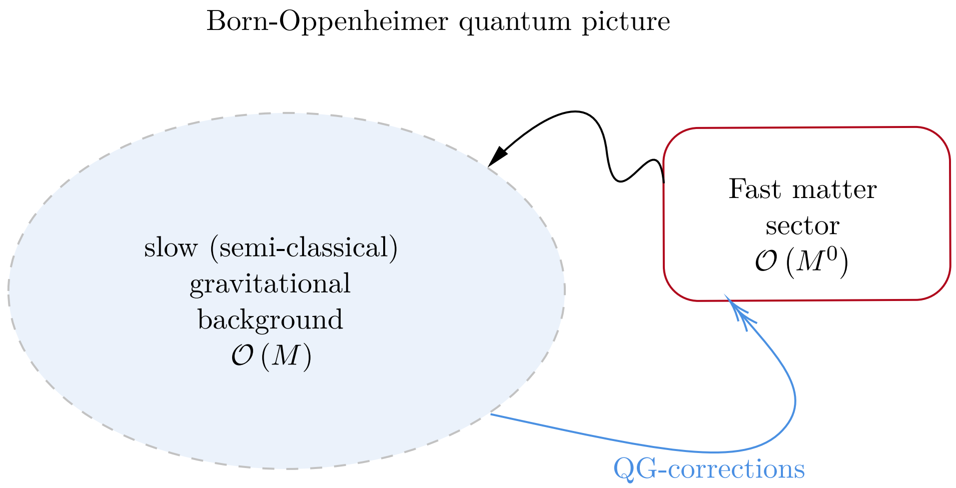

Figure 4.1. Schematic representation of the Born-Oppenheimer picture distinguishing the different scales of the gravitational and matter sectors. The gravitational one is of Planckian order, while the "fast" matter component living on such "slow" background starts at the next order in the expansion parameter. The quantum nature of the gravitational sector will cause a modification to the standard Schrödinger dynamics of the "fast" matter, i.e. it will induce QG effects at the next order.

where X^μ are the Gaussian coordinates, ψ is the function associated with the slow gravitational background, and χ is the function for the fast matter sector (depending parametrically i.e. on the background metric). Following the WKB method, we rewrite (4.7) expanding both ψ and χ in the Planckian parameter M (2.38):

$$\Psi\left(h_{ij},\phi,X^\mu\right) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left(MS_0+P_1+\frac{1}{M}P_2\right)}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left(Q_1+\frac{1}{M}Q_2\right)}\,, \tag{4.8}$$

where again the expansion is performed up to order $1/M$, sufficient for the investigation of quantum gravitational effects. In this notation, the functions $Q_n(\phi, X^\mu; h_{ij})$ are associated with the fast matter sector, and similarly $S_n(h_{ij})$ are the slow background functions.

Following the B-O approach of Sec. 3.4, we make the three following assumptions:

I) We require that

$$\frac{\langle\hat{H}^m\rangle_\chi}{\langle\hat{H}^g\rangle_\psi} = \mathcal{O}\left(\frac{1}{M}\right), \tag{4.9}$$

where $\langle\cdot\rangle$ denotes the average value over the relevant wave function. In other words, we are assuming that the fast matter sector lives at a smaller energy scale with respect to gravity i.e. it is of smaller order in the expansion parameter.

II) We again consider any matter effects to be negligible at the Planck scale, so that the gravitational wave function satisfies the following constraints

$$\hat{H}^g\,\psi(h_{ij}) = 0\,, \tag{4.10}$$

$$\hat{H}^g_i\,\psi(h_{ij}) = 0\,. \tag{4.11}$$

III) The adiabatic condition

$$\frac{\delta Q_n}{\delta h_{ij}} = \mathcal{O}\left(\frac{1}{M}\right), \tag{4.12}$$

must also be implemented, order by order, stating that the functional gradients of the fast χ with respect to the slow coordinates are small; this is in analogy to the B-O approximation in molecular dynamics.

These equations are to be adjoined to the total constraints of the system deriving from (4.5) and (4.6); namely, the system of equations to be expanded order by order reads explicitly:

$$\left[-\frac{\hbar^2}{2M}\left(\mathcal{G}_{ijkl}\frac{\delta}{\delta h_{ij}}\frac{\delta}{\delta h_{kl}} + f_{ij}\frac{\delta}{\delta h_{ij}}\right) + MV_g\right]\psi = 0\,, \tag{4.13}$$

$$2i\hbar\, h_{ij} D_k \frac{\delta}{\delta h_{kj}}\psi = 0\,, \tag{4.14}$$

$$\begin{aligned}\Bigg[-\frac{\hbar^2}{2M}\left(\mathcal{G}_{ijkl}\frac{\delta}{\delta h_{ij}}\frac{\delta}{\delta h_{kl}} + f_{ij}\frac{\delta}{\delta h_{ij}}\right) + MV_g - \frac{\hbar^2}{2\sqrt{h}}\frac{\delta^2}{\delta\phi^2} + U_m \\ + i\hbar W^{-1}\frac{\delta}{\delta T} + i\hbar W W^k\frac{\delta}{\delta X^k}\Bigg]\Psi = 0\,,\end{aligned} \tag{4.15}$$

$$\left(2i\hbar\, h_{ij} D_k \frac{\delta}{\delta h_{kj}} + i\hbar(\partial_i\phi)\frac{\delta}{\delta\phi} + i\hbar(\partial_i T)\frac{\delta}{\delta T} + i\hbar(\partial_i X^k)\frac{\delta}{\delta X^k}\right)\Psi = 0\,, \tag{4.16}$$

4.2.1 The classical limit

The zeroth order is $\mathcal{O}(M)$, where one obtains (omitting the M factor in front):

$$\frac{1}{2}\mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\frac{\delta S_0}{\delta h_{kl}} + V_g = 0\,, \tag{4.17}$$

$$-2h_{ij}D_k\frac{\delta S_0}{\delta h_{kj}} = 0\,. \tag{4.18}$$

corresponding to the HJ equation for gravity in vacuum, and to the diffeomorphism invariance for S_0. Here the function S_0 is real, as discussed in Sec. 3.5, since it corresponds to the classical HJ solution.

We stress that Eq. 4.17 does not include matter contributions since we have considered negligible backreaction and imposed independently the gravitational constraint. These two properties will be crucial in the following cosmological applications of Sec. 4.3 and Sec. 5.3; we will further discuss the role of backreaction at the HJ level in Sec. 5.3.1.

4.2.2 The QFT limit

At the order $\mathcal{O}(M^0)$, the equations give

$$-\frac{i\hbar}{2}\mathcal{G}_{ijkl}\frac{\delta^2 S_0}{\delta h_{ij}\delta kl} + \mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\frac{\delta P_1}{\delta h_{kl}} - \frac{i\hbar}{2}f_{ij}\frac{\delta S_0}{\delta h_{ij}} = 0\,, \tag{4.19}$$

$$-2h_{ij}D_k\frac{\delta P_1}{\delta h_{kj}} = 0\,, \tag{4.20}$$

$$\begin{aligned} &-\frac{i\hbar}{2}\mathcal{G}_{ijkl}\frac{\delta^2 S_0}{\delta h_{ij}\delta kl} + \mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\frac{\delta P_1}{\delta h_{kl}} - \frac{i\hbar}{2}f_{ij}\frac{\delta S_0}{\delta h_{ij}} + U_m - \frac{i\hbar}{2\sqrt{h}}\frac{\delta^2 Q_1}{\delta\phi^2} \\ &\quad + \frac{1}{2\sqrt{h}}\left(\frac{\delta Q_1}{\delta\phi}\right)^2 - W^{-1}\frac{\delta Q_1}{\delta T} - WW^k\frac{\delta Q_1}{\delta X^k} = 0\,, \end{aligned} \tag{4.21}$$

$$-2h_{ij}D_k\frac{\delta P_1}{\delta h_{kj}} - (\partial_i\phi)\frac{\delta Q_1}{\delta\phi} - (\partial_i T)\frac{\delta Q_1}{\delta T} - (\partial_i X^k)\frac{\delta Q_1}{\delta X^k} = 0\,. \tag{4.22}$$

Here, the gravitational constraints simplify Eqs. (4.21) and (4.22). We remember that the quantum matter wave function is at this order

$$\chi_0 = \mathrm{e}^{\frac{i}{\hbar}Q_1}\,, \tag{4.23}$$

so we can combine Eqs. (4.21) and (4.22) in order to reconstruct the total matter Hamiltonian for χ_0, in analogy with Sec. 3.4, resulting in the following:

$$\begin{aligned} \hat{\mathcal{H}}^m\chi_0 &= \int d^3x(NH^m + N^iH^m_i) = i\hbar\frac{\delta}{\delta\tau}\chi_0 \\ &\equiv \int d^3x\left[\Big(NW^{-1} + N^i(\partial_i T)\Big)\frac{\delta}{\delta T} + \Big(NWW^k + N^i(\partial_i X^k)\Big)\frac{\delta}{\delta X^k}\right]\chi_0\,, \end{aligned} \tag{4.24}$$

which describes a functional Schrödinger evolution, when one defines the quantum clock of the theory via the fluid momenta operators. In this sense we have recovered the standard QFT evolution on the assigned background. We remark that definition (4.24) is a generalization of the time derivative implemented in the Kuchař-Torre model when choosing the time parameter as exactly the Gaussian time (2.71), as well as choosing $x^i \equiv X^i$ or both conditions at the same time. Indeed, we here maintain the Gaussian coordinates as functions of the generalized parameters, not implementing a specific coordinate choice with this definition.

4.2.3 The quantum-gravity corrections

Going up to the next order $\mathcal{O}\left(M^{-1}\right)$ one finds (omitting the factor $1/M$ in front of every equation):

$$-\frac{i\hbar}{2}\mathcal{G}_{ijkl}\frac{\delta^2 P_1}{\delta h_{ij}\delta h_{kl}} + \frac{1}{2}\mathcal{G}_{ijkl}\frac{\delta P_1}{\delta h_{ij}}\frac{\delta P_1}{\delta h_{kl}} + \mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\frac{\delta P_2}{\delta h_{kl}} + -\frac{i\hbar}{2}f_{ij}\frac{\delta P_1}{\delta h_{ij}} = 0\,, \tag{4.25}$$

$$-2h_{ij}D_k\frac{\delta P_2}{\delta h_{kj}} = 0\,, \tag{4.26}$$

$$\begin{aligned} &-\frac{i\hbar}{2}\mathcal{G}_{ijkl}\frac{\delta^2 P_1}{\delta h_{ij}\delta h_{kl}} + \frac{1}{2}\mathcal{G}_{ijkl}\frac{\delta P_1}{\delta h_{ij}}\frac{\delta P_1}{\delta h_{kl}} + \mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\frac{\delta P_2}{\delta h_{kl}} + M\mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\frac{\delta Q_1}{\delta h_{kl}} \\ &\quad - \frac{i\hbar}{2}f_{ij}\frac{\delta P_1}{\delta h_{ij}} - \frac{i\hbar}{2\sqrt{h}}\frac{\delta^2 Q_2}{\delta\phi^2} + \frac{1}{\sqrt{h}}\frac{\delta Q_1}{\delta\phi}\frac{\delta Q_2}{\delta\phi} - W^{-1}\frac{\delta Q_2}{\delta T} \\ &\quad - WW^k\frac{\delta Q_2}{\delta X^k} = 0\,, \end{aligned} \tag{4.27}$$

$$-2h_{ij}D_k\frac{\delta P_2}{\delta h_{kj}} - 2Mh_{ij}D_k\frac{\delta Q_1}{\delta h_{kj}} - (\partial_i\phi)\frac{\delta Q_2}{\delta\phi} - (\partial_i T)\frac{\delta Q_2}{\delta T} - (\partial_i X^k)\frac{\delta Q_2}{\delta X^k} = 0\,. \quad (4.28)$$

Here again, the first terms in (4.27) and (4.28) disappear due to the gravitational constraints, leaving terms that contain the functions Q_2 and Q_1. However, noting that the quantum matter wave function at $\mathcal{O}\left(M^{-1}\right)$ is

$$\chi_1 = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left(Q_1 + \frac{1}{M}Q_2\right)}, \quad (4.29)$$

and making use of the adiabatic condition (4.12), we can sum Eqs. (4.27)-(4.28) with the Eqs. (4.21)-(4.22) found at the previous order (i.e. $\mathcal{O}\left(M^0\right)$) for Q_1. Therefore we find for the super-Hamiltonian (scalar) equation

$$\begin{aligned} &\mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\frac{\delta Q_1}{\delta h_{kl}} - \frac{i\hbar}{2\sqrt{h}}\left(\frac{\delta^2 Q_1}{\delta\phi^2} + \frac{1}{M}\frac{\delta^2 Q_2}{\delta\phi^2}\right) + \frac{1}{2\sqrt{h}}\left(\frac{\delta Q_1}{\delta\phi}\right)^2 + U_m \\ &\quad + \frac{1}{M\sqrt{h}}\frac{\delta Q_1}{\delta\phi}\frac{\delta Q_2}{\delta\phi} - \left(W^{-1}\frac{\delta}{\delta T} + WW^k\frac{\delta}{\delta X^k}\right)\left(Q_1 + \frac{1}{M}Q_2\right) = 0\,, \end{aligned} \quad (4.30)$$

where the matter super-Hamiltonian H^m is applied to χ_1 and we have some extra terms, some with the functional derivatives with respect to the Gaussian coordinates. From the supermomentum constraint, with the same procedure, one finds

$$\begin{aligned} &-2h_{ij}D_k\frac{\delta Q_1}{\delta h_{kj}} - (\partial_i\phi)\left(\frac{\delta Q_1}{\delta\phi} + \frac{1}{M}\frac{\delta Q_2}{\delta\phi}\right) - (\partial_i T)\left(\frac{\delta Q_1}{\delta T} + \frac{1}{M}\frac{\delta Q_2}{\delta T}\right) \\ &\quad - (\partial_i X^k)\left(\frac{\delta Q_1}{\delta X^k} + \frac{1}{M}\frac{\delta Q_2}{\delta X^k}\right) = 0\,, \end{aligned} \quad (4.31)$$

i.e. the action of the matter supermomentum $\hat{H}^m_i$ on χ_1 plus extra terms.

Now the time definition (4.24) can clearly be reconstructed: we first multiply (4.30) by N and (4.31) by N^i and sum them, the we integrate over the spatial hypersurfaces Σ obtaining

$$\begin{aligned} &\int d^3x\left[N\left(W^{-1}\frac{\delta}{\delta T} + WW^k\frac{\delta}{\delta X^k}\right) + N^i\left((\partial_i T)\frac{\delta}{\delta T} + (\partial_i X^k)\frac{\delta}{\delta X^k}\right)\right]\chi_1 \\ &\quad \equiv \mathrm{i}\hbar\frac{\delta}{\delta\tau}\chi_1 = \hat{\mathcal{H}}^m\chi_1 + \int d^3x\left[N\mathcal{G}_{ijkl}\frac{\delta S_0}{\delta h_{ij}}\left(-i\hbar\frac{\delta}{\delta h_{kl}}\right)\right. \\ &\quad \left. -2N^k h_{ij}D_k\left(-i\hbar\frac{\delta}{\delta h_{kj}}\right)\right]\chi_1\,. \end{aligned} \quad (4.32)$$

It is evident that the quantum matter dynamics at $\mathcal{O}\left(M^{-1}\right)$ is modified by the terms in (4.32) due to the slow quantum gravitational background, therefore they are quantum gravity contributions. The modified dynamics has the same functional form as the one obtained in (3.92) via the kinematical action implementation. Since we already motivated that those correspond to a unitary dynamics (see Sec. 3.5), the same reason stands in this case and thus the nonunitarity problem is overcome with this approach. We can then think of the kinematical action as a reference frame, which (once fixed) emerges in the formalism as a fluid with the properties discussed above.

Analogy with the kinematical action We here highlight another important observation. As we have seen, the remaining corrective terms in (4.32) exactly mimic the ones of (3.92). Actually, the time definitions (3.81) and (4.24) can be related. Let us take the Gaussian reference fluid contribution with only the time condition $\mathcal{F} \neq 0, \mathcal{F}_i = 0$ that is the incoherent dust (i.e. a fluid with null heat conductivity, which greatly simplifies the equations for this approach); this is compatible with selecting a homogeneous setting in which the supermomentum constraints are identically satisfied. If we also restrict the kinematical action to the form $\partial_t y^\mu \to \dot{T}$ by selecting the homogeneous setting with $N^i = 0$ and time-like direction $n^\mu = (1, \vec{0})$, then the two time definitions exactly coincide; moreover, the modified dynamics is the same both at $\mathcal{O}\left(M^0\right)$ and $\mathcal{O}\left(M^{-1}\right)$.

This property signals that the kinematical action is playing the role of the reference frame, acting as a fast quantum matter component and giving a preferred set of variables suitable for the construction of the time parameter. However, the parallelism is not present in a generic non-homogeneous model with arbitrary foliation, since the two implementations (3.81) and (4.24) would differ. Therefore, we have a correlation between the two approaches, since the kinematical action was added exactly to play the role of a reference system in the previous work.

4.3 A simple example: the FLRW model

In this section, we show a simple cosmological application of the procedure previously analyzed, choosing a model for the universe with suitable characteristics in order to mimic a slow-roll inflation period (see discussion of Chapter 5). We select an isotropic Universe, with a free inflaton field and a cosmological constant that accounts for the almost constant inflaton potential. Evidently, due to the requirement of an isotropic model, the spatial term of the Gaussian coordinates vanishes identically and the reference time coincides with Gaussian time.

In order to deal with a gravity-matter Lagrangian as restricted to a reference frame having $g^{00} = -1$, we must suitably add a corresponding constraint to the total action. If we denote by T the time variable associated with the fixed reference system (i.e., the Gaussian fluid), the constraint to be imposed covariantly reads

$$g^{\mu\nu}\partial_\mu T \partial_\nu T + 1 = 0\,, \tag{4.33}$$

such that the total action reads

$$\mathrm{S} = \int d^4x\sqrt{-g}\frac{c^4}{16\pi G}\left(R - 2\Lambda\right) + \frac{1}{2}g^{\mu\nu}\partial_\mu\phi\,\partial_\nu\phi - \frac{\mathcal{F}}{2}\left(g^{\mu\nu}\partial_\mu T\,\partial_\nu T + 1\right)\,. \tag{4.34}$$

We consider the spatially-flat homogeneous and isotropic Friedmann-Lemaitre-Robertson-Walker (FLRW) universe, see Sec. 1.6.1, i.e. we deal with the ADM line element (in $c = 1$)

$$ds^2 = -N(t)^2 dt^2 + a(t)^2\left(dx^2 + dy^2 + dz^2\right)\,, \tag{4.35}$$

with associated Ricci scalar curvature

$$R = 6\left(\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2}\right). \tag{4.36}$$

Taking equal to unity the fiducial volume over which the spatial integration is performed, and observing that the homogeneity of the model implies $\phi = \phi(t)$, $T = T(t)$, and $\mathcal{F} = \mathcal{F}(t)$, the action (4.34) reads as

$$\mathrm{S} = \int dt \left\{ -\frac{3}{8\pi G}\left(\frac{a\,\dot{a}^2}{2N} + \frac{N\Lambda a^3}{3}\right) + \frac{a^3\dot{\phi}^2}{2N} - \frac{\mathcal{F}a^3}{2}\left(\frac{\dot{T}^2}{N} - N\right)\right\}, \tag{4.37}$$

where the dot denotes differentiation with respect to the time variable t. The spatial component N^i, and so the supermomentum functions H_i, are not present since the supermomentum constraint is automatically satisfied due to symmetry of the model.

Since the Lagrangian term corresponding to the reference frame fixing vanishes identically, its Hamiltonian contribution is only $p_T\dot{T}$, where p_T is the conjugate momentum to the variable T (coinciding with the synchronous time variable). The relation between p_T and the Lagrange multiplier can be found from

$$p_T = \mathcal{F}a^3\frac{\dot{T}}{N}\,, \tag{4.38}$$

where to ensure $\dot{T} = N$, we have to require $p_T = \mathcal{F}a^3$. In the Hamiltonian formulation (4.37) rewrites as

$$\mathrm{S} = \int dt\left\{p_a\dot{a} + p_\phi\dot{\phi} + p_T\dot{T} - NH\right\} \tag{4.39}$$

with

$$H \equiv -\frac{\kappa}{12}\frac{p_a^2}{a} + \frac{\Lambda}{\kappa}a^3 + \frac{p_\phi^2}{2a^3} + p_T\,, \tag{4.40}$$

p_a and p_ϕ denoting the conjugate momenta to a and ϕ respectively. Since we are interested in the WKB expansion in the Planckian parameter M, we use the definition (2.38) to write the Wheeler-DeWitt constraint for this model (up to the fiducial volume set to unit) as

$$\left(\frac{\hbar^2}{48Ma}\partial_a^2 + 4M\Lambda a^3 - \frac{\hbar^2}{2a^3}\partial_\phi^2 - i\hbar\,\partial_T\right)\Psi = 0\,. \tag{4.41}$$

Here we have chosen the natural operator ordering by setting $f_{ij}\delta/\delta h_{ij} = 0$ in (4.5), as the final result will be unaffected; we have also replaced the functional dependence and derivatives with simple functions and partial derivatives only due to the minisuperspace setting.

Following the steps of the previous section, we separate and expand the total wave function of the isotropic universe as (4.8), identifying the functions $Q_n(T,\phi;a)$ for the matter components (scalar field and Gaussian fluid time), while $S_0(a)$ and $P_n(a)$ are for the isotropic background. We implement the same assumptions, so the conditions (4.9) and (4.12) together with the Wheeler-DeWitt constraint for the gravitational sector (the supermomentum one is already satisfied) which reads

$$H^g\,\psi(a) = \left(\frac{\hbar^2}{48aM}\,\partial_a^2 + 4M\Lambda a^3\right)\mathrm{e}^{\frac{i}{\hbar}\left(MS_0 + S_1 + \frac{1}{M}S_2\right)} = 0\,. \tag{4.42}$$

The total super-Hamiltonian constraint, taking contributions from the matter components, is explicitly

$$\begin{aligned}&(\hat{H}^g + \hat{H}^f + \hat{H}^\phi)\,\Psi(\phi, T; a)\\ &= \left(\frac{\hbar^2}{48aM}\,\partial_a^2 + 4M\Lambda a^3 - \frac{\hbar^2}{2a^3}\partial_\phi^2 - i\hbar\,\partial_T\right) e^{\frac{i}{\hbar}\left(MS_0+S_1+Q_1+\frac{1}{M}(S_2+Q_2)\right)} = 0\,.\end{aligned} \tag{4.43}$$

Proceeding order by order, we first obtain the HJ equation for the gravitational background at $\mathcal{O}\left(M^1\right)$:

$$-\left(\partial_a S_0\right)^2 + 192\Lambda a^4 = 0\,, \tag{4.44}$$

which gives the solution for the classical action S_0.

At $\mathcal{O}\left(M^0\right)$, we obtain

$$\mathrm{i}\hbar\partial_a^2 S_0 - 2\partial_a S_0 \partial_a S_1 = 0\,, \tag{4.45}$$

$$\frac{\mathrm{i}\hbar}{48a}\partial_a^2 S_0 - \frac{1}{24a}\partial_a S_0 \partial_a S_1 - \frac{\mathrm{i}\hbar}{2a^3}\partial_\phi^2 Q_1 + \frac{1}{2a^3}\left(\partial_\phi Q_1\right)^2 = -\partial_T Q_1\,, \tag{4.46}$$

which can be rewritten by inserting the first equation into the second one and labeling as $\chi_0 = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}Q_1}$ the matter wave function at this order, as the following:

$$-\frac{\hbar^2}{2a^3}\partial_\phi^2\chi_0 = \hat{H}^m\chi_0 = \mathrm{i}\hbar\,\partial_T\chi_0\,. \tag{4.47}$$

At $\mathcal{O}\left(M^{-1}\right)$ we have

$$\mathrm{i}\hbar\partial_a^2 S_1 - \left(\partial_a S_1\right)^2 - 2\partial_a S_0 \partial_a S_2 = 0\,, \tag{4.48}$$

$$\begin{aligned}&\frac{\mathrm{i}\hbar}{48a}\partial_a^2 S_1 - \frac{1}{48a}\Big(\left(\partial_a S_1\right)^2 + 2\partial_a S_0\partial_a S_2 + 2M\partial_a S_0 \partial_a Q_1\Big) - \frac{\mathrm{i}\hbar}{2a^3}\partial_\phi^2 Q_2\\ &\quad + \frac{1}{a^3}\partial_\phi Q_1 \partial_\phi Q_2 = -\partial_T Q_2\,.\end{aligned} \tag{4.49}$$

Here again, the solution S_2 from the first equation simplifies the form of the second one, leaving

$$-\frac{M}{24a}\partial_a S_0 \partial_a Q_1 - \frac{\mathrm{i}\hbar}{2a^3}\partial_\phi^2 Q_2 + \frac{1}{a^3}\partial_\phi Q_1 \partial_\phi Q_2 = -\partial_T Q_2\,. \tag{4.50}$$

Remembering that the matter wave function at this order is$\chi_1 = e^{\frac{i}{\hbar}\left(Q_1+\frac{1}{M}Q_2\right)}$ and that by hypothesis (4.12) the term $\partial_a Q_2$ is of higher order in the expansion, we can write summing (4.50) with (4.47):

$$i\hbar\,\partial_T\chi_1 = \hat{\mathcal{H}}_m\chi_1 + i\hbar\frac{1}{24a}(\partial_a S_0)\partial_a\chi_1\,. \tag{4.51}$$

The first term on the right-hand side is just the quantum matter Hamiltonian operator $-\hbar^2\partial_\phi^2/2a^3$ of this toy model, while the second one is the quantum-gravity corrective term which is small ($\mathcal{O}\left(M^{-1}\right)$) due to hypothesis (4.12). This modified dynamics would have been the same if we had used the kinematical action time as defined in (3.81). Since we interpret this contribution as a "fast variable" in the sense of a Born-Oppenheimer approximation, the nonphysical character of the emerging synchronous fluid (Sec. 4.1) is overcome.

4.3.1 Solution of the perturbative scheme

We now compute an explicit solution of this minisuperspace application. Starting from the gravitational solutions, at $\mathcal{O}\left(M^1\right)$ Eq. (4.44) gives

$$S_0(a) = -\frac{8\sqrt{3}}{3}\sqrt{\Lambda}\left(a^3 - a_0^3\right), \tag{4.52}$$

where a_0 is the value of the cosmic scale factor at a reference time (e.g., the start of the slow-roll phase); the negative solution has been selected to correspond to an expanding universe. At $\mathcal{O}\left(M^0\right)$, we obtain from (4.45),

$$S_1(a) = \mathrm{i}\hbar \log\left(\frac{a}{a_0}\right). \tag{4.53}$$

Finally, at $\mathcal{O}\left(M^{-1}\right)$ we get from (4.48)

$$S_2(a) = -\frac{\hbar^2}{24\sqrt{3}\sqrt{\Lambda}}\left(a^{-3} - a_0^{-3}\right). \tag{4.54}$$

We now focus on the fast matter sector. For the computation of these functions, it is useful to work in Fourier space, using the previous notation for the conjugated momenta p_ϕ and p_a, so that the general solution takes the form

$$\chi_1(a,\phi,T) = \int dp_\phi \int dp_a\, \tilde{\chi}(p_\phi,p_a,T) f(p_\phi,p_a), \tag{4.55}$$

where f is a generic weight function. At $\mathcal{O}\left(M^0\right)$, the dynamics is described by (4.47), so that the solution corresponds to the natural plane wave for quantum matter on a (classical) curved background:

$$\tilde{\chi_0} = e^{-\mathrm{i}\hbar\frac{p_\phi^2}{2a^3}T}. \tag{4.56}$$

The quantum gravity effects emerge at the next order, where the matter dynamics is described by Eq. (4.51). To solve it, it is convenient to use a rescaled time parameter

$$d\tau = \frac{dT}{a^3}. \tag{4.57}$$

In this way, the dynamics for the fast matter function χ_1 is

$$\mathrm{i}\hbar\,\partial_\tau\tilde{\chi_1} = \frac{\hbar^2 p_\phi^2}{2}\tilde{\chi_1} + \frac{\hbar\, p_a\,(-\tau)^{4/3}}{3(3\Lambda)^{1/6}}\,\tilde{\chi_1}, \tag{4.58}$$

where τ is negative-defined. The wave function evolving via this modified dynamics is the following:

$$\tilde{\chi_1} = \exp\left(-\mathrm{i}\hbar\frac{p_\phi^2}{2}\tau + \mathrm{i}\frac{p_a\,(-\tau)^{7/3}}{7(3\Lambda)^{1/6}}\right). \tag{4.59}$$

One can immediately show from (4.58) that a deformation of the energy spectrum takes place, as described by

$$E = E_0 + \frac{\hbar p_a(-\tau)^{7/3}}{3(3\Lambda)^{1/6}}, \tag{4.60}$$

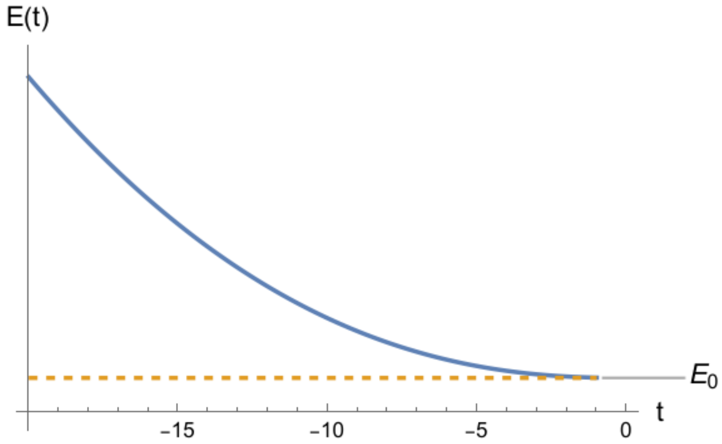

Figure 4.2. Plot of the modified energy spectrum (4.60) with respect to the baseline E_0. Here the QG-induced correction is greatly enhanced for clarity.

i.e. a decreasing function in time, which is plotted in Fig. 4.2. Clearly, this corrective term lives at order $\mathcal{O}\left(M^{-1}\right)$ with respect to the standard QFT spectrum since we are assuming the condition (4.12).

To understand the effects of the quantum gravity corrections, let us investigate the evolving probability density associated to the modified wave function (4.59) for the isotropic universe. As initial condition, we consider for χ a Gaussian wave packet in both degrees of freedom:

$$f(p_a, p_\phi) = \frac{1}{\sqrt{(2\pi)\sigma_a \sigma_\phi}} \exp\left(-\frac{(p_a - p_{0,a})^2}{4\sigma_a^2}\right) \exp\left(-\frac{(p_\phi - p_{0,\phi})^2}{4\sigma_\phi^2}\right), \tag{4.61}$$

where the free parameters $p_{0,a}$ and $p_{0,\phi}$ are the mean values of the Gaussian distribution and σ_a, σ_ϕ are their standard deviations. The expression (4.61) will correspond in principle to a localized probability density; this straightforward choice is contextualized in Chapter 5. To satisfy the adiabatic condition (4.12), we shall consider the regime in which

$$-\frac{1}{M} < p_a < \frac{1}{M}\,, \tag{4.62}$$

so we integrate and normalize the wave packet only in this interval.

Implementing the dynamics (4.58) for (4.61) in Fourier space, we find that the probability density for the fast quantum matter is modified as shown in Fig. 4.3. We stress that the obtained behavior has a very weak dependence (i.e. almost flat) in the scale factor a, since the hypothesis (4.12) requires (4.62). It follows that the quantum gravity effects on the system are of very small intensity, as predicted by the perturbative approach.

Figure 4.4 shows the comparison between such modified evolution and the standard spreading of the Gaussian wave packet that would take place without the QG-induced corrections of Eq. (4.58) for the reference value $\tau = -20$. We observe from this figure that the principal modification to the evolved probability density takes place as $ln(a)$ approaches zero, i.e. towards the reference value $\tilde{a} = 1$.

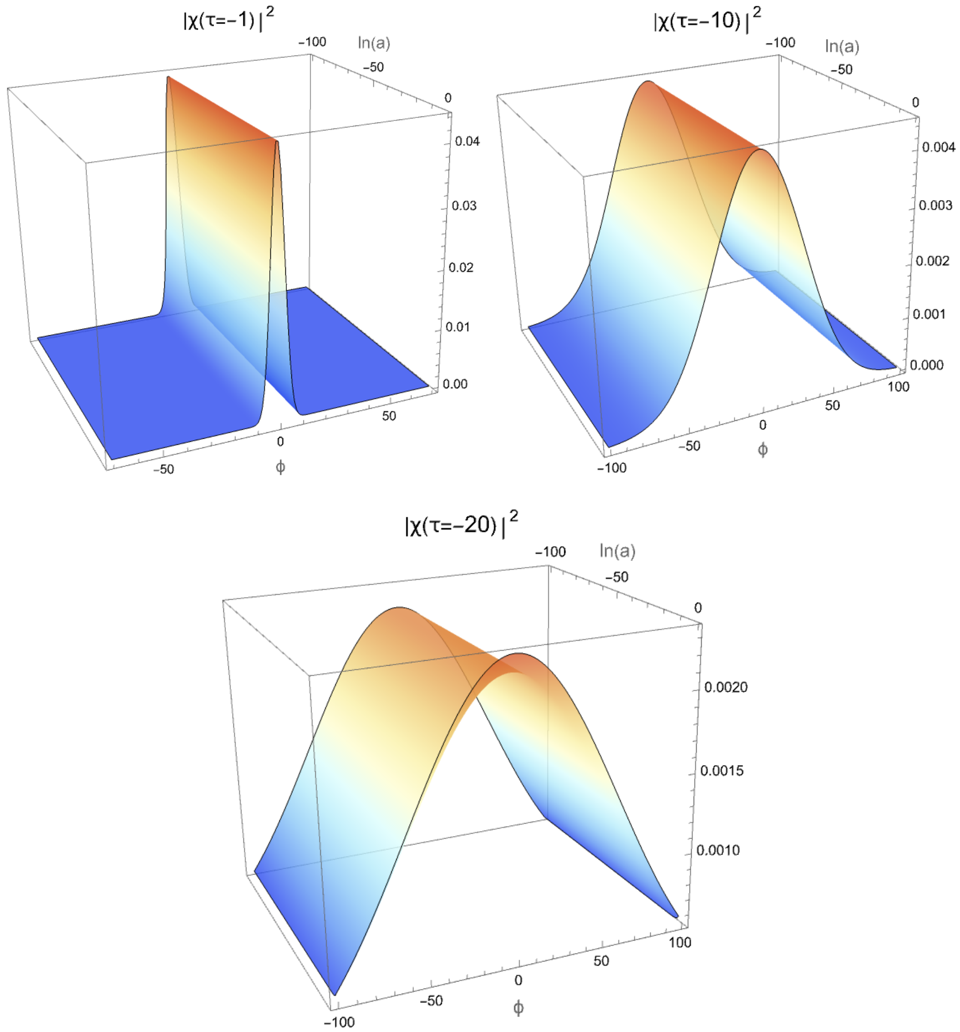

Figure 4.3. Evolution of the normalized probability density associated to the wave packet (4.61) for different values of the rescaled time τ. Reference values in Planck units: $M = 100$, $\Lambda = 10^{-2}$, $ln(a_0) = 10$, $\bar{p}_\phi = 0$, $\sigma_\phi = 3$, $\bar{p}_a = 0$, $\sigma_a = 2 \cdot 10^{-2}$. Here M is set to a larger value with respect to the one in such units, in order to enhance the perturbative treatment in $1/M$. We observe the spreading of the wave packet in time and that the QG-induced corrections cause a deformation along the a axis when a approaches a reference value. The wavefunction has been normalized over a suitable interval of $\ln(a)$. Figures re-elaborated from [91].

To summarize, the QG-corrections in this toy model correspond to a phase shift in energy and modify the evolution of the wave function. The initially localized wave packet undergoes the expected spreading, with a previously unaccounted behaviour along the α direction, more specifically when approaching a reference value a_0 of the scale factor. The predictions of such modified evolution in the cosmological setting are analyzed in the next Chapter.

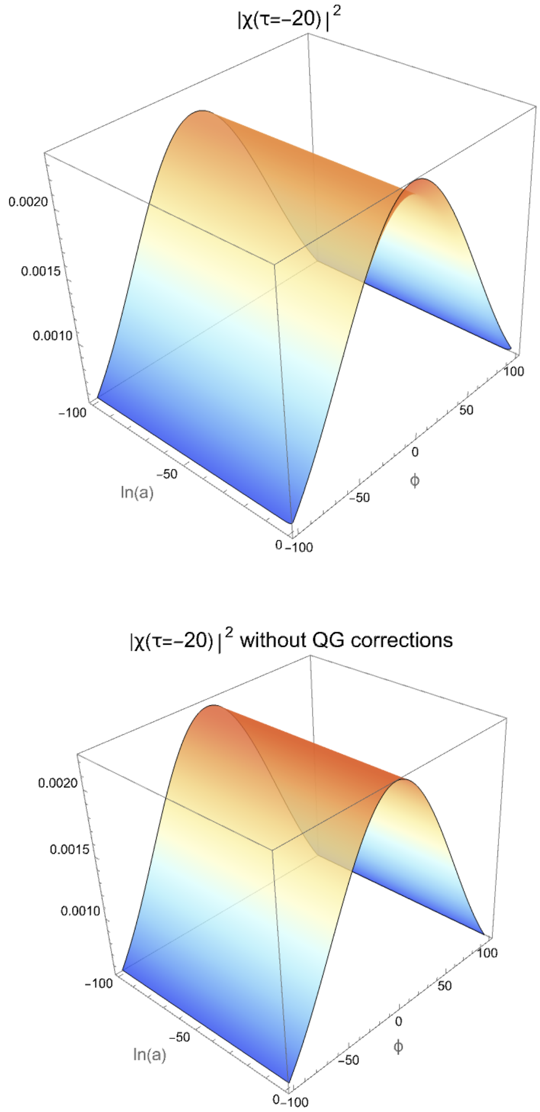

Figure 4.4. Comparison between the two probability densities $|\chi(\tau = -20)|^2$ with and without QG-induced effects. The top figure is obtained evolving the wave packet via the modified evolution (4.58) which contains the QG corrections. The bottom plot refers to the evolution without such effects, i.e. the same of the previous order (the second term on the right-hand side of (4.58) is absent). Reference values in Planck units: $M = 100$, $\Lambda = 10^{-2}$, $ln(a_0) = 10$, $\bar{p}_\phi = 0$, $\sigma_\phi = 3$, $\bar{p}_a = 0$, $\sigma_a = 2 \cdot 10^{-2}$. Figures re-elaborated from [91].

Chapter 5

Predictions in Quantum Cosmology

The previous chapters have dealt with the investigation of quantum-gravity-induced effects on QFT, however such predictions must be confronted with our physical experience. In this respect, Quantum Cosmology aims to study the origin, evolution, and structure of the universe as a whole, focusing on the scale in which the classical description of gravity and spacetime may break down, such as the earliest moments of the Big Bang.

In the present Chapter we focus on the so-called inflationary spectrum, i.e. the power spectrum associated to small quantum fluctuations which after the inflationary expansion formed the large scale structures of our universe, whose remnants can be observed through the CMB. For this purpose we address quantum perturbations of the scalar field only; such case is equivalent to the study of a free massless scalar field fluctuating on a de Sitter background. The classical energy contribution of the scalar field will be identified with a positive cosmological constant Λ term, i.e. the gap between the false and true vacuum energy density. The effects of the quantum-gravity corrections computed in Chapters 3-4 on such spectrum are analyzed in Sec. 5.3,illustrating the results of Ref. [94].

5.1 The early evolution of the Universe and CMB

Cosmological models implement a minisuperspace reduction (see Sec. 1.6) in order to portray a more faithful description of our current universe: according to the Cosmological Principle, the universe appears homogeneous and isotropic at large scales. However, it is also interesting to reduce the model's degrees of freedom while keeping anisotropic features, since they are helpful to describe specific cases such as the Mixmaster universe or the Belinski–Khalatnikov–Lifshitz (BKL) solution [95].

In cosmological settings, one considers a non-stationary metric tensor with non-zero curvature everywhere; matter contributions if present also give a non-vanishing energy-momentum tensor in each space point and at any time instant in the Einsteins' equations[1], see Sec. 1.6.2.

[1]This configuration in general does not admit an asymptotically flat spacetime at spatial infinite, but vanishing behaviors of the curvature can emerge in time.

The early evolution of our Universe is currently described by the Big Bang theory, in which an extremely hot and dense state (i.e. the initial singularity) expanded and cooled down, with the temperature dropping to a point where protons and neutrons could combine to form light atomic nuclei (nucleosynthesis). At the moment of the so-called recombination, when electrons combined with protons to form neutral hydrogen atoms, photons were released creating the so-called cosmic microwave background radiation (CMB). In its original formulation the Big Bang model did not explain a number of observed cosmological facts: the matter over antimatter predominance, the origin of the seed inhomogeneities required to start structure formation, the nature of dark matter, the smallness of any cosmological term, and the large-scale isotropy, homogeneity, and flatness of the Universe [20].

Quantum Cosmology (QC) and the theory of inflation aim to describe such evolution surpassing the classical treatment and to address the above points. The question of the initial singularity is also investigated in QC: some models indeed predict not a universe emerging from a single point, but a Bounce i.e. a universe whose size systematically contracts and then expands [96, 97]. In this view, the entire universe is described by a wave function, which encodes the probabilities of different configurations of the universe. Clearly its evolution in time is described by the Wheeler-DeWitt equation (2.10), while there is an ongoing discussion regarding the appropriate initial conditions for such wave function. In the inflationary paradigm, the initial state underwent a rapid (exponential) expansion known as cosmic inflation; the fluctuations necessary to initiate the formation of large scale structure are nothing else than the small quantum fluctuations of a primordial scalar field (the *inflaton* field), then scaled to relevant sizes due to the expansion. This is the prevailing theory to explain the origin and development of the cosmos and its predictions have been tested against observational data finding crucial evidence supporting it [19].

The CMB, originally understood in the 1940s and first measured (accidentally) in 1964 [98], represents the remnant of the light that suddenly stopped being scattered by charged particles (due to recombination, after the expansion) and started propagating freely. This event happened everywhere at the same cosmic time, following the cosmological principle that the universe is homogeneous and isotropic on large scales; such photons emitted some 13.8 billion years ago arrive to us from every direction. Since such radiation contains relevant data on the the inflationary era, many Earth-based and space experiments focus in the measurement and analysis of such radiation: the COsmic Background Explorer (COBE) [99], the Wilkinson Microwave Anisotropy Probe (WMAP) [100], the PLANCK satellite [101].

To better understand the magnitude of such observations, we recall that the CMB appears today as an almost perfect black body, in the sense that it is very well-described by a Planck spectrum of temperature $T_{\mathrm{CMB}} = 2.72548 \pm 0.00057\,\mathrm{K}$; its peak wavelength is of the order of mm (that is a microwave/radio signal). This corresponds to an emitted spectrum of temperature $k_B T^* \simeq 0.3\,\mathrm{eV}$ ($\lambda^* \simeq \mu\mathrm{m}$) which has been redshifted to cosmic expansion via the redshift parameter

$$z^* = \frac{\lambda^*_{obs}}{\lambda^*_{obs} - \lambda^*_{em}} = 1089.90 \pm 0.23\,. \tag{5.1}$$

However, the CMB is not perfectly isotropic, as described by fluctuations in the observed temperature of the order $\delta T \simeq 500\,\mu\mathrm{K}$. It is precisely this fluctuating behaviour that contains the relevant information about the universe, since anisotropies can be generated before recombination (primary anisotropies, related to the physics of inflation and of the primordial plasma) or from effects occurring during the photons' travel such as gravitational lensing (secondary anisotropies). The evolution of such small fluctuations, imputed to the small quantum fluctuations of a scalar (inflaton) field, is analyzed by the theory of cosmological perturbations, which will be described in more detail in Sec. 5.2. We will then show how the modified dynamics inferred in Chapter 3-4 can influence such evolution, presenting a concrete example in Sec. 5.3.

5.2 Theory of cosmological perturbations

The theory of inflation motivates the primordial inhomogeneities of the universe as emerging from the vacuum fluctuations of a scalar field, the so-called *inflaton* field. One of the most remarkable results of such mechanism is the ability to solve two concerning points of our observations: the horizon problem (causally disconnected regions of the universe presenting similar properties at large scales) and the flatness problem (the spatial curvature parameter of the universe appears to be very close to zero) [1, 95, 102, 103]. This framework can be outlined by considering a spatially flat universe for the background, since any curvature is damped by the exponential expansion, and adding a scalar field living on top. More specifically, one should consider the homogeneous and isotropic FLRW spacetime (see Sec. 1.6.2), i.e. with line element:

$$ds^2 = -N^2(t)\, dt^2 + a^2(t) \left(dx^2 + dy^2 + dz^2\right) \tag{5.2}$$

being a the cosmic scale factor, and insert the inflaton contribution as a minimally coupled inhomogeneous scalar field ϕ slowly rolling down its potential $U(\phi)$.

In the theory of cosmological perturbations, one introduces small linear perturbations for both the metric and for the inflaton, and then decomposes the resulting fluctuations into scalar, vector and tensor sectors and analyzes their Hamiltonian formulation, see for example [102, 17]. Differently from the QFT case, the introduction of such matter fluctuations is highly non-trivial: the perturbed and unperturbed quantities of a given field live in different space-times, since the metric also is fluctuating. Therefore, one has to analyze how such perturbations behave under coordinate transformations and the resulting changes can also be decomposed along the scalar, vector and tensor sectors. In other words, non-physical perturbations could arise as "artifacts" in the model simply due to coordinate changes.

Two different strategies are available to tackle this problem. The first is to select a specific gauge, usually the longitudinal (or conformal Newton) one, which has the following line element

$$ds^2 = a^2(\eta) \left[-(1 + 2\Phi)d\eta^2 + (1 - 2\psi)\gamma_{ij}dx^i dx^j\right] \tag{5.3}$$

where Φ and ψ are metric perturbation variables. In the second strategy, one does not fix the gauge but works with a basis of gauge-invariant variables. Actually, it is possible to define gauge-invariant variables that coincide with the diagonal metric perturbations Φ and ψ in longitudinal gauge [104, 105].

In the following, we will use the second strategy and focus on perturbations of the scalar inflaton field, which are those relevant for the CMB and structure formation. Given the perturbations $\delta\phi$ of such field, their gauge-invariant treatment is obtained by defining

$$v := a\varphi = a\,\delta\phi\,, \tag{5.4}$$

that is a specific case of the Mukhanov–Sasaki (M-S) variable v describing the scalar sector of perturbations [106, 107, 108] (see also the discussion in [109]), when the metric fluctuations are switched off; for a more general treatment we refer to Chapter 6. The variable (5.4) corresponds to the (rescaled) scalar field perturbations computed in the spatially flat gauge (that eliminates spatial metric perturbations). On a de Sitter spacetime, i.e. expanding as $a(\eta) = -1/(H\eta)$, the evolution of this variable will take the form of a time-dependent harmonic oscillator since it will have a time-dependent effective mass [68], see the application of Sec. 5.3.

We here stress that addressing the BO separation discussed above does not alter the gauge invariance of the perturbation theory: in the limit in which the backreaction on the metric scalar perturbation is neglected, the M-S variable is simply (5.4) and its gauge invariance is immediately recovered.

Since the evolution of the inflaton fluctuations is responsible for the formation of primordial structures in the Universe, one must focus on their dynamics. To understand their behavior, let us consider modes with physical wavelength $\lambda_{phys} \equiv a(t)\lambda_0$, λ_0 being the comoving wavelength. It is useful to compare this quantity with the so-called Hubble radius (or micro-physics horizon) $\mathscr{H}^{-1} = a/\dot{a}$, that for any given time is the inverse of the Hubble parameter (using $c = 1$). This horizon represents the scale separating the gravity-dominated regime from the quantum one: the first happens for modes with physical wavelength such that $\lambda_{phys} \gg \mathscr{H}^{-1}$, and the second is the case for $\lambda_{phys} \ll \mathscr{H}^{-1}$. It can be shown that during the period of accelerated expansion predicted by the theory the Hubble radius is constant in the physical coordinates, while λ_{phys} exponentially increases [95, 103]. This means that the quantum fluctuations emerge at early times within the micro-physical scales (i.e., for $\lambda_{phys} \ll \mathscr{H}^{-1}$), rapidly expand going outside the horizon, and propagate until they re-enter the Hubble radius at later times; when inflation is over, the behavior is opposite, since $\mathscr{H}^{-1}$ grows faster than the λ_{phys} [1, 102].

Using the gauge-invariant formalism via the variable (5.4), it is possible to compute the power spectrum relative to the distribution of these primordial fluctuations. N particular one can compute the spectrum $\mathcal{P}_v(k)$, where k specifies the wave number of each Fourier mode associated with the inflaton perturbations. For the evolution of the primordial Universe, it is more convenient to work with the spectrum associated with the comoving curvature perturbation ζ (which is the one leaving its fingerprint on the cosmic microwave background radiation) [110]: indeed, ζ is constant (i.e., it freezes) for all the time in which the perturbations are outside the horizon; therefore, one only needs to compute its spectrum at the end of inflation [95, 103]. In the primordial era of our interest, the two quantities ζ and v are directly related by

$$\zeta = \sqrt{\frac{4\pi G}{\epsilon}}\frac{v}{a}, \tag{5.5}$$

with $\epsilon = -\dot{\mathscr{H}}/\mathscr{H}^2$ being the first slow-roll parameter. In the following, we will focus on the dynamics of the M-S variable v and only at the end use (5.5) to compute the invariant power spectrum.

Upon decomposition in Fourier modes $v_{\mathbf{k}}$, if the quantum amplitudes associated with each $v_{\mathbf{k}}$ are Gaussian distributions, then all the relevant properties of the inflationary perturbations are contained in the two-point correlation function [110]:

$$\Xi(\mathbf{r}) := \langle 0|\hat{v}(\eta, \mathbf{x})\hat{v}(\eta, \mathbf{x}+\mathbf{r})|0\rangle \,, \tag{5.6}$$

where $|0\rangle$ is the vacuum state of the inflaton field, defined via the so called Bunch–Davies condition.

The Bunch-Davies vacuum When dealing with QFT on curved spacetime, the notion of absence of particles is lost due to effects associated to the spacetime curvature, such as the Unruh effect: an accelerated observer provided with a detector would detect particles even in a state which seen as empty in the rest frame [111]. It is then unclear how one should impose suitable conditions for the wave function of the universe to correspond to an initially "empty" state.

The Bunch–Davies vacuum state requirement [1, 110], actually first derived in [112], provides a clear and unambiguous criterion to solve this dilemma. It states that, in the limit $k\eta \to -\infty$ i.e. when the inflaton wavelength is small compared to the curvature of the universe, one must select the state corresponding to the lowest energy state of the harmonic oscillator in Minkowskian vacuum: in other words, a vacuum state that is devoid of particles in the distant past, where the metric appears as Minkowskian at the inflaton scale. The limit is dictated by the observation that, at the beginning of inflation, all the modes of astrophysical interest today have a physical wavelength smaller than the Hubble radius.

We stress that such requirement is not strictly necessary for the computation of the primordial power spectrum, which will instead be computed in the super-Hubble limit $k\eta \to 0^-$. It is however imposed in cosmology to provide initial conditions that are in accord with a field theory description on curved spacetime.

Let us summarize how from the correlation function (5.6) one can proceed to compute the associated power spectrum of primordial perturbations. The expectation value implies integration over $\mathbf{k}$-modes, which can be carried out given the expression (see for example [110])

$$\Xi(\mathbf{r}) = \frac{1}{(2\pi)^3}\int d\mathbf{p}\; e^{-i\mathbf{p}\cdot\mathbf{r}}|f_{\mathbf{p}}|^2 = \frac{1}{2\pi^2}\int_0^{+\infty}\frac{dp}{p}\frac{sin(pr)}{pr}p^3|f_p|^2 \,. \tag{5.7}$$

Here, $f_{\mathbf{p}}$ is the mode function associated with the scalar perturbations, and from (5.7), the power spectrum is defined as

$$\mathcal{P}_v(k) = \frac{k^3}{2\pi^2}|f_k|^2 \,, \tag{5.8}$$

i.e., the Fourier amplitude of $\Xi(0)$ per unit logarithmic interval. As mentioned above, this quantity is then evaluated in the super-Hubble limit $k/(a\mathscr{H}) \ll 1$, when the perturbations essentially freeze. We stress that the vacuum state in (5.6) must be selected as the one corresponding to the ground level of the scalar field Hamiltonian in the limit $k/(a\mathscr{H}) \to \infty$ (or equivalently $\lambda_{phys} \ll \mathscr{H}^{-1}$), also known as the

Bunch–Davies vacuum, see Section 5.3. From (5.8), the spectrum $\mathcal{P}_\zeta(k)$ related to the curvature perturbations ζ can be obtained using (5.5).

In inflationary cosmology, such spectrum provides the initial conditions for the formation of large scale structures. Its parameters can be constrained by observing the properties of the CMB radiation and the large scale structure of our universe. Recent satellite missions, such as WMAP [100] and PLANCK [113, 114], provided an accurate detection of the fluctuation spectrum in the CMB temperature. These observations, and in particular, the Gaussian profile distribution of the fluctuations, properly fulfill the prediction of the inflation paradigm; in this respect, a significant constraint for the spectral index n_s

$$n_s - 1 := \frac{d \ln \mathcal{P}_\zeta}{d \ln k} \tag{5.9}$$

is now available [113]. For completeness, we mention that some recent data analyses suggest the possibility of anomalies in the Gaussianity of the fluctuations [115] and called attention to the possibility to be interpreted via a multi-field inflationary scenario [116, 117], which will not be investigated in this thesis.

5.3 Modified power spectrum of primordial perturbations

Before facing the analysis of inflationary perturbations and how the quantum gravity corrections can affect the associated power spectrum, it is worth stressing some key differences between the present analysis and other similar approaches, as in [109, 52].

In our formulation, apart from the WKB expansion in the Planckian parameter M, we are addressing a BO separation between the "slow" gravitational component and the "fast" matter contribution, with the latter including also the fluid's presence. This separation is justified by virtue of a corresponding scale separation between the energy of the quantum matter dynamics, say in the order of the matter Hamiltonian spectrum, and that one of the Planck order, at which the gravity quantization is expected to manifest itself. In view of this adopted B-O approximation, the backreaction of the quantum matter on the gravitational background is implicitly negligible. In other words, quantum corrections of the gravitational dynamics are clearly present (as implied by the function P_1 in (4.7), associated with a quantum amplitude for the background metric), but they exist independently of the matter's dynamics.

We here consider the slow-rolling phase of inflation, that is when the inflaton can be approximately described as a free massless scalar field (the almost constant potential acts as a cosmological term) [95]. More specifically, we will employ an exact de Sitter phase, thus neglecting the slow-rolling parameter ϵ. This simplified approximated scheme can be useful to obtain insights on the inflaton evolution, such as [68]. The analysis of quantum gravity's effects on the inflationary spectrum is achieved by considering the fluctuations of the scalar field over a quasi-classical background, expressed by the FLRW metric in (5.2).

Due to the homogeneous minisuperspace reduction of the background model, we neglect the supermomentum contributions and start with the superHamiltonian constraint (WDW)

$$\hat{H}_{tot}\Psi(a,T,v_{\mathbf{k}}) = 0\,, \tag{5.10}$$

$$\hat{H}_{tot} = \frac{\hbar^2}{48Ma^2}\partial_a\left(a\partial_a\right) + 4M\Lambda a^3 - i\hbar\partial_T + \frac{1}{2a}\sum_{\mathbf{k}}\left(-\hbar^2\partial^2_{v_{\mathbf{k}}} + \omega_k^2 v_{\mathbf{k}}^2\right)\,. \tag{5.11}$$

Here we have implemented a specific factor ordering, i.e. the Laplace–Beltrami one, which ensures a gauge-invariant treatment. The positive cosmological constant Λ plays the role of the matter potential U_m in (4.15). The momentum $-i\hbar\partial_T$ associated with the Gaussian time T is the only relevant contribution of the reference fluid of Chapter 4 due to the homogeneity requirement. Clearly, the last two terms in (5.11) correspond to the inflaton field fluctuations in the gauge-invariant formalism, being $v_{\mathbf{k}}$ the Fourier modes of the M-S variable (5.4). When such perturbations live over a FLRW background, they behave as time-dependent harmonic oscillators [118, 68, 119] with a frequency depending on the wavenumber modulus only:

$$\omega_k^2 = k^2 - \frac{a^2}{N^2}\left(\dot{\mathscr{H}} - \mathscr{H}\frac{\dot{N}}{N} + 2\mathscr{H}^2\right)\,. \tag{5.12}$$

The WDW constraint corresponds to the vanishing of the operator (5.11) applied to the total system wave function $\Psi(a,T,v_{\mathbf{k}})$. We implement for convenience the logarithmic scale factor,

$$\alpha := \ln\left(\frac{a}{a_0}\right)\,, \tag{5.13}$$

with a_0 being the reference value at the stat of the de Sitter phase, such that the global WDW equation reads

$$\begin{aligned}&\frac{1}{a_0e^{\alpha}}\left(\frac{\hbar^2}{48M}\frac{1}{a_0^2e^{2\alpha}}\partial_\alpha^2 + 4a_0^4e^{4\alpha}\Lambda M\right)\Psi - i\hbar\partial_T\Psi\\ &\qquad + \frac{1}{2a_0e^{\alpha}}\sum_{\mathbf{k}}\left(-\hbar^2\partial^2_{v_{\mathbf{k}}} + \omega_k^2v_{\mathbf{k}}^2\right)\Psi = 0\,.\end{aligned} \tag{5.14}$$

Let us now consider a single Fourier mode identified by a wave number $\mathbf{k}$. Following the scheme discussed above, for each independent mode, the ansatz is taken as

$$\Psi_{\mathbf{k}}(\alpha,T,v_{\mathbf{k}}) = \psi_{\mathbf{k}}(\alpha)\,\chi_{\mathbf{k}}(\alpha,T,v_{\mathbf{k}})\,, \tag{5.15}$$

and then WKB expanded as in (4.7):

$$\psi_{\mathbf{k}}(\alpha) = e^{\frac{i}{\hbar}\left[MS_0(\alpha)+P_1(\alpha)+M^{-1}P_2(\alpha)\right]}\,, \tag{5.16}$$

$$\chi_{\mathbf{k}}(\alpha,T,v_{\mathbf{k}}) = e^{\frac{i}{\hbar}\left[Q_1(\alpha,T,v_{\mathbf{k}})+M^{-1}Q_2(\alpha,T,v_{\mathbf{k}}))\right]}\,. \tag{5.17}$$

Upon substitution into (5.14), one obtains the dynamics dictated by the WDW constraint at each order. We first discuss the solutions pertaining to the gravitational sector, which are readily obtained at the three orders:

$$S_0(\alpha) = -8\sqrt{\frac{\Lambda}{3}}a_0^3\left(e^{3\alpha} - e^{3\alpha_0}\right) , \tag{5.18}$$

$$P_1(\alpha) = \frac{3}{2}i\hbar(\alpha - \alpha_0) , \tag{5.19}$$

$$P_2(\alpha) = \frac{\hbar^2}{64}\sqrt{\frac{3}{\Lambda}}a_0^{-3}\left(e^{-3\alpha} - e^{-3\alpha_0}\right) . \tag{5.20}$$

Here, S_0 solves the HJ equation and so corresponds to the classical limit of the gravitational component, while the next order functions P_1 and P_2 account for quantum gravity effects; α_0 is just the starting value $_0$ written in the logarithmic coordinate.

Turning to the quantum matter sector, we employ the time definition (4.24) to rewrite the first order (i.e. $\mathcal{O}\left(M^0\right)$) as a Schrödinger-like evolution. In agreement with gauge-invariant treatments to the primordial spectrum in literature, we implement the conformal time gauge[2] via $N = a_0\, e^{\alpha}$ so that $T'(\eta) = a_0 \exp\left(\alpha(\eta)\right)$; this is allowed by the fact that the Gaussian time $T(t)$ of Sec. 4.2 is in principle a generic function of time and we can suitably choose the time parameter of the reference fluid. Thus the matter dynamics at $\mathcal{O}\left(M^0\right)$ is described by

$$i\hbar\partial_\eta\chi_{\mathbf{k}}^{(0)} = \left(-\frac{\hbar^2}{2}\partial^2_{v_{\mathbf{k}}} + \frac{1}{2}\omega_k^2(\eta)v_{\mathbf{k}}^2\right)\chi_{\mathbf{k}}^{(0)} , \tag{5.21}$$

which is clearly a time-dependent harmonic oscillator in conformal time.

The time-dependent harmonic oscillator system can be exactly solved by implementing the so-called Lewis–Riesenfeld method of invariants [120, 121, 122, 123]. The method, which is described in detail in Appendix A, allows to construct a wave function of the general form (see Eq. (A.9))

$$\chi_{\mathbf{k}}^{(0)}(\eta, v_{\mathbf{k}}) = \sum_n c_{n,k}\, e^{i\delta_{n,k}(\eta)}\, \phi_{n,\mathbf{k}}(\eta, v_{\mathbf{k}}) , \tag{5.22}$$

where $\phi_{n,\mathbf{k}}$ are appropriately rescaled standard oscillator solutions and $\delta_{n,k}$ and ρ_k are functions defined in (A.10). Clearly, the arbitrary coefficients in those expressions must be set through suitable initial conditions; we fix them via the Bunch-Davies vacuum requirement (see Sec. 5.2), in order to provide a meaningful field description for the inflaton sector on the curved spacetime. Looking at the general form (5.22) in the relevant limit, the coefficients $c_{n,k}$ and the function ρ must satisfy

$$\rho_k(\eta) \xrightarrow[\eta\to-\infty]{} k^{-1/2} , \tag{5.23}$$

$$c_{n,k} = \delta_{0,k} . \tag{5.24}$$

The second condition (5.24) is easily understood observing that the $n = 0$ eigenvalue of the invariant constructed via the Lewis method (see (A.1)) corresponds, for a fixed time, to the lowest-energy state of the oscillator. The first condition, when applied to

[2] This choice allows to write the oscillator's frequency as a direct function of the gauge-invariant variables, eliminating the dependence on the lapse function and Hubble parameter in (5.12).

the specific ρ_k (A.3) of the time-dependent oscillator solution, gives $A = B = \gamma_1 = 1$ so that

$$\rho_k(\eta) = \sqrt{\frac{1}{k} + \frac{1}{\eta^2 k^3}} \tag{5.25}$$

satisfies the required limit.

Substitution into (A.10) gives the $\delta_{n,k}$ functions as

$$\delta_{n,k} = -\left(n + \frac{1}{2}\right) \int d\eta \frac{1}{\rho_k^2(\eta)} = -\left(n + \frac{1}{2}\right) (\eta k - \arctan(\eta k) + c) \, . \tag{5.26}$$

Finally, the solution to Equation (5.21) satisfying the Bunch–Davies condition is:

$$\begin{aligned} {}^{BD}\chi_{\mathbf{k}}^{(0)}(\eta, v_{\mathbf{k}}) =& e^{-\frac{i}{2}(\eta k - \arctan(\eta k))} \left(\frac{k^3}{\pi\hbar\left(\frac{1}{\eta^2} + k^2\right)} \right)^{\frac{1}{4}} \\ & \times \exp\left[\frac{i}{2\hbar} \left(-\frac{1}{\eta^3\left(\frac{1}{\eta^2} + k^2\right)} + i \frac{k^3}{\frac{1}{\eta^2} + k^2} \right) v_{\mathbf{k}}^2 \right] . \end{aligned} \tag{5.27}$$

At this level, we have only computed the solution for the QFT limit, which would correspond to the standard scale-invariant power spectrum of the de Sitter phase (as we will compute below). We can now focus on the next order M^{-1}: here, due to the quantum gravity corrections, the dynamics is no longer that of a time-dependent oscillator but it becomes

$$i\hbar\partial_\eta \chi_{\mathbf{k}}^{(1)} = \left[\frac{i\hbar}{24} \frac{1}{a_0^2 e^{2\alpha}} (\partial_\alpha S_0)\partial_\alpha - \frac{\hbar^2}{2}\partial_{v_{\mathbf{k}}}^2 + \frac{1}{2}\omega_k^2 v_{\mathbf{k}}^2 \right] \chi_{\mathbf{k}}^{(1)} \, . \tag{5.28}$$

We can here use (5.18) and the classical scale factor solution for the de Sitter phase $a_0 e^{\alpha}(\eta) = -\sqrt{\frac{3}{\Lambda}}\frac{1}{\eta}$[3], so that Eq. (5.28) becomes

$$i\hbar\partial_\eta \chi_{\mathbf{k}}^{(1)}(\alpha, \eta, v_{\mathbf{k}}) = \left[\frac{i\hbar}{\eta}\partial_\alpha - \frac{\hbar^2}{2}\partial_{v_{\mathbf{k}}}^2 + \frac{1}{2}\omega_k^2(\eta) v_{\mathbf{k}}^2 \right] \chi_{\mathbf{k}}^{(1)}(\alpha, \eta, v_{\mathbf{k}}) \, . \tag{5.29}$$

Clearly, a general solution to (5.29) is difficult to calculate. However, similarly to previous investigations e.g. [68], we can implement the method of separation of variables and focus on the following class of separable solutions

$$\chi_{\mathbf{k}}^{(1)}(\alpha, \eta, v_{\mathbf{k}}) = \theta(\alpha)\, \Gamma_{\mathbf{k}}(\eta, v_{\mathbf{k}}) \, , \tag{5.30}$$

where we remark that the (quantum) degree of freedom α is in principle independent from the chosen conformal time η, and the classical relation only stands in the appropriate low-energy limit. Such choice is backed by the assumption of negligible backreaction and it will limit the validity of the following results to these specific settings, see the discussion in Sec. 5.3.1.

[3]This expression is easily found from the Friedmann equation (1.83) for zero spatial curvature ($k = 0$) and when only a cosmological constant contribution is dominant in ρ.

Taking into account the form (5.30), Eq. (5.29) is solved for

$$-i\hbar\partial_\alpha\theta(\alpha) = \lambda\,\theta(\alpha)\,, \tag{5.31}$$

$$i\hbar\partial_\eta\Gamma_{\mathbf{k}}(\eta, v_{\mathbf{k}}) = \left(-\frac{\hbar^2}{2}\partial^2_{v_{\mathbf{k}}} + \frac{1}{2}\omega_k^2(\eta)v_{\mathbf{k}}^2 - \frac{\lambda}{\eta}\right)\Gamma_{\mathbf{k}}(\eta, v_{\mathbf{k}})\,, \tag{5.32}$$

where the constant λ identifies the family of solutions in (5.31), giving the eigenvalues of the momentum associated with the (logarithmic) scale factor. Now we are left with solving Eq. (5.32), which is a time-dependent harmonic oscillator with an additional time-dependent "potential". Actually, we can implement a suitable rescaling

$$\Gamma_{\mathbf{k}}(\eta, v_{\mathbf{k}}) = \exp\left[\frac{i}{\hbar}\lambda\log(-\eta)\right]\tilde{\Gamma}_{\mathbf{k}}(\eta, v_{\mathbf{k}}) \tag{5.33}$$

in order to reconnect to the usual time-dependent harmonic oscillator. Therefore, $\tilde{\Gamma}_{\mathbf{k}}$ coincides with the solution $\chi^{(0)}_{\mathbf{k}}$ of the previous order and the $\Gamma_{\mathbf{k}}$ is readily obtained. Now using the solutions of (5.31) and (5.32), we can write the complete matter wave function (5.30) as

$$\chi^{(1)}_{\mathbf{k}}(\alpha, \eta, v_{\mathbf{k}}) = \theta_{p_\alpha}(\alpha)\, e^{\frac{i}{\hbar}p_\alpha\, log(-\eta)}\, \chi^{(0)}_{\mathbf{k}}(\eta, v_{\mathbf{k}})\,, \tag{5.34}$$

which can then be implemented to analyze the quantum-gravity corrected power spectrum.

Before proceeding we stress two important points of this application.

On one hand, we stress that the QG corrections of the present model are extremely small with respect to the accuracy of current fluctuation measurements, since they can be estimated via the square ratio of the inflationary energy scale to the corresponding Planckian one, namely about 10^{-8}. Despite the possibility of detecting such quantum gravity modifications of the spectrum in current or near-future experiments appearing unlikely, their prediction stands as a fundamental conceptual challenge.

On the other hand, the requirement (4.12) imposed in Sec. 4.2 due to the BO approximation scheme translates to $|p_\alpha| < 1/M$ in this specific minisuperspace setting, as we have seen in Sec. 4.3. Therefore, in (5.34) we construct a convolution over all the admissible values of the momentum p_α

$$\chi^{(1)}_{\mathbf{k}}(\alpha, \eta, v_{\mathbf{k}}) = \chi^{(0)}_{\mathbf{k}}(\eta, v_{\mathbf{k}}) \int dp_\alpha g(p_\alpha)\theta_{p_\alpha}(\alpha)e^{\frac{i}{\hbar}\log(-\eta)p_\alpha}\,, \tag{5.35}$$

where $g(p_\alpha)$ is a generic distribution. We here choose a Gaussian weight distribution with deviation σ and zero mean value, i.e.

$$g(p_\alpha) = \frac{1}{(\sqrt{2\pi}\sigma)^{1/2}}e^{-\frac{p_\alpha^2}{4\sigma^2}}\,; \tag{5.36}$$

this choice is reasonable since, as discussed in Sec. 5.2, for the Gaussian case the two-point correlation function (5.6) would be sufficient to describe the whole spectrum. It is also significant if one considered χ emerging from a large number of independent and identically distributed random variables; in this case, the distribution would indeed tend towards the Gaussian one (regardless of the individual distributions) thanks to the central limit theorem.

The matter wave function modified by quantum gravity corrections ends up as

$$\chi^{(1)}_{\mathbf{k},Gauss}(\alpha,\eta,v_{\mathbf{k}}) = \chi^{(0)}_{\mathbf{k}}(\eta,v_{\mathbf{k}}) \left\{ (8\pi\sigma^2)^{1/4} \exp\left[-\frac{\sigma^2}{\hbar^2} \left(\alpha + \log(-\eta)\right)^2 \right] \right\}. \quad (5.37)$$

Here, the effect of quantum gravity corrections has clearly factorized, an aspect which will deeply impact the result of the power spectrum analysis and will be discussed in Sec. 5.3.1 in relation to the separable ansatz (5.30). Indeed, the obtained wave function shall be considered as the "new" vacuum state in order to derive the primordial power spectrum for the order M^{-1} of the prescribed theory, i.e., modified by quantum gravity effects. However, as the modification impacting the wave function (5.37) manifests solely as a time factor, its resultant contribution simplifies the spectrum computation, aligning with the previous order's result. Essentially, the power spectrum associated to (5.37) will be equivalent to the one computed with (5.27) in the absence of quantum gravitational corrections.

To present this result, we have to carefully address the dependence of $\chi^{(1)}$ on the quantum variable α in the proposed paradigm, in light of studying phenomenological implications. Anticipating the content of the next Chapter, we can consider an "averaged" wave function in the form of

$$\bar{\chi}(\eta,v_{\mathbf{k}}) = \int d\alpha |A|^2(\alpha)\, \chi(\alpha,\eta,v_{\mathbf{k}}) \quad (5.38)$$

where $A = e^{iP_1/\hbar}$ is the (quantum) amplitude coming from the lowest-order quantum gravitational component. This choice corresponds to averaging on the quasi-classical gravitational probability density, which in the selected minisuperspace is associated with the logarithmic scale factor α only. It is worth stressing that weighting the matter wave function on the WKB amplitude of the gravitational field is, on the present level, a purely phenomenological procedure. In fact, it is clear that such a wave function can in principle no longer satisfy Eq. (5.28). Nonetheless, we will show in the next Chapter that such a calibrated wave function is actually a solution of the Schrödinger equation when suitable gauge invariance of the BO procedure is taken into account, reserving the details for Sec. 6.2.

Upon substitution of (5.37) and (5.19) into Eq. (5.38), the averaged wave function for each mode becomes

$$\bar{\chi}^{(1)}_{\mathbf{k},Gauss}(\eta,v_{\mathbf{k}}) = \chi^{(0)}_{\mathbf{k}}(\eta,v_{\mathbf{k}}) \left[\hbar \left(\frac{8\pi^3}{\sigma^2} \right)^{\frac{1}{4}} (-\eta)^3 \exp\left(\frac{9\hbar^2}{4\sigma^2} \right) \right]. \quad (5.39)$$

Requiring normalization over the possible $v_{\mathbf{k}}$ values, i.e. dividing by the wave function integrated on such variables, the term in squared brackets clearly factors out of the integration (we stress that it depends only on time and on the specific form of the weight (5.36)). Therefore, we have for the averaged and normalized wave function

$$\bar{\chi}^{(1)}_{\mathbf{k},Gauss} \xrightarrow{integration\ over\ \alpha} \chi^{(0)}_{\mathbf{k}}(\eta,v_{\mathbf{k}}), \quad (5.40)$$

namely, we recover the previous order state.

We now proceed to the computation of the inflationary power spectrum in the described setting, by computing the two-point correlation function of the M-S variable on the the Bunch–Davies state (5.27). For convenience, we rewrite ${}^{BD}\chi^{(0)}_{\mathbf{k}}$ in the following way:

$$ {}^{BD}\chi^{(0)}_{\mathbf{k}}(\eta, v_{\mathbf{k}}) = N_k(\eta) \exp\left(i\delta_{0,k}(\eta) - \Omega_k(\eta) v_{\mathbf{k}}^2\right) , \tag{5.41} $$

where

$$ \Omega_k(\eta) := \frac{1}{2\hbar}\left(\frac{i}{\eta^3\left(\frac{1}{\eta^2}+k^2\right)} + \frac{k^3}{\frac{1}{\eta^2}+k^2}\right) , \tag{5.42} $$

$$ N_k(\eta) := \left(\frac{2}{\pi}\Re(\Omega_k)\right)^{1/4} = \left(\frac{k^3}{\pi\hbar\left(\frac{1}{\eta^2}+k^2\right)}\right)^{\frac{1}{4}} , \tag{5.43} $$

and $\Re(\cdot)$ isolates the real part. In the following, we also isolate the real and imaginary parts of the (complex) variable $v_{\mathbf{k}}$ as

$$ v_{\mathbf{k}} = \frac{1}{\sqrt{2}}(v^R_{\mathbf{k}} + i v^I_{\mathbf{k}}) . \tag{5.44} $$

Then, the two-point correlation function of the complex M-S variable computed on the Bunch–Davies vacuum state (for which we drop the prefix in ${}^{BD}\chi^{(0)}_{\mathbf{k}}$ for readability) corresponds to [110]

$$ \begin{aligned} \Xi(\mathbf{r}) &= \langle 0|v(\eta,\mathbf{x})v(\eta,\mathbf{x}+\mathbf{r})|0\rangle \\ &= \int \prod_{\mathbf{k}} dv^R_{\mathbf{k}} dv^I_{\mathbf{k}} \left(\prod_{\mathbf{k}'} \chi^{(0)*}_{\mathbf{k}'}(\eta, v_{\mathbf{k}'})\right) v(\eta,\mathbf{x})v(\eta,\mathbf{x}+\mathbf{r}) \left(\prod_{\mathbf{k}''} \chi^{(0)}_{\mathbf{k}''}(\eta, v_{\mathbf{k}''})\right) \\ &= \prod_{\mathbf{l}} |N_l(\eta)|^4 \int \prod_{\mathbf{k}} dv^R_{\mathbf{k}} dv^I_{\mathbf{k}} \left(\prod_{\mathbf{k}'} e^{-2\Re(\Omega_{k'})\left[(v^R_{\mathbf{k}'})^2+(v^I_{\mathbf{k}'})^2\right]}\right) v(\eta,\mathbf{x})v(\eta,\mathbf{x}+\mathbf{r}) \\ &= \left(\prod_{\mathbf{l}} \frac{2\Re(\Omega_l)}{\pi}\right) \int \frac{d\mathbf{p}}{(2\pi)^{3/2}} \int \frac{d\mathbf{q}}{(2\pi)^{3/2}} e^{i\mathbf{p}\cdot\mathbf{x}} e^{i\mathbf{q}\cdot(\mathbf{x}+\mathbf{r})} \\ &\quad \times \int \prod_{\mathbf{k}} dv^R_{\mathbf{k}} dv^I_{\mathbf{k}} \left[v_{\mathbf{p}} v_{\mathbf{q}} e^{-2\sum_{\mathbf{k}'} \Re(\Omega_{k'})\left((v^R_{\mathbf{k}'})^2+(v^I_{\mathbf{k}'})^2\right)}\right] . \end{aligned} \tag{5.45} $$

More specifically, we are considering each Fourier mode of the vacuum state, substituting the expression (5.41) in the second equality, and expanding both variables in Fourier modes in the third. The last integral vanishes for $\mathbf{p} \neq \pm\mathbf{q}$, and the same happens for $\mathbf{p} = \mathbf{q}$, since we obtain exponents of the form $\left[(v^R_{\mathbf{p}})^2 - (v^I_{\mathbf{p}})^2\right]$, and the real and imaginary parts contribute the same amounts. Therefore, the surviving contribution is in the case $\mathbf{p} = -\mathbf{q}$:

$$ \begin{aligned} \Xi(\mathbf{r}) = \left(\prod_{\mathbf{l}} \frac{2\Re(\Omega_l)}{\pi}\right) \int \frac{d\mathbf{p}}{(2\pi)^3} e^{-i\mathbf{p}\cdot\mathbf{r}}\, 2 \int \prod_{\mathbf{k}} dv^R_{\mathbf{k}} dv^I_{\mathbf{k}} \Big[(v^R_{\mathbf{p}})^2 \\ \times e^{-2\sum_{\mathbf{k}'} \Re(\Omega_{k'})\left((v^R_{\mathbf{k}'})^2+(v^I_{\mathbf{k}'})^2\right)}\Big] \\ = \int \frac{d\mathbf{p}}{(2\pi)^3}\, e^{-i\mathbf{p}\cdot\mathbf{r}}\, \frac{1}{2\Re(\Omega_p)} , \end{aligned} \tag{5.46} $$

where we remind that $\Omega_p = \Omega_p(\eta)$ as from the definition (5.42). Using (5.7) and the definition (5.8), we obtain a power spectrum of the form

$$\mathcal{P}_v(k) = \frac{k^3}{4\pi^2} \frac{1}{\Re(\Omega_k)}\,, \tag{5.47}$$

and the invariant one associated with the curvature perturbation ζ (5.5)

$$\mathcal{P}_\zeta(k) = \frac{4\pi G}{\epsilon\, a_0^2\, e^{2\alpha}} \mathcal{P}_v(k) = \frac{G}{\pi\epsilon} \frac{k^3}{a_0^2\, e^{2\alpha}} \frac{1}{\Re(\Omega_k)}\,. \tag{5.48}$$

Since as discussed in Sec. 5.1 the perturbations freezed out when crossing the horizon, we now evaluate this quantity in the super-Hubble limit, which in conformal time corresponds to modes for which $k\eta \to 0^-$. In this case, we note from the definition (5.42) that the function $\Re(\Omega_k)$ becomes

$$\Re(\Omega_k(\eta)) \approx k^3\eta^2 \tag{5.49}$$

where we considered $\hbar = 1$ for easier comparison with the literature. When implementing this limit and substituting the classical solution $\alpha(\eta)$, we arrive at the following result for the primordial power spectrum in the de Sitter phase:

$$\mathcal{P}_\zeta(k) = \frac{G\,\mathscr{H}_\Lambda^2}{\pi\epsilon}\bigg|_{k=a\mathscr{H}_\Lambda}\,, \tag{5.50}$$

where $\mathscr{H}_\Lambda = \sqrt{8\pi G\Lambda/3}$ and the slow-roll parameter ϵ is evaluated at the horizon crossing. Clearly, the corresponding spectral index (5.9) results to be null.

At this order, we have recovered the standard QFT spectrum for the primordial fluctuations implementing the Gaussian fluid as a time parameter (4.24). It is evident that the quantum gravity corrections in (5.29) do not modify, but preserve the inflationary power spectrum up to this expansion order. Such result stems from the modified Schrödinger equation (5.28), which presents no coupling between the quantum gravitational degree of freedom α and the perturbation variables $v_{\mathbf{k}}$. Therefore here the correction to the "fast" wave function χ (5.35) factorizes, and due its time-dependent form, does not influence the evolution of the perturbation modes. Actually, we show that the present result stands in any minisuperspace setting with negligible backreaction in the next Subsection.

5.3.1 A general minisuperspace treatment: the role of backreaction

The result presented in the previous section suggests that the quantum gravity-induced corrections on the matter evolution, obtained in the WKB expansion and via the time parameter introduced in (4.24), give as a net effect a time-dependent factor. Such term could be considered *a posteriori* a phase rescaling acting on the matter wave function, as we show here in the general case.

Let us start from the modified dynamics (4.32) analyzed for a generic minisuperspace model in which the supermomentum is identically vanishing. We adopt for convenience the synchronous time $N = 1$ such that the definition (4.24) coincides with the derivative with respect to T, up to a fiducial volume set to unit, but the result here discussed stands for a generic lapse function N. Explicitly, we recall the dynamics up to the order M^{-1}

$$i\hbar\frac{\partial\chi}{\partial T} = \hat{\mathcal{H}}^m\chi - i\hbar\,\mathcal{G}_{ab}\frac{\partial S_0}{\partial h_a}\frac{\partial}{\partial h_b}\chi\,, \tag{5.51}$$

being $\mathcal{G}_{ab}$ the minisupermetric. We now write the matter wave functional in the form

$$\chi(h_a,T,\phi) = \xi_g(h_a)\;\Theta_m(T,\phi)\,, \tag{5.52}$$

analogous to the ansatz (5.30). Clearly this is a stronger requirement and is inherently different from the Born–Oppenheimer separation (4.7), since Θ_m is now assumed to be independent of the generalized minisuperspace coordinate h_a. Such separation is backed by the observation that, in the absence of quantum matter backreaction, we can consider the two sets of degrees of freedom as independent. By substituting (5.52) into (5.51), and dividing by the non-trivial functional ξ_g, we obtain

$$i\hbar\frac{\partial\Theta_m}{\partial T} = \hat{\mathcal{H}}^m\Theta_m - \frac{i\hbar}{\xi_g}\mathcal{G}_{ab}\frac{\partial S_0}{\partial h_a}\frac{\partial \xi_g}{\partial h_b}\,\Theta_m\,. \tag{5.53}$$

Here, S_0 belongs to the classical solution (see (4.17)), thus the corresponding factor is a function of time only: $\partial_{h_a}S_0 = f(T)$, where the form of f depends on the specific cosmological model. Additionally, the modified dynamics cannot induce dependence of Θ on the h_a, since that would be inconsistent with the initial separation (5.52). Then, we can express the factor containing ξ_g as a constant, whose value can depend on the quantum number associated with h_a; i.e., its value is fixed during the dynamics once a specific foliation is selected:

$$\frac{1}{\xi_g}\frac{\partial\xi_g}{\partial h_a} = ik_{(h_a)} \tag{5.54}$$

where for convenience, we have inverted the couple of indices a and b in (5.51), making use of the symmetry of the minisupermetric G_{ab}. The writing $k_{(h_a)}$ is to be understood as a function of the gravitational variable h_a. The solution to (5.54) has a plane wave structure

$$\xi_g(h_a) = e^{ik_{(h_a)}\,h_a}\,. \tag{5.55}$$

The functions (5.55) constitute a complete basis that can be adopted to construct wave packets, which will describe the quantum gravitational contribution to χ.

In what follows, we limit our attention to the plane wave (5.55) associated with a specific value $k_{(h_a)}$; in this case, the modified dynamics take the form

$$i\hbar\frac{\partial\Theta_m}{\partial T} = \hat{\mathcal{H}}^m\Theta_m + \hbar f(T)\,k_{(h_a)}\Theta_m \tag{5.56}$$

We now rewrite the function Θ_m, which is useful for the computation of the corrective effects, as:

$$\Theta_m(T,\phi) = e^{i\Upsilon(T)}\varrho(T,\phi)\,, \tag{5.57}$$

where ϱ has the same degrees of freedom with respect to Θ_m, and a (complex) time-dependent phase Υ has been separated. In the general case, such a phase can acquire different forms depending on the wave number $k_{(h_a)}$ present in (5.54) and (5.55) (or, as we will discuss later, depending on the considered wave packet). It is exactly the phase factor $\Upsilon(T)$ that will account for the quantum gravity corrections, since we will see that ϱ exactly solves the unperturbed matter dynamics at such order. Indeed, by substituting (5.57) into (5.56) and requiring that

$$\frac{\partial \Upsilon(T)}{\partial T} = f(T)\, k_{(h_a)} \tag{5.58}$$

the additional contribution on the right-hand side of (5.56) cancels out via the phase rescaling, and the function ϱ satisfies the unperturbed Schrödinger evolution:

$$i\hbar \frac{\partial \varrho(T,\phi)}{\partial T} = \hat{\mathcal{H}}_m\, \varrho(T,\phi)\,. \tag{5.59}$$

Here, the matter Hamiltonian $\mathcal{H}_m$ is left as a generic expression; for the purpose of the cosmological implementation above, it took the form of a time-dependent harmonic oscillator.

It is then possible to discuss any effects of such quantum gravity contributions to the scalar field's power spectrum. As previously stated, the net effect is encased in the time-dependent phase $\Upsilon(T)$ solution of (5.58), which is actually real-valued, since $f(T)$ follows from the classical solution S_0. The complete matter wave function at $\mathcal{O}\left(M^{-1}\right)$ thus reads

$$\chi(h_a, T, \phi) = e^{ik_{(h_a)}\, h_a}\, e^{ik_{(h_a)} \int dT' f(T')}\, \varrho(T,\phi) \tag{5.60}$$

where the integral in the second term $\int dT' f(T')$ is intended to be between values T_0 and T, for which the WKB approximation holds. We observe that the solution (5.60) has the same shape of the result obtained above. Due to the peculiar morphology of the quantum gravity factors arising from (5.54) and (5.58) (which originally stem from the requirement (5.57)), the effect on the matter spectrum is canceled once the matter wave function is properly normalized. This is the reason for which at this level the quantum gravity corrections preserve the primordial inflationary spectrum.

While at $\mathcal{O}\left(M^{-1}\right)$ no corrections emerge for the inflationary spectrum, this clearly does not mean that a deformation of the scale invariance property cannot come out at the next orders of approximation. However, we here focus attention on a specific point: the absence of a spectral modification is a consequence of the phase form that the quantum gravity corrections take in the matter wave function, and in turn, this feature is induced by the possibility of factorizing such a wave function into a gravitational and a matter component. The physical meaning of this assumption must be searched, in this specific formulation, in the absence of a quantum matter backreaction on the classical gravitational background.

Let us go back to the modified Schrödinger equation (4.32) computed with the Gaussian fluid time in Sec. 4.2. It should be noted that the lowest-order solution S_0 for the gravitational field and in particular the classical momentum terms appearing in the quantum gravity corrections do not depend, by the considered WKB perturbation scheme, on the quantum matter degrees of freedom. It is exactly this point which enters the possibility of factorizing the matter wave function into two independent components (5.52). On the contrary, if the HJ equation (4.17) contained the expectation value of the matter Hamiltonian, then also the classical momentum would be affected on average by the quantum degrees of freedom. Then, the choice of a factorized form for the matter wave function would no longer appear as a natural solution to the perturbed dynamics.

The role played by the matter backreaction (see also the review [62]) can be elucidated in view of Sec. 3.2. When implementing a standard B-O scheme in the WKB approximation order by order in $1/M$ [43],we have seen that the quantum matter expectation value enters both the right-hand side of the HJ equation (4.17) and the Schrödinger equation (4.24). Actually, the phase rescaling of χ needed to remove such contribution from the Schrödinger dynamics induces an opposite change of phase to the gravitational one, with the net effect that the backreaction term is also removed from the HJ equation (Sec. 3.2). This suggests that such a contribution could be neglected in view of the gauge invariance analyzed above. We stress that actually in the B-O procedure the gauge invariance is used to eliminate the "geometric" phase [124] but not to cancel the (fast) electronic eigenvalue contribution in the slow nuclear dynamics [125]. From this point of view, it is more natural to maintain the expectation value contribution both in the HJ equation and in the Schrödinger one. This would lead to a non-trivial coupled integro-partial differential system which could be treated with a self-consistent method.

We here referred to orders M^1 and M^0 of the WKB approximation, but this discussion naturally extends to $\mathcal{O}\left(M^{-1}\right)$. Thus, the inclusion of the matter Hamiltonian term in (4.32) would give a coupled system, that only at the lowest order of approximation in a Hartree self-consistent approach can be reduced to the form discussed in Sec. 4.2. The complete problem naturally introduces dependence of the HJ function S_0 on the matter one (via an integral of the matter's degrees of freedom); this point clarifies the technical content of the discussion above on the role of the matter backreaction in the separability of Eq. (4.32) to some order of approximation. Therefore, we are led to conclude that the proposed WKB expansion in the quantity $1/M$ would result in a modified inflationary spectrum only if one carefully takes into account the matter (average) backreaction on the gravitational quasi-classical background.

One could also discuss the possible presence of macroscopic matter contributions at th HJ level. In the present model, based on a WKB expansion in M (Sec. 2.4), the macroscopic matter (apart from the cosmological constant contribution) is absent. Such sources could only emerge via an *ad-hoc* rescaling of the matter field via the Planckian parameter, resulting in an auxiliary potential $V(\phi)$ inside the HJ Eq. (4.17), as implemented in [52].

To conclude, the present theory always contains the class of separable solutions (5.30) for which the QG corrections reduce to a simple phase contribution, depending on the gravitational HJ equation (4.17). In order to overcome such restriction, will reformulate the scheme in Chapter 6 by allowing for independent variables describing the "slow" quantum gravitational sector (i.e. graviton contributions); there, the modified dynamics with QG corrections will take a form different from (5.51) such that the QG-induced corrections will exclude the class of separable solutions (5.52).

Chapter 6

Beyond WKB: averaging over gravitational fluctuations

In this chapter we explore the possibility of accounting for small graviton fluctuations in the WKB picture, performing a B-O separation inside the gravitational sector as well to characterize a fully classical background from its small quantum fluctuations. The latter are described through independent degrees of freedom and, since we consider tensor perturbations only, correspond to graviton particles. We first reformulate Vilenkin's original WKB proposal in this extended B-O view in Sec. 6.2, showing that one can actually relax the initial hypothesis of the gravitational constraint and make use of the B-O gauge symmetry to recover the QFT limit after an average over the gravitons variables. In this way, the selected gauge condition exactly corresponds to Vilenkin's gravitational equation expanded at the desired WKB order, thus providing an *a posteriori* motivation for such hypothesis.

We then reformulate in Sec. 6.3 the complete gravity-matter system with the Gassian fluid clock in such extended B-O view, in order to compute the QG-induced corrections after such gravitational separation is carried on. The result here presented exactly matches the modified dynamics of Chapter 4 (and so Chapter 3) after the average procedure and selecting a different gauge condition, which does not correspond to the gravitational WDW constraint. We further discuss the meaning of such choice and also show how an effective QFT can be cast also at this order.

This Chapter illustrates the results of the investigations in Refs. [126, 127].

6.1 Motivations for a separation of the quantum gravitational sector

A B-O-like separation of the semiclassical and quantum wave functionals was implemented in [41], see Sec. 2.3, based on the scale separation 1. In such view, the semiclassical component has a "slow" character, and the quantum one is the "fast" component of the coupled system, similarly to the discussions in Sec. 2.4 and Chapters 3-4.

Let us discuss more the implications of such separation. In Vilenkin's proposal, the total wave functional of the gravity and matter system is decomposed as $\Psi(s_a, q_m) = \psi(s_a)\chi(s_a, q_m) = A(s_a)\, e^{iS(s_a)/\hbar}\, \chi(s_a, q_m)$ (see (2.23)), with A and S

real functions and χ is associated to the quantum subsystem. Implementing both the total WDW constraint (2.25) and the gravitational one (2.24) independently actually breaks a symmetry related to the above separation of Ψ in a B-O-like fashion. Indeed, $\Psi = \psi(s_a)\chi(s_a, q_m)$ is invariant under the following rescaling of both components via a "semiclassical" phase $\theta(s_a)$

$$\psi(s_a) \to \psi(s_a) e^{-\frac{i}{\hbar}\theta(s_a)}\,, \tag{6.1a}$$

$$\chi(s_a, q_m) \to e^{\frac{i}{\hbar}\theta(s_a)}\chi(s_a, q_m)\,. \tag{6.1b}$$

The total WDW constraint (2.25) is invariant under such transformation, since the rescalings of both components exactly compensate; however, the gravitational constraint clearly is not. In other words, requiring both constraints to hold at the same time is inconsistent with a true B-O-like formulation of the system. Indeed, in the proposals discussed in Sec. 3.2, the use of a similar rescaling (see (2.54) and (3.36)) is allowed by the fact that the gravitational constraint is not imposed *a priori*; in those cases, different implementations allow to obtain a second equation referring to the semiclassical component ψ only, although with the caveats discussed in Sec. 3.2. This observation represents the starting point if one wants to incorporate the original Vilenkin's proposal with a proper B-O treatment, considering that the semiclassical sector is not truly classical but has an inherent quantum (although "slow") nature. However, there are other limitations of [41] stemming from the WKB expansion in the B-O-like picture.

We first observe that in Ref. [41] the separation between a quasiclassical background system and a "small" quantum one was pursued without taking into account the physical nature of the variables. Let us consider, both for the present discussion and the following application, a minisuperspace model with semiclassical variables h_a and a matter sector described by variables q_m, for a clearer analogy with Sec. 3.1. The WKB expansion in $\hbar$ of the gravitational constraint and the total one in Vilenkin's formulation result in the Eqs. presented in Sec. 2.3, which we here rewrite for clarity

$$\mathcal{G}^{ab}\frac{\partial S}{\partial h_a}\frac{\partial S}{\partial h_b} + V(h_a) = 0\,, \tag{6.2}$$

$$\mathcal{G}^{ab}\frac{\partial}{\partial h_a}\left(A^2\frac{\partial S}{\partial h_b}\right) = 0\,, \tag{6.3}$$

$$i\hbar\partial_\tau\chi = N\hat{H}^Q\chi\,, \tag{6.4}$$

being N is the lapse function. We recall that the time derivative in Eq. (6.4) is defined as

$$\partial_\tau\chi \equiv 2N\mathcal{G}^{ab}\frac{\partial S}{\partial h_a}\frac{\partial\chi}{\partial h_b} = \dot{h}_a\frac{\partial}{\partial h_a}\chi\,, \tag{6.5}$$

using the classical Hamilton's equation associated to variation of p_A (here a dot denotes differentiation with respect to label time). Equation (6.2) is of order $\hbar^0$ and corresponds to the Hamilton-Jacobi equation for the classical limit of gravity. Both Eqs. (6.3) and (6.4) are obtained[1] at order $\hbar$; the former arises from the gravitational

[1]Here we have adopted again the "natural" operator ordering; this choice has no deep physical implications for the conceptual paradigm here.

WDW equation, while the latter yields the desired QFT dynamics for quantum matter, recovered by simply combining an expansion in $\hbar$ with the B-O separation.

Now we are ready to outline four points of the approach [41] which raise some ambiguity in a B-O-like picture and are the main motivations for the present study.

i) The variables h_a do not represent a set of classical gravitational degrees of freedom, because a quantum amplitude $A(h_a)$ is retained at order $\hbar$. Qualitatively, we could write
$$h_a = h_a^0(t) + \delta h_a \,, \tag{6.6}$$
where $h_a^0(t)$ account for the classical gravitational degrees of freedom (with the dependence on the label time t determined by the Hamilton's equations), while δh_a represent quantum corrections of order $\hbar$ to some suitable power. In this chapter's notation, the symbol δ does not indicate functional derivatives but only a (small) quantum fluctuation. Thus, the time differentiation (6.5) should be defined by employing derivatives with respect to h_a^0 only, rather than the full quantum variable h_a.

ii) This also implies that δh_a are independent degrees of freedom with respect to $h_a^0(t)$. Therefore, a description of their dynamics is necessary. This is readily understood if we remember that the small metric perturbations of an isotropic universe (whose only degree of freedom is given by the cosmic scale factor a) have two scalar, two vector, and two tensor components, at both a classical and a quantum level. These degrees of freedom are independent from a and are different in number and morphology from the small quantum fluctuations δa.

iii) Equations (6.3) and (6.4) both live at the same order in $\hbar$ and their separation relies on the assumption that it is *a priori* possible to impose the gravitational WDW constraint independently. However, this assumption does not have a physical motivation in the analysis of Ref. [41], and is inconsistent with a pure B-O approximation, because it violates its typical gauge invariance. In fact, the B-O method separates the whole system into a slow and a fast component. Thus, if we multiply the quantum matter wave functional χ by a phase depending on h_a, the state is invariant provided that we multiply the gravitational component by an inverse phase. This gauge symmetry is broken if we separately impose the gravitational constraint, so that such a procedure appears rather ambiguous.

iv) The functional Schrödinger equation (6.4) is not the right one for quantum matter on a classical curved spacetime, since the matter wave functional χ depends on the quantum fluctuations of the background δh_a. This dependence, which was implicitly neglected in Ref. [41], is problematic for the purpose of recovering QFT on curved spacetime.

We would like to remark that the difficulties i), ii) and iv) were also present also in Ref. [42], while iii) was not, because the equation for the quantum-gravitational amplitude $A(h_a)$ was obtained via a gauge condition (see Ref. [61] for a comparison of the two approaches in Refs. [41] and [42]).

We now move on to address these motivations and reformulate the problem in order to recover the QFT on curved spacetime limit without imposing the gravitational constraint and after averaging over quantum-gravitational effects [126].

6.2 Graviton fluctuations in Bianchi I spacetime

Starting from point (i)) of the previous section, we take the classical cosmological background to be a vacuum diagonal Bianchi I model, which is the simplest case of the Bianchi classification (Sec. 1.6.1). The advantage of this choice over a FLRW model (used for example in Refs. [118, 68, 52, 119, 55]) is that, being a vacuum geometry, no scalar or vector perturbations are present [15, 1] and we are effectively able to separate the tensor gravitational fluctuations from the matter sector.

In the variables α, β_+ and β_- introduced in Sec. 1.6.1, the line element reads

$$ds^2 = -N^2(t)dt^2 + e^{\alpha}(e^{\beta})_{ij}dx^i dx^j, \tag{6.7}$$

with β_{ij} being the a diagonal traceless matrix. The super-Hamiltonian (1.76) for the Bianchi I case has vanishing potential U_B and it reads

$$H^I(\alpha(t), \beta_\pm(t)) = \frac{4}{3M} e^{-\frac{3}{2}\alpha} \left(-p_\alpha^2 + p_+^2 + p_-^2\right), \tag{6.8}$$

where M was defined in (2.38).

According to point ii), we describe the gravitational fluctuations via tensor perturbations only, as guaranteed by the choice of the vacuum Bianchi I model. Thus the "slow" quantum degrees of freedom δh^A correspond to gravitons and are independent from the classical background. In the original analysis of Ref. [41], the existence of these variables was implicitly assumed, as is clear from the presence of a quantum amplitude $A(h_a)$ computed at first order in $\hbar$; a similar feature was found in the analysis of Ref. [42]. The core difference with the formulation of Chapters 3 and 4 is that we here "extend" the B-O picture by further characterizing the gravitational sector into a classical and a "slow" quantum component; in other words, we modify the scheme of Fig. 4.1 by replacing it with Fig. 6.1.

A gauge-invariant formulation can be portrayed also for tensor fluctuations, as done in Sec. 5.3 for scalar ones, via the same Mukhanov-Sasaki formalism. In this case, one introduces the gauge-invariant variables $v_{\mathbf{k}}^{\lambda}$ corresponding to the tensor perturbations in Fourier space, where λ identifies the two polarization states. For the Bianchi I case, the corresponding Hamiltonian (where $N = e^{\alpha}$ in the conformal time η gauge) is [128]

$$NH^{(v^\lambda)} = \sum_{\mathbf{k},\lambda} \frac{1}{2}\left[-\partial^2_{v_{\mathbf{k}}^{\lambda}} + \omega_k^2(\eta)(v_{\mathbf{k}}^{\lambda})^2 + \mathcal{V}_{\lambda,\bar{\lambda}}\right]. \tag{6.9}$$

Clearly, each mode $\mathbf{k}, \lambda$ behaves as a time-dependent harmonic oscillator with

$$\omega_k^2(\eta) = k^2 - z_\lambda''/z_\lambda \tag{6.10}$$

being $z_\lambda(\eta, k_i)$ a function of the background metric and $' \equiv \partial_\eta$. The presence of an interaction potential $\mathcal{V}_{\lambda,\bar{\lambda}}$ should be highlighted: this term is a function of the so-called shear tensor $\sigma_{ij} = \frac{1}{2}(e^{\beta})'_{ij}$ of the background metric [128] and it expresses the mixing of the two polarization modes $(\lambda, \bar{\lambda})$. We stress that such tensor mixing takes place due to the anisotropic nature of spacetime even at the classical level [129] if one considered classical tensor object; this is a stark difference from isotropic models where it does not emerge classically.

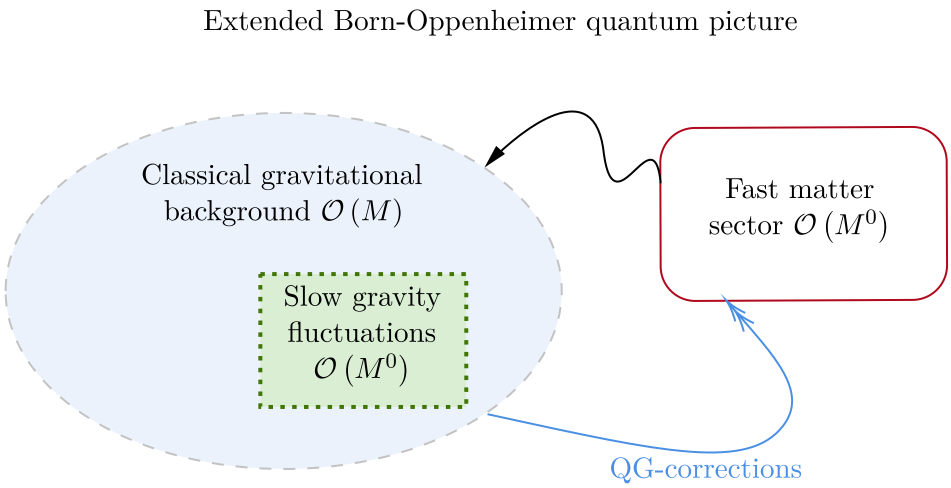

Figure 6.1. Schematic representation of the extended Born-Oppenheimer picture, distinguishing the different scales also within the gravitational component. Here the degrees of freedom for the gravity background are separated into classical ones, and small quantum fluctuations on top. These perturbations start at the next order and are considered "slow" in the B-O picture. Matter retains the same role of a fast quantum component.

Also, since we here neglect the matter backreaction contributions in the B-O approximation, no mixing between scalar and tensor perturbations arises; a treatment of perturbations in a Bianchi I universe coupled to matter, which goes outside the aim of this Chapter, can be found in Refs. [130, 131, 132, 133].

We consider a free test scalar field as the "fast" quantum matter sector (e.g. the inflaton field), whose Hamiltonian in the MS formalism takes the form

$$NH^{(\phi)} = \sum_{\mathbf{k}} \frac{1}{2}\left[-\partial^2_{\phi_{\mathbf{k}}} + \nu_k^2(\eta)\,(\phi_{\mathbf{k}})^2\right]. \tag{6.11}$$

Th pulsation of the time-dependent harmonic oscillator describing each Fourier mode is

$$\nu_k^2(\eta) = k^2 - (e^{\alpha})''/e^{\alpha} \tag{6.12}$$

.

The WDW equation for the full model is

$$\hat{H}\Psi = \left(\hat{H}^I + \hat{H}^{(v^\lambda)} + \hat{H}^{(\phi)}\right)\Psi = 0\,, \tag{6.13}$$

and the wave functional Ψ is again assumed to be separable in the B-O scheme as

$$\Psi = \psi_g(\alpha, \beta_\pm, v^\lambda_{\mathbf{k}})\,\chi_m(\phi_{\mathbf{k}}; \alpha, \beta_\pm, v^\lambda_{\mathbf{k}}) \tag{6.14}$$

and ψ_g is independent of the matter variables $\phi_{\mathbf{k}}$ assuming a negligible backreaction, following the previous Chapters. Given the separation (6.14), the WDW equation (6.13) is clearly invariant under the transformation:

$$\psi_g \to \psi_g e^{-\frac{i}{\hbar}\theta}\,, \quad \chi_m \to e^{\frac{i}{\hbar}\theta}\chi_m\,, \tag{6.15}$$

where the phase $\theta = \theta(\alpha, \beta_\pm, v^\lambda_{\mathbf{k}})$ depends on the gravitational variables only.

As in point iii), we do not require the gravitational sector to satisfy the gravitational constraint *a priori*. The gravitons' evolution will instead be derived on physical grounds by requiring the correct QFT dynamics to arise in the appropriate limit and exploiting the gauge invariance (6.1).

For this purpose we now apply the WKB perturbative scheme in $1/M$ to our model, which allows us to consistently separate the gravity and matter sectors. We emphasize this is equivalent to the (semiclassical) WKB expansion in the Planck constant $\hbar$ used in Ref. [41] up to the order of quantum-gravitational corrections, as discussed in Sec. 3.1.

We first focus on the recovery of the QFT formulation for the matter sector in such picture. Therefore we expand up to order M^0 only

$$\Psi = e^{\frac{i}{\hbar}MS_0}\, e^{\frac{i}{\hbar}\left(P_1+\mathcal{O}\left(M^{-1}\right)\right)}\, e^{\frac{i}{\hbar}\left(Q_1+\mathcal{O}\left(M^{-1}\right)\right)}\,, \tag{6.16}$$

being $S_0 = S_0(\alpha, \beta_\pm)$ and the complex functions $P_n = P_n(v^\lambda_{\mathbf{k}}; \alpha, \beta_\pm)$ and $Q_n = Q_n(\phi_{\mathbf{k}}; \alpha, \beta_\pm, v^\lambda_{\mathbf{k}})$ are associated to the tensor and scalar quantum components of the system, respectively. Let us now examine the WDW equation (6.13) applied to Eq. (6.16) perturbatively examined at each order in $1/M$: at $\mathcal{O}\left(M\right)$ we obtain

$$\frac{4}{3}e^{-\frac{3}{2}\alpha}\left(-\left(\partial_\alpha S_0\right)^2 + \left(\partial_+ S_0\right)^2 + \left(\partial_- S_0\right)^2\right) = 0, \tag{6.17}$$

which is consistent with the classical Bianchi I solution

$$S_0(\alpha, \beta_\pm) = k_\alpha \alpha + k_+\beta_+ + k_-\beta_- \tag{6.18}$$

with $k_\alpha < 0$ such that $k_\alpha^2 = k_+^2 + k_-^2$ corresponding to an expanding universe.

For the $\mathcal{O}\left(M^0\right)$ things are not so trivial. Indeed, we should introduce the time differentiation operator as in Eq. (6.5) to recast Vilenkin's original formulation in this effective B-O scheme. Let us choose $N = e^\alpha$; we can construct such operator using only derivatives with respect to the classical variables $\alpha, \beta_\pm$, such that the issue i of Sec. 6.1 does not arise. We have

$$-i\hbar\partial_\tau = \frac{8}{3}e^{-\frac{1}{2}\alpha}\left(\partial_\alpha S_0\, \partial_\alpha + \partial_+ S_0\, \partial_+ + \partial_- S_0\, \partial_-\right)\,. \tag{6.19}$$

Now using Eqs. (6.19) and (6.18), at $\mathcal{O}\left(M^0\right)$ we find

$$\begin{aligned} &-i\hbar(\partial_\tau e^{\frac{i}{\hbar}P_1})e^{\frac{i}{\hbar}Q_1} - i\hbar(\partial_\tau e^{\frac{i}{\hbar}Q_1})e^{\frac{i}{\hbar}P_1}\\ &\quad + \frac{1}{2}\sum_{\mathbf{k},\lambda}\left[\omega_k^2(v^\lambda_{\mathbf{k}})^2 + \mathcal{V}_{\lambda,\bar\lambda} - \partial^2_{v^\lambda_{\mathbf{k}}}\right]e^{\frac{i}{\hbar}(P_1+Q_1)}\\ &\quad + \frac{1}{2}\sum_{\mathbf{k}}\left[\nu_k^2(\phi_{\mathbf{k}})^2 - \partial^2_{\phi_{\mathbf{k}}}\right]e^{\frac{i}{\hbar}(P_1+Q_1)} = 0. \end{aligned} \tag{6.20}$$

Clearly the quantum matter wave function still depends on the graviton variables (see point iv). In the spirit of effective field theory, we average over quantum-gravitational effects with the aim to recover a functional Schrödinger equation in accordance with the interpretation of Sec. 2.3. To this end, we label $\Gamma_g = \exp(iP_1/\hbar)$

(which is ψ_g at order M^0 only) and multiply Eq. (6.20) by the conjugate $\Gamma_g^* = \exp(-iP_1^*/\hbar)$, obtaining

$$\begin{aligned}&-i\hbar\partial_\tau\left(\Gamma_g^*\Gamma_g\chi_1\right)+i\hbar(\partial_\tau\Gamma_g^*)\,\Gamma_g\chi_1\\&\quad+\frac{1}{2}\sum_{\mathbf{k},\lambda}\Big[\left(\omega_k^2\,(v_{\mathbf{k}}^\lambda)^2\Gamma_g^*+\mathcal{V}_{\lambda,\bar\lambda}\Gamma_g^*-\partial^2_{v_{\mathbf{k}}^\lambda}\Gamma_g^*\right)\Gamma_g\chi_1\\&\quad+\partial_{v_{\mathbf{k}}^\lambda}\left(2(\partial_{v_{\mathbf{k}}^\lambda}\Gamma_g^*)\Gamma_g\chi_1-\partial_{v_{\mathbf{k}}^\lambda}\left(\Gamma_g^*\Gamma_g\chi_1\right)\right)\Big]\\&\quad+\frac{1}{2}\sum_{\mathbf{k}}\left[\nu_k^2\,(\phi_{\mathbf{k}})^2-\partial^2_{\phi_{\mathbf{k}}}\right]\Gamma_g^*\Gamma_g\chi_1=0\,,\end{aligned}\tag{6.21}$$

where $\chi_1 = \exp(iQ_1/\hbar)$ also depends on the $v_{\mathbf{k}}^\lambda$. The effective scheme that we wish to obtain now has a clearer interpretation: integration over the $v_{\mathbf{k}}^\lambda$ modes corresponds to considering an "average effect" of the gravitons. In doing so, we assume that the wave functionals satisfy appropriate boundary conditions such that

$$\int\prod_{\mathbf{k},\lambda}dv_{\mathbf{k}}^\lambda\sum_{\mathbf{k},\lambda}\partial_{v_{\mathbf{k}}^\lambda}\left(2(\partial_{v_{\mathbf{k}}^\lambda}\Gamma_g^*)\Gamma_g\chi_1-\partial_{v_{\mathbf{k}}^\lambda}\left(\Gamma_g^*\Gamma_g\chi_1\right)\right)=0\,.\tag{6.22}$$

Here, we are summing over all contributions to the "border term" corresponding to the different $v_{\mathbf{k}}^\lambda$ modes and then integrate over all of them, such that the final boundary condition does not depend on the graviton variables.

We recall that we still have not made use of the gauge freedom (6.1). We take advantage of this symmetry by imposing the following condition on Γ_g

$$\Gamma_g\left[i\hbar\partial_\tau\Gamma_g^*+\frac{1}{2}\sum_{\mathbf{k},\lambda}\left(\omega_k^2(v_{\mathbf{k}}^\lambda)^2+\mathcal{V}_{\lambda,\bar\lambda}-\partial^2_{v_{\mathbf{k}}^\lambda}\right)\Gamma_g^*\right]=0\,,\tag{6.23}$$

in the spirit of (6.1) representing a gauge freedom, that can be fixed (for example, an analogy is the Lorentz gauge chosen in the electromagnetic interaction). This condition is possible provided that the equation

$$\begin{aligned}&\frac{1}{2\hbar}\sum_{\mathbf{k},\lambda}\left[-i\partial^2_{v_{\mathbf{k}}^\lambda}\theta+\hbar^{-1}(\partial_{v_{\mathbf{k}}^\lambda}\theta)^2-i(\partial_{v_{\mathbf{k}}^\lambda}\theta)\partial_{v_{\mathbf{k}}^\lambda}(\ln\Gamma_g^*)\right]-\partial_\tau\theta\\&\quad=\frac{1}{2}\sum_{\mathbf{k},\lambda}\left[\omega_k^2(v_{\mathbf{k}}^\lambda)^2+\mathcal{V}_{\lambda,\bar\lambda}-\partial^2_{v_{\mathbf{k}}^\lambda}\right]\Gamma_g^*-i\hbar\partial_\tau(\ln\Gamma_g^*)\end{aligned}\tag{6.24}$$

has a solution. It is understood that the boundary condition (6.22) is imposed in the specific gauge set by Eq. (6.23).

Equations (6.21) and (6.23) then guarantee that the "averaged" quantum matter wave functional

$$\widetilde{\Theta}(\phi_{\mathbf{k}};\alpha,\beta_+,\beta_-)=\int\prod_{\mathbf{k},\lambda}dv_{\mathbf{k}}^\lambda\;\Gamma_g^*\,\Gamma_g\,e^{\frac{i}{\hbar}Q_1}\tag{6.25}$$

satisfies the functional Schrödinger equation

$$i\hbar\,\partial_\tau\widetilde{\Theta}=\frac{1}{2}\sum_{\mathbf{k}}\left[\nu_k^2(\phi_{\mathbf{k}})^2-\partial^2_{\phi_{\mathbf{k}}}\right]\widetilde{\Theta}=N\hat{H}^{(\phi)}\widetilde{\Theta}\,,\tag{6.26}$$

therefore recovering QFT on curved spacetime on average. We remark that (6.23) fixes the independent dynamics of gravitons, so the issue ii) is also resolved.

At this point, it is worth briefly discussing the relationship between our analysis and standard QFT on curved spacetime [111, 134]. In that approach, at the one-loop order of approximation, the semiclassical background metric is sourced by the expectation values associated with the quantum components:

$$G_{\mu\nu} = \frac{8\pi G}{c^4}\left(\langle T^{(m)}_{\mu\nu}\rangle + \langle t^{(g)}_{\mu\nu}\rangle\right) , \tag{6.27}$$

where $G_{\mu\nu}$ is the Einstein tensor of (1.1), while $T^{(m)}_{\mu\nu}$ and $t^{(g)}_{\mu\nu}$ denote the energy-momentum tensors of the (renormalized) quantum matter and graviton contributions respectively. The last two are in principle of the same order, although the graviton term is often neglected in QFT applications [111].

In our WKB approach, both backreaction terms are $1/M$ suppressed at leading order [16] and the background is therefore a purely classical vacuum solution described by Eq. (6.17), i.e., the Bianchi I spacetime. The quantum backreaction of the fast (matter) component on the slow one does arise at the next order in the general B-O scheme, in the form of an expectation value of the matter Hamiltonian (under the assumption of gravitons being a “slow” component, there is no contribution of graviton themselves to the average over the fast sector). This backreaction can be removed from the equation governing the matter dynamics and included instead in the gauge condition (6.23) specifying the gravitons’ dynamics by a phase rescaling of both the matter and gravitational wave functions, as elucidated in Sec. 3.2.

In conclusion, we remark that the inclusion of a matter expectation value, which has been here we neglected based on the assumed B-O separation of energy scales, would not alter the final result i.e. the recovery of QFT in the appropriate low-energy limit.

6.2.1 Comparison with gravitational WDW equation

Let us now analyze the WKB dynamics arising when separately imposing the gravitational WDW constraint (as in Ref. [41]). In the conformal time gauge, this equation reads

$$\begin{aligned}\left(\hat{H}^I + \hat{H}^{(v^\lambda)}\right)^\dagger \psi_g^* = \Bigg[&\frac{4}{3M}e^{-\frac{3}{2}\alpha}\left(-p_\alpha^2 + p_+^2 + p_-^2\right)^\dagger \\ &+\frac{1}{2}e^{-\alpha}\sum_{\mathbf{k},\lambda}\left(-\partial^2_{v^\lambda_{\mathbf{k}}} + \omega_k^2 (v^\lambda_{\mathbf{k}})^2 + \mathcal{V}_{\lambda,\bar{\lambda}}\right)^\dagger\Bigg]\psi_g^* = 0\end{aligned} \tag{6.28}$$

where $\psi_g^* = \exp\left(-i(MS_0^* + P_1^*)/\hbar\right)$. At $\mathcal{O}\left(M^0\right)$ and using the Hamilton-Jacobi solution (6.18) for S_0, which is real-valued (so $S_0^* \equiv S_0$), we obtain

$$\begin{aligned}&-\frac{8}{3}e^{-\frac{3}{2}\alpha}\left(\partial_\alpha S_0 \partial_\alpha + \partial_+ S_0 \partial_+ + \partial_- S_0 \partial_-\right) P_1^*\, e^{-\frac{i}{\hbar}P_1^*} \\ &\quad + \frac{1}{2}e^{-\alpha}\sum_{\mathbf{k},\lambda}\Bigg[-i\hbar^{-1}\,\partial^2_{v^\lambda_{\mathbf{k}}} P_1^* + \hbar^{-2}\left(-\partial_{v^\lambda_{\mathbf{k}}} P_1^*\right)^2 \\ &\quad + \left(\omega_k^2\,(v^\lambda_{\mathbf{k}})^2\right)^\dagger + \mathcal{V}^\dagger_{\lambda,\bar{\lambda}}\Bigg]\, e^{-\frac{i}{\hbar}P_1^*} = 0.\end{aligned} \tag{6.29}$$

From Eq. (6.19), this reduces to

$$-i\hbar\partial_\tau\Gamma_g^* = \frac{1}{2}\sum_{\mathbf{k},\lambda}\left(-\partial^2_{v^\lambda_{\mathbf{k}}} + \omega_k^2 (v^\lambda_{\mathbf{k}})^2 + \mathcal{V}_{\lambda,\bar{\lambda}}\right)^\dagger \Gamma_g^* \,. \tag{6.30}$$

The terms on the right-hand side are Hermitian for each mode $\mathbf{k},\lambda$ separately, so Eq. (6.30) multiplied by Γ_g coincides with the condition (6.23). Thus, the gravitons' dynamics imposed by selecting the gauge (6.23) is equivalent to the one following from the gravitational constraint. In other words, requiring on phenomenological grounds that the quantum matter sector follows the Schrödinger dynamics implies that the gravitons' wave functional must satisfy Eq. (6.30).

Let us briefly recap the results of this Chapter until now. In order to address the observations and consequential difficulties listed in points (i)–(iv) of Sec. 6.1, we separated *ab initio* the Bianchi I classical background from its first-order quantum perturbations (the vacuum geometry allowed us to restrict to tensorial perturbations). In this respect, it is worthwhile to clarify that the tensor fluctuations in Refs. [52, 68, 69] were treated on the same level as the matter degrees of freedom (i.e., as a fast contribution in the B-O scheme), whereas in our approach the gravitons are separated in energy scale from matter (i.e., they belong to the slow component). We demonstrated that the functional Schrödinger equation for the matter sector is correctly recovered after averaging over quantum-gravitational effects, fixing a gauge from Eq. (6.1) on the gravitons' sector, whose dynamics corresponds to the one dictated by the gravitational WDW equation only. The possibility to independently impose such constraint was one of the starting assumptions in Ref. [41], although not sufficiently motivated. Since the graviton dynamics cannot be regarded as a gauge-dependent feature, the present study justifies *a posteriori* and on physical grounds the assumption that the gravitational constraint simultaneously holds. In Ref. [41], however, such condition would no longer correspond to a gauge choice, simply because the gauge symmetry was broken from the very beginning.

We have thus far limited our attention to the first two expansion orders, where the nonunitarity issue does not arise. It is meaningful to ask whether such effective picture can be brought to the next order with the reference fluid time of Chapter 4: this is the object of the next section.

6.3 Unifying the Gaussian fluid time approach with averaged graviton fluctuations

The procedure exposed in the previous section allows to take into account small graviton fluctuations in the WKB picture, thus representing an intermediate step towards a more refined treatment of QG. It is interesting to investigate cosmological implications of this treatment, most importantly how the power spectrum of primordial perturbations (Sec. 5.2) is affected. The main goal of this Section is to unify the treatment of Chapter 4 with the model of Sec. 6.2, obtaining a theory in which the reference fluid approach is applied to a gravitational background with "slow" gravitational perturbations (expressed via tensor degrees of freedom) in the B-O picture [127]. We therefore deal with a Bianchi I minisuperspace on which we set gravitons' degrees of freedom, a test scalar matter field and the reference fluid.

As previously discussed, since the Bianchi I model is diagonal in the variables $(\alpha, \beta_{\pm})$ we can choose the ADM splitting in such a way that $N^i = 0$. Doing so ensures a symmetry of the foliation such that the supermomentum constraint is identically satisfied and it is absent from the gravitational action (1.52). Moreover, due to spatial diffeomorphisms invariance, this allows us to impose the Gaussian time condition $\gamma^{00} = -1$ alone in the reference fluid sector (see discussions in Sec. 4.3 and 5.3), thus we have the fluid variable $T(x)$ only.

In analogy with Sec. 5.3, we model the slow-roll inflation period through a scalar field, moving in a region of almost constant potential, thus behaving similarly to a cosmological constant contribution. We thus move away from the minisuperspace Bianchi I background (which, as a vacuum geometry, does not account for energy sources such as Λ) and consider the commonly used FLRW geometry. More specifically, we again describe a pure de Sitter phase by neglecting the slow-roll parameter ϵ, so that the inflaton contribution will correspond to a free massless scalar field on a metric with cosmological constant. In such background, the independence of the scalar and tensorial perturbations allows us to restrict to the tensor sector only, framing the matter contents as test fields not affecting the background. This treatment is inherently different from the one in Sec. 4.3, where the WKB expansion with the Kuchar-Torre fluid clock did not take into account the graviton fluctuations.

Thus, the total Wheeler-DeWitt superHamiltonian of the system is given by:

$$\begin{aligned}\hat{H}^{tot} =& \frac{4}{3M} e^{\frac{3}{2}\alpha} \left[\partial_\alpha^2 - \partial_+^2 - \partial_-^2\right] + \frac{e^{-\alpha}}{2} \sum_{\mathbf{k},\lambda} \left[-\hbar^2 \partial^2_{v^\lambda_{\mathbf{k}}} + \omega_k^2(\eta)(v^\lambda_{\mathbf{k}})^2 + \mathcal{V}_{\lambda,\bar{\lambda}}\right] \\ &+ \frac{e^{-\alpha}}{2} \sum_{\mathbf{k}} \left[-\hbar^2 \partial^2_{\phi_{\mathbf{k}}} + \nu_k^2(\eta)(\phi_{\mathbf{k}})^2\right] - i\hbar W^{-1} \frac{\partial}{\partial T(x)}\end{aligned} \tag{6.31}$$

where both the graviton fluctuations and the scalar matter component are expressed as time-dependent harmonic oscillators, see Sec. 6.2 and Sec. 5.3 respectively.

Following the same ideas of Sec. 4.2, we consider the ansatz (4.8) where now

$$S_0 = S_0(\alpha, \beta_\pm, v^\lambda_{\mathbf{k}})\,, \tag{6.32a}$$

$$P_n = P_n(\alpha, \beta_\pm, v^\lambda_{\mathbf{k}})\,, \tag{6.32b}$$

$$Q_n = Q_n(\phi_{\mathbf{k}}, T; \alpha, \beta_\pm, v^\lambda_{\mathbf{k}}) \tag{6.32c}$$

are complex functions; we neglect terms of order $1/M^2$ or higher for the purpose of investigating the first-order quantum gravitational effects. This separation is once again justified by the assumption that matter and gravity live at different energy scales. This is also the reason why the expansion of χ lacks a term of $O(M)$: in fact, the leading order in this model represents again the pure gravity limit, which coincides with the high-energy one.

We stress that here we do not implement the full set of assumptions I)-III) of Sec. 4.2. More specifically, we consider the following:

- we preserve in full form only the hypothesis I), namely the condition (4.9) where now $H^m = H^\phi + H^f$ and $H^g = H^I + H^{v^\lambda}$, in accordance with the general B-O view.

- The hypothesis (4.10) is not considered here since the validity *a priori* of that equation would clearly break the gauge invariance discussed in Sec. 6.1. As in the previous section, the gravitational dynamics will be recovered through the gauge choice in the WKB formulation at each order.

- The adiabatic condition (4.12) expressing the weak dependence of the matter functions on the gravitational degrees of freedom must now take into account the fact that we have both classical and semi-classical (in the sense of being "slowly" quantized) variables for gravity. In order to reflect this difference and highlight the quantum nature of gravitons, we modify the condition such that:

$$\frac{\partial Q_n}{\partial h_a} = \mathcal{O}\left(\frac{1}{M^2}\right), \tag{6.33}$$

$$\frac{\partial Q_n}{\partial v^\lambda_{\mathbf{k}}} = \mathcal{O}\left(\frac{1}{M}\right) \tag{6.34}$$

  so that all gravitational variables are slow, but the dependence of the Q_n on the classical ones is even weaker than the dependence on the quantum degrees of freedom.

The content of such model is described by the WKB expansion in M of the total constraint $\hat{H}^{tot}\Psi$ using (6.31) and the ansatz (4.7).

It is remarkable that in such formulation one has, in principle, a non-trivial contribution at $\mathcal{O}\left(M^2\right)$ coming from the application of $\hat{H}^{v^\lambda}$:

$$\sum_{\mathbf{k},\lambda} (\partial_{v^\lambda_{\mathbf{k}}} S_0)^2 = 0. \tag{6.35}$$

Since all $v^\lambda_{\mathbf{k}}$ are independent degrees of freedom, this equation reduces to the requirement $\partial_{v^\lambda_{\mathbf{k}}} S_0 = 0$. Thus, the $\mathcal{O}\left(M\right)$ contribution to the wave functional (4.7) must be independent of tensor perturbations and function of the classical background only

$$S_0 = S_0(\alpha, \beta_\pm)\,, \tag{6.36}$$

as assumed in (6.16). This feature reinforces the idea that, while gravitons are indeed slow variables, they still present an inherently quantum nature that differentiates them from the classical background.

At $\mathcal{O}\left(M\right)$ the Wheeler-DeWitt equation corresponds to the HJ equation (6.17) of the gravitational background, which admits the solution (6.18) of the Bianchi I minisuperspace geometry. It is then clear that at the leading order the gravitational wavefunctional ψ represents the cosmological background. Since the quantum matter sector χ has no term of $\mathcal{O}\left(M\right)$, here the leading order of Ψ coincides with the pure gravity limit, as in Chapters 3-4 and Sec. 6.2.

At the next order, all sectors contribute to the Wheeler-DeWitt equation. By multiplying both sides by $N = e^\alpha$, we can write the superHamiltonian constraint in the conformal gauge as:

$$
\begin{aligned}
&-\frac{8}{3}e^{-\frac{\alpha}{2}}\left[\partial_\alpha S_0\partial_\alpha P_1-\partial_+S_0\partial_+P_1-\partial_-S_0\partial_-P_1\right]\\
&\quad+\frac{1}{2}\sum_{\mathbf{k},\lambda}\left[\omega_k^2(\eta)(v_{\mathbf{k}}^\lambda)^2+\mathcal{V}_{\lambda,\bar\lambda}-i\hbar\partial^2_{v_{\mathbf{k}}^\lambda}P_1+(\partial_{v_{\mathbf{k}}^\lambda}P_1)^2\right]\\
&\quad+\frac{1}{2}\sum_{\mathbf{k}}\left[\nu_k^2(\eta)(\phi_{\mathbf{k}})^2-i\hbar\partial^2_{\phi_{\mathbf{k}}}Q_1+(\partial_{\phi_{\mathbf{k}}}Q_1)^2\right]+e^{\alpha}W^{-1}\partial_TQ_1=0.
\end{aligned}
\tag{6.37}
$$

Now labeling the $O(M^0)$ contributions as

$$
\psi_1=e^{\frac{i}{\hbar}P_1}\,,\quad \chi_1=e^{\frac{i}{\hbar}Q_1},
\tag{6.38}
$$

then Eq. (6.37) can be recast in the form:

$$
\begin{aligned}
&\left(\frac{8}{3}i\hbar e^{-\frac{\alpha}{2}}\left[\partial_\alpha S_0\partial_\alpha-\partial_+S_0\partial_+-\partial_-S_0\partial_-\right]\psi_1\right)\chi_1\\
&+\left(\frac{1}{2}\sum_{\mathbf{k},\lambda}\left[\omega_k^2(\eta)(v_{\mathbf{k}}^\lambda)^2+\mathcal{V}_{\lambda,\bar\lambda}-\hbar^2\partial^2_{v_{\mathbf{k}}^\lambda}\right]\psi_1\right)\chi_1\\
&+\psi_1\left(\frac{1}{2}\sum_{\mathbf{k}}\left[\nu_k^2(\eta)(\phi_{\mathbf{k}})^2-\hbar^2\partial^2_{\phi_{\mathbf{k}}}\right]\chi_1\right)+\psi_1\left(-i\hbar\, e^{\alpha}W^{-1}\partial_T\chi_1\right)=0.
\end{aligned}
\tag{6.39}
$$

The above equation does not contain any term coming from the action of $\hat{H}^g$ on χ_1 due to the adiabatic conditions (6.33)-(6.34). In fact, all contributions of this kind are made up of derivatives of Q_1 with respect to the gravitational variables, namely they are moved to the next order; this is even more evident for the next functions Q_n.

We recall that the Born-Oppenheimer separation (6.14) is invariant under local phase shifts of the gravitational and quantum matter wave functionals, see (6.1) where now $\theta=\theta(\alpha,\beta_\pm,v_{\mathbf{k}}^\lambda)$ is function also of the slow degrees of freedom $v_{\mathbf{k}}^\lambda$ (this is possible since the phase θ still commutes with the matter operators). This characteristic gauge freedom can be exploited to impose an additional constraint to our system in the form of a gauge-fixing condition. In particular, we choose to work in the gauge for which the following equation holds:

$$
\begin{aligned}
&\frac{8}{3}i\hbar e^{-\frac{\alpha}{2}}\left[\partial_\alpha S_0\partial_\alpha-\partial_+S_0\partial_+-\partial_-S_0\partial_-\right]\psi_1\\
&\quad+\frac{1}{2}\sum_{\mathbf{k},\lambda}\left[\omega_k^2(\eta)(v_{\mathbf{k}}^\lambda)^2+\mathcal{V}_{\lambda,\bar\lambda}-\hbar^2\partial^2_{v_{\mathbf{k}}^\lambda}\right]\psi_1=0.
\end{aligned}
\tag{6.40}
$$

This requirement can be recast in the form of a differential equation for $\theta(\alpha,\beta_\pm,v_{\mathbf{k}}^\lambda)$, the solution of which identifies the transformation from an arbitrary gauge to the one in which (6.40) holds.

By examining closely the gauge-fixing (6.40), one can see that it coincides with the complex conjugate of (6.23) in which Vilenkin's time construction has been used (we recall that S_0 is independent of the $v_{\mathbf{k}}^\lambda$). Therefore, the physical meaning of the fixed gauge is precisely the same at this order: we recover the gravitational Wheeler-DeWitt equation $\hat{H}^g\psi = \left(\hat{H}^I + \hat{H}^{(v^\lambda_{\mathbf{k}})}\right)\psi = 0$. As a consequence, in this model the super-Hamiltonian constraint of the gravity sector can be seen as a gauge-fixing of the Born-Oppenheimer separation as in Sec. 6.2, instead of an *a priori* imposition that ends up breaking such symmetry.

Let us take a brief detour to discuss the dynamics of the gravitons sector described by the gauge choice (6.40). Clearly, since we wish to implement the Gaussian fluid as a time, such equation appears to be timeless (it does not contain the parameter T at all). However, one can interpret (6.40) as a dynamical evolution using a background (internal) time. The motivation is that, at the level of graviton fluctuations in the WKB expansion, one cannot implement the clock derived from the fast component, which is carried at the next order due to the B-O assumptions. Given the classical background solutions $\alpha(\eta)$, $\beta_\pm(\eta)$ with η being the conformal time, one could recast the contributions with such variables as derivatives with respect to η. More specifically the classical relation

$$p_\alpha = -\frac{3}{8}Me^{\alpha/2}\,\dot{\alpha} = M\partial_\alpha S_0 \tag{6.41}$$

and the chain rule

$$\dot{\alpha}\frac{\partial}{\partial\alpha} = \frac{d\alpha(\eta)}{d\eta}\frac{\partial}{\partial\alpha} = \frac{\partial}{\partial\eta} \tag{6.42}$$

allow, together with the analogous ones for β_+, β_-, to rewrite Eq. 6.40 in the form

$$i\hbar\partial_\eta\psi_1 = \frac{1}{2}\sum_{\mathbf{k},\lambda}\left[\omega_k^2(\eta)(v^\lambda_{\mathbf{k}})^2 + \mathcal{V}_{\lambda,\bar{\lambda}} - \hbar^2\partial^2_{v^\lambda_{\mathbf{k}}}\right]\psi_1 \tag{6.43}$$

where we have absorbed a factor 3 in the time derivative.

From an interpretative standpoint, Vilenkin's hypothesis of the gravitational constraint is recovered through the B-O gauge symmetry, even though the graviton sector here "evolves" via a different clock from the fast component (which will have the reference fluid time). This ambiguity can be eliminated by performing a coordinate transformation (allowed by the diffeomorphisms invariance) such that the quantum field $T(x)$ of the Gaussian fluid corresponds, at each spacetime point, to the conformal time η, i.e. the gravitons and the matter field evolutions are parametrized by the same parameter. The identification $T(x) \equiv \eta$ shall be considered after the gauge fixing, since T is a quantum variable. Even without such correspondence, Eq. 6.40 dictates the behaviour of the graviton fluctuations which we recall have been introduced as arbitrary degrees of freedom.

Once the gauge has been fixed, the $\mathcal{O}\left(M^0\right)$ constraint equation reads:

$$\frac{1}{2}\sum_{\mathbf{k}}\left[\nu_k^2(\eta)(\phi_{\mathbf{k}})^2 - \hbar^2\partial^2_{\phi_{\mathbf{k}}}\right]\chi_1 = i\hbar\; e^\alpha W^{-1}\partial_T\chi_1, \tag{6.44}$$

where we have divided both sides by ψ_1. Since the left-hand side corresponds to $N\hat{H}^\phi\chi_1$ at this order, by integrating over the spatial hypersurface Σ we get the corresponding Hamiltonian:

$$\hat{\mathcal{H}}^\phi\chi_1 = \int_\Sigma d^3x\; N\hat{H}^\phi\chi_1 = i\hbar\int_\Sigma d^3x\; e^\alpha W^{-1}\partial_T\chi_1. \tag{6.45}$$

In the spirit of Chapter 4, we now defining the time derivative in terms of the reference fluid, using the same form of (4.24); we take we take $N^i = 0$ and $N = e^\alpha$ for this minisuperspace setting, so that the only fluid variable left is the Gaussian time T as in Sec. 4.3 and 5.3. This implementation is inherently different from the one used in Sec. 6.2, where we only aimed to recast Vilenkin's formulation [41] in order to take into account the small graviton fluctuations. Thus using

$$\frac{\delta}{\delta\tau} = \int_\Sigma d^3x \; e^\alpha W^{-1} \frac{\partial}{\partial T(x)} \tag{6.46}$$

we recover the Schrödinger functional equation for χ_1, i.e.

$$\hat{\mathcal{H}}^\phi \chi_1 = i\hbar \frac{\delta}{\delta\tau} \chi_1 \,. \tag{6.47}$$

However, at this level we have not properly recovered the standard QFT description since χ_1 still depends on the cosmological perturbations $v^\lambda_{\mathbf{k}}$ of the background. Therefore, we shall implement in some way the averaging procedure of Sec. 6.2 to recover the standard phenomenology as an effective theory.

This point is easily understood at $\mathcal{O}\left(M^0\right)$ since all operators in Eq. (6.47) act on the matter variables alone. Essentially, multiplying both sides by $\psi_1^*\psi_1$ and bringing this factor inside the operators that equation can be recast as

$$\hat{\mathcal{H}}^\phi \left(\psi_1^*\psi_1\chi_1\right) = i\hbar \frac{\delta}{\delta\tau} \left(\psi_1^*\psi_1\chi_1\right) \,. \tag{6.48}$$

With the same reasoning $\hat{\mathcal{H}}^\phi$ and $\delta/\delta\tau$ commute with the integral over the $v^\lambda_{\mathbf{k}}$. Therefore we can define an averaged matter wave functional at this order, in clear analogy to (6.25), where we now integrate over the graviton variables:

$$\widetilde{\Theta}_1(\phi_{\mathbf{k}}, T; \alpha, \beta_\pm) = \int \prod_{\mathbf{k},\lambda} dv^\lambda_{\mathbf{k}} \; \psi_1^*\psi_1\chi_1 \,. \tag{6.49}$$

The resulting $\widetilde{\Theta}_1$ is essentially averaged with the weight $|\psi_1|^2$, corresponding to the first order of gravitons fluctuations. In this way, $\widetilde{\Theta}_1$ retains a dependence on the reference fluid degree of freedom and indeed satisfies

$$\hat{\mathcal{H}}^\phi \widetilde{\Theta}_1 = i\hbar \frac{\delta}{\delta\tau} \widetilde{\Theta}_1 \tag{6.50}$$

which now correctly reproduces the QFT phenomenology, having removed any trace of the gravitons fluctuations.

We stress that, differently from Eq. 4.24, here the reference fluid clock is essentially reduced to a incoherent dust (due to the absence of the Lagrange multiplier $\mathcal{F}_i$ in such minisuperspace setting) and the supermomentum constraint does not appear as a consequence of the ADM foliation with $N^i = 0$. Apart from this technical differences, the physical meaning of the two equations is the same: we have constructed a clock for the fast matter subsystem through the reference fluid, obtaining a functional Schrödinger evolution akin to QFT at this order.

6.3.1 Gauge symmetry order by order

We now move to the order M^{-1}, having

$$\begin{aligned}&\frac{4}{3}e^{-\frac{\alpha}{2}}\Big[i\hbar\left(\partial_\alpha^2-\partial_+^2-\partial_-^2\right)P_1-(\partial_\alpha P_1)^2+(\partial_+ P_1)^2\\&-(\partial_- P_1)^2-2\left(\partial_\alpha S_0\partial_\alpha-\partial_+ S_0\partial_+-\partial_- S_0\partial_-\right)P_2\Big]\\&+\frac{1}{2}\sum_{\mathbf{k},\lambda}\left[-i\hbar\partial^2_{v^\lambda_\mathbf{k}}+2\partial_{v^\lambda_\mathbf{k}}P_1\partial_{v^\lambda_\mathbf{k}}\right](P_2+MQ_1)\\&+\frac{1}{2}\sum_{\mathbf{k}}\left[-i\hbar\partial^2_{\phi_\mathbf{k}}Q_2+2\partial_{\phi_\mathbf{k}}Q_1\partial_{\phi_\mathbf{k}}Q_2\right]+e^\alpha W^{-1}\partial_T Q_2=0.\end{aligned} \tag{6.51}$$

We stress that here we have terms $\partial_{v^\lambda_\mathbf{k}}Q_1$ which were absent in the previous order due to the assumption (6.34); since the function Q_2 in the ansatz is associated to the order $1/M$, the terms $\partial_{v^\lambda_\mathbf{k}}Q_2$ would be of $\mathcal{O}\left(M^{-2}\right)$ and are thus neglected. The lack of contributions of the form $\partial_\alpha Q_1$ (or equivalently with $\beta_\pm$) is instead a consequence of (6.33): to distinguish the fast matter sector from the slow graviton one, we have assumed that the derivative of Q_n with respect to the classical variables is even smaller in the expansion parameter.

As in the previous order, we label the $O(1/M)$ wave functionals as

$$\psi_2=e^{\frac{i}{\hbar}(P_1+\frac{1}{M}P_2)},\qquad \chi_2=e^{\frac{i}{\hbar}(Q_1+\frac{1}{M}Q_2)}. \tag{6.52}$$

Summing Eq. (6.51) with the corresponding $\mathcal{O}\left(M^0\right)$ equation (6.37) we obtain:

$$\begin{aligned}&\frac{8i\hbar}{3}e^{-\frac{\alpha}{2}}\chi_2\left(\partial_\alpha S_0\partial_\alpha-\partial_+ S_0\partial_+-\partial_- S_0\partial_-\right)\psi_2\\&+\frac{4\hbar^2}{3M}e^{-\frac{\alpha}{2}}\chi_2\left(\partial_\alpha^2-\partial_+^2-\partial_-^2\right)\psi_2+\psi_2\left(-i\hbar\, e^\alpha W^{-1}\partial_T\chi_2\right)\\&+\frac{1}{2}\chi_2\sum_{\mathbf{k},\lambda}\left[\omega_k^2(\eta)(v^\lambda_\mathbf{k})^2+\mathcal{V}_{\lambda,\bar\lambda}-\hbar^2\partial^2_{v^\lambda_\mathbf{k}}\right]\psi_2+\frac{1}{2}\psi_2\sum_{\mathbf{k}}\left[\nu_k^2(\eta)\phi_\mathbf{k}^2-\hbar^2\partial^2_{\phi_\mathbf{k}}\right]\chi_2\\&+\frac{1}{2}\psi_2\sum_{\mathbf{k},\lambda}\left[-\hbar^2\partial^2_{v^\lambda_\mathbf{k}}-2i\hbar\partial_{v^\lambda_\mathbf{k}}P_1\partial_{v^\lambda_\mathbf{k}}\right]\chi_2=0.\end{aligned} \tag{6.53}$$

We can see in the last line the presence of terms containing derivatives of the matter functional with respect to the $v^\lambda_\mathbf{k}$. This kind of contribution which was completely absent in the previous order due to the adiabatic conditions (6.33)-(6.34) and here corresponds here to quantum gravitational corrections, attributed to the slow quantum nature of the graviton fluctuations. We remark that the time definition (6.46) has been obtained by imposing the gauge-fixing condition (6.40) through a specific choice of the gauge function θ, which was the degree of freedom associated to the symmetry (6.1). Thus, it would seem that there is no residual gauge freedom for this model.

This is actually not the case since θ in (6.1) allows a "total" rescaling of both wave functions ψ and χ *before* the WKB expansion. Since the two are then expanded in $1/M$, we can apply the same expansion to the phase itself:

$$\theta(\alpha,\beta_\pm,v^\lambda_\mathbf{k})=\sum_{n=1}^{\infty}\left(\frac{1}{M}\right)^{n-1}\theta_n(\alpha,\beta_\pm,v^\lambda_\mathbf{k}), \tag{6.54}$$

where each θ_n is a single-order contribution. It should be noted that such expansion of the phase does not include a contribution of $\mathcal{O}(M)$, i.e. it starts from $n = 1$. The reason is immediately stated: such term is not allowed by the B-O symmetry (6.1) itself, since χ inherently starts from the next order M^0. In other words, a contribution of order M would break the B-O separation; in a sense there is no gauge invariance at the first Planckian order.

We can thus associate the gauge transformation with the following operator

$$\hat{T}(\theta) = e^{\frac{i}{\hbar}\theta} = \prod_{n=1}^{\infty} exp\left[\frac{i}{\hbar}\left(\frac{1}{M}\right)^{n-1}\theta_n\right] \tag{6.55}$$

acting as $\psi \to \hat{T}(\theta)\psi$ and $\chi \to \hat{T}^{\dagger}(\theta)\chi$ respectively. Clearly, $\hat{T}$ is a functional of θ from which one can extract the corresponding single-order transformation

$$\hat{T}_n(\theta_n) = exp\left[\frac{i}{\hbar}\left(\frac{1}{M}\right)^{n-1}\theta_n\right] \tag{6.56}$$

acting at $\mathcal{O}\left(M^{1-n}\right)$ only.

The total gauge transformation (6.55) can be understood as the simultaneous action of all (6.56) on each corresponding wave functional, under which the B-O separation (6.1) is invariant. In essence, each order of expansion in this scheme is characterized by its own gauge freedom, parametrized by θ_n.

Since we are now considering the dynamics up to order M^{-1}, we can express the phase as

$$\theta(\alpha, \beta_\pm, v^\lambda_{\mathbf{k}}) = \theta_1(\alpha, \beta_\pm, v^\lambda_{\mathbf{k}}) + \frac{1}{M}\theta_2(\alpha, \beta_\pm, v^\lambda_{\mathbf{k}})\,. \tag{6.57}$$

Clearly this means that the ψ is transformed as

$$\psi \to e^{\frac{i}{\hbar}\theta}\psi = e^{\frac{i}{\hbar}\theta_1} e^{\frac{i}{\hbar}\frac{1}{M}\theta_2}\psi\,, \tag{6.58}$$

where it is evident that the total gauge transformation can be seen as the composition of two separate rescalings, one of $\mathcal{O}\left(M^0\right)$ and one of $\mathcal{O}\left(M^{-1}\right)$, as in (6.56).

Since we have fixed only the function θ_1 through the condition (6.40), there is a residual gauge freedom at $\mathcal{O}\left(M^{-1}\right)$ associated to θ_2. We consider the gauge fixing which corresponds to the gravitational Wheeler-DeWitt constraint up to order $1/M$, in analogy with Eq. 6.40 of the previous order:

$$\begin{aligned}&\frac{4}{3}e^{-\frac{\alpha}{2}}\left[2i\hbar\left(\partial_\alpha S_0\partial_\alpha - \partial_+ S_0\partial_+ - \partial_- S_0\partial_-\right) + \frac{\hbar^2}{M}\left(\partial^2_\alpha - \partial^2_+ - \partial^2_-\right)\right]\psi_2\\&\quad + \frac{1}{2}\sum_{\mathbf{k},\lambda}\left[\omega^2_k(\eta)(v^\lambda_{\mathbf{k}})^2 + \mathcal{V}_{\lambda,\bar{\lambda}} - \hbar^2\partial^2_{v^\lambda_{\mathbf{k}}}\right]\psi_2 = 0\,.\end{aligned} \tag{6.59}$$

This corresponds to a differential equation for θ_2 once θ_1 has been identified at the $\mathcal{O}\left(M^0\right)$.

Once the condition (6.59) has been imposed, the residual equation at order M^{-1} takes the form:

$$\begin{aligned}&\frac{1}{2}\sum_{\mathbf{k}}\left[\nu^2_k(\eta)\phi^2_{\mathbf{k}} - \hbar^2\partial^2_{\phi_{\mathbf{k}}}\right]\chi_2 - i\hbar\, e^{\alpha}W^{-1}\partial_T\chi_2\\&\quad + \frac{1}{2}\sum_{\mathbf{k},\lambda}\left[-\hbar^2\partial^2_{v^\lambda_{\mathbf{k}}} - 2i\hbar\partial_{v^\lambda_{\mathbf{k}}}P_1\partial_{v^\lambda_{\mathbf{k}}}\right]\chi_2 = 0,\end{aligned} \tag{6.60}$$

where the gravitational wave functional ψ_2, acting as purely multiplicative, has been simplified. Recalling the starting superHamiltonian (6.31) and the time definition (6.46), we can integrate this equation on the ADM spatial hypersurfaces Σ to reconstruct the total Hamiltonian (in this minisuperspace reduction we could also consider a fiducial volume), giving

$$i\hbar\frac{\delta}{\delta\tau}\chi_2 = \hat{\mathcal{H}}^{\phi}\chi_2 + \hat{\mathscr{I}}\chi_2, \tag{6.61}$$

where we defined the operator:

$$\hat{\mathscr{I}} = \frac{1}{2}\int_{\Sigma} d^3x \sum_{\mathbf{k},\lambda}\left[-\hbar^2\partial^2_{v^\lambda_{\mathbf{k}}} - 2i\hbar\partial_{v^\lambda_{\mathbf{k}}}P_1\partial_{v^\lambda_{\mathbf{k}}}\right]. \tag{6.62}$$

The functional Schrödinger evolution (6.61) is now corrected by this operator, produced by the dependence of χ_2 from the $v^\lambda_{\mathbf{k}}$ degrees of freedom. This effect is also related to the form of the function P_1, which is fixed by the $O(M^0)$ gauge-fixing condition (6.40) that is the gravitational WDW equation. Thus, the quantum gravitational corrections on χ_2 depend also on the specific dynamics that gravitons follow on the classical background. The main advantage of the gauge choice (6.59) is to directly obtain a modified dynamics of the matter subsystem which takes into account the whole gravitational sector.

Actually, we could reformulate the term corresponding to the QG-corrections as

$$\begin{aligned}\hat{\mathscr{I}}^{tot} = \int_{\Sigma} d^3x \Bigg[&- 2i\hbar\left(\partial_\alpha S_0\partial_\alpha - \partial_+ S_0\partial_+ - \partial_- S_0\partial_-\right)\\ &-\frac{1}{2}\sum_{\mathbf{k},\lambda}\left(-\hbar^2\partial^2_{v^\lambda_{\mathbf{k}}} - 2i\hbar\partial_{v^\lambda_{\mathbf{k}}}P_1\partial_{v^\lambda_{\mathbf{k}}}\right)\Bigg]\\ = \int_{\Sigma} d^3x &\left[-2i\hbar\left(\partial_\alpha S_0\partial_\alpha - \partial_+ S_0\partial_+ - \partial_- S_0\partial_-\right)\right] + \hat{\mathscr{I}}\,.\end{aligned} \tag{6.63}$$

This redefinition is backed by the observation that, in Eq. (6.51), we have omitted the contributions $\partial_{v^\lambda_{\mathbf{k}}}Q_2$ and $\partial_\alpha Q_1$, $\partial_\pm Q_1$. However, if we consider the complete action of the operator on χ_2 and then select only the terms which survive up to order M^{-1}, we indeed obtain (6.62). Thus we can equivalently rewrite Eq. (6.61) as the following

$$i\hbar\frac{\delta}{\delta\tau}\chi_2 = \hat{\mathcal{H}}^{\phi}\chi_2 + \hat{\mathscr{I}}^{tot}\chi_2 \tag{6.64}$$

by keeping in mind that in this scheme we are addressing only the dynamics up to $\mathcal{O}\left(M^{-1}\right)$.

At this level, we still maintain a dependence on the gravitons degrees of freedom inside the matter wave functional χ_2 and clearly the QG-induced corrections have taken a novel form with respect to (4.32), which did not include such $v^\lambda_{\mathbf{k}}$ variables. We now analyze how to implement the averaging procedure in this expanded scheme, in order to recover the same form (6.25) of an averaged matter wave functional.

6.3.2 Averaging procedure at the next order

Performing an average over the graviton degrees of freedom at the next order M^{-1} is not an immediate task as in Sec. 6.2. Our starting point is the averaged wave functional

$$\widetilde{\Theta}_2(\phi_{\mathbf{k}}, T; \alpha, \beta_\pm) = \int \prod_{\mathbf{k},\lambda} dv^\lambda_{\mathbf{k}}\ \psi^*_2 \psi_2 \chi_2\,. \tag{6.65}$$

To recast (6.61) as an equation for $\widetilde{\Theta}_2$, we multiply it by $\psi^*_2\psi_2 = |\psi_2|^2$, being ψ_2 defined in (6.52). However this factor cannot be brought inside $\hat{\mathscr{J}}$ which contains derivatives with respect to the $v^\lambda_{\mathbf{k}}$ (we remind that the functions S_0, P_n now contain both the classical background variables and the gravitons fluctuations). Therefore, one would argue this averaging procedure cannot be implemented in the gauge for which Eq. (6.61) holds.

Let us show how this concern can be overcome. Eq. 6.61, obtained after imposing the gauge condition (6.59), describes the following evolution at $\mathcal{O}\left(M^{-1}\right)$:

$$i\hbar \frac{\delta}{\delta\tau}\widetilde{\Theta}_2 = \frac{1}{2}\sum_{\mathbf{k}} \left[\nu^2_k(\eta)\phi^2_{\mathbf{k}} - \hbar^2\partial^2_{\phi_{\mathbf{k}}}\right]\widetilde{\Theta}_2 + \int \prod_{\mathbf{k},\lambda} dv^\lambda_{\mathbf{k}}\ \psi^*_2\psi_2 \hat{\mathscr{J}}^{tot}\chi_2 \tag{6.66}$$

The last term clearly is not an operator acting on the whole $\widetilde{\Theta}_2$. However, to make it so we could relax the assumption (6.59) that the WDW gravitational constraint holds. Since we still have the gauge freedom regarding θ_2, we do not wish to drop the associated gauge choice entirely, bust just to modify it. A cumbersome calculation (here omitted for clarity) shows that the following different gauge choice

$$\begin{aligned}
&\frac{4}{3}e^{-\frac{\alpha}{2}}\psi^*_2\left[2i\hbar\left(\partial_\alpha S_0\partial_\alpha - \partial_+ S_0\partial_+ - \partial_- S_0\partial_-\right) + \frac{\hbar^2}{M}\left(\partial^2_\alpha - \partial^2_+ - \partial^2_-\right)\right]\psi_2 \\
&\quad + \frac{1}{2}\sum_{\mathbf{k},\lambda}\psi^*_2\left[\omega^2_k(\eta)(v^\lambda_{\mathbf{k}})^2 + \mathcal{V}_{\lambda,\bar{\lambda}} - \hbar^2\partial^2_{v^\lambda_{\mathbf{k}}}\right]\psi_2 + \frac{i}{\hbar}\sum_{\mathbf{k},\lambda}\psi^*_2\left(\partial^2_{v^\lambda_{\mathbf{k}}}P_1\right)\psi_2 \\
&\quad + (\hat{\mathscr{J}}^{tot})^\dagger\left(\psi^*_2\psi_2\right) = 0
\end{aligned} \tag{6.67}$$

and the boundary condition

$$\int \prod_{\mathbf{k},\lambda} dv^\lambda_{\mathbf{k}} \sum_{\mathbf{k},\lambda}\hbar^2\partial_{v^\lambda_{\mathbf{k}}}\left[\psi^*_2\psi_2\,\partial_{v^\lambda_{\mathbf{k}}}\chi_2 - \partial_{v^\lambda_{\mathbf{k}}}\left(\psi^*_2\psi_2\chi_2\right) + \frac{i}{\hbar}(\partial_{v^\lambda_{\mathbf{k}}}S_1)\psi^*_2\psi_2\chi_2\right] = 0 \tag{6.68}$$

allow to rewrite the Eq. (6.66) as

$$\begin{aligned}
i\hbar\frac{\delta}{\delta\tau}\widetilde{\Theta}_2 &= \hat{\mathcal{H}}^\phi\widetilde{\Theta}_2 + \int_\Sigma d^3x\left[-2i\hbar\left(\partial_\alpha S_0\partial_\alpha - \partial_+ S_0\partial_+ - \partial_- S_0\partial_-\right)\right]\widetilde{\Theta}_2 \\
&= \hat{\mathcal{H}}^\phi\widetilde{\Theta}_2 + \langle\hat{\mathscr{J}}^{tot}\rangle\widetilde{\Theta}_2\,.
\end{aligned} \tag{6.69}$$

We stress that the relevance of this equation is that all all QG-induced corrections due to the gravitons fluctuations have been eliminated through the gauge freedom (which does not correspond to the gravitational WDW anymore) and some appropriate boundary conditions. In other words, the modified dynamics of $\widetilde{\Theta}_2$ perceives only corrections due to the classical background via the term labeled $\langle\hat{\mathcal{H}}^{QG}\rangle$. We observe that the resulting theory is exactly the same of Chapter 4, where the Gaussian reference fluid takes the role of the physical clock but no graviton fluctuations are characterized, in a diagonal Bianchi I minisuperspace model (i.e. $N^i = 0$). Thus we have derived a mathematically consistent model which takes into account both proposals, and the limit of Chapter 4 is directly obtained via the gauge choice (6.67).

The difference between the two gauge choices stands in the "departure" from the idea that the gravitational WDW constraint must at some point be recovered. Indeed, if we only wished to extend the result of the previous order keeping such gravitational constraint, we would end up with the gauge choice (6.59) and the modified dynamics (6.64). In the case of (6.67) instead we are dropping the connection between the B-O gauge freedom and such gravitational equation, leaving the evolution of the gravitons degrees of freedom totally arbitrary.

6.3.3 Effective QFT at $\mathcal{O}\left(M^{-1}\right)$

Actually, it is also possible to recover QFT on average with a different gauge-fixing condition. After some calculations, it is found that with the following equation

$$\begin{aligned}&\frac{4}{3}e^{-\frac{\alpha}{2}}\psi_2^*\left[2i\hbar\left(\partial_\alpha S_0\partial_\alpha-\partial_+S_0\partial_+-\partial_-S_0\partial_-\right)+\frac{\hbar^2}{M}\left(\partial_\alpha^2-\partial_+^2-\partial_-^2\right)\right]\psi_2\\&+\frac{1}{2}\sum_{\mathbf{k},\lambda}\left(\psi_2^*\left[\omega_k^2(\eta)(v_{\mathbf{k}}^\lambda)^2+\mathcal{V}_{\lambda,\bar{\lambda}}-\hbar^2\partial^2_{v_{\mathbf{k}}^\lambda}\right]\psi_2+\left[\hbar^2\partial^2_{v_{\mathbf{k}}^\lambda}-2i\hbar\partial_{v_{\mathbf{k}}^\lambda}P_1\partial_{v_{\mathbf{k}}^\lambda}\right]\psi_2^*\psi_2\right)\\&+i\hbar\sum_{\mathbf{k},\lambda}\psi_2^*(\partial^2_{v_{\mathbf{k}}^\lambda}P_1)\psi_2=0,\end{aligned}\tag{6.70}$$

and integration over the $v_{\mathbf{k}}^\lambda$ with boundary condition

$$\int\prod_{\mathbf{k},\lambda}dv_{\mathbf{k}}^\lambda\sum_{\mathbf{k},\lambda}\hbar^2\partial_{v_{\mathbf{k}}^\lambda}\left[\psi_2^*\psi_2\,\partial_{v_{\mathbf{k}}^\lambda}\chi_2-\partial_{v_{\mathbf{k}}^\lambda}\left(\psi_2^*\psi_2\chi_2\right)+\frac{i}{\hbar}(\partial_{v_{\mathbf{k}}^\lambda}P_1)\psi_2^*\psi_2\chi_2\right]=0,\tag{6.71}$$

brings the constraint equation at $O(1/M)$ to take the simple form

$$i\hbar\frac{\delta}{\delta\tau}\widetilde{\Theta}_2=\hat{\mathcal{H}}^\phi\widetilde{\Theta}_2\,,\tag{6.72}$$

i.e. the ordinary dynamics. With this choice all gravitational corrections are canceled out, recovering QFT as an effective theory also at order $1/M$.

Eq. (6.72) provides an effective description of matter in a quasi-classical background, aligned to the original Vilenkin's proposal [41]. This result proves once again that the extended B-O model recovers (through the gauge (6.70)) Vilenkin's interpretation of QFT on the gravitational background from the full gravity-matter system.

In a sense, the formulation of this Chapter could be seen as a generalization of [41] taking into account the quantum nature of gravity and with a Gaussian fluid clock. However, this is only a limited outcome of our broader investigation: we have developed a consistent theory in the extended B-O picture using a physical clock (the Gaussian reference fluid), which allows to investigate the matter subsystem's modified dynamics with QG-corrections while preserving unitarity i.e. with a reliable physical interpretation.

6.4 Primordial spectrum in the extended B-O picture

Let us now investigate such modified dynamics for the inflaton field in the slow-rolling phase and its associated spectrum. Essentially, we aim to replicate the computation of Sec. 5.3 but in the extended formulation, taking into account the graviton fluctuations in the metric sector.

As already elucidated, the slow-rolling phase is characterized by $V(\phi) \simeq const.$ emerging as a cosmological constant contribution. Clearly, to take into account such term we must change the minisuperspace geometry from the vacuum Bianchi I case to the FLRW one, as in Sec. 5.3. In principle, such geometry allows for (independent) scalar and tensor perturbations of the metric [95, 103]; we here consider the FLRW background to be purely classical and the fluctuations to be of tensor nature, i.e. graviton contributions, in accordance with the model developed in the previous Section. Similarly, we neglect the backreaction of the inflaton scalar field on the spacetime geometry and we mimic an exact de Sitter phase by considering $\epsilon = const.$

Based on these considerations, we use the FLRW line element (5.2) and the gauge-invariant formalism for both the graviton perturbations $v^\lambda_{\mathbf{k}}$ and the inflaton modes $\phi_{\mathbf{k}}$. The background setting is the same as in Sec. 5.3. Over the homogeneous and isotropic background, it is well known that both types of perturbations emerge as time-dependent harmonic oscillators (recalling (5.12), see for example [68]) so that we have the following WDW equation

$$\begin{aligned}\Bigg(\frac{\hbar^2}{48M}e^{-3\alpha}\partial^2_\alpha + 4M\Lambda e^{3\alpha} + \frac{e^{-\alpha}}{2}\sum_{\mathbf{k},\lambda}\left[-\hbar^2\partial^2_{v^\lambda_{\mathbf{k}}} + \nu^2_k(\eta)(v^\lambda_{\mathbf{k}})^2\right] \\ + \frac{e^{-\alpha}}{2}\sum_{\mathbf{k}}\left[-\hbar^2\partial^2_{\phi_{\mathbf{k}}} + \nu^2_k(\eta)(\phi_{\mathbf{k}})^2\right] - i\hbar W^{-1}\frac{\delta}{\delta T(x)}\Bigg)\Psi = 0\end{aligned} \tag{6.73}$$

where

$$\omega^2_k(\eta) = k^2 - \frac{(e^\alpha\sqrt{\epsilon})''}{e^\alpha\sqrt{\epsilon}}\,, \tag{6.74}$$

$$\nu^2_k(\eta) = k^2 - \frac{(e^\alpha)''}{e^\alpha}\,, \tag{6.75}$$

which clearly reduce to the same function in the de Sitter case $\epsilon = const$:

$$\omega^2_k(\eta) = \nu^2_k(\eta) = k^2 - \frac{2}{\eta^2} \tag{6.76}$$

that we label ν^2_k from now on. We note that the graviton superHamiltonian lacks the term $\mathcal{V}_{\lambda,\bar{\lambda}}$ of Sec. 6.2 and 6.3 since no mixing of the two polarization modes is possible in this highly symmetric background. We also stress that the fluid sector $\hat{H}^f$ contains a functional derivative since $T(x^\mu)$ is a function of a generic coordinate system due to the reparametrization procedure.

We consider again the WKB ansatz up to the first order of QG-corrections, i.e.

$$\Psi = e^{\frac{i}{\hbar}(MS_0 + P_1 + \frac{1}{M}P_2)}e^{\frac{i}{\hbar}(Q_1 + \frac{1}{M}Q_2)} \tag{6.77}$$

where the functions S_0 and P_n describe the gravitational sector only, while Q_n is associated to the inflaton variables too, as in (6.32).

The procedure here follows Sec. 5.3, with the addition of the graviton sector. From the expansion at order M, we have the same HJ equation

$$\frac{1}{48}e^{-3\alpha}(\partial_\alpha S_0)^2 - 4\Lambda e^{3\alpha} = 0\,, \tag{6.78}$$

solved by

$$S_0(\alpha) = -8\sqrt{\frac{\Lambda}{3}}\left(e^{3\alpha} - e^{3\alpha_0}\right) \tag{6.79}$$

which coincides with (5.18).

At $\mathcal{O}\left(M^0\right)$, we use the B-O symmetry to impose the gravitational constraint analogous to (6.40) but over the FLRW background:

$$\frac{e^{-2\alpha}}{24}\left(i\hbar\partial_\alpha^2 S_0 - 2\partial_\alpha S_0 \partial_\alpha P_1\right) + \sum_{\mathbf{k},\lambda}\left[-i\hbar\partial^2_{v^\lambda_\mathbf{k}}P_1 + (\partial_{v^\lambda_\mathbf{k}}P_1)^2 + \nu_k^2(v^\lambda_\mathbf{k})^2\right] = 0\,, \tag{6.80}$$

or analogously writing $\psi_1 = e^{\frac{i}{\hbar}P_1}$:

$$\frac{e^{-2\alpha}}{24}\psi_1^*\left(i\hbar\partial_\alpha^2 S_0 + 2i\hbar\partial_\alpha S_0\partial_\alpha\right)\psi_1 + \psi_1^*\sum_{\mathbf{k},\lambda}\left[-\hbar^2\partial^2_{v^\lambda_\mathbf{k}} + \nu_k^2(v^\lambda_\mathbf{k})^2\right]\psi_1 = 0\,. \tag{6.81}$$

We stress that, compared to Sec. 6.3, the background derivative terms take a different form due to the lack of anisotropies and the non-linearity of the classical solution S_0 (6.79) (which was instead the case in (6.18)). As already motivated, this gauge implies a functional Schrödinger dynamics for the averaged inflaton wave functional, see (6.50):

$$i\hbar\, e^\alpha W^{-1}\frac{\delta}{\delta T}\Theta_1 = i\hbar\frac{\delta}{\delta\tau}\Theta_1 = \hat{\mathcal{H}}^\phi\Theta_1 = \frac{1}{2}\sum_{\mathbf{k}}\left[-\hbar^2\partial^2_{\phi_\mathbf{k}} + \nu_k^2\phi_\mathbf{k}^2\right]\Theta_1 \tag{6.82}$$

where Θ_1, defined as in (6.49), is the average of $\chi_1 = e^{\frac{i}{\hbar}Q_1}$ over the graviton modes. The fiducial volume emerging from the spatial integration has been set to 1 for simplicity.

At $\mathcal{O}\left(M^{-1}\right)$ we find

$$\begin{aligned}&\frac{e^{-3\alpha}}{48}\left[i\hbar\partial_\alpha^2 P_1 - (\partial_\alpha P_1)^2 - 2\partial_\alpha S_0\partial_\alpha P_1\right] + \frac{1}{2}\sum_{\mathbf{k},\lambda}\left[-i\hbar\partial^2_{v^\lambda_\mathbf{k}}(P_2 + MQ_1)\right.\\ &\left.+2\partial_{v^\lambda_\mathbf{k}}P_1\partial_{v^\lambda_\mathbf{k}}(P_2+MQ_1)\right] + \frac{1}{2}\sum_{\mathbf{k}}\left[-i\hbar\partial^2_{\phi_\mathbf{k}}Q_2 + 2\partial_{\phi_\mathbf{k}}Q_1\partial_{\phi_\mathbf{k}}Q_2\right]\\ &+e^\alpha W^{-1}\frac{\delta Q_2}{\delta T} = 0.\end{aligned} \tag{6.83}$$

Eq. (6.83) can be summed up with (6.80) and integrated over the spatial hypersurfaces to reconstruct the inflaton Hamiltonian acting on $\chi_2 = e^{\frac{i}{\hbar}(Q_1 + \frac{1}{M}Q_2)}$. However, we recall that we still have the gauge freedom on the graviton sector at this order, so we require for $\psi_2 = e^{\frac{i}{\hbar}(P_1+\frac{1}{M}P_2)}$:

$$\frac{e^{-3\alpha}}{24}\psi_2^*\left[i\hbar\partial_\alpha S_0\partial_\alpha + \frac{\hbar^2}{M}\partial_\alpha^2\right]\psi_2 + \psi_2^*\sum_{\mathbf{k},\lambda}\left[\nu_k^2(v_\mathbf{k}^\lambda)^2 - \hbar^2\partial^2_{v_\mathbf{k}^\lambda}\right]\psi_2 = 0 \tag{6.84}$$

analogously to the previous order. Then the modified dynamics for χ_2 is

$$i\hbar\frac{\delta}{\delta\tau}\chi_2 = \hat{\mathcal{H}}^\phi\chi_2 + \hat{\mathscr{J}}\chi_2\,, \tag{6.85}$$

$$\hat{\mathscr{J}} = \frac{1}{2}\sum_{\mathbf{k},\lambda}\left[-\hbar^2\partial^2_{v_\mathbf{k}^\lambda} - 2i\hbar\partial_{v_\mathbf{k}^\lambda}P_1\partial_{v_\mathbf{k}^\lambda}\right]\,, \tag{6.86}$$

i.e. equivalent to the expressions (6.61) and (6.62) up to the spatial integration. We clarify that the extra terms present in the definition (6.63) are here absent thanks to the isotropic FLRW setting.

Before proceeding to the power spectrum analysis, we need to compute the function P_1 that appears in (6.86), i.e. the exponent of the gravitational solution ψ_1 at order M^0. Its evolution is dictated by (6.81), which as already noted in the previous Section appears to be timeless. However, we can rewrite the terms in the first parenthesis in a suitable way. Recalling the solution (6.79), $\partial_\alpha^2 S_0$ can be readily obtained. For the second term, we use the Hamilton equation for the (classical) variable $\alpha(\eta)$: $\dot\alpha = \partial_{p_\alpha}(NH^{(\alpha)})$ in the conformal case $N = e^\alpha$, being $H^{(\alpha)}$ the FLRW sector of superHamiltonian (6.73), giving

$$\dot\alpha = -\frac{p_\alpha}{24M}e^{-2\alpha}\,. \tag{6.87}$$

Since MS_0 corresponds to the classical action (see the starting ansatz (6.77)), it must also hold that $p_\alpha = M\partial_\alpha S_0$; comparing the two, we are able to rewrite the desired term in the gauge condition as

$$\partial_\alpha S_0\partial_\alpha = -24e^{2\alpha}\dot\alpha\,\partial_\alpha = -24e^{2\alpha}\partial_\eta\,. \tag{6.88}$$

We stress that here, although the graviton gauge sector is timeless, i.e. independent of the Gaussian fluid time T, the classical solution for the background variable α allows to write ∂_α as derivatives with respect to the conformal time η, similarly to Vilenkin's approach (see discussion in Sec. 2.3). The interpretation is the following: Eq. (6.88) can be reconciled with the Gaussian fluid time procedure by noting that, thanks to the reparametrization, the fluid variable is actually $T(x^\mu)$ so we can exploit the diffeomorphism invariance to make T coincide with the synchronous time t and then relate it to the conformal one η by using $\partial_t = e^{-\alpha}\partial_\eta$ (up to a fiducial volume). In other words, we parametrize the wordlines of the fluid such that T is aligned with the synchronous time of the minisuperspace classical background. As a consequence, the evolution of the graviton fluctuations is parametrized by the same clock of the quantum matter field when making use of (6.87). Clearly, such extra steps will not be needed for the quantum inflaton sector, which is directly described by the Gaussian fluid clock.

Now the graviton gauge condition (6.81) takes the form

$$i\hbar\left(\sqrt{3\Lambda}e^{\alpha}+2\partial_\eta\right)\psi_1=\sum_{\mathbf{k},\lambda}\left[-\hbar^2\partial^2_{v^\lambda_{\mathbf{k}}}+\nu_k^2 v^\lambda_{\mathbf{k}})^2\right]\psi_1\,, \tag{6.89}$$

which can be further simplified with the following transformation

$$\begin{aligned}\psi_1\to\bar{\psi}_1&=\psi_1\,exp\left(-\frac{\sqrt{3\Lambda}}{2}\int d\eta\; e^{\alpha(\eta)}\right)\\ &=\psi_1\,exp\left(\frac{\sqrt{3\Lambda}}{2\mathscr{H}_0}\ln(-\eta)\right)=(-\eta)^{\frac{\sqrt{3\Lambda}}{2\mathscr{H}_0}}\psi_1\end{aligned} \tag{6.90}$$

so that we recover exactly the standard time-dependent harmonic oscillator:

$$i\hbar\partial_\eta\bar{\psi}_1=\sum_{\mathbf{k},\lambda}\left[-\hbar^2\partial^2_{v^\lambda_{\mathbf{k}}}+\nu_k^2(v^\lambda_{\mathbf{k}})^2\right]\bar{\psi}_1\,. \tag{6.91}$$

We stress that the transformation from ψ_1 to $\bar{\psi}_1$ is only used as a mathematical tool to compute the solution and will be reverted afterwards; in this sense, it is not implemented as a physical rescaling on the whole system. In analogy with Sec. 5.3, we use the method of invariants ad the Bunch-Davies vacuum requirement to find:

$$\begin{aligned}\bar{\psi}_1(\eta,v^\lambda_{\mathbf{k}})=\prod_{\mathbf{k},\lambda}&\left[\frac{k^3}{\pi\hbar\left(\frac{1}{\eta^2}+k^2\right)}\right]^{\frac{1}{4}}\exp\left[-\frac{i}{2}\left(\eta k-\arctan(\eta k)\right)\right]\\ &\times\exp\left[\frac{i}{2\hbar}\frac{ik^3\eta^3-1}{\eta^3\left(\frac{1}{\eta^2}+k^2\right)}(v^\lambda_{\mathbf{k}})^2\right]\,.\end{aligned} \tag{6.92}$$

Then, it is easy to invert (6.90) to recover the solution for $\psi_1=e^{\frac{i}{\hbar}P_1}$ and obtain the function P_1:

$$\begin{aligned}P_1(\eta,v^\lambda_{\mathbf{k}})=-i\hbar\sum_{\mathbf{k},\lambda}&\left[\frac{1}{4}\ln\left(\frac{k^3}{\pi\hbar\left(\frac{1}{\eta^2}+k^2\right)}\right)-\frac{\sqrt{3\Lambda}}{2\mathscr{H}_0}\ln(-\eta)\right.\\ &\left.-\frac{i}{2}\left(\eta k-\arctan(\eta k)\right)+\frac{i}{2\hbar}\frac{ik^3\eta^3-1}{\eta^3\left(\frac{1}{\eta^2}+k^2\right)}(v^\lambda_{\mathbf{k}})^2\right]\end{aligned} \tag{6.93}$$

We recall that $\hat{\mathscr{J}}$ contains its derivative with respect to $v^\lambda_{\mathbf{k}}$, that is

$$\partial_{v^\lambda_{\mathbf{k}}}P_1=\frac{i}{\hbar}\frac{ik^3\eta^3-1}{\eta^3\left(\frac{1}{\eta^2}+k^2\right)}v^\lambda_{\mathbf{k}}\,. \tag{6.94}$$

6.4.1 Power spectrum result with a Gaussian ansatz

Let us now proceed to the computation of the inflaton solution. Identifying T with the conformal time η, Eq. (6.85) provides the following dynamics with QG corrections:

$$i\hbar\partial_\eta\chi_2=\frac{1}{2}\sum_{\mathbf{k}}\left[-\hbar^2\partial^2_{\phi_{\mathbf{k}}}+\nu_k^2(\phi_{\mathbf{k}})^2\right]\chi_2-\frac{1}{2}\sum_{\mathbf{k},\lambda}\left[\hbar^2\partial^2_{v^\lambda_{\mathbf{k}}}+2i\hbar\partial_{v^\lambda_{\mathbf{k}}}P_1\partial_{v^\lambda_{\mathbf{k}}}\right]\chi_2\,. \tag{6.95}$$

We first decompose χ_2 in Fourier space, considering it as a product of independent modes $\chi_{\mathbf{k}}$ each one depending on $\phi_{\mathbf{k}}$ and $v_{\mathbf{k}}^{\lambda}$; this turns (6.95) into a set of independent equations, one for each $\mathbf{k}$. In analogy with Chapter 5 and other implementations such as [68, 52], we look for a Gaussian solution

$$\chi_{\mathbf{k}} = A_{\mathbf{k}}(\eta, v_{\mathbf{k}}^{\lambda})\, e^{-\frac{1}{2}\Omega_{\mathbf{k}}(\eta)(\phi_{\mathbf{k}})^2} = \mathcal{N}_{\mathbf{k}}(\eta, v_{\mathbf{k}}^{\lambda})\, e^{i\varphi_{\mathbf{k}}(\eta, v_{\mathbf{k}}^{\lambda})} e^{-\frac{1}{2}\Omega_{\mathbf{k}}(\eta)(\phi_{\mathbf{k}})^2} \tag{6.96}$$

where the complex amplitude $A_{\mathbf{k}}$ has been rewritten by means of a (real) magnitude $\mathcal{N}_{\mathbf{k}}$ and a (real) phase $\varphi_{\mathbf{k}}$, and the Gaussian width $\Omega_{\mathbf{k}}$ depends on η alone.

We can further WKB expand those functions by noting that the QG-corrections related to the graviton fluctuations in (6.95) are inherently of order M^{-1}, so it is reasonable to require all the $O(M^0)$ functions to depend on η alone; moreover, we postulate the Gaussian width to be independent of the $v_{\mathbf{k}}^{\lambda}$, as in [68, 52]

$$\mathcal{N}_{\mathbf{k}}(\eta, v_{\mathbf{k}}^{\lambda}) = N_{\mathbf{k}}(\eta)\left[1 + \frac{\mathscr{H}_0^2}{M} G_{\mathbf{k}}(\eta, v_{\mathbf{k}}^{\lambda})\right], \tag{6.97}$$

$$\varphi_{\mathbf{k}}(\eta, v_{\mathbf{k}}^{\lambda}) = \varphi_{\mathbf{k}}^{(0)}(\eta) + \frac{\mathscr{H}_0^2}{M}\varphi_{\mathbf{k}}^{(1)}(\eta, v_{\mathbf{k}}^{\lambda}), \tag{6.98}$$

$$\Omega_{\mathbf{k}}(\eta) = \Omega_{\mathbf{k}}^{(0)}(\eta) + \frac{\mathscr{H}_0^2}{M}\Omega_{\mathbf{k}}^{(1)}(\eta). \tag{6.99}$$

Here the functions are expanded in the factor $\mathscr{H}_0^2/M$ by comparison with the unmodified standard power spectrum, assuring the correct dimensions for all quantities. The compatibility of such assumptions will be shown in Appendix B. Clearly, the Gaussian ansatz for each mode is then

$$\chi_{\mathbf{k}} = N_{\mathbf{k}}\left(1 + \frac{\mathscr{H}_0^2 G_{\mathbf{k}}}{M}\right)\exp\left[i\left(\varphi_{\mathbf{k}}^{(0)} + \frac{\mathscr{H}_0^2}{M}\varphi_{\mathbf{k}}^{(1)}\right) - \frac{1}{2}\left(\Omega_{\mathbf{k}}^{(0)} + \frac{\mathscr{H}_0^2}{M}\Omega_{\mathbf{k}}^{(1)}\right)(\phi_{\mathbf{k}})^2\right], \tag{6.100}$$

where we dropped all dependencies for readability. Inserting it into (6.95), we find for both the Gaussian amplitude and width an equation at order M^0 and one at order M^{-1}, ending up with the following four coupled equations:

$$i\partial_\eta \Omega_{\mathbf{k}}^{(0)} = \left(\Omega_{\mathbf{k}}^{(0)}\right)^2 - \nu_k^2, \tag{6.101}$$

$$i\partial_\eta \Omega_{\mathbf{k}}^{(1)} = 2\Omega_{\mathbf{k}}^{(0)}\Omega_{\mathbf{k}}^{(1)}, \tag{6.102}$$

$$i\partial_\eta N_{\mathbf{k}} - N_{\mathbf{k}}\partial_\eta \varphi_{\mathbf{k}}^{(0)} = \frac{1}{2}N_{\mathbf{k}}\Omega_{\mathbf{k}}^{(0)}, \tag{6.103}$$

$$\begin{aligned} iG_{\mathbf{k}}\partial_\eta N_{\mathbf{k}} + N_{\mathbf{k}}\left[i\partial_\eta G_{\mathbf{k}} - \partial_\eta\varphi_{\mathbf{k}}^{(1)} - G_{\mathbf{k}}\partial_\eta\varphi_{\mathbf{k}}^{(0)}\right] &= \frac{1}{2}N_{\mathbf{k}}\left(G_{\mathbf{k}}\Omega_{\mathbf{k}}^{(0)} + \Omega_{\mathbf{k}}^{(1)}\right) \\ -\frac{1}{2}N_{\mathbf{k}}\sum_\lambda\Big(\partial^2_{v_{\mathbf{k}}^{\lambda}}G_{\mathbf{k}} + i\partial^2_{v_{\mathbf{k}}^{\lambda}}\varphi_{\mathbf{k}}^{(1)} &- 2\xi_k(\eta)\left[\partial_{v_{\mathbf{k}}^{\lambda}}G_{\mathbf{k}} + i\partial_{v_{\mathbf{k}}^{\lambda}}\varphi_{\mathbf{k}}^{(1)}\right]v_{\mathbf{k}}^{\lambda}\Big)\Big]. \end{aligned} \tag{6.104}$$

Eq. (6.101) is identical to the one in [68] (although obtained via a different implementation) and can be readily solved for the Gaussian width, compatible with the Bunch-Davies vacuum condition:

$$\Omega_{\mathbf{k}}^{(0)}(\eta) = \frac{k^3\eta^2}{1 + k^2\eta^2} + \frac{i}{\eta(1 + k^2\eta^2)}. \tag{6.105}$$

In the super-Hubble limit $k\eta \to 0^-$, which is the relevant one for the computation of the primordial spectrum, $\Omega^{(0)}_{\mathbf{k}}(\eta) \sim k^3\eta^2 + \frac{i}{\eta}$ and therefore we can obtain a solution of (6.102) in this limit:

$$\Omega^{(1)}_{\mathbf{k}}(\eta) \sim c_1\eta^2 \left(1 - \frac{2}{3}ik^3\eta^3\right). \tag{6.106}$$

where c_1 is an integration constant.

The normalization of the Gaussian ansatz over both the graviton and inflaton degrees of freedom $\int d\phi_{\mathbf{k}} dv^{\lambda}_{\mathbf{k}}\ \chi^*_{\mathbf{k}}\chi_{\mathbf{k}} = 1$ gives a further restriction for the remaining functions:

$$|N_{\mathbf{k}}|^4 \left(1 + \int dv^{\lambda}_{\mathbf{k}}\, \frac{4\mathscr{H}_0^2}{M} G_{\mathbf{k}}\right) = \frac{\Re(\Omega^{(0)}_{\mathbf{k}})}{\pi} + \frac{\mathscr{H}_0^2}{M}\frac{\Re(\Omega^{(1)}_{\mathbf{k}})}{\pi}. \tag{6.107}$$

having neglected all terms of $O(1/M)$ or higher. It is understood here that the integration over the $v^{\lambda}_{\mathbf{k}}$ is applied only to the functions of order M^{-1}, since the order M^0 in (6.97)-(6.99) is independent of those variables. Here the fourth power is due to the complex nature of the perturbation variables, which has required to treat their real and imaginary parts separately, see [110, 68]. Therefore, the normalization condition splits into

$$N_{\mathbf{k}}(\eta) = \left(\frac{\Re(\Omega^{(0)}_{\mathbf{k}})}{\pi}\right)^{\frac{1}{4}}, \tag{6.108}$$

$$\int dv^{\lambda}_{\mathbf{k}}\ G_{\mathbf{k}}(\eta, v_{\mathbf{k}}) = \frac{\Re(\Omega^{(1)}_{\mathbf{k}})}{4\Re(\Omega^{(0)}_{\mathbf{k}})}. \tag{6.109}$$

We now have all the necessary ingredients to compute the correlation function associated to the inflaton wave function χ_2 in the Gaussian form (6.96). The calculation yields

$$\begin{aligned}\Xi(\mathbf{r}) = \prod_{\mathbf{k}} |N_{\mathbf{k}}|^4 \left(1 + \int dv^{\lambda}_{\mathbf{k}} \frac{4\mathscr{H}_0^2 G_{\mathbf{k}}}{M}\right) \cdot \int \prod_{\mathbf{p}} d\phi_{\mathbf{p}}\ e^{-\sum_{\mathbf{k}'}\left[\Re(\Omega^{(0)}_{\mathbf{k}'}) + \frac{\mathscr{H}_0^2}{M}\Re(\Omega^{(1)}_{\mathbf{k}'})\right](\phi_{\mathbf{k}'})^2} \\ \times\ \phi(\eta,\mathbf{x})\phi(\eta,\mathbf{x}+\mathbf{r})\end{aligned} \tag{6.110}$$

Eq. (6.110) presents some novel contributions with respect to the analogous one obtained in Sec. 5.3 in the non-extended B-O approach, i.e. without taking into account the graviton fluctuations as separate degrees of freedom. Proceeding in the same way for the integration over the real and imaginary parts of $\phi_{\mathbf{p}}$, we find

$$\Xi(\mathbf{r}) = \int \frac{d\mathbf{p}}{(2\pi)^3} e^{-i\mathbf{p}\cdot\mathbf{r}} \frac{1}{2\left[\Re(\Omega^{(0)}_{\mathbf{p}}) + \frac{\mathscr{H}_0^2}{M}\Re(\Omega^{(1)}_{\mathbf{p}})\right]}, \tag{6.111}$$

therefore both $\Omega^{(0)}_{\mathbf{p}}$ and $\Omega^{(1)}_{\mathbf{p}}$ enter the power spectrum compared with (5.47). We can now turn from the inflaton spectrum to the comoving curvature spectrum $P_\zeta(k)$ using the definition of the M-S variable, as in (5.48):

$$\mathcal{P}_\zeta(k) = \frac{Gk^3}{\pi\varepsilon a^2} \frac{1}{k^3\eta^2 + \frac{\mathscr{H}_0^2}{M}c_1\eta^2} \tag{6.112}$$

where we have already applied the super-Hubble limit and we considered $\hbar = 1$ for easier comparison with the literature.

This result can be formulated as a small correction with respect to the standard power spectrum by a Taylor expansion for small $\mathscr{H}_0^2/M$; finally, recalling the classical solution $a(\eta) = -1/(\mathscr{H}_0\eta)$, we obtain at the horizon crossing $k = a\mathscr{H}_0$:

$$\mathcal{P}_\zeta(k) = \frac{G\mathscr{H}_0^2}{\pi\varepsilon}\left[1 - c_1\frac{\mathscr{H}_0^2}{M}\left(\frac{k_0}{k}\right)^3\right], \tag{6.113}$$

where we have made evident a reference wave number k_0, coming from the discretized treatment of the perturbations as time-dependent harmonic oscillators, which recovers the correct dimensions, see [68]. A direct comparison with (5.50) shows that the extended B-O approach has indeed refined the formulation, providing an inflationary spectrum modified via a k-dependent factor: therefore the prediction of the theory does not corresponds anymore to a scale-invariant result.

It is interesting to compare such result also with the modified spectrum derived in [68], with the time parameter described in Sec. 2.4 and without taking into account the graviton fluctuations as generating QG corrections (there instead the tensor fluctuations were considered on the same level as the scalar ones): the result in that formalism brings

$$\mathcal{P}_\zeta(k) = \mathcal{P}_\zeta^{(0)}(k)\left[1 + 0.988\frac{\mathscr{H}_0^2}{M}\left(\frac{k_0}{k}\right)^3\right]. \tag{6.114}$$

Confronting our result with (6.114), we see that through the Gaussian fluid time and extended B-O formalism we have obtained a deviation from the standard spectrum with the same scale dependence $\propto k^{-3}$; this is also in accordance with the results of [135, 136] computed in the de Sitter phase, [137, 138, 52] in the slow-roll approximation, and [139] for power-law inflation, all with a time implementation analogous to 2.4 and without the gravitons treatment here presented.

However, let us note that in (6.113) the integration constant c_1 cannot take negative values due to the normalization condition (6.109). Therefore, the present model predicts a reduction of power at large scales. This is a notable difference from the power enhancement obtained in (6.114) and [136], while it agrees with the results in [137] obtained via the procedure of Sec. 2.4.1. Actually, it has been debated in [140] that the sign of the correction to the primordial spectrum depends on the initial conditions implemented for $\Omega^{(1)}$. In this sense, we stress that our model dictates $c_1 > 0$ by the requirement that both polarizations contribute with the same weight in (6.109), therefore it represents a specific solution. Clearly, this predicted modification is properly scaled to a quantum regime by the presence of the WKB parameter $1/M$.

Chapter 7

Beyond canonical quantization: the de Broglie-Bohm interpretation

We here switch to the alternative description of QM provided by the de Broglie-Bohm pilot-wave theory. Such theory is deterministic, in contrast with the standard formulation, and non-local, being the evolution over time described by the so-called guidance equation. After a brief introduction, we discuss its formulation in QC and how it can lead to novel phenomenologies. More specifically, we illustrate in Sec. 7.3 how to conciliate such picture with a B-O separation of the gravity-matter system, able to compute the effect of small quantum corrections of the gravitational sector to the matter evolution. In Sec. 7.4, we specifically compute its predictions for the inflationary spectrum in a pure de Sitter phase.

This Chapter contains the investigations of Refs. [141, 142].

7.1 Overview of the dBB approach

The de Broglie-Bohm approach (also referred to as pilot-wave theory) dates back to the 1950s and is a deterministic theory, which gives an alternative interpretation of what constitutes trajectories and probabilities in QM.

In this framework, the core elements of the quantum theory are postulated to exist independently of observation or measurement. For the QG case, they are the geometry of the 3d hypersurfaces and their canonical momenta, related to the extrinsic curvature (Sec. 1.5). The quantum evolution of such elements diverges from classical dynamics, since a quantum potential emerges, but it is inherently a deterministic theory: the evolution of particles and their positions in space are determined by the initial conditions and the guiding wave function.

To understand this, let us consider a single-particle non-relativistic quantum dynamics, i.e. the following Schrödinger equation

$$i\hbar\partial_t\Psi(x,t) = \left(-\frac{\hbar^2}{2m}\partial_x^2 + V(x)\right)\Psi(x,t)\,. \tag{7.1}$$

Since the wave function is complex, one can rewrite it as

$$\Psi(x,t) = A(x,t)\, e^{\frac{i}{\hbar}S(x,t)} \tag{7.2}$$

being A and S both real. This is equivalent to the ansatz of Sec. 2.3 used to discuss Vilenkin's original proposal [41], but it now takes a different connotation since we are already starting from a full Schrödinger dynamics (no time definition is needed). Eq. (7.1) then automatically decomposes into two partial differential equations stemming from its real and imaginary parts: we get respectively

$$\frac{\partial S}{\partial t} + \frac{(\partial_x S)^2}{2m} + V - \frac{\hbar^2}{2m}\frac{\partial_x^2 A}{A} = 0\,, \tag{7.3}$$

$$\partial_t A^2 + \frac{1}{m}\partial_x\left(A^2 \partial_x S\right) = 0\,. \tag{7.4}$$

In the Copenhagen interpretation of QM, Eq. (7.4) represents the continuity equation for the probability density A^2 associated to finding the particle at a given position x in time. In this sense, all physical content is given by this equation and the phase (Eq. (7.3)) is irrelevant.

In the dBB interpretation one instead considers both equations. In particular, Eq. (7.3) is essentially a HJ equation with an extra term, that is called *quantum potential*:

$$Q(x,t) = -\frac{\hbar^2}{2m}\frac{\partial_x^2 A}{A}(x,t)\,. \tag{7.5}$$

Here we observe that Q depends only on the form of Ψ; the main role of the amplitude A is indeed to determine the quantum potential here, and secondly to define the probability density. Since Q modifies the equation for S, it will also influence the so-called *guidance equation*

$$p = m\dot{x} = \partial_x S(x,t)\,, \tag{7.6}$$

whose solution describes the (determined) quantum trajectory of the particle in the dBB interpretation. More generally, we can write the guidance equation for a spinless particle as

$$\partial_t q_i(t) = \frac{\hbar}{m}\,\mathrm{Im}\left(\frac{\partial_i \Psi}{\Psi}\right)(q_i,t)\,, \tag{7.7}$$

where q_i are configuration variables.

Clearly, the classical limit is recovered when the quantum potential is negligible: in the regime $Q \to 0$, Eq. (7.3) becomes the standard HJ equation and the physical predictions coincide with the classical behaviour. In this case the set (7.3)-(7.4) can be interpreted as describing an ensemble of classical particles under the influence of a classical potential V, with velocity field $\partial_x S/m$.

The dBB interpretation allows for a simple explanation of the measurement process: observational outcomes are determined by the interactions between the guiding wave function and the measuring apparatus, preserving the unitary evolution of the quantum state. This means that there is no collapse of the wave function.

To sum up, the dBB interpretation provides a fully deterministic view, contrary to QM; however experimental verifications of its predictions can be challenging [143].

7.2 The dBB cosmological picture

This conceptual framework has been applied in QG and QC to various (homogeneous) minisuperspace models, as for example Ref. [144]. Notably, it has been shown that such cosmological models can avoid singularities through quantum effects [145, 146, 147, 148]: indeed the quantum potential assumes significance near the singularity, causing a repulsive force that counters gravitational collapse. The classical limit of this framework is then typically achieved for large scale factors.

To elucidate this point, let us consider a homogeneous and isotropic universe described by a single degree of freedom $a(t)$ (i.e. the scale factor), such as the FLRW model. Given an initial wave function $\Psi_0(a)$ and its evolution in time $\Psi(a,\eta)$ (we here refer to conformal time), we can use (7.2) to extract the phase $S(a,\eta)$. Then, the dBB trajectory is dictated by (see (7.6) and (7.2)):

$$\frac{\partial S}{\partial a} \equiv a'(\eta) = \frac{i}{2|\Psi|^2}\left(\Psi\frac{\partial\Psi^*}{\partial a} - \Psi^*\frac{\partial\Psi}{\partial a}\right) . \tag{7.8}$$

The resulting trajectory might present interesting properties: not only $a(\eta)$ might be non-vanishing (therefore avoiding the singularity), it might be decreasing towards a certain value and then expand again. The latter behaviour corresponds to a Bounce, i.e. a Universe which contracts, reaches a certain minimum volume and then reverts to an expansion. Clearly this would solve the problem of the initial singularity predicted by GR at the Big Bang.

Within the dBB picture, one could also face the question of different clock implementations from the WDW equation. Indeed, different time constructions can lead to varied singularity avoidance and bouncing cosmologies [148, 141]. It is interesting to ask whether such evolutions carry different outcomes for the isotropization of the universe, and how one could take into account cosmological perturbations within the same framework. In this respect, a review of previous results can be found in [145].

Let us now contextualize the dBB interpretation within the early universe evolution. As discussed in Chapter 5, the inflationary theory predicts an accelerated expansion ($\ddot{a} > 0, \dot{a} > 0$), addressing both the horizon and flatness problem. After this phase, the universe undergoes another expanding phase (first dominated by radiation, and then by pressureless matter) and cools down; however in this case GR predicts the expansion to be decelerated ($\ddot{a} < 0$). Since the growth rate slows down, the Hubble radius grows faster than all physical distance scales in the universe:

$$\frac{d\mathscr{H}}{da} = 1 - \frac{\ddot{a}a}{\dot{a}^3} > 1\,, \tag{7.9}$$

which is possible for $\dot{a} > 0$, $\ddot{a} < 0$. We recall from Sec. 5.1 that $\mathscr{H}$ outlines which regions were causal contact with each other. Therefore, this phase alone would not explain the temperature isotropy of the CMB radiation, since it would cause many scales to be outside the Hubble radius in the past and so causally disconnected. It is through the inflationary theory that we recover accordance with the isotropic and almost flat universe that we observe today.

Although the theory of inflation is widely recognized and accepted, we mention here an alternative possibility for the phase preceding the radiation era. One could hypothesize that a contracting decelerating phase occurs, i.e. with $\ddot{a} < 0$ and $\dot{a} < 0$ in (7.9). This would imply a universe immensely large in the past and would overcome the horizon and structure formation concerns [147]. Clearly, this early contraction would need to reconnect with the expansion of today through a Bounce.

While bouncing cosmologies do not necessarily require an inflationary era, this does not preclude compatibility with such mechanisms. In the following Section, we apply the dBB interpretation to a simple cosmological model describing the de Sitter phase of inflation, investigating the trajectories and modified power spectrum of perturbations.

7.3 Born-Oppenheimer separation in the dBB picture

In this Section, we show that it is possible to merge the Born-Oppenheimer-like separation of the gravity-matter system with the dBB picture. The final aim is to analyze the first-order quantum corrections to the inflationary power spectrum deriving from the quantum potential; essentially, we will analyze the cosmological setting of Chapter 5 but through the lens of the dBB picture [142].

We consider the minisuperspace model describing the de Sitter phase, with a WDW equation of the form (in natural units $c = 1$)

$$H = -\frac{1}{48M}\frac{p_a^2}{a} + 4M\Lambda a^3 + H^{\phi}\,. \tag{7.10}$$

Here, the scalar matter content represents the inflation field, whose small fluctuations on the background form the power spectrum to be investigated. For convenience of the analysis, we make a canonical transformation to use a square-root volume variable $v = a^{3/2}$ instead of the scale factor a, obtaining the following super-Hamiltonian for the gravitational background:

$$H = -\frac{3}{64M}p_v^2 + 4M\Lambda v^2 + H^{\phi}\,. \tag{7.11}$$

With the gauge-invariant formalism of Chapter 5, the inflaton sector takes the form:

$$\hat{H}^{\phi} = \frac{1}{2v^{2/3}}\sum_{\mathbf{k}}\left(-\hbar^2\partial^2_{\phi_{\mathbf{k}}} + \omega_k^2(\eta)\phi_{\mathbf{k}}^2\right)\,. \tag{7.12}$$

We stress that the background will be intrinsically different from Chapter 5, since the trajectories of the scale factor will be modified by the quantum potential.

Let us employ the Born-Oppenheimer separation between the gravitational and matter components: $\Psi(v,\phi) = \psi(v)\chi(\phi, v)$. Here the inflaton field is understood as a purely quantum component, while for the gravitational sector we wish to use the dBB picture to compute the modified dynamics with small quantum corrections. Therefore, keeping in mind the form (7.2), we start with the following ansatz:

$$\Psi(v,\phi) = \sqrt{\rho}(v)\, e^{\frac{i}{\hbar}S(v)}\, \chi(\phi, v) \tag{7.13}$$

As previously noted, this ansatz is similar to Vilenkin's one [41]. An important deviation from the treatment of Chapters 3-4 is that here we do not implement a full WKB expansion of the wave function; indeed, the form (7.13) corresponds to a WKB expanded gravitational sector, while we retain the matter component at the purely quantum level.

In the spirit of the BO separation and motivated by the discussion in Sec. 4.2, we implement the following assumptions:

- We consider the gravitational constraint to be satisfied *a priori*, similarly to [41]. As illustrated in Chapter 6, this is equivalent in the canonical picture to performing the extended BO approximation and averaging over the small graviton fluctuations, since the associated gauge reconstructs the gravitational WDW equation at first order.

- To characterize the regime in which the gravitational sector is close to the classical behaviour, we consider it to have a large momentum [21]. This can expressed through its phase by the condition:

$$\partial_v S \gg 1\,. \tag{7.14}$$

  This condition is usually referred to as the *eikonal* approximation [4], which is a simpler case of the WKB one. In other words, by employing the hypothesis (7.14) together with the form (7.13), we effectively use a gravitational WKB scheme, and we will compute its small quantum deviations in the deterministic dBB picture.

- The adiabatic approximation here must be implemented in a different form, since we lack the expansion parameter and also the WKB functions Q_n of the matter sector (see Eq. 4.12). We then impose

$$\partial_v^2\chi \ll (\partial_v\psi)\partial_v\chi\,. \tag{7.15}$$

  In other words, we still express a small dependence of the fast matter sector on the "volume" variable, but the smallness is here expressed with respect to the gravitational wave function itself. We cannot say that $\partial_v\chi$ alone is small, since we do not employ the WKB expansion of the full system; also such choice would discard all the relevant effects that we wish to investigate.

We therefore work with the following system of quantized constraints:

$$\left(\frac{3\hbar^2}{64M}\partial_v^2 + 4M\Lambda v^2\right)\sqrt{\rho}\,e^{\frac{i}{\hbar}S} = 0\,, \tag{7.16}$$

$$\left(\frac{3\hbar^2}{64M}\partial_v^2 + 4M\Lambda v^2 + \hat{H}^\phi\right)\sqrt{\rho}\,e^{\frac{i}{\hbar}S}\chi = 0\,. \tag{7.17}$$

The explicit form of this system is:

$$\begin{aligned}&\frac{3\hbar^2}{64M}\left[\partial_v^2\sqrt{\rho} + 2\frac{i}{\hbar}(\partial_v\sqrt{\rho})\partial_v S + \frac{i}{\hbar}\sqrt{\rho}\,\partial_v^2 S - \frac{\sqrt{\rho}}{\hbar^2}\left(\partial_v S\right)^2\right]e^{\frac{i}{\hbar}S}\\ &\quad + 4M\Lambda v^2\sqrt{\rho}\,e^{\frac{i}{\hbar}S} = 0\,,\end{aligned} \tag{7.18}$$

$$
\begin{aligned}
&\frac{3\hbar^2}{64M}\left[\partial_v^2\sqrt{\rho}+2\frac{i}{\hbar}(\partial_v\sqrt{\rho})\partial_v S+\frac{i}{\hbar}\sqrt{\rho}\,\partial_v^2 S-\frac{\sqrt{\rho}}{\hbar^2}\,(\partial_v S)^2\right]e^{\frac{i}{\hbar}S}\chi\\
&\quad+\frac{3}{32M}\left(\partial_v\sqrt{\rho}\,e^{\frac{i}{\hbar}S}+\frac{i}{\hbar}\sqrt{\rho}(\partial_v S)e^{\frac{i}{\hbar}S}\right)(\partial_v\chi)+\frac{3}{64M}\sqrt{\rho}\,e^{\frac{i}{\hbar}S}\partial_v^2\chi\\
&\quad+4M\Lambda v^2\,\sqrt{\rho}\,e^{\frac{i}{\hbar}S}\,\chi+\frac{1}{2v^{2/3}}\sqrt{\rho}\,e^{\frac{i}{\hbar}S}\sum_{\mathbf{k}}\left(-\hbar^2\partial^2_{\phi_{\mathbf{k}}}+\omega_k^2(\eta)\phi_{\mathbf{k}}^2\right)\chi=0\,.
\end{aligned}
\tag{7.19}
$$

Eq. (7.18) can be used to simplify the total constraint; then, making use of the assumptions (7.15)-(7.14), one finds

$$
\begin{aligned}
&\frac{3}{32M}\left(\frac{i}{\hbar}\sqrt{\rho}(\partial_v S)\partial_v\chi\right)e^{\frac{i}{\hbar}S}\\
&\quad+\frac{1}{2v^{2/3}}\sqrt{\rho}\,e^{\frac{i}{\hbar}S}\sum_{\mathbf{k}}\left(-\hbar^2\partial^2_{\phi_{\mathbf{k}}}+\omega_k^2(\eta)\phi_{\mathbf{k}}^2\right)\chi=0\,.
\end{aligned}
\tag{7.20}
$$

Here, we stress that only the dominant contribution from the gravitational momentum operator acting on Ψ has been taken into account. The other terms which were present in the second line of Eq. (7.19) are negligible in the present B-O picture. More specifically, we have omitted both $\partial_v^2\chi$ due to the adiabatic condition (7.15) with respect to $(\partial_v S)\partial_v\chi$, and the term with $\partial_v\sqrt{\rho}$. The motivation for the latter is that the amplitude is determined by the dBB picture to be

$$
\sqrt{\rho}\propto\frac{1}{|\partial_v S|^{1/2}}
\tag{7.21}
$$

and therefore subdominant (see (7.14)). The relationship (7.21) will be explicitly demonstrated in the computation of the dBB trajectory in the next Section.

To recover a physical description of the inflaton evolution, we must still recover a time parameter from the WDW equation. It is now straightforward to implement the time definition analogous to Vilenkin, i.e. as a composite derivative with respect to label time, up to the Planckian numerical factor (see discussion in Sec. 3.1). The matter evolution is expressed by its dependence on S via

$$
i\hbar\partial_t\chi\equiv-\frac{3}{32M}\frac{i}{\hbar}(\partial_v S)\partial_v\chi\,.
\tag{7.22}
$$

Here a remark is necessary: while such time construction has been discussed to lead to non-unitary effects in Sec. 3.1, we are here using the alternative dBB interpretation, instead of the WKB expansion in the canonical picture. This means that we will find a modified dynamics for the inflaton sector, but this behaviour will be induced by the fact that the gravitational component experiences a non-classical evolution due to the quantum potential, as will be clear in the computation of the dBB trajectories. Therefore this approach is not in contrast with the findings of Chapter 3, but it gives an alternative formulation to study small quantum corrections for the gravity-matter system.

Having performed these steps, we recover a Schrödinger evolution for the inflation field as a time-dependent harmonic-oscillator:

$$
i\hbar\partial_t\chi=\frac{1}{2v^{2/3}}\sum_{\mathbf{k}}\left(-\hbar^2\partial^2_{\phi_{\mathbf{k}}}+\omega_k^2(\eta)\phi_{\mathbf{k}}^2\right)\chi\,.
\tag{7.23}
$$

This is the same formalism of (5.21), with frequency (5.12) in Fourier space i.e.

$$\omega(\eta)^2 = k^2 - \frac{z''}{z}\,. \tag{7.24}$$

To summarize, by considering a BO separation of the scalar inflaton field on top of such (Bohmian) background with the clock (7.22), we have placed ourselves in the same scenario as in Sec. 5.2.

In the next Section we explicitly compute the dBB trajectory for the universe "volume" in this model, resulting in a modified frequency (7.24), and we will analyze the corresponding primordial power spectrum.

7.4 dBB trajectory and power spectrum analysis

We first focus on the gravitational sector alone to derive the dBB trajectory for the scale factor (actually for the variable $v = a^{2/3}$) of the universe in the minisuperspace model of Sec. 7.3.

As stated in Sec. 7.1, the trajectory can be inferred from the guidance equation and it depends on the phase S of $\psi(v) = \sqrt{\rho}(v)e^{\frac{i}{\hbar}S(v)}$. However, the dynamics of $\sqrt{\rho}$ and S are inferred by the real and imaginary parts of the quantized gravitational constraint (7.18) and are actually coupled. We label the two contributions with $\mathcal{C}_{\Re}$ and $\mathcal{C}_{\Im}$ respectively, finding:

$$\mathcal{C}_{\Re} := \frac{3}{64M}\hbar^2\frac{\partial^2\sqrt{\rho}}{\partial v^2} - \frac{3}{64M}\sqrt{\rho}\left(\frac{\partial S}{\partial v}\right)^2 + 4M\Lambda v^2\sqrt{\rho} = 0\,, \tag{7.25}$$

$$\mathcal{C}_{\Im} := \frac{3}{64M}i\hbar\left(2\frac{\partial\sqrt{\rho}}{\partial v}\frac{\partial S}{\partial v} + \sqrt{\rho}\,\frac{\partial^2 S}{\partial v^2}\right) = 0\,. \tag{7.26}$$

We immediately observe that $\mathcal{C}_{\Re}$ (7.25) corresponds in the $\hbar \to 0$ limit to the standard HJ equation

$$\sqrt{\rho}\left[-\frac{3}{64M}\left(\frac{\partial S}{\partial v}\right)^2 + 4M\Lambda v^2\right] = 0\,. \tag{7.27}$$

Indeed the first term of Eq. (7.25), which is of order $\hbar^2$, is the quantum potential giving the deviation from the purely classical solution.

Let us now focus on the imaginary part of the constraint. Recognizing that (7.26) can be rewritten as $\partial_v\left[(\sqrt{\rho})^2\partial_v S\right]/\sqrt{\rho}$, we can immediately solve the amplitude in terms of the phase, i.e.

$$\sqrt{\rho} = \frac{c}{|\partial_v S|^{1/2}} \tag{7.28}$$

being c a numerical constant. This validates the relation (7.21) anticipated in the previous Section. Substituting into (7.25) and dividing by $\sqrt{\rho}$, one is lead to the following equation for $S(v)$:

$$-\frac{3}{64M}(\partial_v S)^2 + 4M\Lambda v^2 = -\frac{9\hbar^2}{256M}\frac{(\partial_v^2 S)^2}{(\partial_v S)^2} + \frac{3\hbar^2}{128M}\frac{\partial_v^3 S}{\partial_v S}\,, \tag{7.29}$$

which is a third-order non-linear inhomogeneous differential equation, of which a closed form is not found. Since we wish to consider the small deviations from the classical behaviour, attributed to the quantum potential and responsible for the right-hand side of (7.29), we look for an approximate solution to (7.29) at leading order:

$$S(v) = S_0(v) + \hbar^2 S_1(v)\,. \tag{7.30}$$

This expression can be interpreted as the WKB expansion of the gravitational phase alone in (7.2). Clearly S_0 must correspond to the (classical) Hamilton-Jacobi solution of (7.27), i.e. for an expanding universe

$$S_0(v) = -\frac{8}{\sqrt{3}} M\sqrt{\Lambda}\, v^2 + \text{const}\,. \tag{7.31}$$

Inserting (7.30) in (7.29), the leading contributions in $\hbar^2$ to $\mathcal{C}_{\Re}$ result in

$$\begin{aligned} -\frac{3}{64M}\Big((\partial_v S_0)^2 + 2\hbar^2(\partial_v S_0)\partial_v S_1\Big) + 4M\Lambda v^2 \\ = -\frac{9\hbar^2}{256M}\frac{(\partial_v^2 S_0)^2}{(\partial_v S_0)^2} + \frac{3\hbar^2}{128M}\frac{\partial_v^3 S_0}{\partial_v S_0}\,. \end{aligned} \tag{7.32}$$

On the right-hand side, only the function S_0 contributes due to the factor $\hbar^2$ in front. Making use of the solution (7.31), for which $\partial_v^3 S_0 = 0$, we arrive at the following expression for S_1:

$$S_1(v) = \frac{1}{256\sqrt{3\Lambda}}\, v^{-2} + \text{const}\,. \tag{7.33}$$

Therefore the gravitational phase in (7.13) at leading order is:

$$S(v) = -\frac{4}{\sqrt{3}} M\sqrt{\Lambda}\, v^2 + \frac{\hbar^2}{256\sqrt{3\Lambda}}\, v^{-2} + \text{const}\,. \tag{7.34}$$

We remark that the presence of a non-zero cosmological constant Λ is compatible with a de Sitter phase: indeed $\Lambda = 0$ would not correspond to a viable solution of the Einstein's equations. If one considered Eq. 7.11 with $\Lambda = 0$, the interpretation would be non-trivial: this case would correspond to a vacuum universe having from (7.27) $S_0 = 0$ at the classical level (actually $S_0(v) = const$, which can be put to zero), but with total phase $S(v) = \hbar^2 S_1(v)$. Therefore the model would yield a "purely quantum" trajectory without the classical background. For this reason, in the following we always consider $\Lambda > 0$.

The Bohmian trajectory for v can now be inferred from the guidance equation

$$\dot{v} = \frac{dv}{dt} = -\frac{3}{32M}\frac{\partial S}{\partial v}\,. \tag{7.35}$$

Using the solution (7.34) one obtains

$$v(t) = \frac{\sqrt{2}}{(3\Lambda)^{1/8}}\left(e^{\sqrt{3\Lambda}(t-t_0)} - \frac{\sqrt{3}\hbar^2}{16\cdot 256 M\sqrt{\Lambda}}\right)^{1/4} \tag{7.36}$$

which is valid in a limited range $t_0 < t_{min} < t < t_{max}$ inside the de Sitter phase (being t_0 the beginning of such phase). By definition of v, the classical regime would correspond to

$$v_0(t) = e^{\frac{\sqrt{3\Lambda}}{4}(t-t_0)} = a_0(t)^{\frac{3}{2}} \equiv \left(e^{\mathscr{H}(t-t_0)}\right)^{3/2} , \tag{7.37}$$

being $a_0(t)$ the classical solution of the de Sitter phase (Sec. 5.3). For simplicity, we have reabsorbed the numerical factor in front inside t_0; we will also consider $t_0 = 0$, effectively putting the origin of coordinate time at the beginning of the de Sitter phase, such that $\mathscr{H} = \sqrt{3\Lambda}/6$.

For the study of the inflationary spectrum, as discussed in Chapter 5, it is more convenient to work in the conformal time gauge $N = a = v^{\frac{2}{3}}$, in which the classical scale factor takes the form $a(\eta) = -1/(\mathscr{H}\eta)$. The dBB trajectory (7.36) now becomes

$$v(\eta) = \left(\frac{2}{3\mathscr{H}}\right)^{\frac{1}{4}} \left[\left(-\frac{1}{\mathscr{H}\eta}\right)^6 - \frac{\hbar^2}{32 \cdot 256\, \mathscr{H}}\right]^{\frac{1}{4}} , \tag{7.38}$$

where again the solution is valid inside an interval $\eta_i < \eta < \eta_f$, since in our analysis the de Sitter model does not correspond to an eternal inflation scenario.

We observe that in both forms (7.36) and (7.38), the action of the quantum potential results in a modified “volume” (actually its square root) which does not vanish in the considered interval, due to the contribution of $\mathcal{O}\left(\hbar^2\right)$, see Figure 7.1. Indeed, Eq. (7.38) vanishes for $\eta^* = -4\sqrt[6]{2}\mathscr{H}M^{1/6}/\hbar^{1/3}$, which falls outside our de Sitter approximation. This result is inherently different from the classical solution, although there is no Bounce.

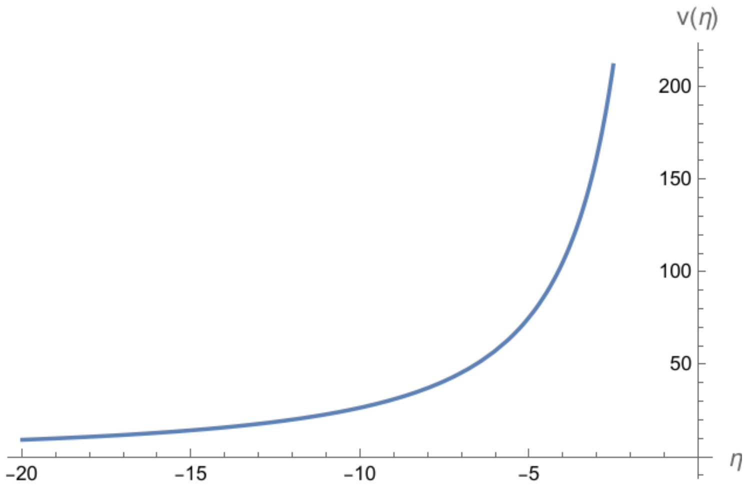

Figure 7.1. Plot of the computed dBB trajectory (7.38) in conformal time. As an effect of the quantum correction, the variable remains above the η axis and does not reach zero. We have used as reference values $\mathscr{H} = 0.02$, $\hbar = 0.001$, $c = 1$.

7.4.1 Inflaton power spectrum on the dBB background

We can now turn to the inflaton sector. The time-dependent harmonic oscillator formalism is characterized by the frequency (7.24), where $k = |\mathbf{k}|$ identifies the mode and $z = a\sqrt{\epsilon}$ with $\epsilon = -\dot{\mathscr{H}}/\mathscr{H}^2$ the first slow-roll parameter.

Clearly, the variable z is influenced by the dBB trajectory, both through $v(\eta)$ and through the parameter ϵ which itself depends on $a(\eta)$ via the Hubble parameter. In this pure de Sitter scheme, we implement a constant ϵ, so that from (7.38) one finds at leading order in $\hbar$

$$\omega(\eta)^2 \simeq k^2 - \frac{2}{\eta^2} + \mu\hbar^2\eta^4 \,, \tag{7.39}$$

where $\mu = \frac{7}{32\cdot 256 M}\mathscr{H}^5$ is a numerical factor. Here again, in the limit $\hbar \to 0$ (7.39) goes to the standard result of cosmological perturbation theory.

To infer the corresponding power spectrum, we recall that the correlation function must be computed on the eigenstates of the oscillator properly satisfying the Bunch-Davies condition (as elucidated in Sec. 5.2). Through the method of invariants (Appendix A), this requires to find the solution to the Ermakov equation (A.2). In this case however, our frequency has a contribution of order $\hbar^2$. In an approximate scheme, we write also the solution to (A.2) expanded in such way, so that

$$\omega^2(k,\eta) = \omega_0^2(k,\eta) + \hbar^2\omega_1^2(k,\eta)\,; \tag{7.40}$$

$$\rho(k,\eta) = \rho_0(k,\eta) + \hbar^2\rho_1(k,\eta) \tag{7.41}$$

where we have dropped the subscript k for readability. From comparison with (7.39) we have that

$$\omega_0^2(k,\eta) = k^2 - \frac{2}{\eta^2}\,, \qquad \omega_1^2(k,\eta) = \mu\eta^4\,. \tag{7.42}$$

As a consequence, also the Ermakov equation splits into a contribution of order $\hbar^0$

$$(\rho_0)'' + \omega_0^2\,\rho_0 = \frac{1}{(\rho_0)^3}\,, \tag{7.43}$$

being $' \equiv \partial_\eta$, and next-order contributions. For the latter, we truncate at the order of first quantum corrections i.e. $\mathcal{O}(\hbar^2)$; this is obtained by Taylor expanding the term $1/\rho^3$ in $\hbar$, which results in:

$$(\rho_1)'' + \omega_0^2\,\rho_1 = -\omega_1^2\,\rho_0 + 3\frac{\rho_1}{(\rho_0)^4}\,. \tag{7.44}$$

Concerning Eq. (7.43), we immediately recognize that its solution is the same one computed in Chapter 5, since the frequency ω_0 (7.42) corresponds to the standard QFT dynamics. So the function ρ_0 is

$$\rho_0 = \sqrt{\frac{1}{k^3\eta^2} + \frac{1}{k}}\,, \tag{7.45}$$

which satisfies the Bunch-Davies vacuum requirement, as discussed in Sec. 5.3.

For ρ_1, we need to solve Eq. 7.44, which is second-order and inhomogeneous. However, we can carry on a qualitative analysis in the limit of small η, in which we aim to compute the spectrum (this regime assures that the inflationary perturbations freeze out, see Sec. 5.2). The term $\omega_0\rho_1$ with $\omega_0^2 \propto 1/\eta^2$ results to be dominant, while $\omega_1^2\rho_0 \sim \eta^3$ and $1/(\rho_0)^4 \sim \eta^4$. Therefore, by neglecting the last term, we deal with the approximate form of Eq. 7.44 in the limit of small η:

$$(\rho_1)'' + \omega_0^2\rho_1 = -\omega_1^2\rho_0\,. \tag{7.46}$$

The general form of the solution to (7.46) is

$$\begin{aligned}\rho_1(k,\eta) =& \frac{c_1}{\sqrt{k}}\left(\frac{sin(k\eta)}{k\eta} - cos(k\eta)\right) + \frac{c_2}{\sqrt{k}}\left(\frac{cos(k\eta)}{k\eta} + sin(k\eta)\right) \\ &- \left(\frac{cos(k\eta)}{k^{1/2}} - \frac{sin(k\eta)}{k^{3/2}\eta}\right)\mathcal{I}_1 - \left(\frac{cos(k\eta)}{k^{3/2}\eta} + \frac{sin(k\eta)}{k^{1/2}}\right)\mathcal{I}_2\,,\end{aligned} \tag{7.47}$$

where c_1, c_2 are numerical constants and we have defined the following integrals

$$\mathcal{I}_1 = \int_1^\eta dy\left[-\frac{\mu\, y^3}{k^{1/2}}\left(\frac{1}{k^3y^2} + \frac{1}{k}\right)^{1/2}\left(\frac{cos(k\,y)}{k} + y\,sin(k\,y)\right)\right]\,, \tag{7.48}$$

$$\mathcal{I}_2 = \int_1^\eta dy\left[\frac{\mu\, y^3}{k^{1/2}}\left(\frac{1}{k^3y^2} + \frac{1}{k}\right)^{1/2}\left(y\,cos(k\,y) - \frac{sin(k\,y)}{k}\right)\right]\,. \tag{7.49}$$

Here we observe that the first line of (7.47) would reconstruct, after the appropriate Bunch-Davies requirement, the same ρ_0 of Chapter 5; therefore, we can consider the two coefficients c_1 and c_2 to be equal to zero, such that ρ_1 purely describes the quantum correction to the previous order solution.

However, for the final state to describe the Bunch-Davies vacuum, the function ρ_1 must go to zero in the relevant limit. Indeed in the Bunch-Davies regime, one considers the inflaton wavelength to be small with respect to curvature (sub-horizon), so that $k_{phys} \gg 1$. In this way, the eigenstate should correspond to the (Minkowskian) lowest energy state of the oscillator. For large values of k it can be shown that (7.47) goes to zero, and we recall that ρ_0 satisfies the requirement by construction; as a consequence, the total function $\rho = \rho_0 + \hbar^2\rho_1$ is compatible with the Bunch-Davies condition.

We are now left with the task of computing the power spectrum from ρ given by (7.45), (7.47). Following the reasoning of Sec. 5.2, we find that the correlation function results in a contribution $\rho^2(k,\eta)$. Subsequently, the power spectrum of curvature perturbations stemming from the inflaton field is

$$\mathcal{P}_\zeta(k) = \frac{k^3}{4\pi^2}\frac{\rho^2(k,\eta)}{2a^2\epsilon}\bigg|_{-k\eta\ll 1} \tag{7.50}$$

computed in the super-Hubble limit, when perturbations are frozen outside the horizon.

Considering the lowest-order contribution ρ_0, we clearly recover the standard scale-invariant result $\mathcal{P}_\zeta^{(0)}(k)$ described in Chapter 5, see (5.50). At leading order, ρ_1 gives a small deviation which can be evaluated by performing a series expansion of the integrals in (7.48)-(7.49). Then, computing the expression in $\eta = 2\pi/\tilde{k} \ll 1$, we find

$$\mathcal{P}_\zeta^{(1)}(k) = \bar{\mu}\,\hbar^2\left(\frac{k}{\bar{\tilde{k}}}\right)^{-4}\left(\frac{\mathscr{H}}{\widetilde{\mathscr{H}}}\right)^{12}\mathscr{P}(k,\tilde{k})\,, \tag{7.51}$$

where $\bar{\mu} \propto 1/M^2$ is a numerical coefficient, $\tilde{k}$ and $\widetilde{\mathscr{H}}$ are reference values for the mode and Hubble parameter in the considered limit, and $\mathscr{P}$ is the following polynomial function in k:

$$\begin{aligned}\mathscr{P}(k,\tilde{k}) = \tilde{k}^{-8}\Big[&20\pi^6 k^6(90-90k^2-35k^4+9k^6)+1152\pi^5\tilde{k}\,k^4(5+3k^2)\\ &-90\pi^4\tilde{k}^2\,k^4(90-90k^2-35k^4+9k^6)-2880\pi^3\tilde{k}^3\,k^2(5+3k^2)\\ &+90\pi^2\tilde{k}^4\,k^2(90-90k^2-35k^4+9k^6)+45\tilde{k}^6(90-90k^2-35k^4+9k^6)\Big]^2\end{aligned} \tag{7.52}$$

For the CMB spectrum, a standard value for $\tilde{k}$ is the pivot scale $\tilde{k} \simeq 0.002\,\mathrm{Mpc}^{-1}$, see for example [149]. A plot of the obtained power spectrum is provided in Figure 7.2.

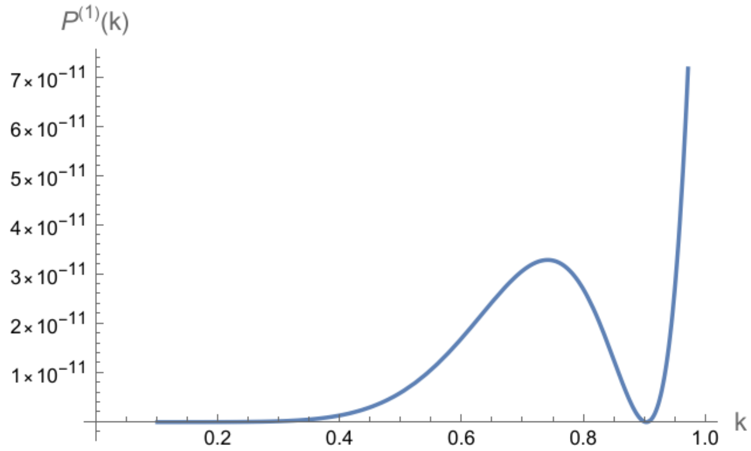

Figure 7.2. Plot of the computed dBB power spectrum (7.51) with reference values $\widetilde{\mathscr{H}} = 2$, $\mathscr{H} = 0.02$, $\tilde{k} = 0.027$ in Planckian-like units $\hbar = 0.001$, $M = 10$, $c = 1$.

The obtained correction is clearly not scale-invariant; moreover, we observe the presence of a minimum at a point much larger than the pivot scale $\tilde{k}$. The presence of the numerical factors $\hbar^2$ and $1/M^2$ in front assures that $\mathcal{P}_\zeta^{(1)}$ constitutes a small deviation from the standard result.

In this context, further investigation could involve computing the dependence of the slow-roll parameter ϵ on the modified evolution of v, here considered negligible at a perturbative level. This approach however would extend beyond the scope of a pure de Sitter phase ($\epsilon = \text{const}$) which was also analyzed in Chapter 5, so preventing a meaningful comparison between the two Born-Oppenheimer formulations. In the analysis of Chapter 5, the quantum-gravity corrections resulted in a time-dependent factor for the quantum state, which canceled out when computing the spectrum. In contrast, the present dBB interpretation describes quantum corrections (which primarily affect the gravitational sector and then the inflaton one) that alter the entire spectrum in a non-factorizable manner. While these deviations diminish as k decreases, they remain significant for large k.

The primordial spectrum can also be characterized by additional observables, describing its scale dependence. The first quantity is the spectral index n_s, defined as

$$\mathcal{P}(k) = A\,k^{n_s-1}\,, \tag{7.53}$$

which therefore can be obtained by

$$n_s = 1 + \frac{\mathrm{d}\, ln\, (\mathcal{P}(k)/A)}{\mathrm{d}\, ln\, k}\,. \tag{7.54}$$

Likewise, one can define the so-called running α_s

$$\alpha_s = \frac{\mathrm{d}\, n_s}{\mathrm{d}\, ln\, k} \tag{7.55}$$

and the running of the running β_s

$$\beta_s = \frac{\mathrm{d}\, \alpha_s}{\mathrm{d}\, ln\, k}\,. \tag{7.56}$$

It is understood that these quantities are evaluated at the horizon exit, i.e. at the pivot scale $k = \tilde{k}$ implemented previously.

In the present analysis, the lowest-order spectrum $\mathcal{P}_\zeta^{(0)}$ reproduces the scale-invariant result, having by definition (7.53) $n_s^{(0)} = 1$ i.e. independent of the scale k, and so the associated runnings would vanish.

The interesting case stems from the next-order result, where the dependence of the power spectrum $\mathcal{P}_\zeta^{(1)}$ on the scale k is expressed by the polynomial in (7.52). Here, we expect the spectral index to depart from unity; computing the corresponding value from the total power spectrum, we now have a polynomial function of k, which is plotted in Figure 7.3.

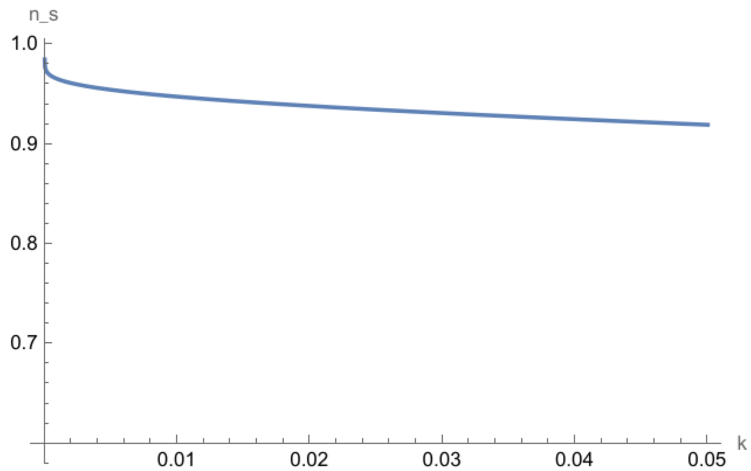

Figure 7.3. Plot of the spectral index n_s corresponding to the power spectrum $\mathcal{P}_\zeta^{(1)}$ in (7.51). Reference values $\tilde{\mathscr{H}} = 2$, $\mathscr{H} = 0.02$, $\tilde{k} = 0.027$ in Planckian-like units ($\hbar = 0.001$, $M = 10$, $c = 1$).

As a consequence, we now have non-trivial runnings α_s and β_s, corresponding again to polynomial functions in the wave number k. A comparison of the two functions provided in Figure 7.4 shows that, while both parameters are compatible with zero in the limit of small k, they actually invert their behavior around $k^* \simeq 0.13$, a value approximately five times larger than the pivot scale here considered.

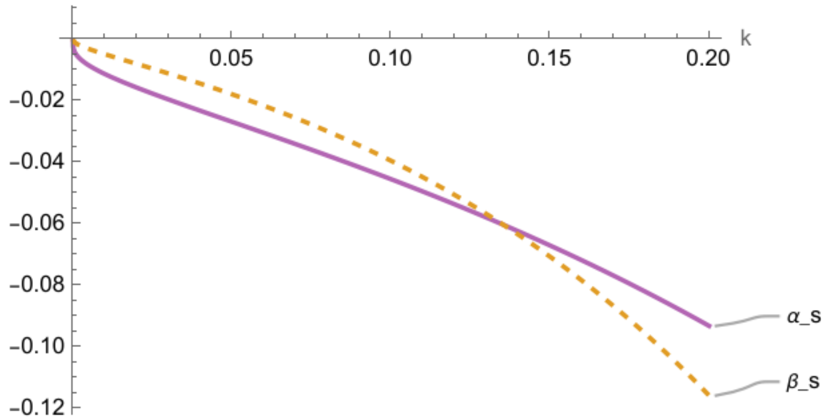

Figure 7.4. Behavior of the runnings α_s an β_s corresponding to the power spectrum $\mathcal{P}_\zeta^{(1)}$ in (7.51). Reference values $\tilde{k} = 0.002$, $\tilde{\mathscr{H}} = 2$, $\mathscr{H} = 0.02$, $\hbar = 0.001$, $M = 10$ in Planckian-like units ($\hbar = 0.001$, $M = 10$, $c = 1$).

Such behavior of the two runnings, also referred to as inversion of the hierarchy, has been deduced by observations by the PLANCK collaboration, see [114]. We stress that here, the deviation of the spectral index and the associated runnings are consequence of the small dBB corrections alone, due to the simplifications of the model here applied. In this sense, they could be overcome by greater-order effect, for example by taking into account the more refined slow-roll approximation, or via other models of inflation; nonetheless, this prediction of the present perturbative model provides interesting insights. Consequently, our interpretation of a gravity-matter B-O-separated picture within the dBB framework demonstrates that relevant quantum effects can occur at the leading order for the power spectrum of primordial perturbations. This framework offers an intriguing opportunity to compare the canonical and dBB schemes within the confines of the B-O approximation's validity.

Conclusions and perspectives

The aim of this thesis was to better characterize the intermediate regime between QG and QFT, in particular to examine the potential quantum gravity effects to QFT on curved spacetime. Indeed, certain physical scenarios, including those within early cosmology and gravitational collapse, present a background metric that cannot be simply interpreted as classical. Rather, it is quasi-classical quantity influenced by quantum fluctuations in the geometry. As we highlighted, this regime has been the scope of a number of investigations [41, 42, 43, 52, 68, 53, 44, 54, 69, 55] focusing on the challenging emergence of a temporal parameter for QFT from the Wheeler-DeWitt equation (2.10).

Our analysis delved into the WKB approach for a "tempus ante quantum" formulation, as elucidated in Sec. 2.2. A large part of our discussion stemmed from the seminal works [41, 42] which explored the acquisition of a standard quantum dynamics for a "small" subsystem within the whole WDW equation; in these studies the matter degrees of freedom were addressed coupled to quasiclassical (gravitational) ones as $\hbar \to 0$ (or $1/M \to 0$).

Actually, the time definitions there proposed lead to an emergent non-unitary dynamics at the first order of quantum-gravitational corrections, i.e. $\mathcal{O}(\hbar)$ or $\mathcal{O}(M^{-1})$ respectively. In the case of the Planckian expansion of Ref. [42], such prediction was immediately noted, while the semiclassical expansion of Ref. [41] did not directly provide such non-unitarity. However, we have showed in Sec. 3.1 that, by an appropriate recasting of the WKB ansatz used in [41] and retuning of the two works' hypotheses, the two models cast the same dynamics with quantum gravitational corrections at first order. As a direct consequence, also Ref. [41] is riddled with potentially non-Hermitian corrections. This outcome can directly be related to the form of the constructed time parameter: the evolution was expressed by the quantum subsystem's dependence on the semiclassical background variables (up to numerical factors). Those semiclassical degrees of freedom were actually considered as classical when using their canonical momenta definition to define the time derivative as a composite one, see Eq. (3.10). Actually, this definition makes a second order derivative of the same form emerge at the next order, thus causing non-unitarity, as motivated in Sec. 3.3.

We have here proposed two "fast" matter clocks incorporated in a B-O-like treatment of the gravity-matter system and their predictions for the modified dynamics in Chapters 3 and 4 respectively. The first formulation is based on the kinematical action, with a more geometrical view but less immediate physical interpretation; this procedure allowed to reinstate a time parameter, different from the internal gravitational variables, and to overcome the non-unitarity concerns of previous treatments. The second formulation is a generalization of Kuchař and Torre's Gaussian reference fluid, which is clearer on a physical ground since it can be formulated as the emergence of a reference system of an observer. In both Chapters we have constructed a general paradigm to determine the quantum gravity corrections to standard QFT treated in the functional representation, adopting these time variables. The key point of the present formulation is in the Born-Oppenheimer separation of the quantum dynamics: we identify a "slow component" with the gravitational degrees of freedom, while the "fast" quantum subset consists of the matter and the reference fluid (or kinematical action) variables. Since the quantum dynamics is WKB expanded in the Planckian parameter M (2.38), the request that the reference sector belongs to the fast component implies that its presence in the Hamilton-Jacobi equation is removed. This way, the violation of the energy conditions which was originally investigated in [57] no longer takes place, and so one could implement the reference fluid as a viable clock. In our analysis, both the kinematical action and the reference fluid describe the quantum matter dynamics, being in this respect a physical time (3.81),(4.24). Their main prediction consists of restoring the unitary character of such modified dynamics at the first order i.e. with QG corrections, see Eqs. (3.92) and (4.32), differently from previous analyses.

However, we also highlighted an important phenomenological difference characterizing the present proposals with respect to previous formulations of the same problem. In fact, the identification of a time variable in [42, 41, 43, 52, 68, 44, 54, 55] is always related to the natural label time, via the (*de facto*) classical dependence of the quantum matter wave functional on the classical gravitational variables. Thus, apart from the nontrivial question of non-unitarity, these studies recovered QFT with a label time dependence and a modified Hamiltonian operator. Our model is instead intrinsically different: the time variable is identified among the fast coordinates, and the matter wave functional is also depending on the gravitational degrees of freedom, which are in principle quantum variables. In other words these variables are never reduced, even in the WKB approximation, to purely classical functions of the space-time slicing. This is coherent with the idea that the so-called "quantum gravity corrections" can be phenomenologically translated only by the dependence of quantum matter on an additional (weakly) quantum set of degrees of freedom.

One then faces the question of how to infer any phenomenology from such a quantum gravity dependence of the QFT dynamics. The question is highly nontrivial from a conceptual point of view, as it happens in almost any implementation of Quantum Gravity and especially of Cosmology [95, 9, 28]. We based our model (see Chapter 6) on the sensible idea that one should somehow average the quantum matter wave functional on quantum gravitational variables. Motivated by the discrepancies outlined in Sec. 6.1, we fundamentally distinguished the classical background degrees of freedom $h_a^0(t)$ from its quantum perturbations δh_a formulated as tensor (graviton) variables, particularly in the context of homogeneous diagonal Bianchi I and FLRW cosmologies. Here we proposed a way to reconstruct *a posteriori* the standard QFT evolution by averaging over the small gravitational fluctuations.

By this averaging procedure, we successfully recovered the functional Schrödinger equation for the matter sector at first order in the WKB expansion, as anticipated by low-energy phenomenology. This is possible by making use of the intrinsic

BO symmetry (6.1) to impose a gauge on the gravitons' sector; furthermore, such equation aligns their dynamics with the gravitational WDW constraint (assumed from the beginning in Ref. [41]). The proposed approach differs from previous treatments [52, 68, 69] in the sense that gravitons are clearly separated in energy scale from matter, due to the adiabatic assumptions.

We stress that the nonunitarity issues analyzed in Refs. [42, 44, 61] may persist at $\mathcal{O}\left(M^{-1}\right)$, contingent upon the choice of time coordinates. To address this point, we actually presented a unified reformulation by considering the "slow" quantum nature of the gravitational variables and at the same time introducing the Gaussian reference fluid clock of Chapter 4. This allowed us to take into account both the observations calling for a quantum treatment of the gravitational sector (Sec. 6.1) and the requirement of unitarity at the next order. We showed in Sec. 6.3 how to reconcile the averaging procedure with such BO formulation and time evolution, by applying the WKB expansion to the geometric phase too. Essentially we motivated that the gauge freedom is present at every order starting from $\mathcal{O}\left(M^{0}\right)$ and thus one can implement independent choices for each phase θ_n. Now the QG-induced corrections clearly take a form depending on the whole gravitational sector, namely both the classical background an the graviton variables. By relaxing the request that the graviton's dynamics is governed by the gravitational WDW equation, we showed that the modified QFT dynamics is recovered at $\mathcal{O}\left(M^{-1}\right)$: in this case the averaged wave functional's evolution presents corrections due to the classical background only (6.69) and coincides with the form (4.32) of Chapters 3,4. Conversely, if one chose the gravitational WDW constraint through the gauge choice (6.59), the matter dynamics before the averaging procedure would be Eq. (6.64), i.e. modified by a different operator with respect to Chapter 4. For the averaged wave functional at $\mathcal{O}\left(M^{-1}\right)$, one can either recover the QG-modified dynamics as in Eq. (4.32) or an effective QFT, depending on the chosen boundary and gauge conditions. This result agrees with the property that in Chapters 3-4 we did not describe the quantum gravitational nature via separate degrees of freedom (we recall the real nature of S_0 corresponding to the classical gravity limit).

Clearly such models must at some point reconnect with our current knowledge and observations of the Universe. For both time proposals of Chapters 3 and 4 we have investigated relevant cosmological settings, showing how the evolution of the fast sector is modified in Sec. 4.2 ; this toy model actually described both proposals, since we have implemented the homogeneous minisuperspace reduction in which the two clocks are equivalent.

We then focused on the first-order QG-effects on the primordial power spectrum of the inflaton field, ultimately responsible for the formation of large scale structures in our universe's history. Considering a pure de Sitter phase and a single scalar inflaton field, we have analyzed the modified dynamics at $\mathcal{O}\left(M^{-1}\right)$ described by the Gaussian fluid clock (analogous to the kinematical action one in this case). Since the net contribution is a time-dependent effect, following the procedure to compute the two-point correlation function (from which the power spectrum is extracted) we find that this term exactly factorizes. We thus recover the previous order result after a normalization requirement is applied. Therefore the inflationary power spectrum is preserved by QG-effects at this order.

Then, we utilized the extended B-O formulation of Chapter 6 for the same analysis, now implementing the Gaussian fluid time and taking into account the quantum nature of the graviton fluctuations. This comprehensive approach leads to QG-induced corrections that depend both on the classical and graviton variables. Following the proposed averaging procedure, we derive a mode-dependent correction to the primordial power spectrum, whose conclusive expression is detailed in Eq. (6.113). Notably, this modified form diverges from the scale-invariant outcome of standard cosmology due to the presence of the factor $\propto k^{-3}$.

While the magnitude of this modification remains inherently small, corroborated by the presence of the perturbation parameter, it serves as a pivotal initial step towards aligning our proposal with current observations, as presented by the PLANCK collaboration [114]. Thus, this prediction stands as probably the major phenomenological result of the present thesis: via the proposed B-O framework for canonical quantum gravity and matter, we are able to derive subtle yet consequential quantum-gravitational corrections to QFT within a low-energy perturbative regime. Notably, these corrections predict non-trivial alterations at the cosmological level, underscoring the significance of our findings.

In the Bohmian approach of Chapter 7 we have demonstrated, through a perturbative scheme in $\hbar$, how to account for modified trajectories of the scale factor of the universe in a de Sitter phase. In this setting, the Gaussian fluid time construction detailed in Chapter 4 has not been implemented, as the dBB approach relies solely on the label time. The modification induced by the quantum potential consequently alters the frequency associated with the time-dependent harmonic oscillator formalism describing the inflaton perturbations. Regarding our attention to the first correction of order $\hbar^2$, we have observed that the associated power spectrum loses its scale-invariance property: the standard result undergoes a small correction, polynomial in the wave number k, due to the effects of the scale factor's modified trajectory.

The present results shed light on the analysis of the fast matter subsystem's evolution in the B-O scheme, considering also the QG-induced effects at the next order. An interesting follow-up of the present investigation would be to include a fast matter backreaction as a mean effect at the HJ level in this formulation, which is intrinsically different from [43] both for the hypotheses implemented and time definition. We remind that the presence of the matter backreaction in [43] is actually removed when one properly rescales also the gravitational wave functional with the geometric phase, as shown in Sec. 3.2.

Actually, we can sort the future perspectives of this thesis into three main lines:

- One could first aim to better characterize cosmological implications of the developed model. More specifically, we could refine the computation for the primordial spectrum of perturbations when implementing both the Gaussian reference fluid clock and the B-O-extended treatment, as in Section 6.4, for example in a slow-rolling approximation. This aspect could lead to non-factorizable modifications to the inflaton evolution and so a modified power spectrum, as in the pure de Sitter phase. A possible inclusion of the matter backreaction at the HJ level, compatible with such scheme, is still up for investigation. In the minisuperspace context, another interesting point of development concerns the physics of black holes: indeed the quantum gravitational corrections could play a relevant role in the so-called evaporation of black holes, i.e. the Hawking radiation [88]. This idea requires to fully understand a minisuperspace treatment of black holes systems in the WKB picture; in this sense, one should develop a novel formalism in order to search for the appropriate formulations of these settings.

- A relevant issue to investigate is the domain of convergence of the presented WKB expansion when the B-O separation is taken into account. Indeed, the first-order QG corrections to the matter dynamics here computed are intrinsically small, in the sense that they are comparable with the small chosen expansion parameter, see also the discussion in Sec. 5.3. However, it is legitimate to ask ourselves what such model would predict at the next-to-next order and so on, with an expansion of both the gravitational and matter components. A more rigorous study of the domain of convergence of such formalism is needed in order to answer this question.

- Finally, we stress that until now we have used a functional approach by considering the WDW equation, which corresponds to a field theoretic description (see Sec. 2.1), within a first quantization formalism i.e. with a functional Schrödinger representation (see also Sec. 3.5). In order to make this model more clearly compatible with the full QFT treatment, one could switch to a formalism more suitable for second quantization methods. A clear example is the path integral approach: in this case, we should provide a direct correspondence between the functional Schrödinger evolution here obtained and the emerging second-quantized theory for gravity and matter, possibly through a saddle-point approximation for the QG sector.

These outlooks are of relevance in the current landscape of QG and call for further investigations. We believe that the present study marks a foundation for future developments of the quantum gravity-matter problem and how a modified dynamics emerges in Born-Oppenheimer-like treatments, particularly in extending the WKB expansion to subsequent orders.

Appendix A

The Lewis-Riesenfeld Invariant Method

We here present a brief overview of the Lewis–Riesenfeld invariant method used in Sec. 5.3 to compute an explicit solution in the cosmological setting of slow-roll inflation. Such method provides an algorithm for computing solutions for a time-dependent quantum system when a specific invariant can be identified, therefore it can be used for the time-dependent harmonic oscillator in (5.21).

Generally speaking, given a system with a generic time-dependent Hamiltonian $\mathcal{H}(t)$, the determination of a Hermitian invariant I (also called Lewis-Riesenfeld invariant) associated with $\hat{\mathcal{H}}(t)$ gives an eigenstate basis that can be used to obtain the solution's wave function. Here, we show the application of this method for the time-dependent quantum harmonic oscillator, for which the method was first developed.

Starting from the time-dependent harmonic Hamiltonian (5.21), one can check that the following is an invariant of evolution:

$$I = \frac{1}{2}\left[\frac{v_{\mathbf{k}}^2}{\rho_k^2} + (\rho_k \pi_{v_{\mathbf{k}}} - \dot{\rho}_k v_{\mathbf{k}})^2\right] \tag{A.1}$$

where ρ_k satisfies the so-called Ermakov equation

$$\ddot{\rho}_k + \omega_k^2 \rho_k = \frac{1}{\rho_k^3} \tag{A.2}$$

and we recall that the time-dependence is inside $\omega_k(\eta)$, as is the case in Sec. 5.3 from the definition (5.12). Explicitly, one can show that the Ermakov equation is solved by the following function

$$\begin{aligned}\rho_k = \gamma_1 \Bigg[& A^2 \frac{(\eta k \sin(\eta k) + \cos(\eta k))^2}{\eta^2 k^3} + B^2 \frac{(\eta k \cos(\eta k) - \sin(\eta k))^2}{\eta^2 k^3} \\ & + \gamma_2 \sqrt{A^2 B^2 - 1}\, \frac{(\eta k \sin(\eta k) + \cos(\eta k))(\eta k \cos(\eta k) - \sin(\eta k))}{\eta^2 k^3}\Bigg]^{\frac{1}{2}}\end{aligned} \tag{A.3}$$

where A, B, and $\gamma_1 = \gamma_2 = \pm 1$ are constants to be appropriately chosen in the cosmological scenario.

We now turn to the computation of the time-dependent oscillator states. From (A.3) one can find the eigenstates of (A.1), which are described for each mode by a quantum index n:

$$\hat{I}\,\phi_{n,\mathbf{k}}(\eta, v_{\mathbf{k}}) = \lambda_n\,\phi_{n,\mathbf{k}}(\eta, v_{\mathbf{k}})\,. \tag{A.4}$$

The expression of such eigenstates can be determined by applying the following unitary transformation:

$$\exp\left(-\frac{i}{2\hbar}\frac{\dot{\rho}_k}{\rho_k}v_{\mathbf{k}}^2\right)\phi_{n,\mathbf{k}} = \frac{1}{\rho_k^{1/2}}\tilde{\phi}_{n,\mathbf{k}}\,, \tag{A.5}$$

that transforms the time-dependent harmonic oscillator problem (5.21) into

$$\left(-\frac{\hbar}{2}\partial^2_{\mathrm{v}_{\mathbf{k}}} + \frac{\mathrm{v}_{\mathbf{k}}}{2}\right)\tilde{\phi}_{n,\mathbf{k}} = \lambda_n\tilde{\phi}_{n,\mathbf{k}} \tag{A.6}$$

being $\mathrm{v}_{\mathbf{k}} = v_{\mathbf{k}}/\rho_k$. Now it is easy to solve this equation, that is a standard (time-independent) quantum harmonic oscillator: the eigenvalues are

$$\lambda_n = \hbar\left(n + \frac{1}{2}\right)\,, \tag{A.7}$$

coinciding with those of the invariant I (see (A.4)), with no explicit dependence on the index mode $\mathbf{k}$. The corresponding eigenstates $\tilde{\phi}_{n,\mathbf{k}}$ must be rescaled back from (A.5) to give those of the invariant I in (A.4), giving

$$\begin{aligned}\phi_{n,\mathbf{k}}(\eta, v_{\mathbf{k}}) = &\left[\frac{1}{(\pi\hbar)^{1/2}2^n n!\,\rho_k(\eta)}\right]^{1/2}\exp\left[\frac{i}{2\hbar}\left(\frac{\dot{\rho}_k(\eta)}{\rho_k(\eta)} + \frac{i}{\rho_k^2(\eta)}\right)v_{\mathbf{k}}^2\right]\\ &\times \mathrm{Hermite}_n\left(\frac{1}{\hbar^{1/2}}\frac{v_{\mathbf{k}}}{\rho_k(t)}\right)\,.\end{aligned} \tag{A.8}$$

where we have the Hermite polynomials. The state basis (A.8) allows one to write the solution for the starting time-dependent harmonic oscillator of our cosmological setting (5.21) as

$$\chi^{(0)}_{\mathbf{k}}(\eta, v_{\mathbf{k}}) = \sum_n c_{n,k}e^{i\delta_{n,k}(\eta)}\phi_{n,\mathbf{k}}(\eta, v_{\mathbf{k}}), \tag{A.9}$$

$$\delta_{n,k}(\eta) = -\left(n + \frac{1}{2}\right)\int d\eta\,\frac{1}{\rho_k^2(\eta)}\,, \tag{A.10}$$

where $c_{n,k}$ are some suitable coefficients fixed by the system's boundary conditions. We thus obtain the wave function describing the evolution of the time-dependent harmonic oscillator system from Eq. (A.9).

Appendix B

Proof of the compatibility of the Gaussian ansatz

Here we wish to prove that the Gaussian ansatz (6.100) and its associated normalization conditions are compatible with the matter equation (6.95). Therefore, we look for a solution of the remaining Eqs. (6.103) and (6.104) of Sec. 6.4.1.

We start with (6.103), which is readily solved by substituting (6.105) and (6.108): it now reduces to an equation in $\varphi^{(0)}_{\mathbf{k}}$ whose solution reads

$$\varphi^{(0)}_{\mathbf{k}}(\eta) = -\frac{1}{6}k^3\eta^3. \tag{B.1}$$

The solution for (6.104) is less immediate. We can rewrite it as a set of two equations, one for each of the two polarization states, that we here label $v^{+}_{\mathbf{k}}$ and $v^{\times}_{\mathbf{k}}$; we recall the two polarizations are independent in the FLRW setting. Let us split both $G_{\mathbf{k}}$ and $\varphi^{(1)}_{\mathbf{k}}$ as

$$G_{\mathbf{k}}(\eta, v_{\mathbf{k}}) = G_{\mathbf{k},+}(\eta, v^{+}_{\mathbf{k}}) + G_{\mathbf{k},\times}(\eta, v^{\times}_{\mathbf{k}}), \tag{B.2}$$

$$\varphi^{(1)}_{\mathbf{k}}(\eta, v_{\mathbf{k}}) = \varphi^{(1)}_{\mathbf{k},+}(\eta, v^{+}_{\mathbf{k}}) + \varphi^{(1)}_{\mathbf{k},\times}(\eta, v^{\times}_{\mathbf{k}}). \tag{B.3}$$

Clearly, this opens the question of how the graviton terms in (6.104) should be distributed between the two. A reasonable choice is an even splitting so that both polarization states act identically, i.e. they obey the same equation. We stress that although $G_{\mathbf{k}}$ and $\varphi^{(1)}_{\mathbf{k}}$ are real, Eq. (6.104) is complex-valued and so are its corresponding sectors for each polarization. Therefore, recalling the solutions for $N_{\mathbf{k}}$, $\Omega^{(0)}_{\mathbf{k}}$ and $\Omega^{(1)}_{\mathbf{k}}$ (see (6.108), (6.105) and (6.106)) in the super-Hubble limit, we obtain from the real and imaginary parts of Eq. (6.104) the following:

$$\partial_\eta G_{\mathbf{k},\lambda} = -\frac{1}{6}k^3\eta^5 - \frac{1}{2}\partial^2_{v^\lambda_{\mathbf{k}}}\varphi^{(1)}_{\mathbf{k},\lambda} - \frac{v^\lambda_{\mathbf{k}}}{\eta}\partial_{v^\lambda_{\mathbf{k}}}\varphi^{(1)}_{\mathbf{k},\lambda}, \tag{B.4}$$

$$-\partial_\eta\varphi^{(1)}_{\mathbf{k},\lambda} = \frac{1}{4}c_1\eta^2 - \frac{1}{2}\partial^2_{v^\lambda_{\mathbf{k}}}G_{\mathbf{k},\lambda} - \frac{v^\lambda_{\mathbf{k}}}{\eta}\partial_{v^\lambda_{\mathbf{k}}}G_{\mathbf{k},\lambda}\,, \tag{B.5}$$

which clearly describe both polarizations via the index λ. Here, the last terms have been rewritten considering the super-Hubble limit of the expression in (6.94), namely

$$\frac{ik^3\eta^3 - 1}{\eta^3\left(\frac{1}{\eta^2} + k^2\right)} \to -\frac{1}{\eta} \tag{B.6}$$

whose imaginary part is infinitesimal for $\eta \to 0^-$, so that the dominant contribution comes from the (divergent) real part.

Let us look for solutions of (B.5) and (B.4) in the form

$$\varphi^{(1)}_{\mathbf{k},\lambda}(\eta, v^\lambda_{\mathbf{k}}) = \bar{\varphi}^{(1)}_{\mathbf{k},\lambda}(\eta) \exp\left[-\frac{1}{2}\sigma_\varphi (v^\lambda_{\mathbf{k}})^2\right], \tag{B.7}$$

$$G_{\mathbf{k},\lambda}(\eta, v^\lambda_{\mathbf{k}}) = \bar{G}_{\mathbf{k},\lambda}(\eta) \exp\left[-\frac{1}{2}\sigma_G(\eta) (v^\lambda_{\mathbf{k}})^2\right]. \tag{B.8}$$

It is important to stress that σ_φ is a free parameter, while the Gaussian width σ_G is function of the conformal time η. Recalling the separation (B.2), we note that up to higher order terms

$$1 + \frac{\mathscr{H}_0^2}{M} G_{\mathbf{k}} = \left(1 + \frac{\mathscr{H}_0^2}{M} G_{\mathbf{k},+}\right)\left(1 + \frac{\mathscr{H}_0^2}{M} G_{\mathbf{k},\times}\right) \tag{B.9}$$

and since both polarizations satisfy the same equations (B.4) and (B.5), then $G_{\mathbf{k},+}$ and $G_{\mathbf{k},\times}$ must have the same functional form.

Therefore, we can now impose the normalization condition (6.109) on $G_{\mathbf{k}}$, recalling (6.105) and (6.106):

$$\int dv^\lambda_{\mathbf{k}}\, G_{\mathbf{k},\lambda} = \sqrt{\frac{c_1}{4k^3}}\,. \tag{B.10}$$

The factor $\bar{G}(\eta)$ is immediately determined as

$$\bar{G}(\eta) = \sqrt{\frac{c_1\, \sigma_G(\eta)}{8\pi k^3}}\,. \tag{B.11}$$

Now plugging (B.7)-(B.8) into (B.4)-(B.5) we obtain ordinary differential equations which, neglecting all terms quadratic in the $v^\lambda_{\mathbf{k}}$, give:

$$\frac{d}{d\eta}\sqrt{\sigma_G} = \sqrt{8\pi k^3}\left(\frac{1}{2}\sigma_\varphi \bar{\varphi} - \frac{\sqrt{c_1}}{6} k^3 \eta^5\right), \tag{B.12}$$

$$-\frac{d}{d\eta}\bar{\varphi} = \sqrt{\frac{c_1\, \sigma_G^3}{8\pi k^3}} + \frac{1}{4} c_1 \eta^2. \tag{B.13}$$

We can determine an explicit solution in our limit of interest $\eta \to 0^-$ by performing a series expansion in η:

$$\sigma_G(\eta) = A_0 + A_1 \eta + O(\eta^2), \tag{B.14}$$

$$\bar{\varphi}(\eta) = B_0 + B_1 \eta + O(\eta^2), \tag{B.15}$$

with A_0, A_1, B_0, B_1 constants depending on the initial conditions. Substituting into Eqs. (B.12) and (B.13) and neglecting all terms of $\mathcal{O}(\eta^2)$ we find

$$A_1 = \sqrt{\frac{8\pi k^3 A_0}{c_1}}\, \sigma_\varphi\, B_0\,, \tag{B.16}$$

$$B_1 = -\sqrt{\frac{c_1}{8\pi}}\left(\frac{A_0}{k}\right)^{3/2}. \tag{B.17}$$

The (approximate) functions are therefore

$$\sigma_G(\eta) = A_0 + \sqrt{\frac{8\pi k^3 A_0}{c_1}}\,\sigma_\varphi\, B_0\, \eta\,, \tag{B.18}$$

$$\bar{\varphi}(\eta) = B_0 - \sqrt{\frac{c_1}{8\pi}}\left(\frac{A_0}{k^3}\right)^{3/2}\eta\;, \tag{B.19}$$

where A_0, B_0 and σ_φ must be positive to obtain well-defined solutions. It is clear from (B.14), (B.15) that $A_0 = \sigma_G(0)$ and $B_0 = \bar{\varphi}(0)$, i.e. they represent the initial conditions of the system.

To conclude, we are now able to insert the solutions (B.18)-(B.19) and (B.11) into the ansatzs (B.7) and (B.8) and compute all the terms relevant for the Gaussian ansatz (6.100) in the super-Hubble limit. In other words, we have shown that a solution of (6.95) exists in the form of a normalized Gaussian (6.100), as implemented in Sec. 6.4.1 to explicitly compute the modified power spectrum.

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