UNIVERSITY OF GENOA

Department of Physics

Doctorate in Physics and Nanosciences
Curriculum: Physics

On the Applications of Semiclassical Gravity in Cosmology and Black Hole Physics

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XXXIV PhD cycle

Abstract

The subject of this Ph.D thesis is the study of the propagation of a free quantum scalar matter field over a classical curved spacetime in the realms of Cosmology and Black Hole Physics. It gathers the original research activity of the author in the framework of Semiclassical Gravity and Quantum Field Theory in Curved Spacetimes.

In a joint work with N. Pinamonti and D. Siemssen, the author shows the existence and uniqueness of local solutions of the semiclassical Einstein equations in cosmological spacetimes, driven by a free quantum massive scalar field arbitrarily coupled with the background curvature. The remarkable result of the work is to show that the source of regularity issues, which prevents to solve the semiclassical problem directly, is an unbounded operator hidden in the expectation value of the quantum stress-energy. However, this operator admits a more regular inverse, which also respects causality. Thus, the application of its inversion formula to the semiclassical equations allows to formulate a well-posed initial-value problem for local solutions in a small interval of time.

In collaboration with N. Pinamonti, S. Roncallo, and N. Zanghì, the semiclassical approach to gravity is applied in the framework of four-dimensional spherically symmetric black holes, which are characterized by dynamical future, outer, trapping horizons. It is shown that the trace anomaly of the quantum stress-energy tensor for a massless, conformally coupled scalar field can be the source of black hole evaporation, after assuming vacuum-like initial conditions in the past and an auxiliary quantum energy condition outside the horizon. As an example, the rate of evaporation induced by the trace anomaly is explicitly evaluated in the Vaidya spacetime.

Finally, in a joint paper with N. Pinamonti, the author studies the problem of stability of semiclassical solutions with higher-order derivative terms in a toy-model, consisting of a quantum scalar field in interaction with a classical scalar field. This toy-model mimics also the evolution induced by semiclassical Einstein equations in physically relevant backgrounds, such as cosmological spacetimes. The main result states that, if the quantum field is massive, then the back-reaction can restore stability on the classical background for wide choices of the renormalization constants, because linear perturbations with past compact spatial support decay polynomially in time at large times.

To my family

Acknowledgements

"Everyone has the friends they deserve."

A very fool person

It could be taken for granted, I know, but the people that deserve my heartfelt thanks, first of all, are my amazing supervisors Nino and Nicola, who have accompanied me in these three difficult years. Your support has never missed, even during the Covid pandemic, when we were forced to speak through a computer screen, always and in any case. When there was something to discuss together, about my Ph.D activity or everything else, I knew that I could count on your help. Several times I have thanked you, and I will never tire of it.

Secondly, my personal acknowledgements go to my (past and current) collaborators Daniel Siemssen and Eleni-Alexandra Kontou, with whom a portion of this work has been realized, for all the discussions we had, and mostly for their patience in supporting me in this initial part of my research career. I am also deeply grateful to Hanno Gottschalk, for inviting me to the University of Wuppertal in the first year of my Ph.D, and for the continuous fruitful exchange of ideas about semiclassical gravity, even during our on-line Zoom seminars about the semiclassical Einstein equations.

Furthermore, I am indebted to Claudio Dappiaggi and Jorma Louko, who have agreed to be the referees of this work. Thanks for the patience in reading this long thesis and for the very helpful comments that have contributed to greatly improving this manuscript.

A special thank goes to my comrade Simone Roncallo. Thanks for our uncountable number of conversations on Microsoft Teams about black holes and evaporation, but not only, and for your help in developing my research project (and possibly others in the future, who knows). Thanks to Nicolai and Daan for our brilliant conversations in Genova and Wuppertal, I hope to have the possibility to collaborate with you again someday. Thanks also to all the members of the LQP community I have the good fortune to know in these three years, such as Nicolò, João (long life to Asinello), Paolo, Lissa, Federico, Rubens, Alessio, for the friendly atmosphere that has arisen in doing mathematical physics. Covid pandemic took us away the possibility to join new in-person conferences: I really hope that everything back to normal very soon. Finally, thanks to Nino's students Matteo ed Augusto, with whom I shared many interesting discussions on Microsoft Teams about geometrodynamics and the Wheeler-DeWitt equation.

But now we come to the "italian acknowledgements".

Un po' là mi state, in realtà, ma grazie infinite ai miei meravigliosi compagni di università che mi hanno accompagnato in questi tre anni di dottorato, e non solo. Grazie ai miei colleghi di simposio, nonché professoroni, Andrea (che dire, Bwwhnn, anzi, stai zitto ***), Lorenzo, che sarà forse l'unica persona a cogliere davvero la citazione a inizio pagina, Davide A. - lo sai, almeno uno di noi deve sopravvivere, e io so su chi puntare - Marco, da cui è sempre un piacere ricevere auguri di morte prematura. Grazie al vecio Cesare, vero discepolo della sacra arte della pausa, per le infinite discussioni avvenute sul terrazzo; a Beatrice, Alice, Nadia, Davide C. per le brevi chiacchierate condivise su Discord a ore per nulla improbabili, Davide S., Denise, Erica e a tutti quanti voi del leggendario DIFI genovese. Tutti non vi posso elencare, ma tranquilli che ci siete anche voi. Una dedica particolare è rivolta ai miei colleghi di scrivania, Luca (prima) e Simone (poi): questi tre anni di dottorato non sarebbe stati gli stessi, senza di voi.

Non meno importanti, un grazie immenso ai miei compagni di liceo: tra gli altri, Cristian, Alessio, Christian, Andrea, Simone, Walter, Mattia, Jacopo, Saverio che ho giusto paccato in quest'ultimo weekend - l'ennesimo - per poter concludere questa tesi. Troppe cose vorrei dirvi, mi limito a ricordare la fortuna incommensurabile che ho avuto, e ho ancora, di poter condividere ancora il tempo insieme a voi, dopo così tanti anni (e potrebbe essere di più, se non fosse per me...).

Ancora, un ringraziamento particolare a Stefano e ai membri della ridente Gymnastic Club sampierdarenese, che mi hanno accompagnato in due anni di rottura muscolare, e a Jacopo e Tommaso, ormai due fratelli acquisiti: anche solo per quell'unica volta all'anno in cui ci vediamo, per me è come fare ritorno a casa.

Infine, ma non per ultima, la mia gratitudine più grande va alla mia famiglia, a cui dedico questo lavoro di tesi, perché più di chiunque altro ha realizzato cosa significhi davvero intraprendere un percorso come questo.

Contents

Introduction

The Only Easy Day Was Yesterday

U.S. Navy SEALs

Semiclassical Gravity and Quantum Field Theory in Curved Spacetimes describe the propagation of a quantum matter field, a free scalar field for instance, over a classical curved spacetime. Solutions of the so-called semiclassical Einstein equations, which govern the interplay between matter and geometry in the semiclassical regime, incorporate the quantum effects due to the back-reaction of the quantum field on the background geometry [BD82; Wal95; For97; HW15]. In this formulation, the classical Einstein tensor of the spacetime is equated to the renormalized quantum stress-energy tensor associated to the quantum matter field, whose expectation value is taken in a certain physical state. Any pair formed by a spacetime and a quantum state satisfying these equations constitutes a solution in Semiclassical Gravity[1].

The semiclassical name attributed to this formulation is due to the nature of the spacetimes satisfying these relativistic equations, because they model physical scenarios where the influence of quantum matter on the spacetime geometry becomes significant. On the one hand, this theory aims to go beyond the scopes of classical General Relativity, which is able to formulate a consistent theory of gravity when it interacts with classical matter contents; on the other hand, it is far from playing the role of a fundamental theory of quantum gravity, because quantum fields "see" only classical geometries in this formulation. In this respect, a semiclassical model of gravity represents a low-energy approximation of an overall quantum gravity, and thus a useful framework where testing physical effects which are expected even at more deepen levels (see [FW96] for the discussion about a potential deduction of Semiclassical Gravity as limit of a theory of quantum gravity). Moreover, a semiclassical theory of gravity should be only valid when fluctuations of the quantum stress-energy tensor are small. This last requirement makes up of the choice of equating probabilistic quantities affecting by fluctuations, such as the expectation values of the quantum stress-energy tensor and the vacuum polarization, with classical sharped objects, such as the Einstein tensor and the scalar curvature of a spacetime. In light of this, the validity of the semiclassical regime has been recently reformulated in the framework of Stochastic Gravity, where the fluctuations of the quantum stress-energy tensor are viewed as a stochastic source for the semiclassical equations - *cf.* [HV20] and references therein.

The formulation of a self-consistent theory of back-reaction is anything but devoid of difficulties, but many progress have been made in recent years thanks to the modern developments in the study of locally covariant quantum field theories in globally hyperbolic spacetimes [BF00; HW01; HW02; BFV03].

[1] This semiclassical definition should not be confused with another semiclassical approach, which consists of performing a WKB approximation of the solution of the Wheeler-De Witt equation, see, e.g., [Kie07].

In the standard formulation of a quantum field theory in flat spacetime, i.e., in the absence of gravitational effects, the canonical quantization procedure, and hence the construction of a Fock space, are founded on the existence of a preferred vacuum state, selected by the Poincaré invariance of the Minkowski spacetime; furthermore, the existence of a Hilbert space associated to the space of "positive frequency solutions" allows a particle interpretation of fields. All these properties are usually absent in arbitrary curved spacetimes in lack of any privileged symmetry, and, a fortiori, without the Poincaré invariance at disposal. Therefore, notions as vacuum and particles are not available within this framework, and, on the contrary, it would be preferable to have a formulation of quantum field theory in curved spacetimes which does not require to select a preferred state [Wal95; HW10].

In view of these difficulties in curved backgrounds, the properties of the quantum theory can be specified at the level of quantum fields, viewed as abstract observables which can be multiplied with each other, instead of being represented as operators acting on a Hilbert space. In this viewpoint, quantum fields must satisfy the canonical commutation relations, and, furthermore, some fundamental conditions, such as locality (they live in bounded region of the spacetimes), covariance (they transform in a precise way under changes of coordinates), and causality (observables evaluated in causally-separated events should commute with each other). Once the rules to construct these composite observables are stated, the correlation functions of the quantum theory are obtained as expectation values in some states [Haa12; BDFY15]. Among the possible choices of quantum states, the class of Hadamard states allows to remove the ultraviolet divergences of the quantum field theory, and thus to obtain finite expectation values of quadratic observables (the quantum stress-energy tensor, for instance). This regularization procedure is performed in a local and covariant way, and generalizes the normal ordering in flat spacetime [KW91; Rad96b; BFK96; FV13].

On the other hand, some conceptual issues remain regarding the possibility to promote Semiclassical Gravity to a well-posed gravitational theory, despite the elegance of its formulation in curved spacetimes. First of all, there exist undoubted difficulties in solving the semiclassical Einstein equations from a more mathematical perspective, even compared to their classical counterparts. In general, semiclassical Einstein equations are non-local and non-linear differential equations, because they always involve a quantum state which is globally constructed on the whole spacetime. Hence, it is strictly coupled to the geometry in a non-local way through certain expectations values appearing inside the equations, such as the renormalized quantum stress-energy tensor and the vacuum polarization. Furthermore, these non-classical contributions give rise to time derivatives of the metric up to the fourth order, different from the classical Einstein equations which contain only second time derivatives. Hence, additional degrees of freedom must be specified when an initial-value problem is formulated. Both those higher-order derivative terms and non-local contributions cannot be neglected in evaluating the back-reaction process, except in some special cases. Therefore, the formulation of a well-posed initial-value problem for the semiclassical Einstein equations, and thus the existence and uniqueness of (physically reasonable) solutions, represent a problematic task in Semiclassical Gravity. Some important results have been obtained quite recently in this direction, for conformally-coupled fields (but not only), and for certain classes of globally hyperbolic spacetimes; see, for instance, [Pin11; PS15a; JA19; San21; GS21; JAM21; JA21; GRS22].

Overcoming these difficulties, and thus investigating the nature of solutions of the semiclassical Einstein equations, would mean to obtain new important insights about the interplay between quantum matter and gravity in several physical contexts, such as in the early stages of evolution of the Universe, or in the vicinity of black holes. It is on these topics that this monograph has focused, and from this point on a synopsis of the main results obtained here is presented, based on author's publications.

The standard paradigm in modern Cosmology to describe the evolution of our Universe in the early stages is constituted by Inflation [Sta80; Gut81; Lin82]. In this picture, a (still not completely clear) phase of exponential acceleration of the Universe happened a few moments later the initial Big Bang singularity (approximately between 10^{-33} and 10^{-32} seconds after the Big Bang), and it led to the formation of large-scale structures of the cosmos seen today. In inflationary Cosmology, one usually assumes that the evolution is driven by classical fields, but it is expected that an improved description of this mechanism is achievable when quantum fields are taken into account at a more fundamental level, by analyzing their interplay with the curvature of the early Universe. Furthermore, it is often argued that the growth of cosmic structures at large scales arise from small density perturbations produced by the fluctuations of quantum fields at a microscopic level [MC81; GP82; Sta82; LL00]. For a discussion about the physical implication of treating quantum fields in Cosmology in the framework of Quantum Field Theory in Curved Spacetimes, see also [Hac10; Hac16].

To simplify the problem, and for ease of comprehension, free quantum scalar fields shall be chosen in this monograph, but generalizations to more realistic fields are viable, despite the technical difficulties in modelling higher spin fields (indeed, a scalar field, sometimes called "inflaton", is often taken into account in the simplest models of Inflation). Therefore, based on all these observations, the inflationary phase is investigated in author's paper [MPS21] according to a semiclassical picture, in which the the Universe is modelled by a Friedmann-LeMaître-Robertson-Walker spacetime at large scales, whose expansion is dictated by the scale factor; on the other hand, the back-reaction of a quantum scalar field upon this spacetime geometry is taken into account for arbitrary values of the coupling with curvature parameter. In this case, contributions with derivatives of the coefficient of the metric up to the fourth order are contained in the expectation values of the stress-energy tensor, and, furthermore, the term with the highest derivative appears in a non-local form. Therefore, all the main issues of a initial-value formulation for Semiclassical Gravity make manifest in this cosmological case. The main result obtained here consists of showing that the non-local highest time derivative enters the semiclassical equations through the application of a linear unbounded operator, which does not depend on the details of the chosen state to evaluate the quantum stress-energy tensor. Remarkably, this unbounded operator admits an inverse, which is more regular than the starting operator, and, furthermore, it respects causality, because it has the form of a retarded operator. Therefore, it is inferred that a well-posed initial-value problem can be formulated after applying the associated inversion formula to the semiclassical Einstein equations, and after choosing four initial conditions for the scale factor. Hence, the proof of local existence and uniqueness of solutions of the semiclassical Einstein equations is finally obtained for small intervals of time, and then a way to find physically reasonable cosmological solutions is now at disposal, even using recursive or numerical methods.

In the framework of Black Hole Physics, the so-called Hawking effect is probably the most famous discovery achieved in Semiclassical Gravity, and represents a first example of how quantum field theory in curved spacetimes can furnish both new insights, and different interpretations, about physical systems previously described in classical relativity. Hawking's prediction showed, in fact, that black holes are not purely absorber of matter and radiation, as expected by General Relativity, but they are able to emit also thermal radiation at large distances, when quantum matter fields come into play. Then, the emission of radiation is usually equated to the evaporation of the black hole, which looses mass at a fixed constant rate proportional to the inverse of its squared mass under the influence of the quantum fields [Haw74; Haw75; Pag76].

However, this equal correspondence between radiation and evaporation is ensured only for static black holes, after assuming some approximations, such as the quasi-static evolution, but it fails when dynamical black holes and apparent horizons are taken into account. In this case, i.e., in the absence of the static symmetry, the power radiated at infinity is not directly related to the negative flux of energy at the horizon, which is, on the contrary, really responsible for the evaporation process. To account for this, a semiclassical description of evaporation is provided in author's papers [MPRZ21; MPRZ22] (see also [Med21]), in which the dynamics of the horizon of a spherically symmetric black hole is locally analyzed by employing the semiclassical Einstein equations as only dynamics equations for the back-reaction. In this view, it is shown that the evolution of the black hole mass can be constrained by the matter content outside and in the causal past of the black hole, without making further approximations on the spacetime. Thus, it is proved that the evaporation of spherically symmetric black holes can be sourced by the quantum trace anomaly of a massless, conformally coupled scalar field, when a quantum energy condition on the stress-energy tensor is assumed outside the horizon. To give some examples, the rate of evaporation of a Vaidya black hole induced by the quantum trace anomaly is evaluated explicitly, and, furthermore, it is found that any static black hole cannot be ever in equilibrium with the back-reaction of any quantum matter field in the semiclassical picture.

As previously pointed out, the semiclassical Einstein equations contain up to fourth-order time derivatives of the metric, in striking contrast with the classical dynamics induced by the Einstein equations. So, in light of this, it is not clear how, and how much, semiclassical solutions can be different from their classical counterparts, and, more importantly, if these non-classical higher order contributions may alter the stability of the back-reacted system. In this respect, it was often argued, mostly in the early eighties, that Semiclassical Gravity represents an unphysical theory of gravity, because it predicts spurious solutions which cannot be expandable about classical relativistic solutions in a perturbative way, or, even worse, which exponentially grow for arbitrary large times, at energy scales closed to the Planck length. Based on these arguments, the validity and the self-consistency of Semiclassical Gravity is usually questioned at fundamental levels, and hence instabilities are sometimes presented as an unavoidable problem affecting such a theory [HW78; Hor80; Sim91; Yam82; Sue92; FW96].

In author's paper [MP22], the issue of runaways solutions is analyzed in a semiclassical toy model in flat spacetime, composed by a quantum scalar field in interaction with a second classical scalar field, which plays the role of a classical background. The approach followed is perturbative, similar to the one employed, e.g., in [Hor80], where the back-reaction process is described by linearized gravitational perturbations over the Minkowski spacetime, satisfying the corresponding linearized semiclassical Einstein equations. In the case of the toy model, the stability of solutions of the semiclassical system against linear perturbations is studied by linearizing the equations over a fixed background theory, formed by a classical scalar field and a free state for the quantum field. Although this semiclassical theory does not model exactly any realistic physical system, it mimics, however, several evolutions driven by the (traced) semiclassical Einstein equations, such as the cases of flat and cosmological spacetimes. In this formal analogy, the background solution is interpreted as one of the degree of freedom of the metric, while the coupling constants are associated to the renormalization freedoms of the underlying semiclassical theory of gravity.

The main result of the work is to show that the semiclassical theory described by this toy model can admit only linear perturbations which decay polynomially in time for large times. This result is achieved by assuming that linear perturbations must have compact spatial support, i.e., they cannot be arbitrarily extended in space, and by taking into account massive quantum fields. In a first step, past compact solutions are constructed through the retarded fundamental solution associated to the linearized semiclassical equations. Then, in a second step, it is proved that there always exist wide ranges of values of the coupling constants which restore the stability of the back-reacted system at large times. In this way, the well-posedness of the initial-value problem associated to the semiclassical equations is always guaranteed for compactly-supported initial data. Moreover, the stability property obtained in this approach is extended to solutions of the linearized semiclassical equations equipped with some compactly-supported smooth source localized in the past. This classical source mimics, e.g., the contribution due to the stress-energy tensor fluctuations usually added to the semiclassical Einstein equations in the stochastic formulation of Semiclassical Gravity.

Outline. The contents of this Ph.D thesis have been divided in four different chapters, to make the analysis as more clear as possible. Each chapter is introduced both by a summary and by an outline of the contents, and is divided into sections, which contain both the novel results and some others inherent the state of art of the subject. In chapter 1, the most relevant tools for Semiclassical Gravity inferred from the literature are listed, and hence divided according to the distinction between General Relativity, Quantum Field theory in Curved Spacetimes, and Semiclassical Einstein Equations. On the contrary, the remaining chapters contain the novel results obtained by the author and his collaborators during his Ph.D activity. In chapter 2, the semiclassical Einstein equations are evaluated in cosmological spacetimes, for massive quantum scalar fields. The central topic consists of showing that an initial-value problem can be always posed for sufficiently small interval of times, taking into account both the non-local contributions and the higher-order derivative terms. In chapter 3, the semiclassical Einstein equations are used to study the issue of black hole evaporation in spherically symmetric dynamical black holes, equipped with apparent horizons. It is shown that the trace anomaly of the quantum stress-energy ensures evaporation when some physically reasonable conditions are assumed outside and in the past of the black hole, in the case of massless, conformally-coupled scalar fields. Eventually, in chapter 4 the issue of stability of linearized semiclassical Einstein equations is investigated in a toy model, which mimics the evolution induced by semiclassical Einstein equations in flat and cosmological spacetimes. It is proved that solutions which decay to zero for large times can be always obtained if massive quantum fields are involved, and spatially compact perturbations are considered, for several values of the renormalization parameters of the model. Finally, a brief summary about differentiation and integration on curved manifolds, the explicit evaluation of some renormalized cosmological observables, and other auxiliary results, are collected in Appendix A, Appendix B, and Appendix C, respectively.

Chapter 1

A Toolkit for Semiclassical Gravity

"Mathematics is the natural language of theoretical physics. It is the irreplaceable instrument for the penetration of realms of physical phenomena far beyond the ordinary experience upon which conventional language is based."

Julian Schwinger

Summary

This first chapter constitutes a summary of the most relevant results in General Relativity and Quantum Field Theory in Curved Spacetimes, in view of a rigorous formulation of a semiclassical theory of gravity. For the sake of brevity, only the results of Differential Geometry relevant for the scopes of this work will be presented here. The material presented in this chapter can be found easily in literature, hence proofs have been omitted from the analysis, with just few exceptions; in this case, references to proofs will be cited throughout the main text. In particular, the main list of references followed by the author are [Wal84; HE73; Poi09; Car19; Sch80], but also [GH07; Fra11; Nak03] and the lectures [Bla21] were considered.

The chapter is organized as follows. In section 1.1 the results of General Relativity are stated: subsection 1.1.1 is devoted to a brief review about both the causal structure of a globally hyperbolic spacetime and the description of the time evolution in the viewpoint of geometrodynamics. Afterwards, in subsection 1.1.2 and subsection 1.1.3 some important notions like geodesic congruence, expansion parameters, and different definitions of energy and mass are gathered, respectively.

In section 1.2 the foundations of a quantum theory for a free scalar field propagating over a background geometry are given: the section starts from the analysis of the Klein-Gordon equation in globally hyperbolic spacetimes (subsection 1.2.1), and hence it proceeds with the quantization of the free scalar field within the framework of algebra of observables (subsection 1.2.2). Then, a description of a physically relevant class of states in curved spacetimes, i.e., Hadamard states, is furnished in subsection 1.2.3. Also, some improved results of microlocal analysis for Hadamard states and singularities in curved backgrounds are presented in subsection 1.2.4, while the construction of both normal-ordered and time-ordered observables is discussed in subsection 1.2.5.

Finally, subsection 1.2.6 and subsection 1.3.3 are devoted to discuss briefly some useful tools in quantum field theories, i.e., the Operator Product Expansion, and quantum energy inequalities, respectively.

Eventually, the main topic of this thesis is presented in section 1.3, that is, the semiclassical Einstein equations, which describe the back-reaction of a quantum matter scalar field over the spacetime geometry. They are obtained in subsection 1.3.1 through the construction of a covariantly-conserved quantum stress-energy tensor, taking advantage of the techniques developed in the previous sections. In particular, subsection 1.3.2 aims to discuss the structure of the trace anomaly of a renormalized quantum stress-energy tensor, which shall play a primary role in chapter 3.

1.1 Spacetimes and Geometry

1.1.1 Causality and globally hyperbolic spacetimes

In a geometric theory of gravitation, the class of dynamical backgrounds is modelled by curved spacetimes, which generalize the concept of flat (or Minkowski) spacetime in Special Relativity.

Definition 1.1.1. A spacetime $(\mathcal{M}, g_{\mu\nu})$[1] is a connected, Hausdorff second-countable orientable four-dimensional smooth manifold $\mathcal{M}$ equipped with a Lorentzian metric tensor $g_{\mu\nu}$ with signature $(-, +, \ldots, +)$.

The invariant volume measure of the spacetime $(\mathcal{M}, g_{\mu\nu})$ shall be denoted by $\mathrm{d}_g x \doteq \sqrt{|\det(g)|}\mathrm{d}^4 x$. Also, $T_p\mathcal{M}$ and $T_p^*\mathcal{M}$ shall identify the tangent space and the cotangent space in a point $p \in \mathcal{M}$, respectively.

In flat spacetime, at each point p is associated a light cone which identifies a future and a past of p. The interior of the future cone represents the chronological future of p, i.e., those events which can be reached by a physical signal starting at p. Thus, the causal future of p is composed by adding to the chronological future the events which lying on the cone itself. Moreover, from the equivalence principle, the tangent space $T_p\mathcal{M}$ is isomorphic to Minkowski spacetime, and hence the causal structure of the manifold $\mathcal{M}$ is locally equivalent to that of the flat case. Therefore, the notion of light cone in a point $p \in \mathcal{M}$ is recovered in arbitrary manifolds, and hence the division of vectors $v \in T_p\mathcal{M}$ in the three different classes:

$$\text{spacelike: } g_p(v, v) > 0, \qquad \text{timelike: } g_p(v, v) < 0, \qquad \text{null: } g_p(v, v) = 0.$$

Spacelike vectors lie outside the light cone of p, whereas causal vectors, timelike and null, lie inside and on the boundary of the light cone, respectively.

To make a precise global designation of future and past, a spacetime given in definition 1.1.1 has to be time orientable, i.e. there should exist a smooth, unit, non-vanishing timelike vector field t^a on $\mathcal{M}$ such that $g(t, t) = -1$. Then, a causal vector v is said to be

$$\text{future-directed: } g_p(v, t) < 0, \qquad \text{past-directed: } g_p(v, t) > 0. \tag{1.1}$$

Hence, a curve $\lambda : I \to \mathcal{M}$ is said to be future (*resp.* past)-directed if its tangent vector $\dot{\lambda}$ is everywhere future (*resp.* past)-directed. It turns out that, if a spacetime is time orientable, then there are only two inequivalent such choices, each called time orientation: choosing a time orientation implies that the spacetime is time oriented.

[1] In this work the abstract index notation explained in [Wal84] is not strictly necessary, so no distinction between Greek and Latin indices will be made.

Fixed a time orientation, the causal structure of a spacetime can be fully characterized as follows.

- $J^{\pm}(p)$ is the causal future/past of $p \in \mathcal{M}$, that is, the union of p and all points $q \in \mathcal{M}$ such that there exists a future-/past-directed, causal curve $\lambda : [a,b] \to \mathcal{M}$ such that $\lambda(a) = p$ and $\lambda(b) = q$;
- $I^{\pm}(p)$ is the chronological future/past of $p \in \mathcal{M}$, that is, the union of all points $q \in \mathcal{M}$ such that there exists a future-/past-directed, timelike curve $\lambda : [a,b] \to \mathcal{M}$ such that $\lambda(a) = p$ and $\lambda(b) = q$.

For subsets of $\mathcal{M}$, one shall define

- $J^{\pm}(U) = \bigcup_{p\in U} J^{\pm}(p)$,
- $I^{\pm}(U) = \bigcup_{p\in U} I^{\pm}(p)$.

On the one hand, a subset is causally convex if $U = J^+(U) \cap J^-(U)$, and spacelike compact if it is closed and there exists another compact subset V such that $U \subset J^+(V) \cup J^-(V)$. On the other hand, two subsets U and V are called causally disjoint (or separated) if

$$\big(J^+(U) \cup J^-(U)\big) \cap V = \emptyset, \tag{1.2}$$

i.e., there is no causal curve connecting the closures of U and V (see fig. 1.1). All these properties always hold locally, because there always exists a convex normal neighborhood of p such that there exists a unique geodesic γ connecting two events q and r entirely contained within the set, for all $q, r \in \mathcal{M}$.

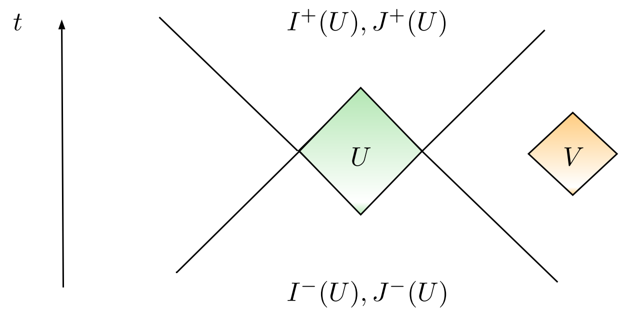

Figure 1.1: Example of two causally disjoint diamonds sets U, V, where V is outside the past and the future of U with respect to a global time function t.

A spacetime $(\mathcal{M}, g_{\mu\nu})$ is said to be causal if it admits no closed causal curves, or, equivalently, if $J^+(p) \cap J^-(p) = \{p\}$ for all $p \in \mathcal{M}$. A physically relevant class of causal spacetimes is identified by globally hyperbolic spacetimes, in which an initial-value problem can be formulated for hyperbolic partial differential equations, i.e., for the equations of motions of matter fields. For such spacetimes, a Cauchy problem is always well-posed, because the entire future and past of the universe can be predicted (or retrodicted) from conditions given at a fixed instant of time. The initial data are always posed on a Cauchy surface, i.e., an hypersurface $\Sigma \subset \mathcal{M}$ which is intersected exactly once by every inextendible timelike curve. Thus, the following definition holds.

Definition 1.1.2. A spacetime $(\mathcal{M}, g_{\mu\nu})$ is said to be globally hyperbolic if one of the following equivalent statements hold:

1. $(\mathcal{M}, g_{\mu\nu})$ admits a Cauchy surface Σ.

2. $(\mathcal{M}, g_{\mu\nu})$ is causal and diamond-compact, i.e., $J^+(p) \cap J^-(q)$ is compact for all $p, q \in \mathcal{M}$.

In this work, there will be interest in investigating cosmological and spherically symmetric spacetimes, so the following Geroch's splitting theorem shall be useful to characterize globally hyperbolic spacetimes [BS03].

Theorem 1.1.1. *Given a global time function t of $\mathcal{M}$, every globally hyperbolic spacetime is isometric to the spacetime $\mathbb{R} \times \Sigma$ endowed with line-element*

$$\mathrm{d}s^2 = -\beta \mathrm{d}t^2 + g_\Sigma,$$

where β is a smooth, strictly positive function, $g_\Sigma(t)$ is a family of Riemannian metrics labelled by t, and $t \times \Sigma$ are smooth spacelike Cauchy surfaces of the form $\{t = const.\}$ which foliate $\mathcal{M}$.

The characterization given in theorem 1.1.1 is a special case of warped products between semi-Riemannian manifolds, which are obtained as deformation of the Cartesian product between two manifolds $\mathcal{M}$ and $\mathcal{N}$ - *cf.* [O'N83]. Given two charts (U, φ), (V, ϕ) parametrized by $\{x^\mu\}_{\mu=1,\dots,m}$, $\{y^\alpha\}_{\alpha=1,\dots,n}$ on the open sets $U \subset \mathcal{M}$, $V \subset \mathcal{N}$, with $m = \dim\mathcal{M}$, $n = \dim\mathcal{N}$, the product manifold $\mathcal{M} \times \mathcal{N}$ with dimension $n + m$ is constructed by the atlas $\bigcup_i U_i \times V_i$ and parametrized by the product chart $(x^\mu(p), y^\alpha(q))$, for all $p \in \mathcal{M}$, $q \in \mathcal{N}$. Thus, the projections

$$\pi : \mathcal{M} \times q \to \mathcal{M}, \qquad \sigma : p \times \mathcal{N} \to \mathcal{N},$$

where $\mathcal{M} \times q = \{(r, q) \in \mathcal{M} \times \mathcal{N} : r \in \mathcal{M}\}$, $p \times \mathcal{N} = \{(p, r) \in \mathcal{M} \times \mathcal{N} : r \in \mathcal{N}\}$, allow to obtain the product metric tensor on $\mathcal{M} \times \mathcal{N}$

$$g_{\mathcal{M}\times\mathcal{N}} \doteq \pi^*(g_\mathcal{M}) + \sigma^*(g_\mathcal{N}),$$

where π^*, σ^* are the pullback of the projection maps. Omitting π and σ. the line-element of the product manifold reads as

$$\mathrm{d}s^2_{\mathcal{M}\times\mathcal{N}} = \mathrm{d}s^2_\mathcal{M} + \mathrm{d}s^2_\mathcal{N},$$

where $\mathrm{d}s^2_\mathcal{M} = g^\mathcal{M}_{\mu\nu} \mathrm{d}x^\mu \mathrm{d}x^\nu$ and $\mathrm{d}s^2_\mathcal{N} = g^\mathcal{N}_{\alpha\beta} \mathrm{d}x^\alpha \mathrm{d}x^\beta$. Hence, given two (pseudo-)Riemannian manifolds $(\mathcal{B}, g_\mathcal{B})$, $(\mathcal{F}, g_\mathcal{F})$ and a positive $f \in C^\infty(\mathcal{B})$, the warped product $\mathcal{M} \doteq \mathcal{B} \times_f \mathcal{F}$ is the product manifold $\mathcal{M} \times \mathcal{B}$ endowed with the metric

$$g_\mathcal{M} \doteq \pi^*(g_\mathcal{B}) + (f \circ \pi)^2 \sigma^*(g_\mathcal{F}).$$

The manifolds $\mathcal{B}$ and $\mathcal{F}$ are called the base and the fiber of $\mathcal{M}$, respectively, while f is the warping function. The set of points $\mathcal{F}_p \doteq \pi^{-1}(p) = p \times \mathcal{F}$ which are projected on the same $p \in \mathcal{B}$ are the fiber over p, while the set of points $\mathcal{B}_q \doteq \sigma^{-1}(q) = \mathcal{B} \times q$ which are projected on the same $q \in \mathcal{F}$ are the leaves over q: both are (pseudo-)Riemannian submanifolds of $\mathcal{M}$. Therefore, the warped product is similar to the Cartesian product, even if the fibers are not isometric to each others. Thus, the line-element of $\mathcal{M}$ is obtained as

$$\mathrm{d}s^2_\mathcal{M} = \mathrm{d}s^2_\mathcal{B} + f^2 \mathrm{d}s^2_\mathcal{F}.$$

Cosmological spacetimes and spherically symmetric black holes presented in section 2.1 and section 3.1, respectively, are constructed as warped products between (pseudo-)Riemannian manifolds.

As stated in theorem 1.1.1, each globally hyperbolic spacetime can be always foliated by Cauchy surfaces $\Sigma_t \doteq \{t = \text{const.}\}$ with respect to a global time function t, which increases along every future-directed causal curve. In this respect, Σ_t are surfaces of simultaneity located at "constant time" t. Thus, the gradient $u_\mu \doteq \nabla_\mu t$ is a future-directed timelike vector according to eq. (1.1), whereas u^μ is a past-directed timelike vector. Therefore, u_μ prescribes a temporal evolution between two points $x_i(t) \in \Sigma_t$ and $x_i(t + \mathrm{d}t) \in \Sigma_{t+\mathrm{d}t}$, labelled by the spatial index i.

Let t^μ be a vector field which identifies the flow of time through $\mathcal{M}$, such that $t^\mu u_\mu = 1$, and let n^μ be the unit normal vector field to Σ_t, according to eq. (A.18). The vector field t^μ can be decomposed as

$$t^\mu = N^\mu + N n^\mu, \tag{1.3}$$

where $N \doteq (n^\rho u_\rho)^{-1}$ is called lapse function, and $N^\mu \doteq h^\mu{}_\nu u^\nu$ is the shift vector, which is orthogonal to n^μ and lays on Σ_t. This last vector is obtained by using the the projection tensor

$$h_{\mu\nu} \doteq g_{\mu\nu}\big|_{\Sigma_t} = g_{\mu\nu} + n_\mu n_\nu, \tag{1.4}$$

such that, given $v^\mu \in T\mathcal{M}$, then $h^\mu{}_\nu v^\nu \in T\Sigma_t$. This tensor is also known as the first fundamental form of the hypersurface Σ_t, i.e., the three-dimensional spatial metric induced by g on Σ_t; furthermore, it satisfies $u^\mu h_{\mu\nu} = 0$ and $h_\rho{}^\rho = 3$.

In the so-called geometrodynamics, General Relativity is viewed as describing the temporal evolution of three-dimensional metrics with respect to the temporal direction prescribed by t. So, $h_{\mu\nu}$ is viewed as the configuration variable which "changes in time" during the evolution along the integral curves of t^μ. On the other hand, both N and N^μ are not dynamical, but specify only how coordinates of Σ_t and $\Sigma_{t+\mathrm{d}t}$ are related within the foliation (see also Figure 1.2). Finally,

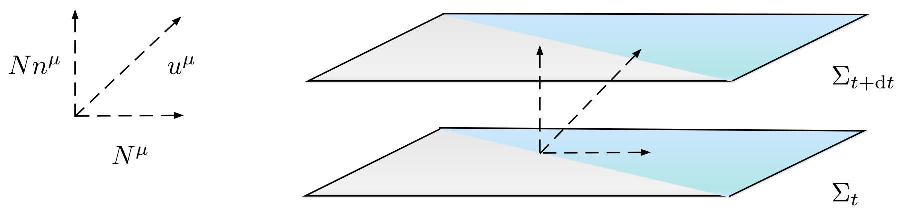

Figure 1.2: An illustration of the foliation between two hypersurfaces $\Sigma_{t+\mathrm{d}t}$ and Σ_t, and the decomposition of the gradient $u^\mu = \nabla^\mu t$ in lapse function N and shift vector N^μ.

the four-dimensional metric can be expressed in terms of the triple $(h_{\mu\nu}, N, N^\mu)$ as

$$g_{\mu\nu}\mathrm{d}x^\mu \mathrm{d}x^\nu = -N^2\mathrm{d}t^2 + h_{\mu\nu}(\mathrm{d}x^\mu + N^\mu \mathrm{d}t)(\mathrm{d}x^\nu + N^\nu \mathrm{d}t). \tag{1.5}$$

The evolution of the first fundamental form is dictated by the so-called extrinsic curvature of Σ_t, that is,

$$K_{\mu\nu} \doteq \frac{1}{2}\mathscr{L}_n h_{\mu\nu}, \tag{1.6}$$

which characterizes the manner in which the hypersurface Σ_t is embedded in the manifold $\mathcal{M}$. In analogy with $h_{\mu\nu}$, $K_{\mu\nu}$ is also called second fundamental form of Σ_t, because it describes the rate of change of $h_{\mu\nu}$ travelling along n^μ. This tensor is symmetric, and it can be written as $K_{\mu\nu} = \nabla_\mu n_\nu + n_\mu \mathcal{L}_n n_\nu$, where the second term always vanishes when the integral curves of the unit normal vector field are geodesics, i.e., when n^μ is parallel-transported even off the hypersurface. In this case, $K_{\mu\nu} = \nabla_\mu n_\nu$ reduces to the covariant derivative of the normal vector to Σ_t. Actually, given the projection tensor $h_{\mu\nu}$, there exists a unique intrinsic covariant derivative D_μ on Σ_t such that $D_\mu h_{\rho\sigma} = 0$ and $K_{\mu\nu} = D_\mu n_\nu$: its action on vectors and one-forms reads as

$$D_\nu V^\mu = h^\mu{}_\rho h_\nu{}^\sigma \nabla_\sigma V^\rho, \tag{1.7}$$
$$D_\nu \omega_\mu = h_\mu{}^\rho h_\nu{}^\sigma \nabla_\sigma \omega_\rho, \tag{1.8}$$

and hence it can be extended to arbitrary (k, l) tensors. Thus, the dynamics of the triple $(\Sigma_t, h_{\mu\nu}, K_{\mu\nu})$ living on a smooth Cauchy surface at constant time Σ_t is governed by the Gauss-Codacci equations:

$$h_\mu{}^\alpha h_\nu{}^\beta h_\rho{}^\gamma R_{\alpha\beta\gamma}{}^\sigma = {}^{(3)}R_{\mu\nu\rho}{}^\sigma + K_{\mu\rho} K_\nu{}^\sigma - K_{\nu\rho} K_\mu{}^\sigma, \tag{1.9}$$
$$D_\alpha K^\alpha{}_\mu - D_\mu K^\alpha{}_\alpha = R_{\rho\sigma} h^\rho{}_\mu n^\sigma, \tag{1.10}$$

where ${}^{(3)}R_{\mu\nu\rho}{}^\sigma \omega_\sigma \doteq [D_\mu, D_\nu]\omega_\rho$ is the three-dimensional Riemann tensor measuring the intrinsic curvature of Σ_t [Wal84].

1.1.2 Geodesic congruences

Given an open region $\mathcal{O} \subset \mathcal{M}$ and fixed $p \in \mathcal{O}$, the concept of geodesic congruences designates a family of causal geodesics whose elements pass one and only one time through p.

To determine the evolution of a timelike geodesic congruence, one needs to know the behaviour in time of the deviation vector ξ^μ between to neighbouring geodesics, with respect to the proper time λ of the reference geodesic. Denoting with $u^\mu = \mathrm{d}x^\mu/\mathrm{d}\lambda$ the unit tangent vector, a timelike geodesic congruence is determined by the following properties:

$$\mathcal{L}_u u = 0, \qquad \mathscr{L}_u \xi = 0, \qquad g_{\mu\nu}\xi^\mu u^\nu = 0.$$

Namely, the deviation vector is orthogonal to u^μ, and hence to the flow of the geodesic; also, the third condition can be always implemented because λ is not unique as affine parameter.

The dynamics of a geodesic congruence is fully characterized by the transverse tensor $B_{\mu\nu} \doteq \nabla_\mu u_\nu$, such that $\mathcal{L}_u \xi^\mu = B^\mu{}_\nu u^\nu$. This tensor measures the rate of geodesic deviation from the u-direction, and it corresponds to the extrinsic curvature (1.6) associated to u. The tensor field B can be decomposed into its algebraically irreducible parts as a sum of tensors orthogonal to u:

$$B_{\mu\nu} = \frac{1}{3}\theta h_{\mu\nu} + \sigma_{\mu\nu} + \omega_{\mu\nu}, \tag{1.11}$$

where

- $h_{\mu\nu} \doteq g_{\mu\nu} + u_\mu u_\nu$ is the transverse metric (see also eq. (1.4));
- $\theta \doteq B^\mu{}_\mu = \nabla^\mu u_\mu$ is called expansion scalar;
- $\sigma_{\mu\nu} \doteq B_{(\mu\nu)} - (1/3)\theta h_{\mu\nu}$ is the symmetric shear tensor;
- $\omega_{\mu\nu} \doteq B_{[\mu\nu]}$ is the antisymmetric vorticity tensor.

Notice that $\sigma_{\mu\nu}\sigma^{\mu\nu} \geq 0$ and $\omega_{\mu\nu}\omega^{\mu\nu} \geq 0$ because the shear and the vorticity are purely spatial. Moreover, the congruence is called irrotational whenever the vorticity vanishes: from Frobenius's theorem, this is, indeed, the case of a congruence which is hypersurface orthogonal to a family of hypersurfaces $\Sigma_f = \{f = \text{const.}\}$. In this case, $u_\alpha = \partial_\alpha f$ and $h_{\mu\nu}$ is the (three-dimensional) induced metric of each Σ_f (for further details on Frobenius's theorem, see [Wal84]).

The equation of motion associated to the geodesic congruence is dictated by the so-called Raychaudhuri's equation

$$\mathcal{L}_u\theta = \frac{\mathrm{d}\theta}{\mathrm{d}\lambda} = -\frac{1}{3}\theta^2 - \sigma_{\mu\nu}\sigma^{\mu\nu} + \omega^{\mu\nu}\omega_{\mu\nu} - R_{\mu\nu}u^\mu u^\nu, \tag{1.12}$$

(it is sometimes referred also as the Landau-Raychaudhuri equation). Its derivation follows directly from the above decomposition of $B_{\mu\nu}$ and the definition of the Ricci tensor $2\nabla_{[\mu}\nabla_{\nu]} = R_{\mu\nu}$ - *cf.* [Wal84; CB08; Poi09]. Hence, under a certain classical energy condition (see subsection 1.1.3), the so-called focussing theorem can be straightforwardly obtained as a manifestation of the attractive nature of gravitation.

Theorem 1.1.2. *Given a hypersurface orthogonal, timelike geodesics congruence and assuming the classical strong energy condition $R_{\mu\nu}u^\mu u^\nu \geq 0$, then $\mathrm{d}\theta/\mathrm{d}\lambda < 0$. Assuming that $\theta = \theta_0 < 0$ on a geodesic of the congruence, then $\theta \to -\infty$ along this geodesic within the proper time $\lambda \leq 3/\theta_0$, namely there exists a caustic where some geodesics converge together.*

Remark 1.1.1. The expansion scalar has a direct physical interpretation in terms of the cross sectional area of a geodesic. Let γ be a geodesic parametrized by the affine parameter λ and $p \in \mathcal{M}$ be a point on the geodesic such that $\lambda(p) = \lambda_p$. Then, the cross section S_p is the three-dimensional set of all points q around p such that another geodesic of the congruence passes through q, and at each point $\lambda = \lambda_p$. Assuming that γ is orthogonal to S_p and labelling with $e^\mu_i \doteq \partial_{y^i}x^\mu$ the basis of vectors associated to a local reference frame (λ, y^i) of γ, the projection operator on γ reads $h^{(\gamma)}_{ij} \doteq e^\mu_i e^\nu_j g_{\mu\nu}$. Then,

$$\theta = \frac{\mathrm{d}}{\mathrm{d}\lambda}\log(\mathcal{V}) = \frac{1}{\mathcal{V}}\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}\lambda}, \tag{1.13}$$

where $\mathcal{V} \doteq \sqrt{|h|}\mathrm{d}^3y$ is cross sectional infinitesimal volume of the geodesic.

A null geodesic congruence can be studied in similar way as before, but after taking into account that the orthogonality condition between ξ and u cannot be imposed. In this case, $g_{\mu\nu}u^\mu u^\nu = 0$, and hence the three-dimensional space of vectors orthogonal to u now includes u itself (in fact, any vector $\xi + cu$, with $c \in \mathbb{R}$, represents the same displacement induced by ξ). To remove this redundant information, one introduces an auxiliary null vector n^μ satisfying $g_{\mu\nu}n^\mu u^\nu = -1$, such that the projected operator and the transverse tensor read now as $\hat{h}_{\mu\nu} \doteq g_{\mu\nu} + u_\mu n_\nu + n_\mu u_\nu$ and $\hat{B}_{\mu\nu} \doteq \hat{h}^\rho_\mu \hat{h}^\sigma_\nu B_{\rho\sigma}$, respectively. Therefore, the irreducible decomposition is

$$\hat{B}_{\mu\nu} = \frac{1}{2}\hat{\theta}\hat{h}_{\mu\nu} + \hat{\sigma}_{\mu\nu} + \hat{\omega}_{\mu\nu}, \tag{1.14}$$

where $\hat{\theta} \doteq h^{\mu\nu}\hat{B}_{\nu\mu}$, $\hat{\sigma}_{\mu\nu} \doteq \hat{B}_{(\mu\nu)} - (1/2)\theta h_{\mu\nu}$, and $\hat{\omega}_{\mu\nu} \doteq \hat{B}_{[\mu\nu]}$. Furthermore, a similar Raychaudhuri's equation holds:

$$\mathcal{L}_u\hat{\theta} = \frac{\mathrm{d}\hat{\theta}}{\mathrm{d}\lambda} = -\frac{1}{2}\hat{\theta}^2 - \hat{\sigma}_{\mu\nu}\hat{\sigma}^{\mu\nu} + \hat{\omega}^{\mu\nu}\hat{\omega}_{\mu\nu} - R_{\mu\nu}u^\mu u^\nu. \tag{1.15}$$

The same results about hypersurface orthogonal congruences and focussing theorem hold in a similar way as in the timelike case, assuming the classical null energy condition $T_{\mu\nu}u^\mu u^\nu \geq 0$ and having $\lambda \leq 2/\hat{\theta}_0$ as null affine time within which a caustic is obtained. In the null case, the expansion $\hat{\theta}$ is associated to the infinitesimal cross sectional area of a geodesic, because the projection tensor is now a two-dimensional metric $\hat{h}_{AB}$, with $A = \theta, \varphi$, due to the ambiguity in the definition of u. Namely,

$$\hat{\theta} = \frac{\mathrm{d}}{\mathrm{d}\lambda}\log(\mathcal{A}) = \frac{1}{\mathcal{A}}\frac{\mathrm{d}\mathcal{A}}{\mathrm{d}\lambda}, \tag{1.16}$$

where $\mathrm{d}\mathcal{A} \doteq \sqrt{|\hat{h}|}\mathrm{d}^2y$. This geometrical interpretation of null expansions parameter shall be used in section 3.1 to define the apparent horizon of a dynamical black hole. For further references and proofs of focussing theorem, see [Wal84; Poi09; CB08].

1.1.3 Energy and mass

Physical conserved quantities associated to a given action S are usually obtained through Noether's theorem [Noe18], which states that each symmetry $(\mathcal{M}, g_{\mu\nu})$ of the action has a corresponding conservation law. Here, symmetry is intended as a an isometry of the spacetime associated to a Killing vector field K^μ (see section A.1).

Consider a source of classical matter described by the action S_m, then the application of Noether's theorem to the diffeomorphism invariance of General Relativity yields the following symmetric, covariantly conserved stress-energy tensor of type (0,2)

$$T_{\mu\nu} \doteq \frac{2}{\sqrt{|\det(g)|}}\frac{\delta S_m}{\delta g^{\mu\nu}}, \qquad \nabla^\rho T_{\mu\rho} = 0. \tag{1.17}$$

Eq. (1.17) has a local interpretation of energy associated to the matter content measured along an integral curve of K^μ. More generally, any generic stress-energy tensor $T_{\mu\nu}$ which is covariantly conserved can be associated to some matter content entering Einstein equations, and thus describing the energy of matter. Denoting with u^μ the four-velocity of an arbitrary timelike curve, a simple example is the stress-energy tensor of a perfect fluid

$$T^{\mu\nu} = (\varrho + p)u^\mu u^\nu + p g^{\mu\nu}, \tag{1.18}$$

where ϱ and p denote the energy density and the pressure of the fluid, respectively. If an equation of state $p = p(\varrho)$ holds, then the fluid is said to be barotropic, while a pressure-free fluid $(p = 0)$ is called dust.

The positivity of the energy density $T_{\mu\nu}u^\mu u^\nu$ of matter is encoded in the so-called energy conditions.

- Weak energy condition: $T_{\mu\nu}u^\mu u^\nu \geq 0$ for all timelike vectors u^μ.
- Null energy condition: $T_{\mu\nu}\ell^\mu \ell^\nu \geq 0$ for all null vectors ℓ^μ.
- Dominant energy condition: $T_{\mu\nu}u^\mu v^\nu \geq 0$ for all future-pointing timelike vectors u^μ, v^ν.
- Strong energy condition: $T_{\mu\nu}u^\mu u^\nu - (1/2)T^\rho{}_\rho u^\mu u_\mu \geq 0$ for all for all timelike vectors u^μ.

The dominant energy condition always implies both the weak and the null energy conditions, and the weak energy condition also implies the null one; on the contrary, the strong energy condition does not imply the weak energy condition, but implies the null one. These energy condition hold for classical matter, but are generally violated by quantum fields, and thus replaced by their quantum counterparts - *cf.* subsection 1.3.3.

The energetic interpretation of $T_{\mu\nu}$ is enforced by the existence of a covariantly conserved current $J^\mu \doteq K_\rho T^{\rho\mu}$, whose covariant derivative vanishes whenever K^μ is a Killing vector, namely $\nabla_\mu J^\mu = 0$. In terms of the Hodge star (A.9), the conservation condition turns to be

$$\mathrm{d}(\star J) = 0, \tag{1.19}$$

with $J = J_\mu \mathrm{d}x^\mu$. Let Σ be a spatial Cauchy surface with normal vector n^μ and three-dimensional induced metric $h_{\mu\nu}$, then the conserved charge associated to J lying on the Σ is constructed as

$$Q_\Sigma \doteq -\int_\Sigma \theta_* (\star J) = -\int_\Sigma n_\nu J^\nu \mathrm{d}_h x, \tag{1.20}$$

where $\mathrm{d}_h x = \sqrt{|\det(h)|}\,\mathrm{d}^3 x$, and θ_* denotes the pull-back to Σ. Then, Q_Σ can be interpreted as the total charge at constant time (the minus sing is just a convention to obtain a positive charge associated to the energy density $\rho = J^0$). After applying Stokes' theorem (A.14) to eq. (1.19) in a bounded region foliated by two Cauchy surfaces Σ_1 and Σ_2 at different times, one obtains that $Q_1 = Q_2$. This means that Q_Σ is both conserved in time and independent from the choice of Σ.

A well-defined notion of energy on Σ holds as conserved charge:

$$E_T \doteq \int_\Sigma T_{\mu\nu} n^\mu \xi_t^\mu \mathrm{d}_h x, \tag{1.21}$$

whenever the existence of a timelike Killing vector ξ_t^μ on $\mathcal{M}$ is ensured, e.g., by the time-translation symmetry of the spacetime. Therefore, $T_{\mu\nu}$ is interpreted as local energy at constant time, and hence E_T represents the conserved total energy of the spacetime. Such a definition of global energy holds in asymptotically flat spacetimes, for instance, and it can be detected at sufficiently large distance from the isolated system. A good definition of total energy for a stationary, asymptotically flatness spacetime is given by the Komar mass [Wal84; Poi09; Car19]

$$E_K \doteq -\frac{1}{8\pi} \lim_{r\to\infty} \int_{\mathbb{S}_t} n_\mu r_\nu \nabla^\mu \xi_t^\nu \mathrm{d}^2\sigma, \tag{1.22}$$

where $\mathbb{S}_t(t,r)$ is a spacelike two-sphere of constant time at spatial infinity $r \to \infty$, with two-dimensional induced metric γ (the volume measure reads $\mathrm{d}^2\sigma = \sqrt{|\det(\gamma)|}\mathrm{d}^2 x = r^2 \sin(\theta)\mathrm{d}\theta\mathrm{d}\varphi$). Furthermore, n_μ and r_ν are the outward-pointing timelike and spacelike normal vectors to $\mathbb{S}_t$, respectively.

Without a global timelike Killing vector field at disposal, as in the case of non-stationary spacetimes, there are several definitions of total energy which can replace the Komar mass (1.22). For instance, whenever an asymptotically flat spacetime admits an asymptotic Cauchy surface at spatial infinity, there is always defined the ADM mass of the spacetime [Poi09; ABIM15; Car19]

$$E_{\mathrm{ADM}} \doteq \frac{1}{16\pi} \lim_{r\to\infty} \int_{\mathbb{S}_t} \left(\partial_j h^j{}_i - \partial_i h^j{}_j\right) r^i \mathrm{d}^2\sigma = -\frac{1}{8\pi} \lim_{r\to\infty} \int_{\mathbb{S}_t} (K - K_0)\,\mathrm{d}^2\sigma. \tag{1.23}$$

In the first definition, h_{ij} denotes the three-dimensional induced metric on Σ, whereas in the second definition $K = \gamma^{AB} K_{AB}$ is the extrinsic curvature (1.6) of $\mathbb{S}_t$ embedded in Σ, while K_0 is the extrinsic curvature of $\mathbb{S}_t$ embedded in the flat spacetime. Furthermore, the ADM mass reduces to Komar mass (1.22) in the stationary case. Finally, another definition of mass is achieved by taking the limit of the two-sphere $\mathbb{S}_t(v,u)$ at null infinity in double-null coordinates (v,u), *cf.* section 3.1. This is the Bondi mass [Poi09]

$$E_B \doteq -\frac{1}{8\pi} \lim_{v\to\infty} \int_{\mathbb{S}(v,u)} (K - K_0)\,\mathrm{d}^2\sigma, \tag{1.24}$$

which describes the outgoing emitted flux at infinity in form of radiation.

A similar notion of positive energy holds also for the gravitational field, in terms of a three-dimensional set of initial data $(\mathcal{M}, h_{ij}, K_{ij})$ (see [ABIM15], Chapter 8 and references therein). Let E_{ADM} be the total energy given in eq. (1.23), and $\vec{P} = (P_1, P_2, P_3)$ be the total linear momentum of $(\mathcal{M}, h_{ij}, K_{ij})$, with

$$P_i \doteq \frac{1}{8\pi} \lim_{r\to\infty} \int_{\mathbb{S}_t} (K_{ij} - K h_{ij})\, r^j \mathrm{d}^2\sigma. \tag{1.25}$$

Then, the so-called total mass of the spacetime $\mathfrak{m} \doteq \sqrt{E_{\mathrm{ADM}}^2 - |\vec{P}|^2}$ fulfils the following positive mass theorem.

Theorem 1.1.3. *Let $(\mathcal{M}, h_{ij}, K_{ij})$ be a three-dimensional asymptotically flat initial data satisfying the dominant energy condition, then $\mathfrak{m} \geq 0$, and $\mathfrak{m} = 0$ if and only if $(\mathcal{M}, h_{ij}, K_{ij})$ can be embedded isometrically in the flat spacetime.*

So defined, $\mathfrak{m}$ has appropriate features to be a good definition of quasi-local mass for an asymptotically flat spacetime, and it is expected that an extended definition of quasi-local mass for non-isolated system should fulfil similarly the positive mass theorem, under the same conditions. There are several definitions of quasi-local mass proposed in literature, see [Sza09] and references therein for all the details. In the study of spherically symmetric spacetimes, *cf.* section 3.1, a crucial role is played by the Hawking quasi-local mass [Haw68; Sch05], which describes the gravitational mass enclosed by a two-dimensional closed surface Σ. Denoting with da the volume measure of Σ, with $\mathcal{A}_\Sigma$ its surface area, and with $\vec{H}$ the mean curvature vector, then

$$M_H(\Sigma) \doteq \sqrt{\frac{\mathcal{A}_\Sigma}{16\pi}} \left(1 - \frac{1}{16\pi} \int_\Sigma |\vec{H}|^2 \mathrm{d}a\right). \tag{1.26}$$

The Hawking mass (1.26) is strictly related to the following Riemann Penrose inequality, which generalizes the positive mass theorem stated in theorem 1.1.3 [Sch05; ABIM15].

Theorem 1.1.4. *Let $(\mathcal{M}, h_{ij})$ be a three-dimensional asymptotically flat spacetime having non-negative scalar curvature R, total mass $\mathfrak{m}$, and outermost horizon Σ with surface area $\mathcal{A}$. Then,*

$$\mathfrak{m} \geq \sqrt{\frac{\mathcal{A}}{16\pi}}, \tag{1.27}$$

where the equality holds if and only if $(\mathcal{M}, h_{ij})$ is isometric to the spatial Schwarzschild spacetime of mass $\mathfrak{m}$ outside their respective horizons.

1.2 Quantum Field Theory in Curved Spacetimes

1.2.1 The free Klein-Gordon field

This section is fully based on some textbooks about Quantum Field Theory in Curved Spacetimes, such as [Wal95; BGP07; BF09; Hac16] (see also [ABIM15], Chapter 10), so the reader is invited to deepen this topic in these much more authoritative references; for further details about the mathematical foundations of this formulation, see, e.g., [KW91; BDH13; BDFY15; Sie15].

A free classical massive Klein-Gordon field $\phi \in C^\infty(\mathcal{M}, \mathbb{R})$ in a curved Lorentzian spacetime $(\mathcal{M}, g_{\mu\nu})$ is described by the action

$$S_0(\phi, g_{\mu\nu}) = \int_\mathcal{M} \mathcal{L}_0(\phi) \mathrm{d}_g x = -\frac{1}{2} \int_\mathcal{M} \left(\nabla_\rho \phi \nabla^\rho \phi + m^2 \phi^2 + \xi R \phi^2\right) \mathrm{d}_g x \tag{1.28}$$

up to the addition of finite real constants, where m denotes the mass of the field, and ξ the coupling parameter to the spacetime scalar curvature R. The evolution of the classical field is dictated by the equation of motion

$$P\phi = 0, \qquad P \doteq \Box_g - m^2 - \xi R, \tag{1.29}$$

where $\Box_g \doteq g^{\mu\nu} \nabla_\mu \nabla_\nu$ denotes the d'Alembert operator on $\mathcal{M}$. In this respect, a scalar field is said to be minimal coupled if $\xi = 0$, otherwise non-minimal coupled if $\xi \neq 0$; in the special case of $\xi = (n-2)/4(n-1)$, the field is said to be conformally coupled, in particular $\xi = 1/6$ in dimension $n = 4$.

Following [Hac16], the space of real (spacelike–compact) solutions of the Klein–Gordon equation (1.29) shall be denoted by

$$\mathrm{Sol}(\mathcal{M}) \doteq \{\phi \in C^\infty(\mathcal{M},\mathbb{R}) : P\phi = 0\} \qquad \mathrm{Sol}_{\mathrm{sc}}(\mathcal{M}) \doteq \mathrm{Sol}(\mathcal{M}) \cap C^\infty_{\mathrm{sc}}(\mathcal{M},\mathbb{R}), \tag{1.30}$$

where

$$C^\infty_{\mathrm{sc}}(\mathcal{M},\mathbb{R}) \doteq \{u \in C^\infty(\mathcal{M},\mathbb{R}) : \exists\, K \text{ compact such that } \mathrm{supp} u \subset J^+(K) \cup J^-(K)\}$$

denotes the set of smooth, real–valued functions with spacelike-compact support, viewed as Fréchet space equipped with the usual seminorms (see also section C.1).

The Klein-Gordon equation (1.29) represents an hyperbolic, partial differential equation in Lorentzian globally hyperbolic spacetimes $(\mathcal{M}, g_{\mu\nu})$, in which $P : C^\infty(\mathcal{M},\mathbb{K}) \to C^\infty(\mathcal{M},\mathbb{K})$ is a linear, second-order differential operator in the class of generalized d'Alembert operators on $\mathcal{M}$, with $\mathbb{K} \doteq \mathbb{R}$ or $\mathbb{C}$. More precisely, P is of the form

$$P = -\sum_{\alpha,\beta=0}^{n-1} g^{\alpha\beta} \frac{\partial^2}{\partial x_\alpha \partial x_\beta} + \sum_{\alpha=0}^{n-1} a_\alpha(x) \frac{\partial}{\partial x_\alpha} + b(x), \tag{1.31}$$

with a_α, b real/complex-valued smooth functions of $x \in \mathcal{M}$. The relevant result about generalized d'Alembert operators P on globally hyperbolic spacetimes consists of the well-posedness of the so-called Cauchy problem associated with such operators. The proof of the following statements can be found in [BGP07] and [BF09], Chapter 3 (see also [Dim80]).

Definition 1.2.1. Let P be a generalized d'Alembert operator (1.31) on a globally hyperbolic spacetime $(\mathcal{M}, g_{\mu\nu})$, and Σ a smooth Cauchy surface with unit normal vector field n. Denoting with $u, \rho \in C^\infty(\mathcal{M},\mathbb{K})$, and $u_0, u_1 \in C^\infty(\Sigma,\mathbb{K})$, the following system of equations

$$\begin{cases} Pu = \rho, \\ u\big|_\Sigma = u_0, \\ \mathcal{L}_n u\big|_\Sigma = u_1 \end{cases} \tag{1.32}$$

is called Cauchy (or initial-value) problem for P with Cauchy data (ρ, u_0, u_1) and initial data (u_0, u_1).

In view of the quantization of the theory, the attention is restricted to compactly supported Cauchy data, i.e., $f, u_0, u_1 \in \mathcal{D}(\mathcal{M},\mathbb{R})$, where $\mathcal{D}(\mathcal{M},\mathbb{R})$ denotes the space of real smooth compactly-supported (or test) functions. This space is equipped with the usual family of semi-norms $\|f\|_\alpha = \sup_{x\in K} |\mathcal{D}^\alpha f(x)|$, for some compact set K, on the Fréchet space $C^\infty(\mathcal{M},\mathbb{R})$ (see section C.1). For Cauchy problems with complex data, one considers the complexification spaces $C^\infty_{\mathbb{C}}(\mathcal{M}) \doteq C^\infty(\mathcal{M},\mathbb{R}) \otimes_{\mathbb{R}} \mathbb{C}$ and $\mathcal{D}_{\mathbb{C}}(\mathcal{M}) \doteq \mathcal{D}(\mathcal{M},\mathbb{R}) \otimes_{\mathbb{R}} \mathbb{C}$.

Any smooth solution $u \in C^\infty(\mathcal{M},\mathbb{R})$ defines a distribution $u \in \mathcal{D}'(\mathcal{M},\mathbb{R})$ on $\mathcal{M}$ through the pairing

$$u[f] \doteq \langle u, f\rangle = \int_{\mathcal{M}} u(x) f(x) \mathrm{d}_g x, \qquad f \in \mathcal{D}(\mathcal{M},\mathbb{R})$$

because $|u(f)| \le c_K \sum_{k\le N} \sup_{x\in K} |\mathcal{D}^\alpha f(x)|$ for some constant c_K and $N \in \mathbb{N}$.

With a slight abuse of notations, a distribution can be identified again by its Kernel u by viewing $C^\infty(\mathcal{M},\mathbb{K})$ as a subspace of $\mathcal{D}'(\mathcal{M},\mathbb{K})$. The global solvability of Cauchy problems in globally hyperbolic spacetimes is formulated in the following theorem [BF09].

Theorem 1.2.1. *Let P be a generalized d'Alembert operator (1.31) on a globally hyperbolic spacetime $(\mathcal{M}, g_{\mu\nu})$, and Σ a Cauchy surface with unit normal vector field n. For all $(\rho, u_0, u_1) \in \mathcal{D}(\mathcal{M}, \mathbb{C}) \oplus \mathcal{D}(\Sigma, \mathbb{C}) \oplus \mathcal{D}(\Sigma, \mathbb{C})$, there exists a unique solution $u \in C^\infty(\mathcal{M}, \mathbb{C})$ of the system of equations (1.32). Furthermore, $supp(u) \subset J^+(K) \cup J^-(K)$, where*

$$K \doteq supp(\rho) \cup supp(u_0) \cup supp(u_1).$$

Thus, for the Klein-Gordon field it follows that each $\phi \in \mathrm{Sol}_{\mathrm{sc}}(\mathcal{M})$ is in one–to–one correspondence with a possible choice of initial data $(u_0, u_1) \in \mathcal{D}(\Sigma, \mathbb{R}) \oplus \mathcal{D}(\Sigma, \mathbb{R})$ on an arbitrary Cauchy surface Σ. It should be stressed that hyperbolic equations such as the ones obtained with P cannot be compactly-supported in the whole spacetime, because a compact support with respect to a time coordinate would spoil the causal propagation on $\mathcal{M}$.

The central argument associated to the causal propagation of Cauchy data in $(\mathcal{M}, g_{\mu\nu})$ is the existence of fundamental solutions in a point $x \in \mathcal{M}$ on globally hyperbolic spacetimes, that is, a distribution $G \in \mathcal{D}'(\mathcal{M}, \mathbb{C})$ such that $PG = \delta_x$, where δ_x denotes the Dirac delta at the point x. The name fundamental is dictated by the character of solutions of the hyperbolic equation $Pu = \rho$ for a given source $\rho \in \mathcal{D}(\mathcal{M}, \mathbb{C})$, which can be constructed from G as $u[\rho] \doteq \langle G, \rho \rangle$ in the distributional sense. Thus, one can define two unique fundamental solutions $G^\pm$ at $x \in \mathcal{M}$ such that

$$P(G^\pm \rho) = \rho, \qquad \mathrm{supp}(G^\pm \rho) \subset J^\pm(\mathrm{supp}\rho). \tag{1.33}$$

Therefore, the partial differential equation $Pu = \rho$ has a unique solution in $u^\pm \in C^\infty(\mathcal{M}, \mathbb{C})$ such that is supported in the future (resp. past) of $\mathrm{supp}\rho$; hence, it is said to be a solution of P with future-compact (resp. past-compact) support.

In the language of quantum field theory, fundamental solutions $G^\pm$ are in one-to-one correspondence to the retarded (resp. advanced) propagator for P at x.

Definition 1.2.2. Let P be a generalized d'Alembert operator (1.31) on a globally hyperbolic spacetime $(\mathcal{M}, g_{\mu\nu})$. The retarded and advanced Green operator are linear maps

$$\begin{aligned} \Delta_{A,R} : \ & \mathcal{D}(\mathcal{M}, \mathbb{K}) \to C^\infty(\mathcal{M}, \mathbb{K}) \\ & f \to \Delta_{A,R} f \end{aligned}$$

such that

$$(\Delta_{R,A} f)(x) = u^\pm[f], \tag{1.34}$$

where $u^\pm[f] = G^\pm[f]$ are solutions of $Pu = f$. They satisfy

$$\hat{P} \circ \Delta_{A,R} = \Delta_{A,R} \circ \hat{P} = \mathbb{I}_{\mathcal{D}(\mathcal{M}),\mathbb{K}}, \qquad \mathrm{supp}(\Delta_{A,R}) \subset J^\pm(\mathrm{supp} f). \tag{1.35}$$

Moreover, $(\Delta_{R,A})^* = \Delta_{A,R}$ whenever P is formally self-adjoint, i.e., $\langle f_1, Pf_2 \rangle = \langle Pf_1, f_2 \rangle$ for $f_1, f_2 \in \mathcal{D}(\mathcal{M})$. Thus, P admits unique advanced and retarded Green operators on $(\mathcal{M}, g_{\mu\nu})$[2].

As $C^\infty(\mathcal{M}, \mathbb{K}) \subset \mathcal{D}'(\mathcal{M}, \mathbb{K})$, the operators $\Delta_{R,A}$ can be extended by continuity to the continuous linear bi–distributions

$$\begin{aligned} \varphi : \ & \mathcal{D}(\mathcal{M}, \mathbb{K}) \to \mathcal{D}'(\mathcal{M}, \mathbb{K}) \\ & \Delta_{A,R} \mapsto \Delta_{A,R}(f_1, f_2) \doteq \langle f_1, (\Delta_{A,R}) f_2 \rangle, \qquad f_1, f_2 \in \mathcal{D}(\mathcal{M}). \end{aligned}$$

[2]The reader should be careful of the conventions used in this monograph for Green operators in definition 1.2.2, which descend from the definition of P given in the equation of motion (1.29): different definitions of retarded and advanced propagators as fundamental solutions may be found elsewhere!

Here, the same symbols for operators and bi-distributions are employed again with a slight abuse of notations. Thus, one can define the causal (or Pauli-Jordan) propagator

$$\Delta \doteq \Delta_R - \Delta_A, \qquad \mathrm{supp}(\Delta f) \subset J^+(\mathrm{supp} f) \cup J^-(\mathrm{supp} f), \tag{1.36}$$

such that it is bi-solution of the Klein-Gordon equation (1.29). If P is formally self-adjoint, then the causal propagator is formally skew–adjoint, i.e., $\langle f_1, \Delta f_2\rangle = -\langle \Delta f_1, f_2\rangle$. Moreover, viewed as linear and continuous application $\Delta : \mathcal{D}(\mathcal{M}, \mathbb{R}) \to C^\infty_{\mathrm{sc}}(\mathcal{M}, \mathbb{R}) \subset C^\infty(\mathcal{M}, \mathbb{R})$, then Δ satisfies the so-called time-slice property [BDFY15; Wal95].

Lemma 1.2.1. *Let $u_f \in C^\infty_{sc}(\mathcal{M}, \mathbb{R})$ be a solution of $Pu = 0$, i.e., $u_f \in Sol(\mathcal{M})$, with compactly-supported initial data (u_0, u_1) on a Cauchy surface Σ, and Σ' another Cauchy surface in the future of Σ. Then there exists $f \in C^\infty_{sc}(\mathcal{M}, \mathbb{R})$ such that*

$$u_f = \Delta f, \qquad \mathit{supp} f \subset J^+(\mathit{supp} f) \cup J^-(\mathit{supp} f) \tag{1.37}$$

up to $f + Ph$, with $h \in C^\infty_{sc}(\mathcal{M}, \mathbb{R})$.

Namely, solutions of the Klein-Gordon equation whose initial data are localized within $\mathrm{supp} f$ are causally propagated on $\mathcal{M}$ through Δ.

For illustrative purposes, it is instructive to evaluate the advanced and retarded fundamental solutions in the four-dimensional Minkowski spacetime $(\mathcal{M}, \eta_{\mu\nu})$, which are solutions of the hyperbolic equation

$$(\Box_\eta - m^2)\Delta_{R,A} = \delta_x \tag{1.38}$$

according to definition 1.2.2. Assuming that $\Delta_{R,A}$ are tempered distributions $\mathcal{S}'(\mathcal{M})$, where $\mathcal{S}(\mathcal{M})$ denotes the Schwartz space on $(\mathcal{M}, \eta_{\mu\nu})$, then eq. (1.38) can be solved in momentum space by applying the Fourier transform; in $\mathbb{R}^4$ and $\mathbb{R}^3$,

$$\hat{f}(p) = \mathcal{F}\{f\} \doteq \int_{\mathbb{R}^4} f(x) \mathrm{e}^{ip\cdot x} \mathrm{d}^4 x, \qquad f(x) = \mathcal{F}^{-1}\{\hat{f}\} = \frac{1}{(2\pi)^4}\int_{\mathbb{R}^4} \hat{f}(p)\mathrm{e}^{-ip\cdot x}\mathrm{d}^4 p, \tag{1.39}$$

$$\tilde{f}(t,\vec{p}) = \mathcal{F}_{\vec{x}}\{f\} \doteq \int_{\mathbb{R}^3} f(t,\vec{x})\mathrm{e}^{i\vec{p}\cdot\vec{x}}\mathrm{d}^3\vec{x}, \qquad f(t,\vec{x}) = \mathcal{F}^{-1}_{\vec{x}}\{\tilde{f}\} = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\tilde{f}(t,\vec{p})\mathrm{e}^{-i\vec{p}\cdot\vec{x}}\mathrm{d}^3\vec{p}. \tag{1.40}$$

For translational invariance, $\Delta_{R,A}(x,y) = \Delta_{R,A}(x-y)$, and hence

$$\Delta_{R,A}(x,y) = \frac{1}{(2\pi)^4}\int \hat{\Delta}_{R,A}(p)\mathrm{e}^{ip_0(t_x - t_y)}\mathrm{e}^{-i\vec{p}\cdot(\vec{x}-\vec{y})}\mathrm{d}p,$$

where $\hat{\Delta}_{R,A}(p)$ satisfy $(p^2 + m^2)\hat{\Delta}_{R,A}(p) = 1$ from eq. (1.38). Denoting with $\omega_0^2 \doteq |\vec{p}|^2 + m^2$, on-shell poles of the propagators are located in $p_0^2 - \omega_0^2 = 0$, in which the inverse of $\Box_\eta$ is not formally defined. Thus, the retarded (resp. advanced) solutions are obtained by standard results in complex analysis through an epsilon regularization: in this prescription, the poles are moved an infinitesimal distance ϵ off the real axes, and thus the contour of the integration is closed either on the upper or in the lower complex plane according to the temporal support of the solution. In the end, one obtains that

$$\hat{\Delta}_{R,A}(p) = \lim_{\epsilon\to 0^+}\frac{1}{(p_0 \mp i\epsilon)^2 - |\vec{p}|^2 - m^2} = \frac{1}{(p_0 \mp i0^+)^2 - |\vec{p}|^2 - m^2}. \tag{1.41}$$

Hence, denoting with $\Theta(t)$ the temporal Heaviside function, they read in the spatial Fourier domain as

$$\tilde{\Delta}_{R,A}(t_x - t_y, \vec{p}) = \begin{cases} \mp\frac{\sin(\omega_0(t_x - t_y))}{\omega_0}\Theta\left(\pm(t_x - t_y)\right) & \text{if } \pm(t_x - t_y) > 0, \\ 0 & \text{otherwise,}\end{cases} \tag{1.42}$$

after applying both Cauchy's integral formula and the residue theorem to the contour of integration. In this last evaluation, the factor $\pm 2\pi i$ is determined according to the orientation of the contour, either counter-clockwise for the retarded solution, or clockwise for the advanced solution. Moreover, by direct computation

$$\Delta_{R,A}(x,y) = \pm\Theta\left(\pm(t_x - t_y)\right)\Delta(x,y), \qquad \tilde{\Delta}(t_x - t_y, \vec{p}) = -\frac{\sin(\omega_0(t_x - t_y))}{\omega_0}, \tag{1.43}$$

as expected from the support of the causal propagator (1.36).

Finally, there exists another fundamental solution which appears when time-ordered fields are involved (see subsection 1.2.5), that is the Feynman propagator associated to the two-point function of the Minkowski vacuum state (1.52). It satisfies

$$(\Box_\eta - m^2)\Delta_F = i\delta_x$$

in units $\hbar = 1$, and reads

$$\Delta_F(x,y) \doteq \begin{cases} \Delta_+(x,y) & \text{if } x \notin J^-(y), \\ \Delta_+(y,x) & \text{if } x \in J^-(y), \end{cases}$$

or, equivalently,

$$\Delta_F(x,y) = \Theta(t_x - t_y)\Delta_+(x,y) + \Theta(t_y - t_x)\Delta_+(y,x) = \Delta_+(x,y) + i\Delta_A(x,y). \tag{1.44}$$

Similarly to the evaluation of $\Delta_{R,A}$ made before, one can evaluate Δ_F in the momentum space using the inverse Fourier transform, which yields

$$\Delta_F(x,y) = \lim_{\epsilon\to 0^+} \frac{i}{(2\pi)^4}\int_{\mathcal{M}} \frac{\mathrm{e}^{-ip(x-y)}}{p_0^2 - p^2 - m^2 + i\epsilon}\mathrm{d}^4 p, \tag{1.45}$$

where the epsilon prescription is chosen to recover the definition given in eq. (1.44). In this case, the poles of the propagator are located in $z_\pm = \pm(\omega_0 - i\epsilon)$, where z is the complex variable associated to p_0, and thus the contour of integration is closed in the upper plane when $t_x > t_y$, and in the lower plane when $t_x < t_y$, respectively.

Notably, $\Delta(x,y) = 0$ whenever $x, y \in \mathcal{M}$ are spacelike separated, because the causal propagator viewed as extended bi-distribution $\Delta(f_1, f_2) = \Delta_R(f_1, f_2) - \Delta_A(f_1, f_2)$ vanishes if $\mathrm{supp} f_1 \cap (J^+(\mathrm{supp} f_2) \cup J^-(\mathrm{supp} f_2))$ is empty. Due to both this support property and the antisymmetric nature of $\Delta(x,y)$, the causal propagator represents a natural local commutator function for quantum fields. The classical counterpart of this quantum commutator function is a symplectic form (or Poisson bracket) of a classical phase space. More precisely, let

$$\mathscr{S}(\mathcal{M}) \doteq \mathcal{D}(\mathcal{M}, \mathbb{R})/\mathcal{I}_P, \tag{1.46}$$

be the vector space of the linear on–shell observables associated to a free Klein-Gordon field ϕ, where $\mathcal{I}_P$ is the closed ideal generated by Pf, $f \in \mathcal{D}(\mathcal{M}, \mathbb{R})$, such that $[f] \in \mathscr{S}(\mathcal{M})$. Then, each smeared classical field $\phi(f) = \langle \phi, f\rangle \in \mathscr{S}'(\mathcal{M})$ corresponds to a classical configuration $\phi(x)$. Thus, it can be shown that the pair $(\mathscr{S}(\mathcal{M}), \sigma_\Delta)$ is a well-defined symplectic space, where

$$\sigma_\Delta : \mathscr{S}(\mathcal{M}) \times \mathscr{S}(\mathcal{M}) \to \mathbb{R}$$
$$\sigma_\Delta([f_1],[f_2]) = \sigma_\Delta(\phi_1, \phi_2) \doteq \langle f_1, \Delta f_2\rangle = \int_{\mathcal{M}} f_1(x)\Delta(x,y)f_2(y)\mathrm{d}_g x$$

is a (non-degenerated anti-symmetric) symplectic form induced by the causal propagator Δ. Hence, $(\mathscr{S}(\mathcal{M}), \sigma_\Delta)$ realizes the classical phase space of the free Klein-Gordon field. Actually, given an arbitrary Cauchy surface Σ with future-pointing unit normal vector field n and induced metric h, this definition of phase space is equivalent to the construction provided by the following symplectic form

$$\sigma_{\mathrm{Sol}}(\phi_1, \phi_2) = \langle \phi_1, \phi_2 \rangle_{\mathrm{Sol}} \doteq \int_\Sigma n^\mu J_\mu(\phi_1, \phi_2) \mathrm{d}_h x, \qquad J_\mu \doteq \phi_1 \nabla_\mu \phi_2 - \phi_2 \nabla_\mu \phi_1, \tag{1.47}$$

for $\phi_1, \phi_2 \in \mathrm{Sol}(\mathcal{M})$ with spacelike–compact overlapping supports. In σ_{Sol}, the covariant conservation equation $\nabla_\mu J^\mu = 0$ implies from the divergence (Stokes') theorem (A.22) that it does not depend on the choice of Σ (see also subsection 1.1.3). Indeed, the symplectic spaces $(\mathscr{S}(\mathcal{M}), \sigma_\Delta)$ and $(\mathrm{Sol}_{\mathrm{sc}}(\mathcal{M}), \sigma_{\mathrm{Sol}})$ are isomorphic through Δ, where $\mathrm{Sol}_{\mathrm{sc}}(\mathcal{M})$ was defined in eq. (1.30), but the former does not depend on the covariant splitting described in theorem 1.1.1. Eventually, it holds that

$$\Delta(x, y)\big|_{\Sigma \times \Sigma} = 0, \qquad \mathcal{L}_n \Delta(x, y)\big|_{\Sigma \times \Sigma} = \delta_\Sigma,$$

and

$$\phi(f) = \langle \phi, f \rangle = \sigma_{\mathrm{Sol}}(\phi, \Delta f), \qquad \forall \phi \in \mathrm{Sol}.$$

The last results have a direct interpretation in the Dirac (or canonical) quantization procedure in Minkowski spacetime, because they reproduce the "equal-time" commutation relations

$$[\phi(x), \phi(y)] = 0, \qquad [\pi_\phi(x), \phi(y)] = \delta_\Sigma(x, y),$$

where $\pi_\phi \doteq \mathcal{L}_n \phi$ denotes the canonical momentum density. For further details about the Klein-Gordon phase space, see [KW91; Wal95; Hac16].

1.2.2 Quantization of the free scalar field

In this section, the quantization of ϕ is performed in an arbitrary globally hyperbolic spacetime by constructing the algebra of quantum observables. Different from other approaches, this viewpoint can be fruitfully adopted to study semiclassical theories of gravity, which involve both normal-ordered and interacting observables in curved spacetimes, such as $:\phi^2:$, and $:T_{\mu\nu}:$. References about this topic can be found, e.g., in [BDFY15; BF09; FGKT20; Hac16].

In this approach, physical observables are viewed as abstract self-adjoint objects which generate a *-algebra $\mathcal{A}$, i.e., a vector space equipped with an associative product and an anti-linear map $a \mapsto a^*, a \in \mathcal{A}$, called involution, such that $(a^*)^* = a$ and $(ab)^* = b^* a^*$ for $a, b \in \mathcal{A}$; it is also called unital if it contains a multiplicative unit $\mathbb{I}$. A subset $G \subset \mathcal{A}$ generates $\mathcal{A}$ if an arbitrary $a \in \mathcal{A}$ can be expressed as a finite complex linear combination of products of elements in G, called generators. In order to formulate a good quantum field theory, the algebra $\mathcal{A}$ must satisfy some fundamental requirements, gathered in the so-called Haag-Kastler axioms [Haa12; Dim80]. Let $\mathcal{O}_1, \mathcal{O}_2 \in \mathcal{I}$ be relatively-compact subsets of $\mathcal{M}$, then the following statements hold.

1. **Locality**. The *-algebra $\mathcal{A}(\mathcal{O}_1)$ is interpreted as the local algebra of observables in the region $\mathcal{O}_1$ of the spacetime.

2. **Isotony**. If $\mathcal{O}_1 \subset \mathcal{O}_2$, then $\mathcal{A}(\mathcal{O}_1) \subset \mathcal{A}(\mathcal{O}_2)$.

3. **Nets of local observables**. Given a set of subsets $\{\mathcal{O}_n\}_{n \in I}$ such that $\mathcal{O}_n \subseteq \mathcal{O}_{n+1}$ and $\bigcup_{n \in I} \mathcal{O}_n = \mathcal{M}$, then the universal algebra $\mathcal{A}(\mathcal{M})$ of local observables on $\mathcal{M}$ is the inductive limit of the local algebras on $\{\mathcal{O}_n\}_{n \in I}$.

4. **Microcausality**. Let $\mathcal{O}_1, \mathcal{O}_2$ be causally separated, *cf.* eq. (1.2), then
$$[\mathcal{A}(\mathcal{O}_1), \mathcal{A}(\mathcal{O}_2)] = \{0\}.$$
5. **Time-slice axiom**. If $\mathcal{O}_1 \subset \mathcal{O}_2$ contains a Cauchy surface Σ of $\mathcal{O}_2$, then the embedding $i : \mathcal{O}_1 \hookrightarrow \mathcal{O}_2$ is an isomorphism.

The first three axioms state that any observable of the theory can be always measured in a limited region of the spacetime, and thus the observables of the whole theory are obtained by the union of the observables living in single bounded regions of the spacetime. The microcausality (or Einstein causality) means that the algebras cannot influence each other whenever two regions are causally uncorrelated, i.e., they cannot be related by any physical interaction. Finally, the last axiom is of deterministic nature, and implies that the evolution of observables is always uniquely determined by the initial data assigned on Σ in every globally hyperbolic spacetime (see lemma 1.2.1).

For the free Klein-Gordon theory, the *-algebra $\mathcal{A}(\mathcal{M}, g_{\mu\nu})$ is called CCR algebra and is generated by a unit $\mathbb{I}$ and by the set of smeared quantum fields $\{\phi(f)\}$, $f \in \mathcal{D}(\mathcal{M})$, together with all their composite operators[3]. On the one hand, the impossibility of measuring the field strength in a point $x \in \mathcal{M}$ in physical situations avoids to treat $\phi(x)$ as an operator at x, but rather to average it with a (smooth) compactly-supported in bounded regions $U \subset \mathcal{M}$. On the other hand, a natural criterion to select a Hilbert space on which ϕ can act as operator is generally absent in curved spacetimes, in lack of a preferred "vacuum" and in presence of unitarily inequivalent representations of the commutation relations.

Based on these statements, each smeared field $\phi(f)$ is viewed as a $\mathcal{A}$-valued distribution on $U \subset \mathcal{M}$ of the form
$$\phi(f) \doteq \langle \phi, f \rangle = \int_U \phi(x) f(x) \mathrm{d}_g x, \tag{1.48}$$
which satisfies the following properties.

1. Linearity.
2. *-involution: $\phi^*(f) = \phi(\bar{f})$.
3. On-shell condition $\phi(Pf) = 0$.
4. $[\phi(f_1), \phi(f_2)] = i\Delta(f_1, f_2)\mathbb{I}$,

where the causal propagator $\Delta(f_1, f_2)$ encodes the commutator function of the quantum theory (see subsection 1.2.1). If the third property is dropped, then $\mathcal{A}(\mathcal{M}, g_{\mu\nu})$ is an off-shell algebra. Finally, states $\omega : \mathcal{A}(\mathcal{M}, g_{\mu\nu}) \to \mathbb{C}$ are linear, positive, and normalized functionals on $\mathcal{A}(\mathcal{M}, g_{\mu\nu})$. Hence, correlation functions are obtained as
$$\omega(\phi(f_1) \cdots \phi(f_n)) \doteq \langle \phi(f_1) \cdots \phi(f_n) \rangle_\omega = \omega_n(f_1, \ldots, f_n), \tag{1.49}$$
where $(f_1, \ldots, f_n) \in \mathcal{D}(\mathcal{M}) \times \cdots \times \mathcal{D}(\mathcal{M})$[4]. At this stage, the canonical formulation of quantum field theories, in terms of Hilbert and Fock spaces, is recovered by the so-called GNS construction [BDFY15]: each state ω gives rise to a GNS triple $(\mathcal{H}_\omega, \pi_\omega, |\Omega_\omega\rangle)$, where $\mathcal{H}_\omega$ is a Hilbert space, $\pi_\omega : \mathcal{D}_\omega \subset \mathcal{H}_\omega \to \mathcal{B}(\mathcal{D}_\omega)$ is a representation mapping state vectors in the linear space of operators

[3]In the rest of the section, only real-valued smooth elements shall be considered, thus the following notations shall be adopted for $C^\infty(\mathcal{M}) = C^\infty(\mathcal{M}, \mathbb{R})$, $\mathcal{D}(\mathcal{M}) = \mathcal{D}(\mathcal{M}, \mathbb{R})$ etc.

[4]Only n-point correlation functions $\omega_n \in \mathcal{D}'(\mathcal{M}^n)$ which are continuous in the usual topology of $\mathcal{D}(\mathcal{M})$ will be considered in this work.

$\mathcal{B}(\mathcal{D}_\omega)$ which leaves $\mathcal{D}_\omega$ invariant, and $|\Omega_\omega\rangle$ is a cyclic vector such that $\omega(a) = \langle\Omega_\omega|\pi_\omega(a)|\Omega_\omega\rangle$ for all $a \in \mathcal{A}$. When applied to $\mathcal{A}(\mathcal{M}, g_{\mu\nu})$, the GNS construction yields the following representation of smeared field operators (1.48)

$$\hat{\phi}_\omega(f) \doteq \pi_\omega\big(\phi(f)\big) : \mathcal{D}_\omega \to \mathcal{H}_\omega,$$

viewed as an operator-valued distribution on f. However, the GNS representations corresponding to different states are not unitarily equivalent in a quantum field theory with infinite degrees of freedom, and hence there exist infinite inequivalent and irreducible Hilbert space representations of the same algebra.

In this work, one shall consider quasi-free (or Gaussian) states, whose n-point correlation functions can be decomposed as

$$\omega_n(f_1, \ldots, f_n) = \begin{cases} 0 & \text{for odd } n, \\ \sum_{partitions} \omega_2(f_{i_1}, f_{i_2}) \cdots \omega_2(f_{i_{n-1}}, f_{i_n}) & \text{for } n = 2,4,\ldots, \end{cases} \tag{1.50}$$

where partitions refer to all possible decompositions of the set $\{1,2,\ldots,n\}$ into $n/2$ pairwise disjoint subsets of two elements $\{i_j, i_k\}$. Therefore, quasi-free states are fully characterized by their two-point functions $\omega_2 \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$, which are always of the form

$$\langle\phi(f_1)\phi(f_2)\rangle_\omega = W_s(f_1, f_2) + \frac{i}{2}\Delta(f_1, f_2), \tag{1.51}$$

where the antisymmetric part $\Delta(f_1, f_2)$ is fixed by the causal propagator (1.36). The symmetric part $W_s(f_1, f_2)$ constitutes the unique degree of freedom for the state, and it characterizes the state in the following way [BDFY15].

Proposition 1.2.1. *Let $W_s \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ be a bi-distribution on $\mathcal{M}$ which satisfies the following properties:*

$$W_s(f_1, f_2) = W_s(f_1, f_2), \qquad W_s(Pf_1, f_2) = W_s(f_1, Pf_2) = 0,$$
$$W_s(f_1, f_1) \geq 0, \qquad |\Delta(f_1, f_2)|^2 \leq 4W_s(f_1, f_1)\, W_s(f_2, f_2).$$

Then W_s defines a positive quasi-free state with two-point distribution given by eq. (1.51).

In general, there are no further criteria to select W_s, and hence a reference quasi-free state, in an arbitrary curved spacetime; furthermore, different choices of states lead to unitarily inequivalent quantum theories. In the case of flat spacetime, the preferred choice of the Minkowski vacuum state is dictated by both the Poincaré symmetry of the spacetimes and the positivity of the energy, which naturally select the maximally symmetric state minimizing the energy. Actually, a class of "physically reasonable" states which generalizes the Minkowski vacuum state can be also selected in curved spacetimes, but this topic is left to be investigated in subsection 1.2.3.

Quasi-free states allow to recover the canonical Fock representation constructed on a one-particle Hilbert space, such that the GNS smeared field $\hat{\phi}_\omega(f)$ can be expressed in terms of creation and annihilation operators $a(\vec{p}), a^\dagger(\vec{p})$. Following [KW91; Wal95], the quantization is performed in the classical phase space $(\mathrm{Sol_{sc}}(\mathcal{M}), \sigma_{\mathrm{Sol}})$, where $\mathrm{Sol_{sc}}(\mathcal{M})$ is the space of solutions of the Klein-Gordon equation with spatial compact support given in eq. (1.30), and σ_{Sol} is the symplectic form defined in eq. (1.47). Also, it is based on the choice of a inner product μ, i.e., a positive, symmetric bilinear map $\mu : \mathrm{Sol_{sc}}(\mathcal{M}) \times \mathrm{Sol_{sc}}(\mathcal{M}) \to \mathbb{R}$ such that, for all $\phi_1, \phi_2 \in \mathrm{Sol_{sc}}(\mathcal{M})$,

$$\frac{1}{4}|\sigma_{\mathrm{Sol}}(\phi_1, \phi_2)|^2 \leq \mu(\phi_1, \phi_1)\mu(\phi_2, \phi_2).$$

For each choice of μ, one can always obtain an Hilbert space $\mathfrak{H}$ and a linear map $K : \mathrm{Sol}_{\mathrm{sc}}(\mathcal{M}) \to \mathfrak{H}$ such that

$$\langle K\phi_1, K\phi_2\rangle = \mu(\phi_1, \phi_2) + \frac{i}{2}\sigma_{\mathrm{Sol}}(\phi_1, \phi_2),$$

which corresponds to the structure of a quasi-free state given in eq. (1.51). The pair $(\mathfrak{H}, K)$ denotes a one-particle Hilbert space, in which performing the quantization procedure after choosing a inner product μ or, equivalently, the two-point function of a quasi-free state ω_2. On the one hand, in the GNS representation $(\mathcal{H}_\omega, \pi_\omega, |\Omega_\omega\rangle)$ induced by ω_2 the Hilbert space corresponds to the Fock space

$$\mathcal{H}_\omega = \bigoplus_{n\geq 0} \mathfrak{H}^{\otimes_s n} = \mathbb{C} \oplus \mathfrak{H} \oplus (\mathfrak{H} \otimes_s \mathfrak{H}) + \dots .$$

Furthermore, the representation π_ω is determined by the canonical creation and annihilation operators $a, a^\dagger$ on $\mathcal{H}_\omega$ appearing in the canonical quantization procedure, which satisfy

$$[a(\phi_1), a(\phi_2)] = 0, \qquad [a(\phi_1), a^\dagger(\phi_2)] = \langle K\phi_1, K\phi_2\rangle.$$

On the other hand, the following smeared operator on $\mathcal{H}_\omega$

$$\hat{\phi}_\omega(f) \doteq ia(K(\Delta f)) - ia^\dagger(K(\Delta f))$$

is the quantum field operator weighted by $f \in \mathcal{D}(\mathcal{M})$ in the Heisenberg picture; in the flat spacetime $(\mathcal{M}, \eta_{\mu\nu})$ and according to the canonical quantization, it can be naively represented at the point $x \in (\mathcal{M}, \eta_{\mu\nu})$ as

$$\hat{\phi}(x) = \frac{1}{(2\pi)^3}\int_{p^2=-m^2} \frac{\mathrm{d}^3\vec{p}}{\sqrt{2\omega_0}} \left(a_{\vec{p}}\,\mathrm{e}^{ipx} + a^\dagger_{\vec{p}}\,\mathrm{e}^{-ipx}\right), \qquad \omega_0 = \sqrt{\vec{p}^2 + m^2},$$

in the Fourier modes expansion. Finally, $|\Omega_\omega\rangle$ is the cyclic vector state such that $a(\phi)\,|\Omega_\omega\rangle = 0$, $\phi \in \mathrm{Sol}_{\mathrm{sc}}(\mathcal{M})$, and

$$\langle\phi(f_1)\phi(f_2)\rangle_\omega = \langle\Omega_\omega|\hat{\phi}_\omega(f_1)\hat{\phi}_\omega(f_2)|\Omega_\omega\rangle\,, \qquad f_1, f_2 \in \mathcal{D}(\mathcal{M}).$$

In this construction, elements of the Hilbert space $\mathfrak{H}$ are the "positive frequencies" ϕ_f^+ of the solutions $\phi_f = \Delta f \in \mathrm{Sol}_{\mathrm{sc}}(\mathcal{M})$ obtained by the causal propagator Δ. Actually, for different choices of inner products $\mu_1 \neq \mu_2$, it may happen that the corresponding one-particle Hilbert spaces $(\mathfrak{H}_1, K_1)$ and $(\mathfrak{H}_2, K_2)$ are unitarily inequivalent, thus different interpretations for "vacuum" and "particles" arise in curved spacetimes.

1.2.3 Hadamard states

Contrary to the case of flat spacetime, where the Poincaré invariance selects a vacuum state uniquely as preferred reference state, in a curved spacetime there is not in principle a preferred notion of "vacuum" dictated by the symmetries of the spacetime. However, a guiding principle to select physically reasonable states in curved spacetimes is that Wick normal-ordered fields like $:\phi^2:$ and $:T_{\mu\nu}:$ should acquire finite expectation values when evaluated on ω. In globally hyperbolic spacetimes, where at least a (pure) Hadamard state always exists [FSW78; FNW81], the set of Hadamard states represents a preferred class where computing normal-ordered fields, because they share the same ultraviolet singular structure of the massive Minkowski vacuum state. Denoting with $x' = (t', \vec{x}'), x = (t, \vec{x}) \in (\mathcal{M}, \eta_{\mu\nu})$, and $\sigma^0_\epsilon \doteq (x' - x)^2 + 2i\epsilon(t' - t) + \epsilon^2$, the two-point function of the Minkowski vacuum reads in the sense of distributions as

$$\begin{aligned}\langle 0|\phi(x')\phi(x)|0\rangle = \Delta_+(x',x) &= \frac{1}{(2\pi)^3}\lim_{\epsilon\to 0^+}\int_{\mathbb{R}^4}\delta(p^2+m^2)\Theta(p_0)\mathrm{e}^{-ip(x'-x)}\mathrm{e}^{-\epsilon p_0}\mathrm{d}^4p \\ &= \frac{1}{4\pi^2}\lim_{\epsilon\to 0^+}\left(\frac{1}{\sigma^0_\epsilon(x',x)}+\frac{m^2}{2}\frac{I_1\big(m\sqrt{(x'-x)^2}\big)}{m\sqrt{(x'-x)^2}}\log\big(m^2\sigma^0_\epsilon(x',x)\big)\right)+\mathcal{W}_+(x'-x),\end{aligned} \tag{1.52}$$

where

$$\mathcal{W}_+(x'-x) \doteq -\frac{m}{4}\sum_{k\geq 0}[\psi(k+1)+\psi(k+2)]\,\frac{1}{k!(k+1)!}\left(\frac{m^2(x'-x)^2}{4}\right)^k. \tag{1.53}$$

Here, $\psi(z)$ and $\Theta(z)$ denote the Digamma and the Heaviside functions, respectively.

To obtain a concrete realization of Hadamard states in arbitrary curved spacetime, it is convenient to introduce a notation due to Synge to represent the coinciding-point limits of bitensors $B(x',x)$, i.e.,

$$[B](x) \doteq \lim_{x'\to x} B(x',x), \tag{1.54}$$

see [PPV11; Hac16]. Covariant derivatives in different points x and x' always commute with each other, and furthermore they are related by the identity $[B_{;\mu'}] = [B]_\mu - [B_{;\mu}]$[5]. Moreover, let $\mathcal{O}\subset\mathcal{M}$ be a convex geodesic neighbourhood, and $\gamma : [\tau_0,\tau_1]\to\mathcal{M}$ the unique geodesic connecting two points $x,x'\in\mathcal{M}$, with $\gamma(\tau_0) = x$, $\gamma(\tau_1) = x'$, and tangent vector $v = \mathrm{d}\gamma/\mathrm{d}\tau$. Then, the one half of the (signed) squared geodesic distance $\sigma(x',x)$ between x' and x, or Synge's world function, is defined as

$$\begin{aligned}\sigma(x',x) &\doteq \pm\frac{1}{2}[s(x',x)]^2, \\ s(x',x) &\doteq \int_{\tau_0}^{\tau_1}\sqrt{g_{\mu\nu}(\gamma(\tau))v^\mu(\tau)v^\nu(\tau)}\mathrm{d}\tau = (\tau_1-\tau_0)\sqrt{g_{\mu\nu}(\gamma(\tau))v^\mu(\tau)v^\nu(\tau)},\end{aligned} \tag{1.55}$$

where the integral was performed because the integrand is constant along γ whenever τ is an affine parameter of the geodesic. Here, the plus and the minus signs holds for spacelike and timelike separations, respectively, while $\sigma(x',x)$ vanishes in the null case. Moreover, it satisfies the following identities:

$$\sigma_{;\mu}\sigma^{;\mu} = 2\sigma, \qquad [\sigma] = 0, \qquad [\sigma_{;\mu}] = 0, \qquad [\sigma_{;\mu\nu}] = g_{\mu\nu}.$$

In flat spacetime, the geodesic is a straight line, and hence $\sigma^0(x',x) = (1/2)\eta_{\mu\nu}(x',x)^\mu(x',x)^\nu$.

Another relevant bitensor is the parallel propagator $g^\mu_{\nu'} \doteq e^\mu_a e^a_{\nu'}$, where e^μ_a denotes the (parallel-transported) tetrad on the geodesic, such that the dual basis is $e^a_\mu = \eta^{ab}e^\mu_b$ and $g_{\mu\nu} = \eta_{ab}e^a_\mu e^b_\nu$, with $a,b = 0,\ldots,3$. The role of the parallel propagator is to transport a vector from x to x' along the unique geodesic connecting these points: for instance $B^{\mu'}(x') = g^{\mu'}_\mu(x',x)B^\mu(x)$. The parallel propagator satisfies the following identities:

$$[g^\mu_{\nu'}] = \delta^\mu_\nu, \qquad g^\mu_{\nu';\rho}\sigma^{;\rho} = 0, \qquad g^\mu_{\rho'}\sigma^{;\rho'} = -\sigma^{;\mu}.$$

The last bitensor which should be mentioned is the van Vleck-Morette determinant

$$\Delta_\sigma(x',x) \doteq -\frac{\det(-\sigma_{\mu\nu'}(x',x))}{\sqrt{\det(g)}\sqrt{\det(g')}}, \tag{1.56}$$

[5] To avoid confusion, one usually denotes tensors evaluated at x and x' with unprimed and primed indices, respectively. Moreover, the partial and the covariant derivatives with respect to the (primed) index μ are denoted by a colon , and a semicolon ; before the index, respectively.

which describes when the geodesic is focusing ($\Delta_\sigma > 1$) or defocusing ($\Delta_\sigma < 1$). With the initial condition $[\Delta_\sigma] = 1$, the van Vleck-Morette determinant satisfies the following transport equation

$$4 = \sigma^\mu_\mu + \sigma^\mu (\log(\Delta_\sigma))_{,\mu}.$$

in four-dimensional spacetimes, and, furthermore, the following covariant expansion at small distances: $\Delta_\sigma = 1 + (1/6) R_{\mu'\nu'} \sigma^{\mu'} \sigma^{\nu'} + \ldots$.

Given the Synge's world function (1.55), one is ready to present the definition of Hadamard states in curved spacetimes. This paragraph is fully based on the results presented in [KW91; BDFY15; Mor03; Hac16; Sie15] and in the references therein, to which the reader is suggested to refer for all the details.

Preliminarily, it is essential to introduce the so-called Hadamard parametrix, which characterizes the singular structure of two-point function of the Minkowski vacuum, and hence it is universally shared by all Hadamard states (in this framework, parametrix means that it satisfies the Klein-Gordon equation (1.29) up to a smooth reminder). Given a convex neighbourhood $\mathcal{O} \subset \mathcal{M}$ and two points $x, x' \in \mathcal{O}$, the Hadamard parametrix is defined as

$$h_{0^+}(x', x) \doteq \lim_{\varepsilon \to 0^+} \frac{u(x', x)}{\sigma_\varepsilon(x', x)} + \sum_{j \geq 0} v_j(x', x) \sigma(x', x)^j \log\left(\frac{\sigma_\varepsilon(x', x)}{\lambda^2}\right), \tag{1.57}$$

where the limit $\varepsilon \to 0^+$ is taken in the distributional sense, $\sigma_\varepsilon(x', x) = \sigma(x', x) + \mathrm{i}\epsilon(t(x') - t(x))$, t is any time function, and $\lambda > 0$ is a length scale. Contrary to a quantum state, which is globally defined over $\mathcal{M}$, the Hadamard parametrix is constructed in a local and covariant way, because only geometry of the spacetime enters eq. (1.57). Moreover, the definition of h_{0^+} does not depend on the choice of the time function, but only on the scale λ.

The so-called Hadamard coefficients $u(x', x)$, $v_j(x', x)$ are real-valued symmetric bi-scalars fixed by the geometry and the equation of motion. On the one hand, $u(x', x) = \sqrt{\Delta_\sigma(x', x)}$ is equal to the square root of the Van Vleck-Morette determinant (1.56). On the other hand, $v(x', x)$ is usually represented by a series expansion in the world function (1.55)

$$v(x', x) = \sum_{j \geq 0} v_j(x', x) \sigma(x', x)^j, \tag{1.58}$$

which, in fact, does converge only in analytic spacetimes. Thus, the definition of a Hadamard state reads as follows.

Definition 1.2.3. Let $(\mathcal{M}, g_{\mu\nu})$ be a globally hyperbolic spacetime, and h_{0^+} the Hadamard parametrix (1.57) constructed in a convex neighbourhood $\mathcal{O} \subset \mathcal{M}$. A quasi-free state ω on the Klein-Gordon CCR algebra $\mathcal{A}(\mathcal{M}, g_{\mu\nu})$ is said to be Hadamard if the Kernel of its two-point function $\omega_2 \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ is locally of the form

$$\langle \phi(x') \phi(x) \rangle_\omega \doteq H_{0^+}(x', x) + \mathcal{W}(x', x) = \frac{1}{8\pi^2} \left(h_{0^+}(x', x) + w(x', x) \right), \qquad x', x \in \mathcal{O}. \tag{1.59}$$

The smooth coefficient $w(x', x)$ characterizes the state, and it must be chosen in such a way that ω_2 is a positive and symmetric bi-solution of the Klein-Gordon equation. For sufficiently regular spacetimes, the series given in eq. (1.58) can be viewed as asymptotic expansion such that

$$\langle \phi(x') \phi(x) \rangle_\omega - H_N(x', x) \in C^N(\mathcal{O} \times \mathcal{O}), \qquad N = 0,1, \ldots,$$

where

$$H_N(x', x) \doteq \frac{1}{8\pi^2} \lim_{\varepsilon \to 0^+} \frac{u(x', x)}{\sigma_\varepsilon(x', x)} + \sum_{j=0}^{N} v_j(x', x) \sigma(x', x)^j \log\left(\frac{\sigma_\varepsilon(x', x)}{\lambda^2}\right) \tag{1.60}$$

is called truncated Hadamard parametrix. Namely, the coefficient $w(x', x)$ which arises from the subtraction is only C^N-regular.

The Hadamard coefficients fulfil the following Hadamard recursive relations

$$(\Box_x \sigma - 4)\, u + 2u_{;\mu}\sigma^{;\mu} = 0, \tag{1.61}$$
$$P_x u + 2v_{0;\mu}\sigma^{;\mu} + (\Box_x \sigma - 2)\, v_0 = 0, \tag{1.62}$$
$$P_x v = 0, \tag{1.63}$$

where P_x denotes the Klein-Gordon operator acting on the x-variable. Thus, coefficients v_j are recursively computed afterwards by:

$$P_x v_0 + 2v_{1;\mu}\sigma^{;\mu} + v_1 \Box_x \sigma = 0, \tag{1.64}$$
$$P_x v_j + 2(j+1)v_{j+1;\mu}\sigma^{;\mu} + v_{j+1}(j+1)\,(2j + \Box_x \sigma) = 0. \tag{1.65}$$

Actually, if one is interested in evaluating the back-reaction of a quantum free field though the semiclassical Einstein equations, then it is sufficient to compute the coinciding limits of such coefficients and of their covariant derivatives. In four dimensions,

$$[v_0] = \frac{1}{2}[P_x u] = \left(m^2 - \left(\xi - \frac{1}{6}\right) R\right), \qquad [v_{j+1}] = \frac{1}{2(j+1)(j+2)}[P_x v_j],$$

and in particular

$$\begin{aligned}[v_1] &= \frac{m^4}{8} + \frac{(6\xi-1)m^2 R}{24} + \frac{(5\xi-1)\Box R}{120} + \frac{(6\xi-1)^2 R^2}{288} + \frac{R_{\mu\nu\rho\sigma}R^{\mu\nu\rho\sigma} - R_{\mu\nu}R^{\mu\nu}}{720} \\ &= \frac{m^4}{8} + \frac{(6\xi-1)m^2 R}{24} + \frac{(5\xi-1)\Box R}{120} + \frac{(6\xi-1)^2 R^2}{288} + \frac{C_{\alpha\beta}{}^{\gamma\delta}C_{\gamma\delta}{}^{\alpha\beta} + R_\mu{}^\nu R_\nu{}^\mu - \frac{1}{3}R^2}{720},\end{aligned} \tag{1.66}$$

where $C_{\alpha\beta\gamma\delta}$ is the Weyl tensor, $R_{\mu\nu\rho\sigma}$ is the Riemann tensor, $R_{\mu\nu}$ is the Ricci tensor, and R is the Ricci scalar[6]. For an expressions of Hadamard coefficients in arbitrary dimensions, see, e.g., [DF08]. Notably, only the coinciding limit $[v_1](x)$ of the biscalar $v_1(x', x)$ is needed to perform the construction of a covariantly conserved quantum stress–energy tensor in curved spacetimes, see subsection 1.3.2.

1.2.4 Microlocal formulation

More recently, thanks to Radzikowski's seminal works [Rad96b; Rad96b], an equivalent characterization of Hadamard states in globally hyperbolic spacetimes was obtained by studying the form of the wave front set of their two-point functions, in the framework of microlocal analysis [Hör03; SVW02; Gér19] (see also [BDFY15; BVDH14]). On physical grounds, a microlocal formulation of the quantum field theory recovers a local energy positivity condition in curved spacetimes, in which the absence of a global timelike Killing vector field prevents to formulate a global energy spectrum condition as in Minkowski spacetime.

More generally, the regularity of a distribution u is usually associated to its decaying properties in momentum space, but a notion of Fourier transform (1.39) is not at disposal in arbitrary curved spacetimes in lack of the translational invariance symmetry. The theory of microlocal analysis for distributions allows to overcome this problem, and to study locally the singular behaviour

[6] The notation of [DFP08; Hac16] is employed here, and thus the explicit value of $[v_1]$ differs from the coefficient $[v_1]_c$ appearing, e.g., in [Wal78b] for a factor 2.

of a distribution without referring to a global notion of "decay at infinity". In this section, the microlocal techniques are introduced in Euclidean case $\mathcal{M} = \mathbb{R}^d$, but they can be generalized also to curved manifolds in a second step.

The analysis of the singular behaviour of a distribution $u \in \mathcal{D}'(U)$, with U an open set of $\mathbb{R}^d$, starts from the definition of its singular support. Let u_U be a smooth restriction of a distribution $u \in \mathcal{D}'(\mathbb{R}^d)$ to U, i.e., a smooth function u_U such that $u[f] = u_U[f]$ for all $f \in \mathcal{D}(U)$. Then, the singular support $\mathrm{singsupp}(u)$ of u identifies the set of points having no open neighbourhoods X to which the restriction u_X of u is a smooth function. Moreover, if u is multiplied by a a smooth compactly-supported function $f \in \mathcal{D}(U)$, with $f(x) \neq 0$, then $fu \in \mathcal{E}'(U)$ is a compactly-supported distribution. Furthermore, this product is also smooth, i.e., $fu \in \mathcal{D}(U)$, whenever its Fourier transform $\mathcal{F}\{fu\}$ decays rapidly in any direction $p \in \mathbb{R}^n$ (see [BF09], Section 4.3).

Therefore, a Fourier analysis allows to establish what are the decaying directions of a distribution u.

Definition 1.2.4. Let $u \in \mathcal{D}'(U)$ be a distribution in $U \subset \mathbb{R}^d$, and denote with Γ an open conical neighbourhood of $p \in \mathbb{R}^n \backslash \{0\}$, i.e., if $p' \in \Gamma$, then $\lambda p' \in \Gamma$ for all $\lambda \in \mathbb{R}$. A pair $(x, p) \in U \times (\mathbb{R}^n \backslash \{0\})$ is a regular direction for u if there exists a smooth compactly-supported function f, with $f(x) \neq 0$, and some constant $c_N \in \mathbb{R}$ such that

$$|\mathcal{F}\{fu\}(p')| \leq \frac{c_N}{(1 + |p'|)^N} \tag{1.67}$$

for all $N \in \mathbb{N}$ and for all $p' \in \Gamma$.

If $\mathrm{singsupp}(u)$ is not empty, then there exists at least one direction in which $\mathcal{F}\{fu\}$ is not rapidly decreasing. In particular, the pair (x, p) is a singular direction of u if there is no conical neighbourhood V in which eq. (1.67) holds for all $p \in V$. Based on these statements, a spectral analysis of singularities aims to detect both the singular points and the singular directions associated to each singular point. In this respect, all the smooth compactly-supported functions f which do not vanish in $x \in U$ must be considered to fully detect a singularity of u.

Let $\Sigma_x(u)$ be the complement of the space of all regular directed points of u, i.e., the set of all non-zero $p \in \mathbb{R}^n$ such that (x, p) is a singular direction for u; in particular $\Sigma_x(u)$ is empty whenever $x \notin \mathrm{singsupp}(u)$. Then, the definition of wave front set follows.

Definition 1.2.5. The wave front set $\mathrm{WF}(u)$ of $u \in \mathcal{D}'(U)$, with $U \subset \mathbb{R}^d$, is the closed subset of $U \times \mathbb{R}^n \backslash \{0\}$ constructed as

$$\mathrm{WF}(u) \doteq \bigsqcup_{x \in U} \Sigma_x(u) = \{(x, p) \in U \times \mathbb{R}^n \backslash \{0\} : p \in \Sigma_x(u)\}. \tag{1.68}$$

Actually, the wave front set is a refinement of the singular support, because it localizes a singularity both in the position space and in momentum space; indeed, $\mathrm{singsupp}(u)$ is the projection of $\mathrm{WF}(u)$ onto its first component, and, furthermore, u is smooth if and only if $\mathrm{WF}(u)$ is empty.

In the viewpoint of Differential Geometry, the notion of wave front set in curved manifolds is recovered after proving that $\mathrm{WF}(u)$ transforms covariantly under diffeomorphisms as subset of T^*U for an open and non-empty $U \subset \mathbb{R}^d$. Namely, $\mathrm{WF}(\phi^* u) = \phi^* \mathrm{WF}(u)$, where $\phi : V \to U$ is a diffeomorphism on an open set $V \subset \mathbb{R}^d$. Thus, the definition of $\mathrm{WF}(u)$ to distributions $u \in \mathcal{D}'(\mathcal{M}, \mathbb{C})$ is directly obtained on an atlas (U_i, φ_i), $i \in \mathbb{N}$ using a partition of unity (χ_i), such that $\sum_i \chi_i = 1$. Therefore,

$$\mathrm{WF}(u) \doteq \bigcup_i \phi_i^* \mathrm{WF}(u_i), \qquad u_i \doteq \left(\phi_i^{-1}\right)^* (\chi_i u),$$

and hence $\mathrm{WF}(u)$ turns to be a conic subset of the cotangent space $T^*\mathcal{M}$ on the local chart (x, p) of $T^*\mathcal{M}$. Namely,

$$\mathrm{WF}(u) \doteq \{(x, p) \in T^*\mathcal{M}\backslash\{\mathbf{0}\} : p \in \Sigma_x(u)\},$$

where $\mathbf{0} \doteq (y,0) \in T^*\mathcal{M}$ denotes the zero section of $T^*\mathcal{M}$. For the proofs and further details and properties about wave front sets of distributions on manifolds, see [BFK96].

Before concluding this general survey about wavefront sets, two final results should be presented, namely the theorem of propagation of singularities, and the Hörmander's criterion for multiplying distributions.

Let P be a partial differential operator with smooth coefficients, σ_P its principal symbol, and $\mathrm{Char}(P) = \sigma_P^{-1}(0) \cap T^*\mathcal{M}\backslash\{\mathbf{0}\}$ the characteristic manifold of P, i.e., the set on non-vanishing directions which are zeros of σ_P. For generalized d'Alembert operators in Lorentzian spacetimes of the form (1.31),

$$\mathrm{Char}(P) = \mathcal{N} \doteq \{(x, p) \in T^*\mathcal{M}\backslash\{\mathbf{0}\} : \sigma_P = -g^{\mu\nu}p_\mu p_\nu = 0\} \tag{1.69}$$

is the set of light cones on $\mathcal{M}$, while each bi-characteristic strip

$$\mathcal{C}_P = \{(x, p) \in T^*\mathcal{M} : p \text{ is a non-zero null vector at } x\} \tag{1.70}$$

is the lift to $T^*\mathcal{M}$ of the null geodesics parametrized by eq. (A.19) (more generally, bi-characteristic strips correspond to the flow lines of the Hamiltonian flow associated to σ_P, which is the geodesic flux in this case). Then, the following theorem holds [DH72].

Theorem 1.2.2. *Let P be a partial differential operator on $\mathcal{M}$ with real-valued principal symbol σ_P. If $u, \rho \in \mathcal{D}'(\mathcal{M}, \mathbb{R})$ satisfies $Pu = \rho$, then, $WF(Pu) \subset Char(P) \cup WF(\rho)$, and $WF(u)\backslash WF(\rho)$ is a union of bicharacteristic strips of the form given in eq. (1.70) on $T^*\mathcal{M}\backslash WF(\rho)$.*

Therefore, the singularities of $u \in \mathcal{D}'(\mathcal{M}, \mathbb{R})$ travel along null geodesics on the light cones, because its wave front set contains only null vectors, and the solutions inside them; hence, the name "wavefront" for $\mathrm{WF}(u)$.

Finally, given two distributions $u, v \in \mathcal{D}'(\mathcal{M}, \mathbb{C})$, the notion of wavefront set is essential to understand the multiplicative operation $u \cdot v$ [Hör03]. In $\mathbb{R}^d$, a well-defined product between distributions can be always achieved when there exists a smooth compactly-supported function f such that $f = 1$ near x, and $\mathcal{F}(fu * fv)$ is fast decaying at x. Thus, on $\mathcal{M}$, one demands that locally the singular directions of the two distributions do not sum up to 0. More precisely, let

$$\Gamma_1 \oplus \Gamma_2 \doteq \{(x, k_1 + k_2) \subset T^*\mathcal{M} : (x, k_1) \in \Gamma_1, (x, k_2) \in \Gamma_2\},$$

be the direct sum of two closed cones Γ_1, Γ_2 of $x \in \mathcal{M}$, and $u, v \in \mathcal{D}'(\mathcal{M}, \mathbb{C})$ two distributions with wavefront sets $\mathrm{WF}(u)$ and $\mathrm{WF}(v)$, respectively. Then, according to the Hörmander's criterion for multiplying distributions, if

$$\mathrm{WF}(u) \oplus \mathrm{WF}(v) = \{(x, k + p) : (x, k) \in \mathrm{WF}(u), (x, p) \in \mathrm{WF}(v)\}$$

does not intersect the zero section, i.e, $k + p \neq 0$ for all $(x, k) \in \mathrm{WF}(u)$, $(x, p) \in \mathrm{WF}(v)$, then the product map

$$\begin{aligned} \psi_{\text{prod}} :\ & \mathcal{D}'(\mathcal{M}, \mathbb{C}) \times \mathcal{D}'(\mathcal{M}, \mathbb{C}) \to \mathcal{D}'(\mathcal{M}, \mathbb{C}) \\ & (u, v) \mapsto \psi_{\text{prod}}(u, v) \doteq u \cdot v \end{aligned}$$

is well-defined in the cone $\Gamma \doteq \Gamma_1 \cup \Gamma_2 \cup (\Gamma_1 \oplus \Gamma_2) \subset T^*\mathcal{M}\backslash\{\mathbf{0}\}$.

For illustrative purposes, it is instructive to analyze the wavefront sets of some notable distributions on $\mathbb{R}$: for examples, the Dirac delta has wavefront set $\mathrm{WF}(\delta) = (0,k)$ for all $k \in \mathbb{R}\backslash\{0\}$, because $\mathcal{F}\{f\delta\} = \hat{f}(0)$ is not fast decaying. Thus, the product of two Dirac delta does not satisfy the above condition: if $(0,k) \in \mathrm{WF}(\delta)$, then $(0,-k) \in \mathrm{WF}(\delta)$ for all k, and hence $\mathrm{WF}(\delta) \oplus \mathrm{WF}(\delta)$ always intersects the zero section. The same conclusion holds also for the Heaviside function Θ, whose wavefront set $\mathrm{WF}(\Theta) = (0,k)$ is equal to $\mathrm{WF}(\delta)$ (actually, δ is the distributional derivative of Θ). Besides, let

$$u_\pm \doteq \mathbb{P}\left(\frac{1}{x}\right) \mp i\pi\delta_x = \frac{1}{x \pm i0^+} = \lim_{\epsilon\to 0^+} \frac{1}{x \pm i\epsilon} \tag{1.71}$$

be the distributions consisting of the principal value of $1/x$ summed up with the "jump" in $x = 0$, and let

$$\mathcal{F}\left\{\frac{1}{x \pm i0^+}\right\} = \mp 2\pi i \Theta(\pm p)$$

be their Fourier transforms. From eq. (1.71)

$$u_+ - u_- = -2i\pi\delta_x,$$

which means that the wavefront set of δ_x can be split in the wavefront sets of $u_\pm$. Thus, $\mathrm{WF}(u_\pm) = \{0\} \times \mathbb{R}_\pm$, and hence $\mathrm{WF}(u_\pm) \oplus \mathrm{WF}(u_\pm) = \{0\} \times \mathbb{R}_\pm$, respectively; therefore, power distributions $u_\pm^n$ can be obtained in $\mathcal{M}$. On the contrary, $\mathrm{WF}(u_+) \oplus \mathrm{WF}(u_-) = (0, \pm(k+p))$ always intersects the zero section when $k > 0$, $p < 0$ and $|p| = |k|$ for all k.

Microlocal analysis and wavefront sets allow to formulate the notion of Hadamard state in the realm of Quantum Field Theory in Curved Spacetimes (see subsection 1.2.3). Studying the form of the Minkowski vacuum two-point function $\Delta_+(x,x')$ given in eq. (1.52), which depends on both $\Theta(p_0)$ and $\delta(p^2+m^2)$, one infers that

$$\begin{aligned}\mathrm{WF}(\Delta_+) =& \{(x,x',p,-p) \in T^*\mathcal{M}^2\backslash\{\mathbf{0}\} : p_0 > 0, p^2 = -m^2\} \cup \\ & \{(x,x',p,-p) \in T^*\mathcal{M}^2\backslash\{\mathbf{0}\} : p_0 > 0, (x-x')^2 = 0\}.\end{aligned}$$

Here, $p_0 > 0$ encodes locally the energy positivity condition, while the pair (x,x') is in $\mathrm{WF}(\Delta_+)$ whenever x and x' are connected by a null geodesic with cotangent vector p. More generally, an equivalent characterization of globally Hadamard states stated in definition 1.2.3 is dictated by the form of the wavefront set of their two-point functions [BDFY15].

Theorem 1.2.3. *Let $(\mathcal{M}, g_{\mu\nu})$ be a globally hyperbolic spacetime, and let ω be a quasi-free state on the Klein-Gordon CCR algebra $\mathcal{A}(\mathcal{M}, g_{\mu\nu})$*[7]*. Denote with*

$$\overline{V}_x^+ = \{k \in T_x^*\mathcal{M} : k \cdot v > 0 \ \forall v \in V_x^+\}, \qquad x \in \mathcal{M}, \tag{1.72}$$

and with $k \rhd 0$ a covector in $\overline{V}_x^+$. The following statements are equivalent:

1. *ω is Hadamard in the sense of eq. (1.59).*
2. *The two-point function ω_2 fulfils the so-called microlocal spectrum condition on $\mathcal{M}$, i.e.,*

$$WF(\omega_2) = \{(x_1,k_1,x_2,-k_2) \in \left(T^*(\mathcal{M})^2\backslash\{\mathbf{0}\}\right) : (x_1,k_1) \sim_\gamma (x_2,k_2),\ k_1 \rhd 0\}, \tag{1.73}$$

where $(x_1,k_1) \sim_\gamma (x_2,k_2)$ means that x_1 and x_2 can be connected by a null geodesic γ such that k_1 is tangential to γ at x_1, and k_2 is the parallel transport of k_1 along γ at x_2.

[7] *Actually, the result stated in this theorem holds also for non quasi-free states, as proved in [San10] (the author is grateful to C. Dappiaggi for pointed it out).*

Moreover, if ω' is another Hadamard state on $\mathcal{A}(\mathcal{M}, g_{\mu\nu})$, then $\omega_2 - \omega_2' \in C^\infty(\mathcal{M}\times\mathcal{M})$.

Furthermore, from the propagation of singularity theorem 1.2.2, two other local-to-global results due to Radzikowski hold [Rad96a; Rad96b].

Theorem 1.2.4. *Let $(\mathcal{M}, g_{\mu\nu})$ be a globally hyperbolic spacetime, and let ω be a quasi-free state on the Klein-Gordon CCR algebra $\mathcal{A}(\mathcal{M}, g_{\mu\nu})$.*

- *If ω_2 is locally of Hadamard form, i.e., it has the form of eq. (1.59) in a neighbourhood of a Cauchy surface, then ω is globally Hadamard over $\mathcal{M}$.*
- *If the microlocal spectrum condition stated in eq. (1.73) for ω holds locally, then it holds also globally.*

More generally, let (x_1, k_1) and (x_2, k_2) be two pairs in $T^*(\mathcal{M})\backslash\{\mathbf{0}\}$ such that $(x_1, k_1) \sim_\gamma (x_2, k_2)$ according to the definition given in theorem 1.2.3, then the wave front sets of the propagators associated to the Klein-Gordon equation read as follows [BF09].

- **Two-point functions**. From theorem 1.2.3 and denoting with $\Delta_-(x, x') \doteq \Delta_+(x', x)$,
$$\mathrm{WF}(\Delta_\pm) = \{(x_1, k_1, x_2, -k_2) \in \left(T^*(\mathcal{M})^2\backslash\{\mathbf{0}\}\right) : \pm k_1 \triangleright 0\}.$$
- **Retarded and advanced propagators**. From eq. (1.42),
$$\mathrm{WF}(\Delta_{R,A}) = \mathrm{WF}(\delta) \cup \{(x_1, k_1, x_2, -k_2) \in \left(T^*(\mathcal{M})^2\backslash\{\mathbf{0}\}\right) : x_2 \in J^\pm(x_1), k_1 \neq 0\}.$$
- **Causal propagator**. From eq. (1.36),
$$\mathrm{WF}(\Delta) = \{(x_1, k_1, x_2, -k_2) \in \left(T^*(\mathcal{M})^2\backslash\{\mathbf{0}\}\right) : k_1 \neq 0\}.$$
- **Feynman propagator**. From eq. (1.44),
$$\begin{aligned}&\mathrm{WF}(\Delta_F) = \mathrm{WF}(\delta)\cup\\ &\{(x_1, k_1, x_2, -k_2) \in \left(T^*(\mathcal{M})^2\backslash\{\mathbf{0}\}\right) : k_1 \triangleright 0 \text{ if } x_1 \notin J^-(x_2), \text{ and } k_1 \triangleleft 0 \text{ if } x_1 \in J^-(x_2)\}.\end{aligned}$$

According to the form of the wavefront set given in eq. (1.73), $\Delta_\pm^2$ is well-defined as distributions, unlike $\Delta_+ \cdot \Delta_-$, as happened for the distributions $u_\pm$ defined in eq. (1.71). In a similar way, the product $\Delta_F \cdot \Delta_F$ cannot be extended directly to the diagonal $x' = x$, and hence a suitable procedure to extend such distribution to the diagonal is required, see subsection 1.2.5. In this case, from the viewpoint of the Hörmander's criterion, $\mathrm{WF}(\Delta_F) \oplus \mathrm{WF}(\Delta_F)$ intersects the zero section through $\mathrm{WF}(\delta) \oplus \mathrm{WF}(\delta)$.

Moreover, in the case of the Minkowski vacuum given in eq. (1.52), the distribution Δ_+^n can be expressed in the so-called Källén-Lehmann spectral representation, i.e., as an integral over the squared mass M^2 depending on a real and positive spectral density $\varrho(M^2)$. In view of the translational invariance of the flat spacetime, denoting with x the difference between two events in $(\mathcal{M}, \eta_{\mu\nu})$, it can be shown that

$$\Delta_+^n(x) = \int_{n^2m^2}^\infty \varrho_n(M^2)\Delta_+(x, M^2)\mathrm{d}M^2, \tag{1.74}$$

where

$$\varrho_n(M^2) = \frac{1}{(2\pi)^{3(n-1)}}\int_{\mathbb{R}^{3n}} \mathrm{d}^3\vec{q}_1 \dots \mathrm{d}^3\vec{q}_n \prod_{k=1}^n \frac{1}{2\omega_{\vec{q}_k}}\delta^{(3)}\left(\sum_{k=1}^n \vec{q}_k\right)\delta\left(\sum_{k=0}^n \omega_{\vec{q}_k} - M^2\right), \tag{1.75}$$

$\omega_{\vec{q}_k} \doteq \sqrt{|\vec{q}_k|^2 + m^2}$, and $\Delta_+(x, M^2)$ denotes the two-point function of the Minkowski vacuum state (1.52) for a scalar field with mass M.

Remark 1.2.1. In [GW19; Gér19] the microlocal spectrum condition given in eq. (1.73) for a quasi-free Hadamard state is formulated in terms of the characteristic manifold $\mathcal{N}$ of a generalized d'Alembert operator (1.31) given in eq. (1.69). Under the action of the cone defined in eq. (1.72), $\mathcal{N}$ splits into the upper/lower energy shells as

$$\mathcal{N} = \mathcal{N}^+ \cup \mathcal{N}^-, \qquad \mathcal{N}^\pm \doteq \mathcal{N} \cap \{\pm k \in \overline{V}_x^\pm\}$$

(the definition of $\overline{V}_x^-$ can be obtained by adapting eq. (1.72) to the past case). Then, an equivalent definition of Hadamard states in terms of microlocal spectrum condition is

$$\mathrm{WF}'(\omega_2) \subset \mathcal{N}^+ \times \mathcal{N}^+, \tag{1.76}$$

where

$$\mathrm{WF}'(u) \doteq \{(x_1, k_1, x_2, k_2) \in \left(T^*(\mathcal{M})^2 \backslash \{\mathbf{0}\}\right) : (x_1, k_1, x_2, -k_2) \in \mathrm{WF}(u)\} \tag{1.77}$$

denotes the dual of $\mathrm{WF}(u)$, for $u \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$.

Before concluding this microlocal survey, a more refined notion of wavefront set, and hence a sharpened version of the microlocal spectrum condition, can be introduced by replacing the wavefront set WF by the analytic wave front set WF_a, according to the references [Hör03; HW01; SVW02; GW19; Gér19].

Definition 1.2.6. Let X be an open subset of $\mathbb{R}^d$ and $u \in \mathcal{D}'(X, \mathbb{R})$. The analytic wavefront set $\mathrm{WF}_a(u)$ of u is defined to be the complement of the set of regular points (x_0, p_0) in $X \times (\mathbb{R}^d \backslash \{0\})$, such that there is a neighbourhood $U \subset X$ of x_0, a conic neighbourhood Γ of k_0, and a bounded sequence of compactly-supported distributions $u_N \in \mathcal{E}'(X)$ which is equal to u in U, which satisfies the estimation

$$|\hat{u}_N(p)| \leq c^{N+1} \left(\frac{N+1}{|p|} \right)^N \tag{1.78}$$

for some constant c, with $N \in \mathbb{N}$, and for all $p \in \Gamma$.

In this definition, the bounded sequence u_N can be always chosen of the form $f_N u$, where $f_N \in \mathcal{D}(K, \mathbb{R})$ is a sequence of smooth compactly-supported functions on a compact subset K of X, such that $\mathrm{WF}_a(u) \cap (K \times F) = \emptyset$ for some closed cone F (see Lemma 8.4.4 in [Hör03] for the details). If $\mathrm{WF}_a(u)$ is empty, then u is strongly real analytic; moreover, $\mathrm{WF}_a(u)$ transforms as a subset of T^*X under analytic diffeomorphisms, thus it can be extended to real analytic manifolds in a similar way to $\mathrm{WF}(u)$. Therefore, the analytic version of the microlocal spectrum condition formulated as in eq. (1.76) holds.

Definition 1.2.7. A quasi-free state ω on the Klein-Gordon CCR $\mathcal{A}(\mathcal{M}, g_{\mu\nu})$ is an analytic Hadamard state if its two-point function obeys the following analytic microlocal spectrum condition:

$$\mathrm{WF}'_a(\omega_2) \subset \mathcal{N}^+ \times \mathcal{N}^+, \tag{1.79}$$

where the notation WF' was introduced in eq. (1.77).

Moreover, if ω' is another analytic Hadamard state, then $\omega_2 - \omega'_2$ is real analytic (see proposition 2.8 in [GW19]). Therefore, one can formulate an analytic version of theorem 1.2.3 for analytic Hadamard states.

Theorem 1.2.5. *Let $(\mathcal{M}, g_{\mu\nu})$ be a globally hyperbolic spacetime, and let ω be a quasi-free state on the Klein-Gordon CCR algebra $\mathcal{A}(\mathcal{M}, g_{\mu\nu})$. Then the following statements are equivalent:*

1. *ω is an analytic Hadamard state in the sense of eq. (1.59), with $\mathcal{W}(f, g) \in \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ real and analytic.*

2. *The two-point function ω_2 fulfils the analytic microlocal spectrum condition on $\mathcal{M}$, i.e.,*

$$WF_a(\omega_2) = \{(x_1, k_1, x_2, -k_2) \in \left(T^*(\mathcal{M})^2 \backslash \{\mathbf{0}\}\right) : (x_1, k_1) \sim_\gamma (x_2, k_2),\ k_1 \rhd 0\}, \tag{1.80}$$

As stated by theorem 6.3 in [SVW02], examples of analytic quasi-free Hadamard states are the Minkowski vacuum state, whose two-point function was given in eq. (1.52), and the KMS thermal state ω^β with respect to a selected Minkowski time at inverse temperature β (see, e.g., [Haa12; GPV17; BDGV19] and references therein). Recalling the Schwartz space $\mathcal{S}(\mathcal{M})$ on the Minkowski spacetime $(\mathcal{M}, \eta_{\mu\nu})$, the two-point function of a KMS state for a massive quantum scalar field defines a tempered bidistribution $\Delta_\beta \in \mathcal{S}'(\mathcal{M} \times \mathcal{M})$ of the form

$$\Delta_\beta(f, g) = \frac{1}{(2\pi)^3} \int \frac{\epsilon(p_0)\delta(p^2 + m^2)}{1 - \mathrm{e}^{\boldsymbol{\beta}^\mu p_\mu}} \hat{f}(-p)\hat{g}(p)\mathrm{d}^4 p, \qquad f, g \in \mathcal{S}(\mathcal{M}), \tag{1.81}$$

where $\boldsymbol{\beta}^\mu \doteq \beta e^\mu$, and whose Kernel reads in the spatial momentum space as

$$\langle\phi(x)\phi(x')\rangle_\beta = \Delta^+_\beta(x - x') = \frac{1}{(2\pi^3)} \int_{\mathbb{R}^3} \frac{\mathrm{d}^3\vec{p}}{2\omega_0} \left(\frac{\mathrm{e}^{-i\omega_0(t-t')}}{1 - \mathrm{e}^{-\beta\omega_0}} + \frac{\mathrm{e}^{i\omega_0(t-t')}}{\mathrm{e}^{\beta\omega_0} - 1} \right) \mathrm{e}^{i\vec{p}\cdot\vec{x}}, \tag{1.82}$$

with $\omega_0 = \sqrt{|\vec{p}|^2 + m^2}$. After regularizing the KMS two-point function by subtracting the Minkowski vacuum state (1.52) instead of the Hadamard parametrix, the smooth part reads

$$\mathcal{W}_\beta(x - x') \doteq \Delta_\beta(x - x') - \Delta_+(x - x') = \frac{1}{(2\pi)^3} \int_{\mathcal{M}} \frac{\delta(p^2 + m^2)}{\mathrm{e}^{\beta|p_0|} - 1} \mathrm{e}^{ip(x-x')}\mathrm{d}^4 p. \tag{1.83}$$

Thus, both the smooth parts $\mathcal{W}_+(f, g)$ given in (1.53) and $\mathcal{W}_\beta(f, g)$ result to be real analytic distributions [SVW02].

1.2.5 Wick and interacting observables

The CCR algebra $\mathcal{A}(\mathcal{M}, g_{\mu\nu})$ of the free smeared Klein-Gordon fields constructed in subsection 1.2.1 contains only finite composite quantum observables evaluated at different points in the spacetime. On the contrary, it does not include non-linear normal-ordered Wick fields, such as $:T_{\mu\nu}:$, $:\phi^n:$, $n \geq 2$, etc.. Therefore, a suitable prescription to extend the previous *-algebra to a new enlarged algebra $\mathcal{A}_{\text{Wick}}(\mathcal{M}, g_{\mu\nu})$ which contains also this class of quantum observables is needed for the scope of Semiclassical Gravity. To this aim, the class of Hadamard states introduced in subsection 1.2.3 allows to extend the usual normal-ordering procedure in Minkowski spacetime to curved spacetimes.

The motivation in constructing normal-ordered fields arises because the expectation values of quadratic observables such as

$$\phi^2(x) \doteq \lim_{x' \to x} \phi(x')\phi(x) \tag{1.84}$$

in a given state ω usually blows up in the coinciding point limit $x' \to x$, due to the singular structure of the two-point function ω_2. A well-known solution to this problem is to subtract this divergent part, and hence taking the coinciding point limit. In flat spacetime this subtraction is usually provided by the the Minkowski vacuum state (1.52), in such a way that the regularized form of eq. (1.84) reads

$$:\phi^2:(x) = \lim_{x' \to x} \left(\phi(x')\phi(x) - \Delta_+(x', x)\mathbb{I}\right). \tag{1.85}$$

According to the discussion made in subsection 1.2.3, this regularization can be generalized to curved spacetimes using the class of Hadamard states. The natural normal-ordering prescription to obtain finite expectation values of Wick observables is the Hadamard point-splitting regularization [BF00; HW01; HW02] (see also [Mor03; Hac16]). In this regularization procedure, the divergences contained in $H_{0^+}(x,x')$ are subtracted from the two-point function before computing the coinciding point limits of the composite operator, and thus obtaining a finite expectation value in the state ω. More precisely, given a convex, geodesic neighbourhood $\mathcal{O}\subset\mathcal{M}$, $x,x'\in\mathcal{O}$, and two bi-differential operators $\mathfrak{D}_{1,2}$ on $C^\infty(\mathcal{O})$, the expectation value of the normal-ordered observable $:(\mathfrak{D}'_1\phi)\,(\mathfrak{D}_2\phi):$ is

$$\langle :(\mathfrak{D}'_1\phi)\,(\mathfrak{D}_2\phi):\rangle_\omega = \lim_{x'\to x}\mathfrak{D}'_1\mathfrak{D}_2\left(\omega_2(x',x)-H_{0^+}(x',x)\right) = \left[\mathfrak{D}'_1\mathfrak{D}_2\mathcal{W}\right], \tag{1.86}$$

where $\mathfrak{D}'_1$ acting on x' is viewed as implicitly parallel-transported in the limit prescription.

The regularization procedure implemented by eq. (1.86) may involve only the truncated version of the Hadamard parametrix (1.60), if one is interested in constructing normal-ordered observables only of order $N\in\mathbb{N}$, depending on the order of differentiation of $\mathfrak{D}_1,\mathfrak{D}'_2$. In particular, for every $N\in\mathbb{N}$ the difference

$$\lim_{x'\to x}\left(H_{0^+}(x',x)-H_N(x',x)\right)$$

is a C^N-regular function (see [BGP07]), and hence subtracting the truncated Hadamard parametrix H_N from the two-point function is sufficient to obtain finite expectation values of Wick polynomials up to a finite order N (see also [Chr76; Chr78]). In this respect, it is not always necessary to evaluate eq. (1.86) in Hadamard states, but only in sufficiently regular states, which ensure a sufficiently regular function $\mathcal{W}(x',x)$. This strategy shall be used to obtain cosmological observables in subsection 2.2.1 and Appendix B, using the truncated Hadamard parametrix of order 1.

According to the Hadamard point-splitting prescription, Wick polynomials in the Wick algebra $\mathcal{A}_{\text{Wick}}(\mathcal{M},g_{\mu\nu})$ turn to be normal-ordered fields with respect to H_{0^+}, composed by Wick powers which can be multiplied with each other. For instance, the normal-ordering applied to $\phi^2(x')\phi^2(x)$ yields

$$:\phi^2(x'):_H:\phi^2(x):_H\;=\;:\phi^2(x')\phi^2(x):_H+4:\phi(x')\phi(x):_H H_{0^+}(x',x)+2H^2_{0^+}(x',x)\mathbb{I}. \tag{1.87}$$

where $H^2_{0^+}$ is always well-defined as distribution. On the one hand, this regularization procedure fully generalizes the usual Wick normal-ordering theorem formulated in flat spacetime in terms of creation and annihilation operators, which is equivalent to subtract the two-point function of the Minkowski vacuum, as in eq. (1.85). On the other hand, unlike the flat case, only local geometry enters in the regularized expectation value evaluated in eq. (1.86), because H_{0^+} is fully determined by the Klein-Gordon equation (1.29) and by the geometry of the spacetime. Therefore, those non-linear quantum observables are local and covariant, and thus they can be promoted to quantum fields in curved spacetimes. Shortly, given an isometric embedding of the spacetime

$$\begin{aligned}\psi:\;\mathcal{M}&\to\mathcal{M}'\\ \psi^*g'&=g,\end{aligned}$$

preserving the causal structure, i.e., if x,x' are causally-related in $\mathcal{M}$, then $\psi(x)$, $\psi(x')$ are causally-related in $\mathcal{M}'$, ϕ is local and covariant field if there exists a natural isomorphism α_ψ : $\mathcal{A}_{\text{Wick}}(\mathcal{M},g_{\mu\nu})\to\mathcal{A}_{\text{Wick}}(\mathcal{M},g_{\mu\nu})'$ such that $\alpha_\psi\left(\phi'(f)\right)=\phi(f\circ\psi^{-1})$ [HW01; BFV03].

After imposing further physical requirements, such as scaling behaviour, commutation relations, smooth dependence on the metric g, the mass m, and the coupling parameter ξ, etc., it was shown in [HW01; HW02] that any prescription to obtain local and covariant Wick observables in curved spacetimes is not unique, but depends on some arbitrary choices of real constants C_n, with $n\in\mathbb{N}$. This ambiguity is due to the property of the Hadamard parametrix (1.57), which is not invariant under a rescale of the metric $g \mapsto \lambda^2 g$, on account of the arbitrary choice of the length scale λ^2 in the logarithmic divergence. Namely,

$$h_{0^+}[g] \mapsto \lambda^2 \left(h_{0^+}[g] + v[g] \log(\lambda^2)\right).$$

Thus, the presence of $\log(\lambda^2)$ implies that Wick monomials fail to scale homogeneously, and hence their explicit expressions depend unavoidably on some degrees of freedom inherited from the arbitrariness of λ. In fact, such freedoms of Wick polynomials are labelled by the renormalization constants of the theory. Moreover, the same freedom occurs also when different regularization prescriptions are prescribed instead of the Hadamard point-splitting procedure given in eq. (1.86). For instance, in the case of the Wick power $:\phi^n:_H$, the following relation holds between two different constructions:

$$:\tilde{\phi}^n:_H \;=\; :\phi^n:_H + \sum_{i=0}^{n-2} \binom{n}{i} C_{n-i} :\phi^i:_H, \tag{1.88}$$

where C_n are real non-vanishing polynomials depending on the metric g, on the Riemann tensor and on its covariant derivatives, on the mass m^2, and on the coupling parameter ξ. Also, the local curvature terms scale as $C_n \mapsto \mu^n C_n$, span a finite dimensional space for every $n \in \mathbb{N}$, and, furthermore, represent the renormalization freedoms of the quantum field theory in flat and curved spacetimes, which are universal and hence fixed once and forever [BFV03]. Finally, they cannot be explicitly evaluated within the theory, but they can only be inferred either from more fundamental theories, or from physical experiments. For instance, when $n = 2$,

$$:\tilde{\phi}^2:_H = :\phi^2:_H + (\alpha_1 R + \alpha_2 m^2)\mathbb{I}, \qquad \alpha_1, \alpha_2 \in \mathbb{R}. \tag{1.89}$$

On the algebra of Wick polynomials $\mathcal{A}_{\mathrm{Wick}}(\mathcal{M}, g_{\mu\nu})$ one can also construct time-ordered products of Wick powers in n factors, viewed as distribution on $\mathcal{M}^n$ valued in $\mathcal{A}_{\mathrm{Wick}}(\mathcal{M}, g_{\mu\nu})$. In particular, the time-ordering of the products among fields

$$T_n\left(\phi^{k_1}(x_1)\cdots\phi^{k_n}(x_n)\right), \qquad n, k_1, \ldots, k_n \in \mathbb{N}, \tag{1.90}$$

is provided by a time-ordering map T_n which implements the causal factorization rule, see [HW01; HW02] and [ABIM15], Chapter 10. For instance, if $n = 2$ and $k_1 = k_2 = 1$, then

$$T_2\left(\phi(x_1)\phi(x_2)\right) = \begin{cases} \phi(x_1)\phi(x_2) & \text{if } x_1 \notin J^-(x_2), \\ \phi(x_2)\phi(x_1) & \text{if } x_1 \in J^-(x_2). \end{cases} \tag{1.91}$$

In flat spacetime, its expectation value in the Minkowski vacuum state yields the Feynman propagator defined in eq. (1.44). However, the above formula (1.91) provides a well-defined distribution $T_2\left(\phi(f_1)\phi(f_2)\right)$ when $\mathrm{supp} f_1 \cap \mathrm{supp} f_2 \neq \emptyset$, where $f_1, f_2 \in \mathcal{D}(\mathcal{M})$ in the sense of eq. (1.48), but it fails when extended to the coinciding limit $x_1 \to x_2$.

The issue of extending a time-ordered product given in eq. (1.90) to the diagonal, namely the construction of a time-ordered map T_n everywhere in the spacetime, corresponds to define a renormalization scheme for the quantum theory [BS80]. In order to obtain a well-posed time-ordered map, and hence constructing interacting observables, T_n has to satisfy some further physical requirements listed in [HW02], such as locality, covariance, scaling, symmetry under permutation, etc. In a similar way as for the case of normal-ordered fields, it turns out that any time-ordered map satisfying all these properties is unique up to the addition of local and covariant freedoms, depending on the mass of the field and on the curvature of the spacetime; they correspond, indeed, to the counterterms characterising two different renormalization schemes at n-perturbative order (hence, they are said renormalization constants of the model). Thus, the construction of the time-ordered products is taken recursively by extending the map T_n at each n, specifying the form of the renormalization counterterms at each recursive step. For all the details about the topic, see [HW01; HW02; HW03; BF00; FR16].

The issue of constructing time-ordered products in terms of extension of distributions to the diagonal was originally solved by Epstein and Glaser in [EGJ65] in the framework of causal perturbative interacting theories in flat spacetime. Afterwards, this renormalization procedure has been generalized by Brunetti and Fredenhagen to curved manifolds in [BF00], taking advantage of all techniques developed in microlocal analysis on globally hyperbolic spacetimes. In this monograph, the discussion will be made in $\mathbb{R}^d$, in view of the applications used in Minkowski spacetime in chapter 4; in this case, thanks to the the translation invariance, extending to the diagonal corresponds to extend the distribution to the origin.

Remark 1.2.2. Actually, there are different methods to treat the singularity of the Feynman propagator located in the diagonal, and thus proceeding with the construction of a renormalized time-ordered product. For example, in flat spacetime popular approaches are multiplicative and additive renormalizations: in the former case, divergences are removed by a redefinition of the "bare" quantities, while, in the latter case, counterterms are added in the Lagrangian to compensate the diverging contributions in the effective action. Moreover, other procedures such as the Pauli-Villars renormalization and the dimensional regularization are often employed in Theoretical Physics for regularizing Feynman diagrams in momentum space[8].

The crucial role to achieve that extension is played by Steinmann's scaling degree of a distribution [Ste71]: let $u \in \mathcal{D}'(\mathbb{R}^d \backslash \{0\})$, then the scaling degree of u measures how much u diverges near the origin, i.e.,

$$\mathrm{sd}(u) \doteq \inf\{\delta \in \mathbb{R} : \lim_{\lambda \to 0^+} \lambda^\delta u(f_\lambda) = 0\}, \tag{1.92}$$

where $f_\lambda(x) \doteq \lambda^{-d} f\left(\frac{x}{\lambda}\right)$ for all $f \in \mathcal{D}'(\mathbb{R}^d \backslash \{0\})$, and hence

$$u(f_\lambda) = \int_{\mathbb{R}^d} u(\lambda x) f(x) \mathrm{d}^d x.$$

In this view, one also defines the divergence degree $\mathrm{div}(u) \doteq \mathrm{sd}(u) - d$. For example, by direct computation, the scaling degree of the Dirac delta δ is equals to d, and turns to be $d + |\alpha|$ for its derivatives $\partial^\alpha \delta$, where α is some multi-index; furthermore, if one considers the four-dimensional Feynman propagator in Minkowski spacetime (1.45), then the evaluation of $\lambda^\delta \Delta(f_\lambda)$ yields a factor $\lambda^{\delta-4+2}$, and hence $\mathrm{sd}(\Delta_F) = 2$, $\mathrm{sd}(\Delta_F^n) = 2n$.

Moreover, a distribution $u_e \in \mathcal{D}'(\mathbb{R}^d)$ is said to be an extension of $u \in \mathcal{D}'(\mathbb{R}^d \backslash \{0\})$ if it coincides with u on $\mathcal{D}(\mathbb{R}^d \backslash \{0\})$. Provided the definitions of scaling degree given in eq. (1.92) and extension of a distribution, the following theorem holds.

Theorem 1.2.6. *Let $u_e \in \mathcal{D}'(\mathbb{R}^d)$ be an extension of $u \in \mathcal{D}'(\mathbb{R}^d \backslash \{0\})$, such that $u_e(f) = u(f)$ for all $f \in (\mathbb{R}^d \backslash \{0\})$.*

1. *If $sd(u) < d$, then there exists a unique extension u_e such that $sd(u_e) = sd(u)$.*

2. *If $d \leq sd(u) < \infty$, let*

$$\mathcal{D}_\rho(\mathbb{R}^d) = \{f \in \mathcal{D}(\mathbb{R}^d) : \partial^\alpha f(0) = 0, |\alpha| \leq \rho\},$$

[8] Discussing accurately strengths and weaknesses of all these approaches to renormalization would require great effort, and in fact it goes beyond the scopes of this monograph; a pedagogical introduction to all these methods in the framework of interacting quantum theories can be found in Fredenhagen's QFT lectures notes [Fre10].

be the space of test functions, together with its derivatives, which vanish in the origin up to order $\rho \geq 0$, where $\rho = sd(u) - d$ denotes the degree of divergence of u. Then, there exists a unique extension u_e such that $sd(u_e) = sd(u)$ in $\mathcal{D}_\rho(\mathbb{R}^d)$. Namely, all the extensions u_e of u are distributions such that

$$u'_e = u_e + \sum_{|\alpha|\leq\rho} c_\alpha \partial^\alpha \delta_x, \qquad u_e, u'_e \in \mathcal{D}'(\mathbb{R}^d), \tag{1.93}$$

where the constants c_α correspond to the renormalization freedoms of the model.

3. *If $sd(u) = \infty$, then u is not extensible.*

In flat spacetime, the renormalization of the powers of the Feynman propagator at a finite order n can be performed by taking advantage of the Källén-Lehmann spectral representation of Δ_+^n given in eq. (1.74).

Proposition 1.2.2. *Let $(\mathcal{M}, \eta)$ be the four-dimensional Minkowski spacetime, and let Δ_+ the two-point function of the vacuum state (1.52). Then, extensions of powers of the Feynman propagator Δ_F^n on $\mathcal{D}(\mathcal{M})$ read in the Källén-Lehmann spectral representation as*

$$\Delta_F(x)^n = (\Box_\eta + a)^{n-1} \int_{n^2m^2}^\infty \varrho_n(M^2) \frac{1}{(M^2+a)^{n-1}} \Delta_F(x, M^2) \mathrm{d}M^2, \qquad a > -n^2m^2, \tag{1.94}$$

viewed in the distributional sense, where the spectral density $\varrho_n(M^2)$ was given in eq. (1.75), and $\Delta_F(x, M^2)$ denotes the Feynman propagator (1.45) with mass M.

Proof. From the definition of the Feynman propagator (1.44), Δ_F reduces to Δ_+ outside and in the future of $x = 0$. Thus, using the representation of Δ_+^n in eq. (1.74)

$$\Delta_F(x)^n = \int_{n^2m^2}^\infty \varrho_n(M^2) \Delta_F(x, M^2) \mathrm{d}M^2$$

outside $x = 0$. As $\Delta_F(x, M^2)$ is solution of $\left(\Box_\eta - M^2\right) \Delta_F(x, M^2) = i\delta_x$, then

$$(\Box_\eta + a)\, \Delta_F(x, M^2) = \left(M^2 + a\right) \Delta_F(x, M^2) + i\delta_x, \qquad a \in \mathbb{R},$$

and hence

$$\Delta_F(x)^n = \int_{n^2m^2}^\infty \varrho_n(M^2) \frac{(\Box_\eta + a)^{n-1}}{(M^2+a)^{n-1}} \Delta_F(x, M^2) \mathrm{d}M^2 \quad \in \mathcal{D}'\left(\mathcal{M} \backslash \{0\}\right).$$

Firstly, from the decaying behaviour of $\hat{\Delta}_F(x, M^2)$ as M^{-2} inferred from eq. (1.45), the above integral always exist for $a > -n^2m^2$. According to theorem 1.2.6, as $\mathrm{sd}(\Delta_F^n) = 2n$, the unique extensions of the above representation of Δ_F^n in $\mathcal{D}(\mathbb{R}^4)$, with $\rho = 2n - 4$, are of the form

$$\Delta_F(x)^{n\prime} = \int_{n^2m^2}^\infty \varrho_n(M^2) \frac{(\Box_\eta + a)^{n-1}}{(M^2+a)^{n-1}} \Delta_F(x, M^2) \mathrm{d}M^2 + \sum_{|\alpha|\leq\rho} c_\alpha \partial^\alpha \delta_x, \qquad c_\alpha \in \mathbb{C}.$$

Indeed, the $n-1$ second order differential operators $\Box_\eta + a$ can be integrated by parts in $\mathcal{D}_\rho(\mathbb{R}^4)$ over test functions $f \in \mathcal{D}_\rho(\mathbb{R}^4)$, and only total derivatives arise in the integration, since $\partial^\alpha f(0) = 0$ up to order $2n - 4$. Therefore, the regularized $\Delta_F^n \in \mathcal{D}'(\mathbb{R}^4)$ can be also written as

$$\Delta_F(x)^n = (\Box_\eta + a)^{n-1} \int_{n^2m^2}^\infty \varrho_n(M^2) \frac{1}{(M^2+a)^{n-1}} \Delta_F(x, M^2) \mathrm{d}M^2,$$

in the sense of distributions, where a replaces the constants c_α as renormalization freedom of Δ_F^n. To verify this last statement, it is sufficient to show that changing the value of a corresponds to change the renormalization constants, namely

$$W(a,b,n-1) \doteq \frac{(\Box_\eta + a)^{n-1}\Delta_F(x,M^2)}{(M^2+a)^{n-1}} - \frac{(\Box_\eta + b)^{n-1}\Delta_F(x,M^2)}{(M^2+b)^{n-1}} = \sum_{\alpha\leq\rho} \tilde{c}_\alpha \partial^\alpha \delta_x \tag{1.95}$$

for $a, b \in \mathbb{R}$ and $\tilde{c}_\alpha \in \mathbb{C}$. This proof can be achieved by induction on $n \geq 2$ starting from the case $n = 2$, which yields

$$W(a,b,1) = \frac{(\Box_\eta + a)\Delta_F(x,M^2)}{M^2+a} - \frac{(\Box_\eta + b)\Delta_F(x,M^2)}{M^2+b} = \frac{b-a}{(M^2+a)(M^2+b)} i\delta_x$$

after using $\left(\Box_\eta - M^2\right)\Delta_F(x,M^2) = i\delta_x$. Then, assuming as inductive hypothesis that eq. (1.95) holds, one obtains at the n-th step

$$\begin{aligned} W(a,b,n) &= \frac{(\Box_\eta + a)^n\Delta_F(x,M^2)}{(M^2+a)^n} - \frac{(\Box_\eta + b)^n\Delta_F(x,M^2)}{(M^2+b)^n} = \\ &= W(a,b,n-1) + \frac{(M^2+b)^n(\Box_\eta+a)^{n-1} - (M^2+a)^n(\Box_\eta+b)^{n-1}}{(M^2+a)^n(M^2+b)^n} i\delta_x, \end{aligned}$$

and hence the proof follows, because the second term is a polynomial in $\partial^\alpha\delta_x$ up to order ρ (the highest-order derivative term $\Box_\eta^{n-1}\delta_x$ is of order $2n-4$).

□

Once Wick fields and their time-ordered products are at disposal in $\mathcal{A}_{\text{Wick}}(\mathcal{M}, g_{\mu\nu})$, interacting observables can be obtained in the framework of a perturbative interacting quantum field theory, described by a Lagrangian of the form $\mathcal{L}_0 + \mathcal{L}_I$, where $\mathcal{L}_0$ is the free Lagrangian associated to the Klein-Gordon action (1.28), and $\mathcal{L}_I$ is an interaction Lagrangian depending on a coupling parameter λ. The fundamental ingredient is the so-called local S-matrix of an interacting theory, which is defined in units $\hbar = 1$ as

$$S(f) \doteq \mathbf{1} + \sum_{n\geq 1} i^n \int_{\mathcal{M}^n} f(x_1)\cdots f(x_n) T\left(\mathcal{L}_I(x_1)\cdots\mathcal{L}_I(x_n)\right)\sqrt{|\det(g)|}\mathrm{d}^n x_1 \ldots \mathrm{d}^n x_n, \tag{1.96}$$

where $f \in \mathcal{D}(\mathcal{M})$ is an interaction cut-off, and $S^{(0)} = \mathbf{1}$ is the starting element of the series. Following [HW01; HW02; FL14] (see also [HW15]), the construction of $S(f)$ can be performed from the viewpoint of a *-algebra after taking into account the local interacting action

$$V \doteq \int_U \mathcal{L}_I(x) f(x) \mathrm{d}_g^4 x, \tag{1.97}$$

where the cut-off function $f \in \mathcal{D}(U)$ identifies the support of V in the globally hyperbolic region $U \subset \mathcal{M}$ of the spacetime. Let $\mathcal{A}_{\text{Wick}}(\mathcal{M}, g_{\mu\nu})(U)$ be the sub-algebra of $\mathcal{A}_{\text{Wick}}(\mathcal{M}, g_{\mu\nu})$ containing the normal-ordered observables smeared in a compact subset of U. Then, the local S-matrix can be represented as a formal power series

$$S(V) = T\left(\exp(iV)\right) = \sum_{n\geq 0} \frac{i^n}{n!} T\left(V^n\right) \tag{1.98}$$

composed by elements in the *-algebra $\mathcal{A}_{\text{Wick}}(\mathcal{M}, g_{\mu\nu})[[\lambda]]$ of formal power series with values in $\mathcal{A}_{\text{Wick}}(\mathcal{M}, g_{\mu\nu})$ (in this context, formal means that $S(V)$ is not expected to converge as series in λ). Moreover, the local S-matrix satisfies the causal factorization condition

$$S(V_1 + V_2 + V_3) = S(V_1 + V_2) S^{-1}(V_2) S(V_2 + V_3), \qquad V_1 \succ V_2 \succ V_3,$$

where the symbol $V_1 \succ V_2$ means $J^+(\mathrm{supp}V_1) \cap J^-(\mathrm{supp}V_2) = \emptyset$.

The presence of the cut-off removes the infrared divergences of the perturbative quantum theory which would appear otherwise in an S-matrix supported everywhere over $\mathcal{M}$. Furthermore, fixed a Cauchy surface $\Sigma \subset \mathcal{M}$ containing the initial data of the field, it localizes the interaction in U, such that $f = 1$ in U, and $U \cap \Sigma$ is also a Cauchy surface. Physically, it corresponds to say that the interacting model approaches a free theory for sufficiently large times in the past, namely that a free quantum in-field is considered. In this formulation, the interaction is dictated by the interacting Lagrangian $\mathcal{L}_I$ starting from a certain initial time fixed by Σ. Eventually, the so-called adiabatic limit $f \to 1$ is taken to remove the mathematical step of switching the interaction, so that $U \to \mathcal{M}$, and ϕ is intended as an interacting field in Bogoliubov's sense (see [HW03] for a procedure to take the adiabatic limit in globally hyperbolic spacetimes).

Remark 1.2.3. At this stage, it should be stressed that the strong adiabatic limit $f \to 1$ may not exist in general interacting quantum theories at level of states, hence the terminology weak adiabatic limit when this limit is performed at level of correlation functions. The existence of interacting states in the adiabatic limit was achieved, for instance, in the vacuum and in the thermal case in [EG73] and [FL14], respectively, whereas it was proved in [DFP18] that the return-to-equilibrium property for KMS states in perturbative interacting quantum theories fails in this limit, but is guaranteed only for spatial compact Lagrangians. For further discussions about adiabatic limits in interacting theories, see [Lin13; BDGV19].

Thus, based on Bogoliubov's original ideas [BS80], an interacting observable can be represented perturbatively at the n-th order as a formal power series of operator-valued distributions of the free theory living on the CCR algebra $\mathcal{A}(\mathcal{M}, g_{\mu\nu})$ through the so-called Bogoliubov map [GHP16]

$$\phi_{\mathrm{int}} = R_V(\phi) \doteq S(V)^{-1} T\left(S(V)\phi\right). \tag{1.99}$$

For instance, in the case of ϕ^2 the expansion of eq. (1.99) reads

$$\phi^2_{\mathrm{int}} = R_V(\phi^2) = \phi^2 + i\left(T\left(V\phi^2\right) - V\phi^2\right) + \frac{1}{2}\left(T\left(V^2\right)\phi^2 - 2V^2\phi^2 - T\left(VV\phi^2\right) + VT(V\phi^2)\right) + \dots \tag{1.100}$$

By definition, one can verify that ϕ_{int} respects causality, i.e., $J^+(\mathrm{supp}V) \cap \phi_{\mathrm{int}} = \emptyset$, and it reduces to the free observable outside U, i.e., before switching the interaction provided by V; furthermore, it solves the interacting Klein-Gordon equation at the first order in V, namely

$$\phi_{\mathrm{int}}(Pf) = \phi(Pf) + iR_V\left(\frac{\delta V}{\delta\phi}(f)\right),$$

which corresponds to the Schwinger–Dyson equation for the operator ϕ [BS80].

1.2.6 The Operator Product Expansion

According to subsection 1.2.5, the construction of Wick observables takes advantage of the existence of Hadamard states in which the normal-ordered regularization procedure is provided. On the other hand, a choice of state in curved spacetime always implies that some prescriptions for selecting preferred states with peculiar properties should be provided. Actually, this requirement is in contrasts with the fundamental principles of a quantum theory in curved background, where the idea of reference states remain intrinsically ambiguous. Based on this arguments, Hollands and Wald proposed in [HW10] a new framework where formulating a local and covariant quantum field theory on curved spacetimes without any reference to the choice of a state, but founded on the well-posedness of the Operator Product Expansion.

The Operator Product Expansion (OPE, for short) was firstly introduced by Wilson and Zimmermann in [Wil69; WZ72; Zim73] to analyse the short-distances behaviour of composite operators, and it represents now a useful tool in the contexts of High Energy Theory and AdS/CFT correspondence to study interacting and renormalizable quantum theories (for a physical introduction about this topic, see, e.g., [Col86], Chapter 10). Later, it was rigorously formulated in [HW07] for perturbative interacting quantum field theories in curved spacetime, and further deepened in [Frö21] (see also the references cited therein). The OPE consists of as an asymptotic expansion of n local quantum observables in some neighbourhood of the diagonal $x_1 = \cdots = x_n$ of the form

$$\langle \mathcal{O}_{i_1}(x_1) \cdots \mathcal{O}_{i_n}(x_n) \rangle_\omega \sim \sum_k C^k_{i_1 \cdots i_n}(x_1, \ldots, x_n, y) \, \langle \mathcal{O}_k(y) \rangle_\omega \,, \tag{1.101}$$

where $\sim$ in understood in the sense of an asymptotic relation in the limit that $x_1, \ldots, x_n \to y$, and the sum includes all the composite operators of the theory. On the one hand, the set of coefficients

$$\mathbf{C}(\mathcal{M}) = \{ C^k_{i_1 \cdots i_n}(x_1, \ldots, x_n, y) \} \tag{1.102}$$

is state-independent, but it captures the fundamental properties of the underlying quantum theory (the list of these properties is stated in [HW10]); on the other hand, the local fields $\{\mathcal{O}_k(y)\}$ correspond to a collection of new generators of the enlarged CCR algebra in the form of normal-ordered Wick monomials regularized according to the Hadamard point-splitting procedure seen in subsection 1.2.5. Moreover, they are associated to the smooth part $\mathcal{W}(f, g)$ of the Hadamard state (1.59), and hence their expectation values depend intrinsically on the choice of ω. Thus, from an axiomatic point of view, the existence of an asymptotic OPE for a quantum field theory replaces the necessity of a reference state, which is intrinsically non-local, with a short-distance regularity condition for the observables of the theory, which is instead entirely local in its essence. In an algebraic viewpoint, the OPE dictates what kind of relations between the generators of the algebra must be satisfied by an interacting quantum theory.

From a more practical point of view, it would be of interest to understand if a n-point correlation function could be generally reconstructed though its OPE (1.101) in a certain point $y \in \mathcal{M}$, starting from the evaluation of the expectation values of local fields $\langle \mathcal{O}_k(y) \rangle_\omega$. Such a reconstruction issue is, indeed, feasible, at least in principle, because the coefficients (1.102) do not depend on the chosen state, but they can be obtained purely from the properties of the quantum model. At this stage, it has pointed out in [Med18] that the reconstruction of a correlation function is guaranteed when it is associated to an analytic Hadamard state, i.e., a state ω satisfying the analytic microlocal spectrum condition stated in theorem 1.2.5. In this particular case, the smooth part $\mathcal{W}(f, g)$ is a real analytic distribution, and thus its distributional Kernel can be expanded in Taylor series whose radius of convergence is infinite over $\mathcal{M}$; on the contrary, if this smooth part is not an analytic in $y \in \mathcal{M}$, then the reconstruction may not be unique, as shown in [Med18] through a counter-example.

To see an example, let $\omega_2(x', x)$ be the two-point function of an analytic Hadamard state (see subsection 1.2.4) in Minkowski spacetime, whose singular part is fixed by the two-point function $\Delta_+(x', x)$ of the Minkowski vacuum state given in eq. (1.52). Thus, let $\tilde{\mathcal{W}} \doteq \omega_2 - \Delta_+$ be the smooth part of the two-point function according to this normal-ordering prescription. Then, using eq. (1.86) with H_{0^+} replaced by Δ_+, the Operator Product Expansion of ω_2 reads

$$\omega_2(x', x) = \Delta_+(x', x) + \left\langle :\phi^2: \right\rangle_\omega + \sum_{n=1}^N \frac{1}{n!} \left\langle :\phi \, \partial_{\mu_1, \ldots, \mu_n} \phi: \right\rangle_\omega (x' - x)^{\mu_1, \ldots, \mu_n} . \tag{1.103}$$

in account of the translational invariance of the spacetime. The local fields in eq. (1.103) are related to the smooth part $\tilde{\mathcal{W}}(x', x)$ in the coinciding limit $x' \to x$ through the following relation in Fourier space

$$\langle :\phi\, \partial_{\mu_1,\dots,\mu_n}\phi: \rangle_\omega = \lim_{x'\to x}\prod_{i=1}^{n}\partial_{\mu_i}\tilde{\mathcal{W}}(x',x) = (-i)^n\int_{\mathbb{R}^4}\frac{d^4p}{(2\pi)^4}\prod_{i=1}^{n}p_{\mu_i}\hat{\tilde{\mathcal{W}}}(p), \qquad \hat{\tilde{\mathcal{W}}}(p) \doteq \mathcal{F}\{\tilde{\mathcal{W}}(x,x)\}, \tag{1.104}$$

where $\mathcal{F}$ denotes the Fourier transform according to the conventions given in eq. (1.39) (notice that the above integral vanishes for odd n, as consequence of the translational invariance). Namely, local fields correspond to the n-th moment of the function $\hat{\tilde{\mathcal{W}}}(x',x)$ according to the definition stated in [GS21] (see also remark 1.2.4 below).

Now, let Δ_β^+ be the KMS thermal two-point function (1.82), and $\mathcal{W}_\beta$ its real analytic smooth part given in eq. (1.83). In this special case, eq. (1.103) simplifies as follows,

$$\Delta_\beta^+(x'-x) = \Delta_+(x'-x) + \sum_{n=0}^{N}\frac{1}{n!}\mathfrak{M}_\beta(n)(x'-x)^n,$$

where $\mathfrak{M}_\beta(n)$ corresponds to the n-th moment (1.104) of Δ_β^+. On the one hand, in the massless case $(m=0)$

$$\hat{\mathcal{W}}_\beta^{(m=0)}(p) = \frac{2\pi}{2p(e^{\beta p}-1)}(\delta_p+\delta_{-p}), \qquad p \doteq |\vec{p}|,$$

and hence the n-th moment reduces to

$$\mathfrak{M}_\beta^{(m=0)}(n) = \frac{(-1)^n}{2\pi^2}\int_0^\infty p^{2+2n-1}\frac{1}{e^{\beta p}-1}dp.$$

Performing the change of variable $z=\beta p$, and denoting with

$$\mathcal{M}\{f\}(s) \doteq \int_0^\infty z^{s-1}f(z)dz, \qquad z\in\mathbb{C}$$

the one-dimensional Mellin transform of f, then

$$\mathfrak{M}_\beta^{(m=0)}(n) = \frac{(-1)^n}{2\pi^2\beta^{2(n+1)}}\mathcal{M}\left\{\frac{z^2}{e^z-1}\right\}(2n) = \frac{(-1)^n}{2\pi^2\beta^{2(n+1)}}\Gamma(2n+2)\zeta(2n+2),$$

where $\Gamma(z)$ and $\zeta(z)$ denote the Euler Gamma and the Riemann zeta function, respectively.

On the other hand, in the massive case

$$\hat{\mathcal{W}}_\beta(w) = \frac{2\pi}{2\omega\,(e^{\beta w}-1)}(\delta_w+\delta_{-w}), \qquad w = p^2+m^2.$$

Thus, in a similar way as before,

$$\mathfrak{M}_{\beta,m}(n) = \frac{(-1)^n}{2\pi^2}\int_m^\infty w^n\sqrt{w^2-m^2}\frac{1}{e^{\beta w}-1}dw,$$

and hence

$$\begin{aligned}\mathfrak{M}_{\beta,m}(n) &= \frac{(-1)^n m^2}{2\pi^2}\sum_{k\geq 1}\frac{\partial^{2n}}{\partial\beta_k^{2n}}\frac{K_1(\beta_k)}{\beta_k}\\ &= \frac{(-1)^n m^2}{2\pi^2}\sum_{k\geq 1}\left(\Gamma(2n+1)\frac{K_1(\beta_k)}{(\beta_k)^{2n}}+\frac{1}{\beta_k}\sum_{l\geq 0}^{2n}\binom{2n}{l}K_{2l-2n+1}(\beta_k)\right),\end{aligned}$$

where $\beta_k \doteq \beta k$, and $K_n(z)$ is the Bessel modified function of the second type (see, e.g., [AS65]).

Remark 1.2.4. The problem of reconstruction a physical state from a tower of moments was also addressed by Gottschalk and Siemssen in [GS21] in the framework of Cosmology, and in an independent way of the argument stated here for OPEs (actually, the n-th moment of the massless KMS thermal state evaluated before is in agreement with the one obtained in [GS21], Section 4.3).

In this work, the authors study the issue about existence and uniqueness of the semiclassical Einstein equations in cosmological spacetimes (see chapter 2) in terms of moments of a two-point function, and they prove existence of maximal/global solutions to this set of equations for vacuum-like or thermal-like states. However, a similar problem in the reconstruction of a generic state from its moments solving the semiclassical equations arises, because it is not clear, in general, which tower of such moments belong to physical states with positive two-point functions.

1.3 The Semiclassical Einstein Equations

1.3.1 The quantum stress-energy tensor

The evaluation of a quantum stress-energy tensor associated to a quantum field, such as the free Klein-Gordon field, is essential to formulate a theory for the back-reaction of quantum matter upon the spacetime geometry. In this model, it is expected that such a matter content influences the spacetime through the semiclassical Einstein equations

$$G_{\mu\nu} = 8\pi \left\langle :T_{\mu\nu}: \right\rangle_\omega \tag{1.105}$$

in units convention $G = c = 1$. On the one hand, the left-hand side of the semiclassical Einstein equations is well-known from classical General Relativity, whereas, on the other hand, the right-hand side has to be carefully treated in in the framework of a Quantum Field Theory in Curved Spacetimes (see section 1.2). As for the previous sections, the contents of this subsection have been already deepened in other several monographs, such as [BD82; Wal95; Sie15; Hac16], so they shall be mostly recalled here in form of a review.

There are different ways to obtain a renormalized quantum stress-energy tensor $:T_{\mu\nu}:$ of a quantum scalar field, which replaces the usual classical stress-energy tensor entering the classical Einstein equations. For instance, either in a Lagrangian approach, as explained in [BD82], or using the construction of the Wick observable $:T_{\mu\nu}:$ on curved spacetimes, as made, e.g., in [Hac16]. According to the results presented in subsection 1.2.3 and subsection 1.2.5, the second approach shall be adopted in this section to construct a conserved quantum stress-energy tensor in a local, covariant and state-independent way (see also [HW01; Mor03; HW05]).

Historically, Wald introduced in [Wal77] a list of five axioms which $:T_{\mu\nu}:$ had to satisfy in order to enter a semiclassical theory of gravity, in the face of the different renormalization schemes to obtain a renormalized stress-energy tensor. Here, they shall be presented in a more modern reformulation than the original one, according to [Wal95; BFV03; Hac16].

- **First axiom**. Given two states ω, ω' such that

  $$\left\langle \phi(x')\phi(x) \right\rangle_\omega - \left\langle \phi(x')\phi(x) \right\rangle_{\omega'} \in \mathcal{C}^\infty(\mathcal{M} \times \mathcal{M}),$$

  then $\left\langle :T_{\mu\nu}: \right\rangle_\omega - \left\langle :T_{\mu\nu}: \right\rangle_{\omega'}$ is given by a suitable point-splitting prescription for obtaining $:T_{\mu\nu}:$ on $\mathcal{M}$. For Hadamard states, this is the Hadamard point-splitting regularization stated in (1.86).

- **Second axiom**. $\left\langle :T_{\mu\nu}: \right\rangle_\omega$ is local and covariant in the following sense. Let $(\mathcal{M}, g_{\mu\nu})$, $(\mathcal{M}, g_{\mu\nu})'$ be two globally hyperbolic spacetimes, and $\mathcal{O} \subset \mathcal{M}$, $\mathcal{O}' \subset \mathcal{M}'$ two open subsets. Given $x \in \mathcal{O}$, denote with $\chi : \mathcal{O} \hookrightarrow \mathcal{O}'$ any isometric embedding preserving both orientation and time orientation, such that $x' = \chi(x) \in \mathcal{O}'$. Let α_χ be the related canonical

$\star$-isomorphism between the two local CCR algebras $\mathcal{A}(\mathcal{O}, g_{\mu\nu})$ and $\mathcal{A}(\mathcal{O}, g_{\mu\nu})'$, which can be identified though the isometry; thus, $\omega = \omega' \circ \alpha_\chi$. Then, the stress-energy tensor evaluated at x in ω is equal to the the stress-energy tensor evaluated at x' in ω'.

- **Third axiom**. $\langle :T_{\mu\nu}: \rangle_\omega$ is covariantly conserved, i.e.,

$$\nabla^\mu \langle :T_{\mu\nu}: \rangle_\omega (x) = 0. \tag{1.106}$$

- **Fourth axiom**. $\langle :T_{\mu\nu}: \rangle_\omega$ vanishes in the Minkowski vacuum state.
- **Fifth axiom**. $\langle :T_{\mu\nu}: \rangle_\omega$ does not contain derivatives of the metric of order higher than two.

On the one hand, the first three axioms are essential to formulate a well-posed semiclassical theory of gravity in accordance with eq. (1.105) and the discussions made in the previous sections. On the other hand, the fourth axiom is not fundamental in Semiclassical Gravity, because a preferred choice of “vacuum” is actually ambiguous in curved spacetimes, and hence it can be omitted. Finally, the fifth axiom is the most problematic statement: it was introduced in order to obtain an initial-value formulation for the semiclassical Einstein equations which was similar to the classical case, and hence avoiding the problem of runaway solutions in higher-order theories of gravity (see subsection 4.1.1). However, even Wald himself realized that it cannot be satisfied, e.g., in massless theories, and hence it must be discard [Wal78b].

The classical stress-energy tensor of a free Klein-Gordon field obtained as functional derivative of the action given in eq. (1.28), i.e.,

$$T_{\mu\nu} \doteq \frac{2}{\sqrt{|\det(g)|}} \frac{\delta S_0(\phi, g_{\mu\nu})}{\delta g^{\mu\nu}} \tag{1.107}$$

is

$$T_{\mu\nu} = \nabla_\mu \phi \nabla_\nu \phi - \frac{1}{2} g_{\mu\nu} \left(\nabla_\rho \phi \nabla^\rho \phi + m^2 \phi^2 \right) + \xi \left(G_{\mu\nu} \phi^2 - \nabla_\mu \nabla_\nu \phi^2 + g_{\mu\nu} \nabla_\rho \nabla^\rho \phi^2 \right). \tag{1.108}$$

Its quantum counterpart $:T_{\mu\nu}:$ can be obtained by replacing the classical field with their normal-ordered quantum observables. Since $\nabla_\mu \phi \nabla_\nu \phi = (1/2) \nabla_\mu \nabla_\nu \phi^2 - \phi \nabla_\mu \nabla_\nu \phi$, one just needs to construct the Wick observables $\Psi \doteq :\phi^2:$ and $\Psi_{\mu\nu} \doteq :\phi \nabla_\mu \nabla_\nu \phi:$. According to the Hadamard point-splitting regularization and the form of the Hadamard state given in eq. (1.59),

$$\begin{aligned} \langle :\phi^2: \rangle_\omega (x) &= \lim_{x' \to x} \left(\langle \phi(x') \phi(x) \rangle_\omega - H_{0^+}(x', x) \right) = \lim_{x' \to x} \mathcal{W}(x', x), \\ \langle :\phi \nabla_\mu \nabla_\nu \phi: \rangle_\omega (x) &= \lim_{x' \to x} \nabla^{(x)}_\mu \nabla^{(x)}_\nu \left(\langle \phi(x') \phi(x) \rangle_\omega - H_{0^+}(x', x) \right) = \lim_{x' \to x} \nabla^{(x)}_\mu \nabla^{(x)}_\nu \mathcal{W}(x', x), \end{aligned} \tag{1.109}$$

and hence

$$\langle :T_{\mu\nu}: \rangle_\omega (x) = \lim_{x' \to x} D_{\mu\nu} \mathcal{W}(x', x), \tag{1.110}$$

where

$$D_{\mu\nu} = (1 - 2\xi) g_\mu^{\mu'} \nabla_{\mu'} \nabla_\nu - 2\xi \nabla_\mu \nabla_\nu + \xi G_{\mu\nu} + g_{\mu\nu} \left\{ 2\xi \Box_g + \left(2\xi - \frac{1}{2} \right) g_\rho^{\rho'} \nabla_{\rho'} \nabla^\rho - \frac{1}{2} m^2 \right\} \tag{1.111}$$

is the bi-differential operator which realizes the point-splitting of $:T_{\mu\nu}:$, and $\mathcal{W}(x', x)$ is the smooth part of the Hadamard state ω. In this expression, unprimed and primed indices denote covariant derivatives in the points x and x', respectively, while $g_\nu^{\nu'}$ is the bitensor of parallel transport [Mor03; Hac16].

According to the construction of the Wick observables Ψ, $\Psi_{\mu\nu}$, there is a finite number of renormalization freedoms inside the definition of $:T_{\mu\nu}:$, and thus a finite number of renormalization constants to fix. In this case,

$$:\tilde{T}_{\mu\nu}: = :T_{\mu\nu}: + c_1 m^4 g_{\mu\nu} + c_2 m^2 G_{\mu\nu} + \alpha I_{\mu\nu} + \beta J_{\mu\nu}, \qquad c_1, c_2, \alpha, \beta \in \mathbb{R}. \tag{1.112}$$

The last two contributions are conserved local tensors obtained by taking R^2 and $R_{\alpha\beta}R^{\alpha\beta}$ as Lagrangian densities [Wal78b; Hac16], namely

$$I_{\mu\nu} \doteq \frac{1}{\sqrt{|\det(g)|}} \frac{\delta}{\delta g^{\mu\nu}} \int_{\mathcal{M}} R^2 \mathrm{d}_g x = -g_{\mu\nu}\left(\frac{1}{2}R^2 + 2\Box_g R\right) + 2\nabla_\mu \nabla_\nu R + 2RR_{\mu\nu} \tag{1.113}$$

$$\begin{aligned} J_{\mu\nu} &\doteq \frac{1}{\sqrt{|\det(g)|}} \frac{\delta}{\delta g^{\mu\nu}} \int_{\mathcal{M}} R_{\alpha\beta}R^{\alpha\beta} \mathrm{d}_g x \\ &= -\frac{1}{2} g_{\mu\nu}\left(R_{\alpha\beta}R^{\alpha\beta} + \Box_g R\right) + \nabla_\mu \nabla_\nu R - \Box_g R_{\mu\nu} + 2R_{\alpha\beta}R^{\alpha}{}_{\mu}{}^{\beta}{}_{\nu}, \end{aligned} \tag{1.114}$$

where $\Box_g$ denotes the d'Alembert operator built over g. For conformally flat spacetimes like the cosmological ones, $I_{\mu\nu} = 3J_{\mu\nu}$. These higher-order derivative tensors span the whole space of conserved fourth order local curvature tensors - *cf.* [Sie15], Proposition 7.1. In the Lagrangian approach, adding $I_{\mu\nu}$ and $J_{\mu\nu}$ in the semiclassical equations (1.105) corresponds to modify the Einstein-Hilbert Lagrangian with higher-order curvature contributions, such that

$$\begin{aligned} \mathcal{L}(g_{\mu\nu}, \phi) &= \mathcal{L}_{EH}(g_{\mu\nu}) + \mathcal{L}_{MG}(g_{\mu\nu}) + \mathcal{L}_0(\phi) \\ &= \frac{R - 2\Lambda}{16\pi} + \alpha R^2 + \beta R_{\mu\nu}R^{\mu\nu} - \frac{1}{2}\left(\nabla_\varrho \phi \nabla^\varrho \phi + (m^2 + \xi R)\phi^2\right) \end{aligned} \tag{1.115}$$

in units convention $G = c = 1$.

Remark 1.3.1. There is a third local curvature tensor which can be added, in principle, to the renormalization freedoms of $:T_{\mu\nu}:$ in eq. (1.112). This is

$$K_{\mu\nu} \doteq \frac{1}{\sqrt{|\det(g)|}} \frac{\delta}{\delta g^{\mu\nu}} \int_{\mathcal{M}} R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta} \mathrm{d}_g x, \tag{1.116}$$

and it is provided by adding the higher-order term $R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta}$ in the Lagrangian (1.115), see [Ste78]. However, using the generalized Gauss-Bonnet-Chern theorem [Alt95], one infers that in four dimensions

$$R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta} - 4R_{\alpha\beta}R^{\alpha\beta} + R^2 \tag{1.117}$$

is a total functional derivative of the metric, and thus it does not contributes to equations of motion when added to the Einstein-Hilbert action. Hence, the following relation holds

$$K_{\mu\nu} = I_{\mu\nu} - 4J_{\mu\nu}. \tag{1.118}$$

Therefore, $K_{\mu\nu}$ can be removed from the list of local curvature tensors. The internal consistency is confirmed after proving that the regularized Einstein-Hilbert quantum gravity theory at one loop order automatically yields a renormalization freedom expressed in terms of R^2 and $R_{\alpha\beta}R^{\alpha\beta}$, and without $R_{\alpha\beta\gamma\delta}R^{\alpha\beta\gamma\delta}$, see [HV74].

1.3.2 The trace anomaly

As firstly discussed in [Wal78b], the differential operator obtained in eq. (1.111) is not covariantly-conserved anymore, because a the geometric Hadamard bidistribution $H_{0^+}(x', x)$ does not fulfil the equation of motion associated to the Klein-Gordon operator (see the remark 1.3.2 below). However, with a proper choice of the renormalization freedoms associated to Ψ and $\Psi_{\mu\nu}$ [HW05], or alternatively, after adding the total derivative term $(1/3)g_{\mu\nu}P$ in eq. (1.108) [Mor03], one can obtain a renormalized quantum stress-energy tensor $:T_{\mu\nu}:$ which is also covariantly conserved. Its expectation value reads

$$\langle :T_{\mu\nu}: \rangle_\omega = [D_{\mu\nu}\mathcal{W}] + \frac{1}{4\pi^2} g_{\mu\nu}[v_1] + c_1 m^4 g_{\mu\nu} + c_2 m^2 G_{\mu\nu} + \alpha I_{\mu\nu} + \beta J_{\mu\nu}, \tag{1.119}$$

where $[v_1](x)$ is the coinciding point limit of the Hadamard coefficient $v_1(x', x)$ given by eq. (1.66), while the state-dependent contribution given in eq. (1.110) can be expressed in terms of the expectation values evaluated in eq. (1.109). With the addition of the contribution proportional to $[v_1]$, the quantum stress-energy tensor given in eq. (1.119) yield the conservation equation (1.106). Thanks to this construction, the expectation value of the quantum stress-energy tensor given in eq. (1.119) can enter the right-hand side of the semiclassical Einstein equations (1.105). On the other hand, this set of partial differential equations involves up to fourth-order derivatives of the metric, due to the presence of the local conserved tensors $I_{\mu\nu}$ and $J_{\mu\nu}$ appearing in $\langle :T_{\mu\nu}: \rangle_\omega$, in striking contrast with their classical counterparts (see chapter 4).

The price to pay to obtain a covariantly conserved expectation value of $:T_{\mu\nu}:$ is the violation of the classical conformal invariance of $T_{\mu\nu}$ (see [Duf77] for a general review about this topic). This is reflected in the additional local term proportional to $[v_1]$, which depends only on the geometry of the spacetime, but not on the choice of the Hadamard state, and it cannot be removed by choosing the renormalization constants in eq. (1.112). In fact, it corresponds to the so-called trace anomaly of the quantum stress-energy tensor. Namely, the four-dimensional trace of $\langle :T_{\mu\nu}: \rangle_\omega$ does not vanish for a massless, conformally coupled field, i.e., when $m = 0$ and $\xi = 1/6$, unlike its classical counterpart on-shell. For a free scalar field ϕ, it reads

$$\langle :T_\rho{}^\rho: \rangle_\omega^{(\mathrm{an})} = \frac{1}{4\pi^2}[v_1] = \lambda \left(C_{\alpha\beta}{}^{\gamma\delta} C_{\gamma\delta}{}^{\alpha\beta} + R_\mu{}^\nu R_\nu{}^\mu - \frac{1}{3}R^2 \right), \tag{1.120}$$

where

$$\lambda \doteq \frac{1}{720(4\pi^2)}. \tag{1.121}$$

The contributions depending on m^4, $m^2 R$, and $\Box_g R$ appearing in $\langle :T_\rho{}^\rho: \rangle_\omega$ through $[v_1]$ were removed by the anomalous contribution, because they actually can be reabsorbed in the renormalization freedoms of the semiclassical theory, in accordance with eq. (1.112). Indeed, in the case of $\langle :T_\rho{}^\rho: \rangle_\omega$, the renormalization scalar freedom is [HW05]

$$Q = 4c_1 m^4 - c_2 m^2 R + \gamma \Box_g R, \tag{1.122}$$

where $\gamma = -(6\alpha + 2\beta)$ is obtained by the relation $I^\mu{}_\mu = 3J^\mu{}_\mu = -6\Box_g R$. In the special case of massless, conformally coupled fields, the term $\Box_g R$ can be always cancelled by choosing properly the renormalization constant γ, thus meeting the requirement that curvature terms do not contain non-classical higher-order derivatives of the metric: in fact, in this special case and at the level of the trace, Wald's fifth axiom holds. In the end, the trace of the quantum stress-energy tensor for an arbitrary quantum scalar field can be written as

$$\langle :T_\rho{}^\rho: \rangle_\omega = \left(3\left(\xi - \frac{1}{6} \right) \Box - m^2 \right) \langle :\phi^2: \rangle_\omega + \frac{1}{4\pi^2}[v_1] + 4c_1 m^4 - c_2 m^2 R + \gamma \Box_g R, \tag{1.123}$$

where $[v_1]$ was given by eq. (1.66), and $\langle :\phi^2: \rangle_\omega$ was evaluated in eq. (1.109) in the Hadamard point-splitting regularization.

Remark 1.3.2. The same anomalous contribution proportional to $[v_1]$ appears both in $\langle :T_{\mu\nu}: \rangle_\omega$ and in $\langle :T_\rho{}^\rho: \rangle_\omega$, after using the following identities

$$[P_x H_{0^+}] = -\frac{3}{4\pi^2}[v_1], \qquad [(P_x H_{0^+})_{;\mu'}] = -\frac{1}{4\pi^2}[v_1]_{;\mu}$$

in the notation for bitensors explained in subsection 1.2.3. For further details about the computation, see [Mor03; Hac16].

Eventually, the formula of the trace given in eq. (1.123) enters the traced semiclassical Einstein equations, which read as

$$-R + 4\Lambda = 8\pi G \langle :T_\rho{}^\rho: \rangle_\omega \tag{1.124}$$

after restoring both the Newton constant G and the cosmological constant Λ. Hence, changing c_1 and c_2 in eq. (1.122) corresponds to a renormalization of the "bare" Λ and G, respectively (about this point, see also the seminal analysis made in [UD62]). On the contrary, the remaining constant γ has no classical interpretation, because it is associated to a contribution of modified gravity which depends locally on the fourth-order derivative of the metric.

1.3.3 Quantum energy inequalities

As anticipated in subsection 1.1.3, classical pointwise energy conditions in General Relativity are often violated by both classical fields and their quantum counterparts. Several reviews can be found in literature about quantum energy inequalities, but a good starting point to introduce the topic may be represented by Fewster's lectures [Few12] and Kontou and Sanders' review [KS20], where many recent results of physical interest are cited. In fact, the brief recap presented in this subsection is mostly based on these papers and on the references therein.

At a quantum stage, a good definition of positive local energy density $\langle :T_{00}(f): \rangle_\omega \geq 0$ is fundamentally incompatible with the usual postulates of local field theory, even for states with vanishing vacuum expectation values [EGJ65]. However, the phenomenology of negative energy in quantum field theory should not surprise the reader who is familiar with the Casimir effect [Cas48]. Indeed, it represents one of the most famous experiment in which negative energy was measured, in form of vacuum polarization induced by electromagnetic fields. Although pointwise energy conditions are usually violated by quantum fields, a notion of positive energy can be often recovered in an averaged sense, after smearing the expectation values of the quantum stress-energy tensor with non-negative sampling functions. The seminal results obtained in flat spacetime by Ford and Roman in [For91; FR95; FR97] (see also the discussion in [FW96] by Flanagan and Wald) confirmed that the negative energy arising from the expectation value of the energy density in arbitrary physical quantum states can be bounded from below, and thus made vanished in sufficiently large interval of times.

More generally, a quantum energy condition for the energy density $\varrho = T_{\mu\nu}t^\mu t^\nu$ measured by a timelike geodesic with tangent vector t^μ has the form of

$$\langle :\varrho(f): \rangle_\omega \geq -\langle Q(f) \rangle_\omega \,, \tag{1.125}$$

where $f \in \mathcal{D}(\mathcal{M})$ is a suitable positive sampling function, while the operator $Q(f)$ can be unbounded from below (for an explicit example of quantum energy inequality applied to the local energy density $\langle :T_{00}: \rangle_\omega$ in four-dimensional flat spacetime, see, e.g., [FE98]). Following the statements described in subsection 1.2.3, the left-hand side of eq. (1.125) is the expectation of a Wick observable associated to the renormalized quantum stress-energy tensor given in eq. (1.119), thus it is evaluated in a Hadamard state ω according to the Hadamard point-splitting regularization described in eq. (1.86). As this prescription is local and covariant, $Q(f)$ depends only on the spacetime geometry, and hence the right-hand of eq. (1.125) does not depend on the chosen state

ω, but it is an absolute bound on the energy. On the contrary, whenever the regularization is prescribed by subtracting a reference state ω_0, the associate inequality is a different quantum energy condition, and thus the operator $Q(f)$ may depend on the choice of both the quantum states ω and ω_0 (for an explicit example, see, e.g., [Few00]).

Therefore, an absolute quantum energy condition which does not involve the choice of a particular reference state, and thus giving a direct bound on the renormalized quantum stress-energy tensor, should be preferable in curved spacetimes. This result was achieved in [FS08] for massive scalar fields and n-dimensional globally hyperbolic spacetimes, where the following theorem was proved on timelike worldline and worldvolumes[9].

Theorem 1.3.1. *Let Σ be a n-dimensional timelike submanifold Σ with induced metric $h_{\mu\nu}$ of a globally hyperbolic spacetime $(\mathcal{M}, g_{\mu\nu})$ which can be covered by a single hyperbolic coordinate chart, i.e., a coordinate system $x_0, \dots x_{n-1}$ such that ∂_0 is a future-pointing timelike vector field, and all causal covectors u_0 on Σ satisfy*

$$c|u_0| \geq \sqrt{\sum_{j=0}^{n-1} u_j^2},$$

where the speed of light c is associated to the time coordinate x_0. Denote with $\kappa : \Sigma \to \mathbb{R}^n$, $\kappa(p) = \left(x^0(p), \dots, x^{n-1}(p)\right)$ the corresponding hyperbolic coordinate map. Let $\mathfrak{D}$ be a partial differential operator at most of order one with smooth real-valued coefficients in a neighbourhood of Σ, and

$$\tilde{H}_k(x, x') \doteq \frac{1}{2} \left(\mathfrak{H}_k(x, x') + \mathfrak{H}_k(x', x) + i\Delta(x, x') \right),$$

where

$$\mathfrak{H}_k(x, x') = H_k(x, x') + \frac{1}{8\pi^2} \sum_{j=0}^{k} w_j(x, x') \sigma(x, x')^j$$

is the Hadamard series composed by the sum of the truncated Hadamard parametrix (1.60) and a smooth reminder of orders k, with $k = max\{n + 3{,}5\}$.

Then, for any $f \in \mathcal{D}(\Sigma)$ and any Hadamard state of the form given in eq. (1.59) the following inequality holds:

$$\int_\Sigma f^2(x) \left((\mathfrak{D} \otimes \mathfrak{D})(\omega_2 - H_{0^+}) \right)(x, x) \sqrt{|h|} \mathrm{d}^n x \geq -\mathcal{B}_A > -\infty, \tag{1.126}$$

where

$$\mathcal{B}_A \doteq 2 \int_{\mathbb{R}^+ \times \mathbb{R}^{n-1}} \frac{\mathrm{d}^n p}{(2\pi)^n} \mathcal{F} \left\{ |h_\kappa|^{1/4} f_\kappa \otimes |h_\kappa|^{1/4} f_\kappa \theta_\kappa^* \left(\mathfrak{D} \otimes \mathfrak{D} \tilde{H}_k \right) \right\} (-p, p), \tag{1.127}$$

h_κ is the determinant of $\kappa^* h$, and θ_κ^* is the pull-back of the function to Σ.

Eq. (1.126) can be applied to the renormalized quantum stress-energy tensor, according to the results presented in subsection 1.3.1 and subsection 1.3.2. In this case, the bi-differential operator was defined in eq. (1.111), and, furthermore, the following integral

$$\int_\Sigma f(x)^2 \left(c_1 m^4 g_{\mu\nu} + c_2 m^2 G_{\mu\nu} + \alpha I_{\mu\nu} + \beta J_{\mu\nu} + \frac{1}{4\pi^2} [v_1] g_{\mu\nu} \right)(x) \sqrt{|\det(h)|} \mathrm{d}^n x$$

has to be added in $\mathcal{B}_A$ to take into account both the renormalization freedoms and the anomalous trace of $\langle :T_{\mu\nu}: \rangle_\omega$ given in eqs. (1.112) and (1.120), respectively.

[9]The author thanks E.A. Kontou for indicating him this theorem in literature.

Remark 1.3.3. The application of eq. (1.126) in four-dimensional spacetimes is rather different in case of null worldlines, because quantum energy inequalities may not hold along null geodesics, as explained in [FR03], where an example of violation of null quantum energy inequalities in Minkowski spacetime was shown.

The application of eq. (1.126) to the quantum stress-energy tensor is an example of averaged energy condition, i.e., a quantum energy inequality applied to the stress-energy tensor of a matter theory and averaged over a certain region of the spacetime. A special case are the averaged weak energy conditions, which are usually non-local constraints of the form [WY91]

$$\liminf_{\lambda\to\infty} \int_{\mathbb{R}} f(t/\lambda)^2 k^\mu k^\nu \left\langle :T_{\mu\nu}: \right\rangle_\omega (\gamma(t)) \mathrm{d}t \geq 0, \tag{1.128}$$

where $k = \dot{\gamma}(t)$ is the tangent vector to the affine-parametrized timelike (or null) geodesic γ, and f is a real-valued smooth function having compact support in the domain of γ. In a similar way than quantum energy inequalities, conditions like eq. (1.128) can also hold outside the limit and employing a specific sampling function for a restricted class of vacuum-like reference states. The sampling functions are often positive and smooth everywhere in their domain, and also decay sufficiently fast at infinity. Some common choices are quasi-free functions or compactly supported test functions having exponential decay in Fourier space, for instance. Although classical fields, and hence their quantum version, usually violate pointwise energy conditions, averaged energy conditions can hold in more general terms, even in the non-minimally coupled case and for different values of ξ. For further references and examples about this topic, see, e.g., [WY91; FO06; FO08; FFR10; Kon15].

Chapter 2

Semiclassical Gravity in Cosmological Spacetimes

" I am not aware of any sensible theory of how classical gravity could interact with quantum matter, and I can't imagine how such a theory might work."

Alan Guth

Summary

The content of this chapter is fully based on author's publication [MPS21], where a proof about the existence and uniqueness of local solutions of the semiclassical Einstein equations is provided in cosmological spacetimes, for arbitrary values of the coupling parameter ξ in the Klein-Gordon equation (1.29). The importance of studying the well-posedness of an initial-value problem lies in the fact that it would guarantee the fundamental result of having a well-behaved evolution of our Universe starting from its initial conditions, fixed at the beginning of the Inflation. Once this result is achieved, the evolution of the very early Universe could be thus investigated in details, even from a numerical point of view, in order to deeply understand how quantum matter fields have significantly influenced the cosmological geometry in the inflationary phase.

Previously, significant results were obtained in [Pin11; PS15a] for the conformally-coupled case, while in [GS21] a different approach to solve eqs. (1.105) was proposed in terms of a sequence of "moments" for the quantum state. Numerical analyses of the semiclassical Einstein equations in cosmology have been made by Anderson in the past in [And83; And84; And85; And86], and more recently by several authors in [Hac16; MW20; GRS22].

The key point of the analysis performed by the author and his collaborators consists of showing that the problematic non-local term in the traced semiclassical equations is contained in the vacuum polarization, and it is independent of the choice of the sufficiently regular state in which computing the renormalized stress-energy tensor. This high-order derivative contribution appears in form of a non-local, retarded, and unbounded operator, which indeed forbids a direct analysis of the equation: in particular, standard recursive approaches to approximate the solution fail to converge. However, after partial integration of the semiclassical Einstein equations, it is proved that an inversion formula for this operator can be given, and the (retarded) inverse happens to be more regular than the direct operator. Thus, the found inversion formula is applied to the traced

semiclassical Einstein equations, which acquire the form of a fixed point equation. Therefore, the proof of local existence and uniqueness of the solution of the semiclassical Einstein equations is achieved by applying the Banach fixed point theorem.

This chapter is organized as follows. In section 2.1 the class of Friedmann-LeMaître-Robertson-Walker spacetimes (FLRW for shorts) and the formulation of a quantum field theory in the cosmological framework are presented, with a brief mention to the mechanism of Inflation, see subsection 2.1.1 and subsection 2.1.2; moreover, some cosmological solutions of the semiclassical Einstein equations, which models the evolution of the early universe under quantum matter effects are reviewed in subsection 2.1.3. Then, it is shown in section 2.2 that eqs. (1.105) admit a well-posed local initial-value problem in cosmological spacetimes, for arbitrary values of the coupling parameter ξ. In this respect, a discussion about the existence of sufficiently regular states where computing $\langle :T_\rho{}^\rho: \rangle_\omega$, $\langle :\varrho: \rangle_\omega$, and $\langle :\phi^2: \rangle_\omega$ is given in subsection 2.2.1 and subsection 2.2.2 (see also appendix B). All these results are fully based on author's publication. Thus, a proof of the existence and uniqueness of local solutions is discussed in subsection 2.2.3, subsection 2.2.4, and subsection 2.2.5, with particular emphasis on how to obtain a contraction map from the inversion a non-local, unbounded operator hidden inside the vacuum polarization, which represents the source of the regularity issues in the semiclassical problem.

2.1 Cosmological Spacetimes

2.1.1 FLRW spacetimes and Inflation

The content of this section is devoted to present the geometric setup of cosmological spacetimes, and to give some basic informations about inflation. These topics are covered by standard text-books about Cosmology, see, e.g., [Dod03; Muk05; Wei08].

According to the cosmological principle and recent observations, our universe is homogeneous and isotropic at large scales and it is essentially spatially flat (here, "large" means scales of the size of galaxy super-clusters, i.e., of the order of 10^8 light-years). Hence, it can be accurately described by a flat Friedmann-Lemaître-Robertson-Walker spacetime $(\mathcal{M}, g_{\mu\nu})$ where $\mathcal{M} = I_t \times \Sigma$, $I_t \subset \mathbb{R}$ is an interval of time and Σ is a three dimensional Euclidean space. The line element of the spacetime is given in cosmological coordinates (t, x^1, x^2, x^3) by

$$\mathrm{d}s^2 = -\mathrm{d}t^2 + a(t)^2 \sum_{i=1}^{3} \mathrm{d}x^i \mathrm{d}x^i, \tag{2.1}$$

where the Euclidean coordinates $\vec{x} = (x^1, x^2, x^3)$ are the comoving coordinates of an isotropic observer while t denotes cosmological time. The strictly positive function $a(t)$ is the scale factor which is the unique degree of freedom of the spacetime. It describes the "history" of our universe and is determined by solving the Einstein equations.

Every flat FLRW spacetime is conformally flat as can be seen writing the metric (2.1) with respect to the conformal time

$$\tau \doteq \tau_0 + \int_{t_0}^{t} \frac{\mathrm{d}\eta}{a(\eta)}. \tag{2.2}$$

In local conformal coordinates $(\tau, \vec{x})$, the metric is

$$\mathrm{d}s^2 = a(\tau)^2 \Big(-\mathrm{d}\tau^2 + \sum_{i=1}^{3} \mathrm{d}x^i \mathrm{d}x^i \Big), \tag{2.3}$$

i.e., FLRW spacetimes are conformally related to the Minkowski spacetime by a conformal transformation whose conformal factor is $a(\tau)$. In this work, one shall consider the scale factor $a(\tau)$

as a function of the conformal time, and such that the Hubble rate $H \doteq \dot{a}/a$ is a strictly positive function, as suggested by experiments. Namely, the cosmological observations shows an expanding universe in time; hence, H_0 denotes the Hubble constant, that is, the Hubble function measured today [1].

Remark 2.1.1. As already pointed out for instance in [ANA15], the semiclassical Einstein equations for $\xi \neq \frac{1}{6}$ involves always up to four time derivatives of the scale factor $a(\tau)$, due to the mass dimension of the stress-energy tensor as composite operator, which is equal to four. Thus, in the case of strong solutions, $a(\tau)$ has to be at least a C^4 function.

The request of having an homogeneous and isotropic solution imposes constraints on the stress-energy tensor which sources the Einstein equations: both in comoving and in conformal coordinates, it must have the form of a perfect fluid (1.18) with respect to a comoving geodesic. Therefore, $T_\mu{}^\nu = \mathrm{diag}(-\varrho, p, p, p)$, in which the relation between energy density ϱ and pressure p is dictated by the equation of state $p = w\rho$, where $w = 0{,}1/3, -1$ for matter, radiation, and dark energy, respectively.

In FLRW spacetimes, the Einstein equations reduce to the so-called Friedmann equations

$$H^2 = \frac{8\pi G}{3}\varrho + \frac{\Lambda}{3}, \qquad \frac{\ddot{a}}{a} = -\frac{4\pi}{3}(\varrho + 3p). \tag{2.4}$$

Since the stress-energy tensor is covariantly conserved, i.e., $\nabla_\mu T^\mu{}_\nu = 0$, the dynamics of a can be equivalently determined by the traced Einstein equations

$$-R + 4\Lambda = 8\pi T_\rho{}^\rho, \tag{2.5}$$

together with an initial condition which corresponds to the validity of the first Friedmann equation at an initial time $\tau = \tau_0$, i.e.,

$$H(\tau_0)^2 = \frac{8\pi}{3}\varrho(\tau_0) + \frac{\Lambda}{3}. \tag{2.6}$$

To perform a semiclassical analysis, it is convenient to adopt this second set of equations, in order to employ the traced semiclassical Einstein equations given in (1.124) as a dynamical equation for the vacuum polarization $\langle :\phi^2: \rangle_\omega$.

The mechanism of inflation was introduced in [Gut81; AS82; Lin82; Sta82] to pose some initial condition on the evolution of our Universe and solve some phenomenological puzzles arising from cosmological observations. The main issues concern the so-called horizon and flatness problems: in the first case, the early Universe is assumed to be highly homogeneous, even if it is formed by causally separated regions in the past; in the second case, the initial value of the Hubble constant H_0 must be carefully fine-tuned to obtain a flat universe like the one we observe today.[2]

A immediate solution to this class of problems is to hypothesize a very early phase of huge expansion, in which the so-called comoving Hubble radius $\mathcal{R} \doteq (aH)^{-1}$ has been decreased very fast, that is, $\mathrm{d}\mathcal{R}/\mathrm{d}t < 0$; thus, the Universe has been strongly accelerated during the expansion, with $\ddot{a} > 0$, under the action of a "repulsive gravity". On the one hand, this mechanism allows that different regions of the universe which where in causal contact which each other in the past

[1] Derivatives with respect to conformal time will be denoted by primes and derivatives with respect to cosmological times by dots, i.e., for the first derivatives of a time-dependent function f we write f' and $\dot{f}$, respectively.

[2] There exist, actually, other cosmological arguments which can be explained by Inflation, such as the absence of magnetic monopoles or the anisotropy of the cosmic background radiation observed today; moreover, an inflationary phase is able to give an origin to the Hubble expansion assumed for our Universe, and a plausible reason to motivate why it became so big and so manifold in its inner components.

appear causally disconnected today; on the other hand, it explains why the Universe has been driven towards a flat configuration immediately after the beginning of its expansion, because it destroys possible spatial curvature present at the early stages.

To obtain a repulsive gravity, i.e., $\ddot{a} > 0$, from the first Friedmann equation given in eq. (2.4) one must obtain that $\varrho + 3p < 0$, namely the classical energy conditions must be violated during inflation. Such a violation happens, e.g., when the universe is dominated by the cosmological constant Λ: in this case, $p_\Lambda = -\varrho_\Lambda$, and the solution of the Einstein equations is a de Sitter space with scale factor

$$a_\Lambda(t) = \frac{1}{H_\Lambda} \exp(H_\Lambda t), \qquad H_\Lambda = \sqrt{\frac{8\pi\varrho_\Lambda}{3}}, \tag{2.7}$$

see [Muk05].

The motivation to consider quantum field theory in curved cosmological spacetimes is founded on the idea that the interplay between matter-energy content and gravity can be described by quantum matter fields interacting with the spacetime geometry. In this viewpoint, the quantum stress-energy tensor associated to a quantum matter field, and entering the semiclassical Einstein equations (1.105), has driven the evolution of the Universe in the early stages, in particular during the inflationary phase. The simplest way to introduce an inflationary phase into the expanding Universe is to assume that an effective scalar field ϕ, the so-called "inflaton field", firstly drove the de Sitter quasi-exponential expansion, in which the "vacuum energy density" of ϕ played the role of cosmological constant. Hence, the same field drove the Universe into a phase of decelerated expansion, dominated by radiation first, then by matter. Besides, both the cosmic microwave background anisotropies and the primordial density perturbations could be originated from the small-scale quantum fluctuations of ϕ. In this viewpoint, the related scalar perturbations have been given rise to the seeds of structure formation at large scales during the inflationary phase, see [MC81; GP82; MFB92; Sta82] and the monographs [LL00; Dur20]. For some general accounts about the present status of inflationary cosmology, see, e.g., [Bau11; Lin15; CMRV19].

One of the first realistic models of inflationary Universe was proposed by Starobinsky in [Sta80]. In this paper, he showed that a semiclassical analysis provided by eqs. (1.105) can give a class of solutions in which the evolution of our early Universe is described by a de Sitter initial state with constant curvature (see subsection 2.1.3). In addition, this model of inflation avoids the so-called graceful exit problem posed by Guth in [Gut81]: in fact, at a certain state in the history of the Universe, there should exist a mechanism which allows to exit from the inflationary phase and to reach a new stage. In Guth's model, now known as "old inflation", the classical scalar field is located in a local, but not global, minimum of its potential $V(\phi)$ during the inflationary phase, that is, a supercooled false vacuum state. However, as the rate of decay is too shorter than the expansion rate, the false vacuum never disappears, and hence the inflationary phase continues to persist eternally (see [Gut07] for a more recent 6review about eternal inflation). A solution to this problem was found by Linde in [Lin82], and then by Albrecht and Steinhardt shortly after in [AS82], in a new formulation of inflation. In this improved model, the false decaying state slowly rolls down into the true vacuum state in such a way that inflation comes to the end due to a spontaneous symmetry breaking. Thus, in the slow-roll approximation $\dot{\phi} \ll V(\phi)$, one can obtain an equation of state associated to the stress-energy tensor of the inflaton ϕ which mimics a cosmological constant: $p_\phi = w_\phi \varrho_\phi$, where $w_\phi \simeq -1$. Hence, a new phase of reheating follows, in which the new quantum fields which start to populate the Universe are produced (see fig. 2.1).

Since both old and new inflation assume some initial configuration for the Universe, such as thermal equilibrium and homogeneity from the very beginning, Linde proposed in [Lin83] a new scenario called chaotic inflation, in which the slow-rolling mechanism was driven by the quantum fluctuations of the inflaton field, without assuming thermal equilibrium. This scenario may happen, in principle, for different behaviours of the potential $V(\phi)$ having a flat region, such as the one considered in the action (1.28), namely

$$V(\phi) = -\frac{1}{2}m^2\phi^2 - \frac{1}{2}\xi R\phi^2. \tag{2.8}$$

For further examples of potentials, see, e.g., [Far96], while see [GBL95] for other different regimes describing inflationary cosmology.

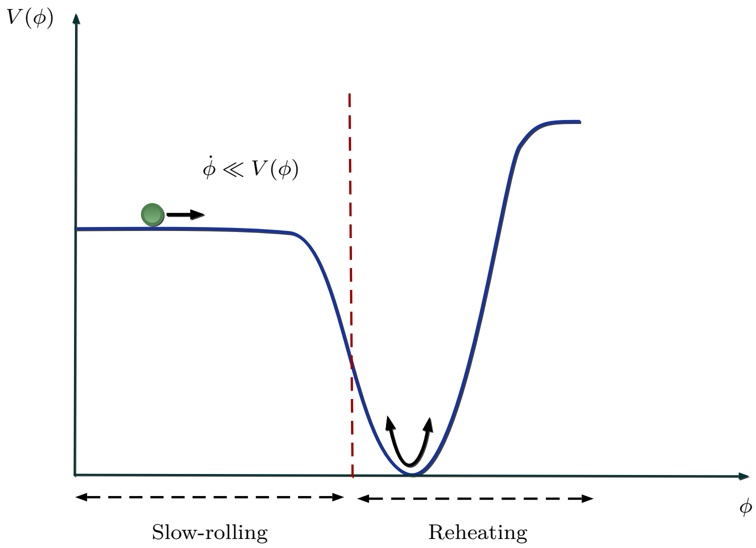

Figure 2.1: Example of a slow-rolling inflationary potential. The inflaton field rolls down into the true vacuum state under the influence of the quantum fluctuations; when the inflaton field reaches the new global minimum, the inflationary phase ends and the reheating stage starts (this picture takes inspiration from [Bau11]).

2.1.2 Quantum field theory in cosmological spacetimes

As it is expected that a consistent model of inflation should be driven by a quantum scalar field, it becomes significant to obtain a coherent formulation of a quantum fields propagating over a cosmological geometry. In this direction, many progress has been made in the last years about the algebraic construction of perturbative interacting quantum theories on curved spacetimes, with applications to Cosmology, see [LR90; Sch10; Sie15; Hac16]; other results based on the particle creation approach can be found, e.g., in the monographs [BD82; MW07]. See also [ADLS21] for a recent analysis about the validity of quantum fields as operator-valued distributions across the Big Bang.

The essential object which must be constructed for this goal is the two-point function associated to a (Hadamard) quantum state ω. Owing to the spatial translational and rotational symmetries of flat FLRW spacetimes, the two-point function of a cosmological quasi-free state is expected to depend on $|\vec{x}' - \vec{x}|$ in the spatial direction. Hence, it can be decomposed in spatial Fourier modes, thus partially recovering the modes decomposition usually provided in the flat spacetime. Furthermore, the conformally flatness allows to write the Klein-Gordon operator in conformal time τ as

$$P = \frac{1}{a^3}\left(\partial_\tau^2 - \vec{\nabla}_{\vec{x}}^2 + a^2m^2 + a^2\left(\xi - \frac{1}{6}\right)R\right)a, \tag{2.9}$$

where $\vec{\nabla}^2_{\vec{x}} = \sum_i \partial_i^2$ denotes the spatial Laplacian operator with respect to the comoving coordinates (x^1, x^2, x^3). Therefore, the two-point function of any homogeneous and isotropic quantum state is always of the form

$$\begin{aligned}\langle \phi(x')\phi(x)\rangle_\omega &= \omega_2(\tau', \tau, |\vec{x}' - \vec{x}|)\\ &= \lim_{\epsilon\to 0^+} \frac{1}{(2\pi)^3 a(\tau')a(\tau)} \int_{\mathbb{R}^3} \left((\gamma(k)+1)\overline{\zeta}_k(\tau')\zeta_k(\tau) + \gamma(k)\zeta_k(\tau')\overline{\zeta}_k(\tau)\right) \mathrm{e}^{\mathrm{i}\vec{k}\cdot(\vec{x}'-\vec{x})}\mathrm{e}^{-\epsilon k}\mathrm{d}\vec{k}\end{aligned} \tag{2.10}$$

viewed in the sense of distributions, where $k \doteq |\vec{k}|$. Here, the coefficient $\gamma(k)$ is polynomially bounded in $L^1(\mathbb{R}^+)$ and fixed on the Cauchy surface $\Sigma_0 : \tau - \tau_0 = 0$. Thus, any quasi-free, pure, homogeneous and isotropic state is fully constructed by the initial conditions for the modes ζ_k. Moreover, after a reparametrisation in terms of the initial data for the state, the two-point function of a Gaussian pure state can be obtained from eq. (2.10) by imposing $\gamma(k) = 0$, and it reads

$$\Delta_+^{\mathrm{FLRW}}(\tau', \tau, |\vec{x}' - \vec{x}|) = \lim_{\epsilon\to 0^+} \frac{1}{(2\pi)^3 a(\tau')a(\tau)} \int_{\mathbb{R}^3} \overline{\zeta}_k(\tau')\zeta_k(\tau)\mathrm{e}^{\mathrm{i}\vec{k}\cdot(\vec{x}'-\vec{x})}\mathrm{e}^{-\epsilon k}\mathrm{d}\vec{k}. \tag{2.11}$$

The temporal modes ζ_k fulfil the equation

$$\zeta_k''(\tau) + \Omega_k^2(\tau)\zeta_k(\tau) = 0, \qquad \Omega_k^2(\tau) \doteq k^2 + a^2m^2 + \left(\xi - \frac{1}{6}\right) Ra^2, \tag{2.12}$$

and, furthermore, they satisfy the normalization condition

$$\zeta_k'\overline{\zeta}_k - \zeta_k\overline{\zeta}_k' = \mathrm{i}. \tag{2.13}$$

Eq. (2.13) is needed to fix the Wronskian to be constant and purely imaginary, and thus it allows to recover the “equal–time” commutation relations between the fields and their canonical momenta in the Dirac quantization procedure, *cf.* section 1.2.1.

To obtain a well-defined state in a time interval $[\tau_0, \tau_1]$, $\tau_1 > \tau_0$, one can consider only cases where $\Omega_k^2 > 0$ for every k: this assumption can be always provided by assuming suitable initial conditions for the Ricci scalar and restricting the time interval accordingly, once the parameters m^2 and ξ are fixed.

In accordance with the formulation of quantum theory in curved spacetimes, where there is not any a priori prescription to fix a quantum state, eq. (2.12) and the condition (2.13) do not fix the modes uniquely, and there is no preferred choice to select the correct ζ_k that describe the actual physics of the system. Furthermore, given a set of modes ζ_k satisfying the above statements, a new family of modes can be always constructed using a Bogoliubov transformation $\tilde{\zeta}_k = \alpha(k)\zeta_k + \beta(k)\overline{\zeta}_k$, where $\alpha(k)$ $\beta(k)$ are the time-independent Bogoliubov coefficients: they satisfy $|\alpha(k)|^2 - |\beta(k)|^2 = 1$ after imposing the normalization condition (2.13) on $\tilde{\zeta}_k$. A choice of α and β corresponds to fix two degrees of freedom, such as the phase of α and the modulus of β, because $\beta(k)$ can be always chosen to be real due to the invariance of the state under a change of phase of ζ_k.

Remark 2.1.2. All the results presented in this section can be generalized to the whole class of Robertson-Walker spacetimes. The line-element of a Robertson-Walker spacetime $(\mathcal{M}^\kappa, g^\kappa_{\mu\nu})$ reads in spatial polar coordinates as

$$\mathrm{d}s_\kappa^2 = -\mathrm{d}t^2 + a(t)^2\left(\frac{\mathrm{d}r^2}{1-\kappa r^2} + r^2\left(\mathrm{d}\theta^2 + \sin^2\theta\mathrm{d}\varphi^2\right)\right), \tag{2.14}$$

where $\kappa = 0, \pm 1$ denotes the sign of the constant curvature associated to the homogeneous Riemannian hypersurfaces Σ^κ. The corresponding spacetime $\mathcal{M}^\kappa$ is called flat when $\kappa = 0$ and closed (*resp.* open) when $\kappa = \pm 1$. The symmetry group $\mathbf{G}^\kappa$ is $\mathbf{E}(3)$ when $\kappa = 0$, it is $\mathbf{O}(4)$ when $\kappa = 1$, and it is $\mathbf{O}(1{,}3)$ when $\kappa = -1$ (in the closed case, the metric (2.14) covers only half of the spacetime).

Using a generalized version of the spatial Fourier transform, evaluated with respect to an orthonormal basis of eigenfunctions of the Laplacian operator in $L^2(\Sigma^\kappa)$, one can obtain a full characterization of the two-point functions of homogeneous and isotropic states similar to what has been made in the FLRW case - *cf.* [LR90; JS02; Kus09].

Any solution of the modes equation (2.12) satisfying eq. (2.13) can be parametrized as

$$\zeta_k(\tau) = \rho(\tau)\mathrm{e}^{i\theta(\tau)}, \qquad \theta(\tau) = \int_{\tau_0}^{\tau} \frac{1}{2\rho(\eta)}\mathrm{d}\eta, \tag{2.15}$$

where ρ and θ are some real functions. The initial data $\theta(\tau_0) = 0$ can be assumed without loss of generalities because each mode is always fixed up to a global phase, and hence the initial conditions for the modes are fully specified by $\rho(\tau_0)$ and $\rho'(\tau_0)$. Equivalently, the state can be also characterized by two other real functions $\Phi(k)$, $E(k)$ and a sign $s \in \{-1, +1\}$, which are related by

$$\Phi(k) = |\zeta_k(\tau_0)|^2 = |\rho(\tau_0)|^2, \qquad E(k) = |\zeta_k'(\tau_0)|^2 = |\rho'(\tau_0)|^2 + \frac{1}{4\Phi(k)}, \qquad \mathrm{sign}\left(\mathrm{Re}\left(\zeta_k'(\tau_0)\right)\right) = s, \tag{2.16}$$

and they satisfy the following inequalities

$$E(k) \geq \frac{1}{4\Phi(k)} \geq 0.$$

In other words,

$$\rho_k(\tau_0) = \sqrt{\Phi(k)}, \qquad \rho_k'(\tau_0) = s\sqrt{E(k) - \frac{1}{4\Phi(k)}}.$$

According to the choice of $\rho(\tau_0)$ and $\rho'(\tau_0)$, different class of cosmological states can be constructed. For example, a relevant class of solutions are the adiabatic states introduced by Parker in [Par69; PF74] (see also [LR90]), to minimise particle creation effects using a WKB-type approximation for $\zeta_k(\tau)$:

$$\zeta_k(\tau) = \frac{1}{\sqrt{2\omega_k(\tau)}} \exp\left(i \int_{\tau_0}^{\tau} \omega_k(\eta)\mathrm{d}\eta\right). \tag{2.17}$$

By inserting this ansatz inside eq. (2.12) the following equation holds:

$$\omega_k^2(\tau) = \Omega_k^2(\tau) + \frac{3}{4}\left(\frac{\omega_k'(\tau)}{\omega_k(\tau)}\right)^2 - \frac{1}{2}\frac{\omega_k''(\tau)}{\omega_k(\tau)}, \tag{2.18}$$

which can be solved iteratively starting from the 0-th order adiabatic mode

$$\zeta_k^{(0)}(\tau) = \frac{1}{\sqrt{2\omega_k^{(0)}}} \exp\left(i \int_{\tau_0}^{\tau} 2\omega_k^{(0)}(\eta)\mathrm{d}\eta\right), \tag{2.19}$$

$$\zeta_k^{(0)}(\tau_0) = \frac{1}{\sqrt{2k_0}}, \qquad \zeta_k^{(0)\prime}(\tau_0) = \frac{ik_0}{\sqrt{2k_0}} - \frac{1}{4}\frac{k_0^{2\prime}}{k_0^2\sqrt{2k_0}} \tag{2.20}$$

where $\omega_k^{(0)} = \Omega_k$, $\omega_k^{(0)}(\tau_0) = k_0 \doteq \sqrt{\Omega_k(\tau_0)}$. In this recursive procedure, the N-th frequency $\omega_k^{(N)}$ defines the adiabatic state of order N $(\zeta_k^{(N)}, \partial_\tau\zeta_k^{(N)})$. It has been shown in [Jun95; JS02] using microlocal arguments that the UV-singularity approaches the Hadamard parametrix in the limit of large N.

An important case of state which is related to the 0-th order adiabatic state is the so-called conformal vacuum, whose two-point function is given by

$$\omega_2^c(\tau',\tau,|\vec{x}'-\vec{x}|) = \lim_{\epsilon\to 0^+} \frac{1}{(2\pi)^3 a(\tau')a(\tau)} \int_{\mathbb{R}^3} \overline{\chi}_k(\tau')\chi_k(\tau) \mathrm{e}^{\mathrm{i}\vec{k}\cdot(\vec{x}'-\vec{x})} \mathrm{e}^{-\epsilon k} \mathrm{d}\vec{k}, \tag{2.21}$$

where modes χ_k are obtained by the following initial data

$$\chi_k(\tau_0) = \frac{1}{\sqrt{2k_0}} \mathrm{e}^{\mathrm{i}k_0\tau_0}, \qquad \chi_k'(\tau_0) = \frac{\mathrm{i}k_0}{\sqrt{2k_0}} \mathrm{e}^{\mathrm{i}k_0\tau_0}, \tag{2.22}$$

with $k_0 = \sqrt{\Omega_k(\tau_0)}$ and Ω_k given in eq. (2.12). The parameter of the theory m^2 and ξ are fixed in such a way that k_0 is strictly positive for every k, after restricting the possible initial conditions a_0 and a_0''. These initial data are essentially the modes of the Minkowski vacuum state in the conformal spacetime (2.3), and thus they are Hadamard states in the massless, conformally coupled case [Pin09].

The regularity of the pure conformal vacuum state is sufficient to evaluate the vacuum polarization $\langle :\phi^2: \rangle_\omega$ in cosmological spacetimes, because the state-dependent function obtained after subtracting the conformal vacuum singularity is continuous in time (a careful analysis of the internal structure of $\langle :\phi^2: \rangle_\omega$ shall be made in subsection 2.2.2). Furthermore, modes equation (2.12) can be solved perturbatively by imposing the initial conditions (2.22) and by constructing χ_k as a convergent Dyson series (see also [PS15a; Sie15]).

Proposition 2.1.1. *Consider the FLRW spacetime $(\mathcal{M}, g_{\mu\nu})$ with $a \in C^2(\mathcal{M})$, constructed in such a way that $\Omega_k^2(\tau_0)$ in (2.12) is strictly positive, a solution χ_k of eq. (2.12) which satisfies the initial conditions (2.16) can be obtained explicitly on $[\tau_0, \tau_1]$ as*

$$\chi_k = \sum_{n\geq 0} \chi_k^{(n)}, \tag{2.23}$$

where $\chi_k^{(n)}$ for $\tau > \tau_0$ are obtained recursively. The recursive step is for $n > 0$

$$\chi_k^{(n)}(\tau) = -\int_{\tau_0}^{\tau} \frac{\sin(k_0(\tau-\eta))}{k_0} V(\eta)\chi_k^{(n-1)}(\eta)\mathrm{d}\eta, \qquad \chi_k^{(0)}(\tau) = \frac{1}{\sqrt{2k_0}}\mathrm{e}^{\mathrm{i}k_0\tau}, \tag{2.24}$$

where $k_0 = \Omega(\tau_0)$ and $V(\tau)$ is the perturbation potential

$$V(\tau) \doteq \Omega_k^2(\tau) - k_0^2 = m^2(a^2-a_0^2) + \left(\xi - \frac{1}{6}\right)(Ra^2 - R_0 a_0^2), \qquad a_0 = a(\tau_0), \quad R_0 = R(\tau_0). \tag{2.25}$$

The following bound holds

$$|\chi_k^{(n)}| \leq \frac{1}{\sqrt{2k_0}n!}\left(\frac{1}{k_0}\int_{\tau_0}^{\tau}|V(\eta)|\mathrm{d}\eta\right)^n \leq \frac{1}{\sqrt{2k_0}n!}\frac{(\tau-\tau_0)^n}{k_0^n}\|V\|_\infty^n. \tag{2.26}$$

Hence, the series (2.23) converges absolutely and

$$|\chi_k(\tau)| \leq \frac{1}{\sqrt{2k_0}}\exp\left(\frac{\|V\|_{1,[\tau_0,\tau]}}{k_0}\right), \qquad |\chi_k'(\tau)| \leq \left(\sqrt{\frac{k_0}{2}} + \frac{\|V'\|_{1,[\tau_0,\tau]}}{\sqrt{2}k_0^{3/2}}\right)\exp\left(\frac{2\|V\|_{1,[\tau_0,\tau]}}{k_0}\right), \tag{2.27}$$

where the norm $\|\cdot\|_{1,[\tau_0,\tau]}$ *is the ordinary* L^1 *norm on the interval* $[\tau_0,\tau]$*. Furthermore,*

$$\begin{aligned} |(\chi_k-\chi_k^{(0)})| &\leq \frac{\|V\|_{1,[\tau_0,\tau]}}{\sqrt{2}k_0^{3/2}}\exp\left(\frac{\|V\|_{1,[\tau_0,\tau]}}{k_0}\right), \\ |(\chi_k-\chi_k^{(0)})'| &\leq \left(\frac{\|V\|_{1,[\tau_0,\tau]}}{\sqrt{2k_0}}+\frac{\|V'\|_{1,[\tau_0,\tau]}}{\sqrt{2}{k_0}^{3/2}}\right)\exp\left(\frac{2\|V\|_{1,[\tau_0,\tau]}}{k_0}\right). \end{aligned} \tag{2.28}$$

Proof. Equation (2.12) equipped with initial conditions (2.16) form a well posed Cauchy problem hence an unique χ solution exists. Furthermore, since eq. (2.12) is of the form of eq. (C.4), one may apply the results of lemma C.2.1. In particular, (C.8) implies that

$$\chi_k(\tau) = -\Delta_R^{k_0} * V\chi_k + \chi_k^{(0)}, \tag{2.29}$$

where $\chi_k^{(0)} = \frac{1}{\sqrt{2k_0}}e^{ik_0\tau}$. Hence

$$(1-\mathcal{R})\chi_k = \chi_k^{(0)}, \tag{2.30}$$

where the linear operator $\mathcal{R}$ is such that $\mathcal{R}\chi_k = -\Delta_R^{k_0} * V\chi_k$. Then χ_k is obtained in terms of $\chi_k^{(0)}$ by applying the inverse of $(1-\mathcal{R})$ on both side of eq. (2.30). Actually,

$$\chi_k = \sum_{n\geq 0}\mathcal{R}^n\chi_k^{(0)} = \sum_{n\geq 0}\chi_k^{(n)}$$

and since $\chi_k^{(n)} = \mathcal{R}^n\chi_k^{(0)}$ eq. (2.24) follows. Notice that $\mathcal{R}^n f$ converges for $f\in L^\infty$ in the interval $[\tau_0,\tau_1]$, so the last equality holds without further conditions. In particular, expanding $\mathcal{R}^n\chi_k^{(0)}$, one gets

$$\chi_k^{(n)}(\tau_{n+1}) = (-1)^n\int_{\tau_0\leq\tau_1\leq\dots\leq\tau_{n+1}}\prod_{j=1}^n\left(\frac{\sin(k_0(\tau_{j+1}-\tau_j))}{k_0}V(\tau_j)\right)\chi_k^{(0)}(\tau_1)\mathrm{d}\tau_1\dots\mathrm{d}\tau_n,$$

and hence eq. (2.26). Absolute convergences of the series $\sum_{n\geq 0}\chi_k^{(n)}$ to χ_k together with its first and second derivatives can now be obtained analyzing the explicit form of $\mathcal{R}$ and using (2.29). The first estimates in eq. (2.27) and in eq. (2.28) can be obtained by an application of Grönwall lemma as in lemma C.2.1 from the inequalities

$$\begin{aligned} |\chi_k(\tau)| &\leq \frac{1}{\sqrt{2k_0}}+\int_{\tau_0}^\tau\frac{|V(\eta)|}{k_0}|\chi_k(\eta)|\mathrm{d}\eta, \\ |(\chi_k-\chi_k^{(0)})(\tau)| &\leq \frac{1}{\sqrt{2}}\int_{\tau_0}^\tau\frac{|V|}{k_0^{3/2}}\mathrm{d}\eta+\int_{\tau_0}^\tau\frac{|V(\eta)|}{k_0}|(\chi_k-\chi_k^{(0)})(\eta)|\mathrm{d}\eta \end{aligned}$$

which are obtained directly from (2.29). The second estimates in eq. (2.27) and in eq. (2.28) descend from the first estimates and applying Grönwall lemma to the inequalities

$$\begin{aligned} |\chi_k'(\tau)| &\leq \sqrt{\frac{k_0}{2}}+\int_{\tau_0}^\tau\frac{|V'(\eta)|}{k_0}|\chi_k(\eta)|\mathrm{d}\eta+\int_{\tau_0}^\tau\frac{|V(\eta)|}{k_0}|\chi_k'(\eta)|\mathrm{d}\eta, \\ |\chi_k-\chi_k^{(0)}|' &= \int_{\tau_0}^\tau\frac{|V|}{k_0}|\chi_k-\chi_k^{(0)}|'\mathrm{d}\eta+\int_{\tau_0}^\tau\frac{V'}{k_0}|\chi_k|\mathrm{d}\eta+\int_{\tau_0}^\tau\frac{V}{\sqrt{2k_0}}|\chi_k|\mathrm{d}\eta. \end{aligned}$$

These inequalities are obtained directly from

$$\begin{aligned} &\chi_k' = -\Delta_R^{k_0} * V\chi_k' - \Delta_R^{k_0} * V'\chi_k + \chi_k^{(0)\prime}, \\ &(\chi_k-\chi_k^{(0)})' = -\Delta_R^{k_0} * V(\chi_k-\chi_k^{(0)})' - \Delta_R^{k_0} * V'\chi_k - \Delta_R^{k_0} * V(\chi_k^{(0)})' \end{aligned}$$

which is the first derivative of eq. (2.29). □

Another physically reasonable argument to construct quantum states can be provided in terms of minimization of energy, in order to partially recover the notion of vacuum state as zero-point energy state for the spacetime. In the cosmological case, one is interested in minimizing the energy density per mode associated to T_{00}, i.e.,

$$\varrho(\zeta_k, \bar{\zeta}_k) = \frac{1}{2a^4}\left(|\zeta_k'|^2 + \left(k^2 + a^2m^2 - (6\xi - 1)a^2H^2\right)|\zeta_k|^2 + aH(6\xi - 1)\left(|\zeta_k|^2\right)'\right), \tag{2.31}$$

see Appendix B for the derivation of eq. (2.31).

In [ANA15], the "instantaneous vacuum" requirement is imposed to construct a physically preferred state, such that the renormalized energy density $\langle :\varrho: \rangle_\omega$ per modes vanishes identically mode by mode. This density has been obtained from eq. (2.31) by the adiabatic point-splitting regularization, using the modes defined iteratively in eq. (2.17). As discussed also in subsection 2.2.1, at least a fourth-order adiabatic state is needed to evaluate the renormalized energy density in the adiabatic regularization scheme. Thus, it was shown that a unique instantaneous vacuum state can be obtained, and hence providing a natural candidate for an hypothetical ground state at a fixed instant of time.

Besides, another possible candidate to be promoted as energetic ground state is the state of low energy obtained in [Olb07], which is defined as the cosmological quantum state which has minimal smeared energy density:

$$\Delta W = \frac{1}{2}\int_I f^2(\tau)\left(\varrho(\zeta_k, \bar{\zeta}_k) - \varrho(\chi_k, \bar{\chi}_k)\right) \tag{2.32}$$

where $I \subset \mathbb{R}$, $f \in \mathcal{D}(\mathcal{M})$, and the modes ζ_k are obtained as linear superposition $\zeta_k = A_k\chi_k + B_k\bar{\chi}_k$ of some reference modes χ_k. Thus, it was shown that in the minimal coupling case, i.e., $\xi = 0$, the corresponding state of low energy satisfy the Hadamard condition given any sampling function f (this smearing definition is, indeed, in accordance with the constructions of quantum energy inequalities, see subsection 1.3.3). Actually, the difference $\varrho(\zeta_k, \bar{\zeta}_k) - \varrho(\chi_k, \bar{\chi}_k)$ can be always minimized at a fixed instant of time by carefully varying of the Bogoliubov coefficients A_k, B_k, and whenever $\xi \in [0,1/6]$ - *cf.* [Sie15], Section 6.2.5.

Finally, a last interesting class of cosmological quantum states was found in [DHP11], which generalizes the notion of KMS thermal states in flat spacetime, *cf.* eq. (1.82). Given a pure state (2.11) defined by modes ζ_k, a generalised thermal state is characterized by the following two-point function

$$\Delta_F^{\mathrm{FLRW}}(x', x) = \frac{1}{(2\pi)^3 a(\tau')a(\tau)}\int_{\mathbb{R}^3}\left(\frac{\bar{\zeta}_k(\tau')\zeta_k(\tau)}{\mathrm{e}^{\beta k_F} - 1} + \frac{\bar{\zeta}_k(\tau)\zeta_k(\tau')}{1 - \mathrm{e}^{-\beta k_F}}\right)\mathrm{e}^{\mathrm{i}\vec{k}\cdot(\vec{x}' - \vec{x})}\mathrm{e}^{-\epsilon k}\mathrm{d}\vec{k}, \tag{2.33}$$

where $k_F \doteq \sqrt{k^2 + m^2a(\tau_F)^2}$ for some "freeze–out time" τ_F and "freeze–out temperature" $T_F = a(\tau_F)/\beta$; for massive fields, it corresponds to a quantum state which was at thermal equilibrium in the hot early universe, when the scale factor had the specific value $a(\tau_F)$.

2.1.3 Semiclassical analysis for conformally coupled fields

The application of the semiclassical Einstein equations in Cosmology represents a fruitful topic in which investigating how our Universe has been evolved in the early stages under the influence of quantum fields and particle creation effects. In this respect, many results matching with recent observations have been already provided, such as those related to the cosmic microwave background radiation and supernova data - *cf.* [PR99; PR01; Hac10; Hac16] and references therein.

A seminal analysis of eqs. (1.105) made in cosmological spacetimes was performed by Starobinsky in [Sta80], followed by [Vil85], for conformally-coupled fields. This semiclassical analysis was discussed later by Simon in [Sim92] in light of the validity of semiclassical theories involving higher-order derivative terms, such as $\Box_g R$, which may be origin of unphysical solutions (see section 4.1). For an investigation of the dynamics in FLRW spacetimes induced only by the trace anomaly, see also [Wal78a; FHH79; Kok10], while further numerical works were made by Anderson in [And85; And86]. A very recent numerical work about semiclassical cosmological models associated to Minkowski-like states and massless scalar fields with general coupling to curvature can be found in [GRS22], and it takes advantage of the formulation of cosmological semiclassical Einstein equations as infinite-dimensional dynamical system presented in [GS21]. Finally, a review about the backreaction problem in Cosmology using semiclassical and stochastic gravity can be found in [HV20]. See also [ST21] for a discussion about the several approaches to backreaction in Cosmology.

In this subsection, one shall review the analysis made in [DFP08; Hac10; DHMP10], which generalize the original Starobinsky model of inflation. On the one hand, the initial-value problem formulated in Starobinsky and Vilenkin's papers predicted a period of exponential expansion of the early Universe in form of a de Sitter solution driven by both the trace anomaly (1.120) and higher-order derivative terms like $\Box_g R$. On the other hand, in [DFP08; Hac10; DHMP10] explicit state-dependent contributions to eqs. (1.105) have been introduced in the back-reaction problem, such as the vacuum polarization and the renormalization constants associated to the Wick square $:\phi^2:$. Notably, these non-classical contributions yield a dynamical realisation of dark energy. Further improvements of these analysis were made in [Hac16] at level of thermal energy density, from both a analytical and numerical point of view.

According to subsection 2.1.1, it is convenient to use the traced semiclassical Einstein equations eq. (1.124) to obtain the dynamics of $H(t)$. Alternatively, since the quantum stress-energy tensor in a FLRW spacetime is of perfect fluid type when evaluated on homogeneous and isotropic states, *cf.* [Zsc14], Lemma 2.9., the semiclassical problem can be expressed in terms of the following differential equations

$$\frac{1}{H}\partial_t \langle :\varrho: \rangle_\omega + 4 \langle :\varrho: \rangle_\omega = - \langle :T_\rho{}^\rho: \rangle_\omega , \qquad H^2 = \frac{8\pi}{3} \langle :\varrho: \rangle_\omega , \tag{2.34}$$

in units $G = c = 1$. In this viewpoint, one is interested in computing the renormalized energy density $\langle :\varrho: \rangle_\omega \doteq \langle :T_{00}: \rangle_\omega$, in order to compare own results with measurements. For an explicit computation of the renormalized energy density, see Appendix B. On the one hand, the first equation in eq. (2.34) is obtained by combining the covariant conservation of $\langle :T_{\mu\nu}: \rangle_\omega$ and the evaluation of the traced stress-energy tensor of perfect fluid (1.18). On the other hand, the second equation, which corresponds to the first Friedmann equation, involves up to the third-order derivatives of the scale factor, according to the following proposition.

Proposition 2.1.2. *The renormalized quantum energy density $\langle :\varrho: \rangle_\omega$ involves up to the third-order derivatives of $a(t)$ with respect to the comoving reference system labelled by ∂_t.*

Proof. This statement can be proved using a reductio ad absurdum argument: assume that $\langle :\varrho: \rangle_\omega$ involves a term of the form $a_1 \dddot{H}$, which depends on up the fourth-order derivative of a. Then, also the renormalized quantum pressure $\langle :p: \rangle_\omega$ involves terms of the form $a_2 \dddot{H}$ from the definition of $\langle :T_\rho{}^\rho: \rangle_\omega = - \langle :\varrho: \rangle_\omega + 3 \langle :p: \rangle_\omega$, which contains the higher-order derivative term $\gamma \Box_g R$. Therefore, it holds that

$$a_2 = \frac{1}{3}(\gamma + a_1).$$

From the conservation equation $\partial_t \langle :\varrho: \rangle_\omega + 3H(\langle :\varrho: \rangle_\omega + \langle :p: \rangle_\omega) = 0$, and up to remaining terms which depend up to $a^{(3)}$, one obtains that

$$a_1 \ddddot{H} + H(\gamma + 4a_1)\dddot{H} + O(a^{(3)}) = 0,$$

which implies that $a_1 = 0$. □

In the original works due to Starobinski and Vilenkin [Sta80; Vil85], an evolution equation for the Hubble function was obtained from $\langle :\varrho: \rangle_\omega$. Hence, it was shown that this equation yields both a flat solution, which is stable in time, and a de Sitter-like solution, which admits unstable growing modes in time. In [DFP08], eq. (1.124) was studied for free conformally-coupled fields, taking into account the renormalization freedoms of the theory, see eq. (1.122). Then, it reads

$$\begin{aligned} -6\left(\dot{H} + 2H^2\right) = -8\pi m^2 \left\langle :\phi^2: \right\rangle_\omega - \frac{1}{30\pi}\left(\dot{H}H^2 + H^4\right) + 4c_1 m^4 \\ - 6c_2 m^2 \left(\dot{H} + 2H^2\right) + \gamma\left(\dddot{H} + 6\ddot{H}H + 4\dot{H}^2 + 12\dot{H}H^2\right) \end{aligned} \tag{2.35}$$

up to the addition of a factor $(16\pi)^{-1}$ which can be reabsorbed in the renormalization constant c_1 . The coefficient $[v_1]$ associated to the trace anomaly in cosmological spacetimes was evaluated in eq. (B.22). Furthermore, the higher-order derivative term proportional to $\Box_g R$ can been removed by carefully choosing the renormalization freedom γ. Following Starobinsky and Vilenkin's original papers, the massless case is considered in the high-curvature limit $R \gg m^2$, and the cosmological equation reduces to

$$\dot{H}(H^2 - H_c^2) = -H^4 + 2H_c^2 H^2, \tag{2.36}$$

where $H_c = \sqrt{180\pi}$. At this level, the choice of the quantum state is irrelevant, since the state-dependent contribution vanishes in the massless, conformally coupled case. Eq. (2.36) admits the same critical points already viewed in the original papers, i.e., the Minkowski spacetime $H = 0$ and the de Sitter space $H_+ = \sqrt{2}H_0$. However, different from the original papers, both of these critical points turn out to be stable according to the choice by hand of a renormalization constant at the initial time t_0.

The generalization to massive fields consists on taking into account both the vacuum polarization and all the other renormalization constants of the theory. This analysis can be provided for different choices of quantum states, such as the zeroth-order adiabatic state defined by eq. (2.19) or the approximate KMS thermal states (2.33) in the limit $T \ll m$. In [Hac10], the following four solutions of the semiclassical problems are obtained for the Hubble function:

$$H_\pm^2 \doteq H_*^2 \pm \sqrt{H_*^4 - \frac{C_1}{a^4} - \frac{C_2}{a^3} - C_3}. \tag{2.37}$$

Here, all the constants depend both on the number of quantum fields involved and on the renormalization constants of the model. These solutions are due to an effective quantum energy density (up to a factor $8\pi/3$) inside the total energy density of the Universe. They can also have the same asymptotically stable fixed points seen in the massless case, for suitable choices of the renormalization constants which can be matched to fit the currently measurements of the Hubble constant H_0. See Figure 2.2. Notably, both the lower and the upper branch provide a quantum theoretical realisation of dynamical dark energy at late times, and, furthermore, the upper branch displays the behaviour of a Big Bang spacetime at early times. However, this branch deviates from the currently observations from Λ-CDM model, contrary to the lower branch. Therefore, it is expected that a certain mechanism which allows to switch from the upper branch to the lower one could be realized in more refined semiclassical models involving higher-order derivative terms. In this respect, the lower branch shows a non-Big Bang singularity when H_-^2 becomes negative, but it can be always avoided by carefully choosing the renormalization constant C_3 in eq. (2.37). In fact, such a unphysical singularity, in which $\dot{H}$ diverges, corresponds to a regime in which the approximations made here break down.

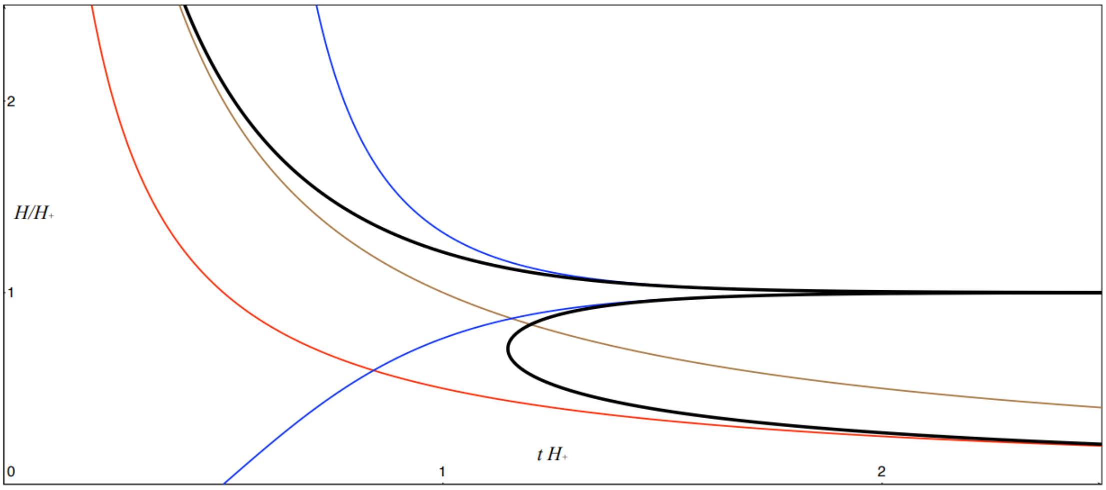

Figure 2.2: Plot of the normalized Hubble function H/H_+ as function of the normalized cosmological time t/H_+ in a FLRW filled by classical radiation (red line) and classical radiation with cosmological constant (blue line), respectively. The black lines composed by the two branches $H_\pm$ denote the semiclassical model incorporating also quantum effects [DFP08; Hac10] (*copyright by N. Pinamonti*).

Finally, it is worth to mention the results obtained in [Pin11; PS15a] about the well-posedness of the initial-value problem for the traced semiclassical Einstein equations in the conformal coupling case $\xi = 1/6$: in this case, the semiclassical equation for $H(\tau)$

$$\frac{\mathrm{d}H}{\mathrm{d}\tau} = \frac{a}{H_c^2 - H^2}\left(H^4 - 2H_c^2 H^2 + 240\pi^2\left(m^2 \left\langle :\phi^2: \right\rangle_\omega + \beta m^2 R + \frac{4\Lambda}{8\pi}\right)\right). \tag{2.38}$$

is written in normal form, namely, the term with the highest derivative of the scale factor is isolated at the left-hand side of the equation. This is due to the behaviour of the vacuum polarization, which can be estimated by only up to first order derivatives of a in $[\tau_0, \tau_1]$ for every τ_1 when $\xi = 1/6$; the same holds also in the special case $H = H_c$, which represents a singularity in the derivative of H as expected from eq. (2.36). As a result of this, eq. (2.38) can be solved directly, and both local and global unique solutions $H(t)$ can be obtained. However, a different analysis is necessary to handle the formulation of an initial-value problem for the semiclassical Einstein equations for arbitrary values of ξ, due to presence of higher-order derivative terms. This issue is treated in the following sections, in which the main results of author's publication [MPS21] are gathered; in particular, the full evaluation of the vacuum polarization for arbitrary $\xi \in \mathbb{R}$ shall be carried out in subsection 2.2.2, whereas the regularity issue associated to the highest-order derivative in the vacuum polarization shall be discussed in subsection 2.2.4, *cf.* remark 2.2.3.

2.2 Initial-value Formulation for Local Solutions

2.2.1 Sufficiently regular states

According to subsection 1.2.3, a guiding principle to select sufficiently regular quantum states is to require that they give finite expectation values for observable like $:\phi^2:$ and the renormalized energy density $:\varrho: \doteq :T_{00}: = -:{T_0}^0:$ associated to the energy density per modes (2.31). Furthermore, in order to have well-defined semiclassical Einstein equations, these functions may depend on the derivative of a up to the third order. These conditions are met, e.g., by adiabatic states of fourth order or by the instantaneous vacuum states considered in subsection 2.1.2. This requirement imposes some constraints on the degrees of freedoms of the quasi-free, pure, homogeneous and isotropic state parametrized by the functions Φ, E, and s defined in eq. (2.16).

More precisely, in view of eq. (1.123), the relevant observables that have to be controlled are the Wick square $:\phi^2:$ and the energy density $:\varrho:$. Their expectation values can be obtained following the analyses performed in [Sch10; EG11; Deg13; Sie15; Hac16] (see also Appendix B), and in the state (2.11) they take the form

$$\begin{aligned}\langle:\phi^2:\rangle_\omega &= \frac{1}{(2\pi)^3 a^2}\int_{\mathbb{R}^3}\left(|\zeta_k|^2 - C^{\mathcal{H}}_{\phi^2}(\tau,k)\right)\mathrm{d}\vec{k} + \frac{w(\tau)^2}{8\pi^2 a^2}\log\left(\frac{w(\tau_0)}{a(\tau)}\right) - \frac{w(\tau_0)^2}{16\pi^2 a^2} + \alpha_1 m^2 + \alpha_2 R,\\ \langle:\varrho:\rangle_\omega &= \frac{1}{(2\pi)^3 a^4}\int_{\mathbb{R}^3}\left(\frac{|\zeta_k'|^2}{2} + \left(k^2 + a^2 m^2 - (6\xi-1)\,a^2 H^2\right)\frac{|\zeta_k|^2}{2} + aH\,(6\xi-1)\,2\mathrm{Re}(\overline{\zeta}_k\zeta_k')\right.\\ &\quad \left. - C^{\mathcal{H}}_{\varrho}(\tau,k)\right)\mathrm{d}\vec{k} \quad - \frac{H^4}{960\pi^2} + \left(\xi - \frac{1}{6}\right)^2\frac{3H^2 R}{8\pi^2} + \tilde{\beta}_1 m^4 - \tilde{\beta}_2 m^2 {G_0}^0 + (\tilde{\beta}_3 - \frac{\tilde{\beta}_4}{3}){I_0}^0,\end{aligned} \tag{2.39}$$

where

$$w(\tau) \doteq \sqrt{\Omega(\tau)^2 - k^2} = a\sqrt{m^2 + \left(\xi - \frac{1}{6}\right)R} \tag{2.40}$$

from eq. (2.12). Here, α_i and $\tilde{\beta}_i$ are (redefinitions of the) renormalization constants of the theory. Furthermore, the functions $C^{\mathcal{H}}_{\phi^2}(\tau,k)$ and $C^{\mathcal{H}}_{\varrho}(\tau,k)$ are subtracted before the k-integration to implement the point splitting regularization mode-wise: recalling $k_0^2 = \Omega_k^2(\tau_0)$ and the perturbative potential (2.25), one defines

$$\begin{aligned} C^{\mathcal{H}}_{\phi^2}(\tau,k) &\doteq \frac{1}{2k_0} - \frac{V(\tau)}{4k_0^3},\\ C^{\mathcal{H}}_{\varrho}(\tau,k) &\doteq \frac{k}{2} + \frac{a^2m^2 - a^2H^2(6\xi-1)}{4k} - \frac{a^4m^4 + 12\left(\xi-\frac{1}{6}\right)m^2a^4H^2 + a^4\left(\xi-\frac{1}{6}\right)^2 2{I_0}^0(\tau)}{16k(k^2+\frac{a^2}{\lambda^2})},\end{aligned} \tag{2.41}$$

where $2{I_0}^0 = 216H^2\dot{H} - 36\dot{H}^2 + 72H\ddot{H}$ corresponds to the 00-component of the local curvature tensor $I_{\mu\nu}$ which encompasses part of the renormalization freedom of $:T_{\mu\nu}:$, *cf.* eq. (1.112). Also, λ is the length scale present in the Hadamard singularity (1.57). Notice that $\Omega_k(\tau_0)^2$ is strictly positive thanks to the choice of initial conditions for the spacetime taken into account.

Definition 2.2.1. A pure homogeneous and isotropic quasi-free state whose two-point function is constructed as in eq. (2.11) with modes ζ_k is said to be sufficiently regular if

$$|\zeta_k^2(\tau_0)| - C^{\mathcal{H}}_{\phi^2}(\tau_0,k) \in L^1\left(k^2\mathrm{d}k\right)_{(0,\infty)}, \quad \frac{\mathrm{d}}{\mathrm{d}\tau}\left[|\zeta_k^2|(\tau) - C^{\mathcal{H}}_{\phi^2}(\tau,k)\right]_{\tau=\tau_0} \in L^1\left(k^2\mathrm{d}k\right)_{(0,\infty)} \tag{2.42}$$

and

$$\begin{aligned}\Bigg[&\frac{|\zeta_k'|^2}{2} + \left(k^2 + a^2m^2 - (6\xi-1)\,a^2H^2\right)\frac{|\zeta_k|^2}{2}\\ &+ aH\,(6\xi-1)\,2\mathrm{Re}(\overline{\zeta}_k\zeta_k') - C^{\mathcal{H}}_{\varrho}(\tau,k)\Bigg]_{\tau=\tau_0} \in L^1\left(k^2\mathrm{d}k\right)_{(0,\infty)}.\end{aligned} \tag{2.43}$$

As will be shown in subsection 2.2.3, it is just sufficient to demand the regularity stated in definition 2.2.1 at initial time in order to ensure the finiteness of the expectation values of $:\phi^2:$ and $:\varrho:$, namely the observables appearing in the semiclassical version of eqs. (2.5) and (2.6).

Remark 2.2.1. To check if a state given in (2.11) is sufficiently regular, one has to control on the derivatives of the scale factor up to the third order, because no fourth order derivative of the metric appear in $C_\varrho^{\mathcal{H}}(\tau_0, k)$, in $C_{\phi^2}^{\mathcal{H}}(\tau_0, k)$ and in $\partial_\tau C_{\phi^2}^{\mathcal{H}}(\tau_0, k)$, and the same holds for the corresponding finite contributions. For instance, adiabatic states of fourth order are sufficiently regular in the sense of definition 2.2.1.

2.2.2 The vacuum polarization

If one is interested in studying solutions of the traced semiclassical Einstein equations (1.124), then the control of the time evolution of the vacuum polarization $\langle{:}\phi^2{:}\rangle_\omega$ is one of the main problems to be faced. This expectation value is constructed with modes ζ_k, which satisfy the initial conditions (2.16), and chosen in such a way that point splitting regularization works, namely (2.42) and (2.43) hold.

In particular, one needs to know how the state depends on the scale factor a and on the initial conditions a_0, a_0', a_0'' and $a_0^{(3)}$, and, furthermore, if the Lipschitz continuity for all the internal contributions can achieved in terms of Gateaux differentiability. For a brief review about these topics, see section C.1. To control $\langle{:}\phi^2{:}\rangle_\omega$, one can compare the modes ζ_k with the modes χ_k associated to the conformal vacuum (2.21) given by the initial data (2.22), in which ${:}\phi^2{:}$ acquires a finite expectation value. However, the regularity of the conformal vacuum is not sufficient to give finite time derivatives control the derivative of $\langle{:}\phi^2{:}\rangle_\omega$: this issue shall be taken into account in the point-splitting regularization.

To address the issue of regularity, the expectation value of ${:}\phi^2{:}$ and of its time derivative is decomposed in the regular state ω, namely it is quasifree and its two-point function is constructed as in eq. (2.11) with modes ζ_k satisfying eqs. (2.42) and (2.43). Then,

$$\langle{:}\phi^2{:}\rangle_\omega = \frac{Q_s}{a^2} + \frac{Q_c}{a^2} + \frac{Q_0}{a^2}, \qquad \partial_\tau \left(a^2 \langle{:}\phi^2{:}\rangle_\omega\right) = Q_s^d + Q_c^d + Q_0^d, \tag{2.44}$$

where the state dependent contribution is contained in the following

$$Q_s \doteq a^2 \langle{:}\phi^2{:}\rangle_\omega - a^2 \langle{:}\phi^2{:}\rangle_{\omega^c} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(|\zeta_k|^2 - |\chi_k|^2\right) \mathrm{d}\vec{k},$$
$$Q_s^d \doteq \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\partial_\tau |\zeta_k|^2 - \partial_\tau |\chi_k|^2 + \frac{V'(\tau_0)}{4k_0^3} \cos(2k_0(\tau - \tau_0))\right) \mathrm{d}\vec{k},$$

and the subtraction of $C_{\phi^2}^{\mathcal{H}}$ in (2.41) taken before the k-integration is visible in the following contributions

$$Q_c \doteq \lim_{\epsilon\to 0^+} \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left[|\chi_k|^2 - \left(\frac{1}{2k_0} - \frac{V(\tau)}{4k_0^3}\right)\right] \mathrm{e}^{-\epsilon k} \mathrm{d}\vec{k},$$
$$Q_c^d \doteq \lim_{\epsilon\to 0^+} \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left[\partial_\tau |\chi_k|^2 + \left(\frac{V'(\tau)}{4k_0^3} - \frac{V'(\tau_0)}{4k_0^3} \cos(2k_0(\tau - \tau_0))\right)\right] \mathrm{e}^{-\epsilon k} \mathrm{d}\vec{k}.$$

Remark 2.2.2. As pointed out before, the subtraction considered in Q_c^d differs from $\partial_\tau C_{\phi^2}^{\mathcal{H}}$ by a contribution which is compensated in Q_s^d. This extra subtraction is necessary because the conformal vacuum ω^c, namely the Gaussian state constructed with the modes χ_k is not regular enough to give finite time derivatives of $\langle{:}\phi^2{:}\rangle_{\omega^c}$, because

$$\partial_\tau \left(a^2 \langle{:}\phi^2{:}\rangle_{\omega^c}\right)(\tau_0) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{V'(\tau_0)}{4k_0^3} \mathrm{d}\vec{k}$$

diverges logarithmically for large k.

Finally, the other two contributions Q_0 and Q_0^d are obtained from eq. (2.44) as the reminder. Both are functions of a and its derivatives and contain the finite reminder of the $C_{\phi^2}^{\mathcal{H}}$ subtraction discussed in eq. (2.39):

$$Q_0 \doteq a^2 \left\langle :\phi^2: \right\rangle_{\omega^c} - Q_c = \frac{w(\tau)^2}{8\pi^2} \log\left(\frac{w(\tau_0)}{a(\tau)}\right) - \frac{w(\tau_0)^2}{16\pi^2} + \alpha_1 m^2 a^2 + \alpha_2 a^2 R,$$
$$Q_0^d \doteq \frac{\partial_\tau w(\tau)^2}{8\pi^2} \log\left(\frac{w(\tau_0)}{a(\tau)}\right) - \frac{aHw(\tau)^2}{8\pi^2} + \alpha_1 m^2 \partial_\tau(a^2) + \alpha_2 \partial_\tau(a^2 R), \tag{2.45}$$

where α_1 and α_2 are renormalization constants, and $w(\tau)$ was defined in eq. (2.40).

According to the results presented in Appendix C, the desired Lipschitz continuity with respect to the potential (2.25) is achieved in the following propositions by studying the functional derivatives of all these operators in V.

Proposition 2.2.1. *Consider a cosmological spacetime and an interval of time $[\tau_0, \tau_1]$ over which Ω_k^2 given in eq. (2.12) is positive. Consider the following non-linear operators acting on C^2-functions which vanish at τ_0, namely on $D^2 \doteq \{V \in C^2[\tau_0, \tau_1] \mid V(\tau_0) = 0\}$*

$$Q_c[V](\tau) = \lim_{\epsilon\to 0^+} \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left[|\chi_k|^2 - \left(\frac{1}{2k_0} - \frac{V(\tau)}{4k_0^3}\right)\right] \mathrm{e}^{-\epsilon k} \mathrm{d}\vec{k},$$
$$Q_c^d[V](\tau) = \lim_{\epsilon\to 0^+} \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left[\partial_\tau |\chi_k|^2 + \left(\frac{V'(\tau)}{4k_0^3} - \frac{V'(\tau_0)}{4k_0^3} \cos(2k_0(\tau - \tau_0))\right)\right] \mathrm{e}^{-\epsilon k} \mathrm{d}\vec{k},$$

where χ_k is the solution of eq. (2.12) with initial data (2.22), and thus it implicitly depends on V. Consider also the following operator

$$\mathcal{T}_{\tau_0}[f] \doteq -\frac{1}{8\pi^2} \int_{\tau_0}^{\tau} f'(\eta) \log(\tau - \eta) \mathrm{d}\eta, \qquad f \in D^2. \tag{2.46}$$

It holds that the functionals

$$Q_f[V] \doteq Q_c[V] - \mathcal{T}_{\tau_0}[V], \qquad Q_f^d[V] \doteq Q_c^d[V] - \mathcal{T}_{\tau_0}[V']$$

admit the Gateaux differential at V or V'. Furthermore, Q_f is continuous with respect to the uniform norm on the interval $[\tau_0, \tau]$ and the same holds for its first functional derivative, hence Q_f can be extended to continuous functions which vanish at τ_0, namely to $D^0 \doteq \{V \in C[\tau_0, \tau_1] \mid V(\tau_0) = 0\}$.

If V is contained in $B_\delta(0)$, a ball of radius δ centred at 0 in $C[\tau_0, \tau_1]$, then

$$\|Q_f[V]\|_\infty \leq C_\delta \|V\|_\infty, \qquad \|\delta Q_f[V, W]\|_\infty \leq C'_\delta \|W'\|_\infty, \qquad V \in B_\delta(0) \cap D^0 \subset C[\tau_0, \tau].$$

Similarly, Q_f^d is continuous with respect to the uniform norm of the derivative on the interval $[\tau_0, \tau_1]$ and it can then be extended to $D \doteq \{V \in C^1[\tau_0, \tau_1] \mid V(\tau_0) = 0\}$. For $V \in D$ and if V' is contained in $B_\delta(0) \subset C[\tau_0, \tau_1]$ then

$$\|Q_f^d[V]\|_\infty \leq C_\delta \|V'\|_\infty, \qquad \|\delta Q_f^d[V, W]\|_\infty \leq C'_\delta \|W'\|_\infty, \qquad V \in D,\ V' \in B_\delta(0),$$

where the constants C_δ, C'_δ depend smoothly on δ and are bounded uniformly in time for $\tau - \tau_0 < \epsilon$ for some $\epsilon > 0$.

Proof. From proposition 2.1.1, $\chi = \sum_n \chi^n$ is well-defined. Then, $Q_c[V]$ and $Q_c^d[V]$ can be decomposed in contributions which are homogeneous in V of various degrees

$$Q_c[V] = \sum_{n\geq 0} L_n[V], \qquad Q_c^d[V] = \sum_{n\geq 0} L_n^d[V],$$

where both zeroth order contributions vanish because of the form of $\chi_k^{(0)}$ given in eq. (2.24). Furthermore,

$$L_1 = \lim_{\epsilon\to 0^+} \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} \left[(\overline{\chi}_k^1\chi_k^{(0)} + \chi_k^1\overline{\chi}_k^0) + \frac{V(\tau)}{4k_0^3}\right] \mathrm{e}^{-\epsilon k}\mathrm{d}\vec{k},$$
$$L_1^d = \lim_{\epsilon\to 0^+} \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} \left[\partial_\tau(\overline{\chi}_k^1\chi_k^{(0)} + \chi_k^1\overline{\chi}_k^0) + \left(\frac{V'(\tau)}{4k_0^3} - \frac{V'(\tau_0)}{4k_0^3}\cos(2k_0(\tau-\tau_0))\right)\right] \mathrm{e}^{-\epsilon k}\mathrm{d}\vec{k},$$

while for $n \geq 2$ the limit $\epsilon \to 0$ can be taken before the k-integration, hence

$$L_n[V] = \sum_{l=0}^{n} \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} \overline{\chi_k^{n-l}}\chi_k^l \mathrm{d}\vec{k}, \qquad L_n^d[V] = \partial_\tau L_n[V].$$

To study the form of L_1 and of L_1^d, recalling the definition of χ^1, integrating by parts, and using the condition $V(\tau_0) = 0$ yield

$$\overline{\chi}_k^1\chi_k^{(0)} + \overline{\chi}_k^0\chi_k^1 = -\frac{V(\tau)}{4k_0^3} + \frac{1}{4k_0^3}\int_{\tau_0}^{\tau} \cos\left(2k_0(\tau-\eta)\right) V'(\eta)\mathrm{d}\eta,$$
$$\partial_\tau\left(\overline{\chi}_k^1\chi_k^{(0)} + \overline{\chi}_k^0\chi_k^1\right) = -\frac{V'(\tau)}{4k_0^3} + \frac{V'(\tau_0)\cos(2k_0(\tau-\tau_0))}{4k_0^3} + \frac{1}{4k_0^3}\int_{\tau_0}^{\tau} \cos\left(2k_0(\tau-\eta)\right) V''(\eta)\mathrm{d}\eta.$$

Here, only the construction of $L_1^d[V]$ shall be discussed, because L_1 can then be obtained in a similar way. So,

$$L_1^d[V](\tau) = \lim_{\epsilon\to 0} \frac{1}{8\pi^2}\int_{\tau_0}^{\tau} \mathrm{d}\eta\, V''(\eta) \int_{w_0}^{\infty} \mathrm{d}k_0 \left[\cos\left(2k_0(\tau-\eta)\right)\frac{1}{k_0} - \cos\left(2k_0(\tau-\eta)\right)\frac{k_0-k}{k_0^2}\right] \mathrm{e}^{-2\epsilon k_0},$$

where $w_0 \doteq \sqrt{k_0^2 - k^2} = \sqrt{a^2(\tau_0)m^2 + \left(\xi - \frac{1}{6}\right)a^2 R(\tau_0)}$ is the k-independent part of $\Omega_k(\tau_0)$. The k_0-integration in the second contribution gives

$$f_1(w_0(\tau-\eta)) \doteq \int_{w_0}^{\infty} \cos(2k_0(\tau-\eta))\frac{k_0-k}{k_0^2}\mathrm{d}k_0.$$

Since $\frac{(k_0-k)}{k_0^2} = \frac{w_0^2}{k_0^2(k_0+k)}$, $f_1 \in C^1(\mathbb{R})$, and hence both f_1 and $\partial_\tau f_1$ are bounded on compact time intervals. The k_0-integration in the first contribution can be performed and in the limit $\epsilon \to 0$, and yields

$$\mathrm{Ci}(2w_0(\tau-\eta)) = -\int_{w_0}^{\infty} \frac{\cos(2k_0(\tau-\eta))}{k_0}\mathrm{d}k_0.$$

Here, $\mathrm{Ci}(z)$ is the cosine integral function which can be expanded as [AS65]

$$\mathrm{Ci}(z) = \gamma + \log(z) + \int_0^z \frac{\cos(t)-1}{t}\mathrm{d}t,$$

where γ is the Euler-Mascheroni constant. Then,

$$L_1^d[V](\tau) = -\frac{1}{8\pi^2}\int_{\tau_0}^{\tau} \mathrm{d}\eta V''(\eta)\mathrm{Ci}(2w_0(\tau-\eta)) - \frac{1}{8\pi^2}\int_{\tau_0}^{\tau} \mathrm{d}\eta V''(\eta) f_1(w_0(\tau-\eta)).$$

Integrating by parts and recalling the definition of $\mathcal{T}$, one gets

$$L_1^d[V] - \mathcal{T}_{\tau_0}[V'] = -\frac{1}{8\pi^2}(\gamma + \log(2w_0) + f_3(0))V'(\tau) + \frac{1}{8\pi^2}(\gamma + \log(2w_0) + f_3(w_0(\tau-\tau_0)))V'(\tau_0)$$
$$- \frac{w_0}{8\pi^2}\int_{\tau_0}^{\tau} \mathrm{d}\eta V'(\eta) f_3'(w_0(\tau-\eta)),$$

where $f_3(x) \doteq f_1(x) + f_2(x) \in C^1(\mathbb{R})$ because the function

$$f_2\,(z) \doteq \mathrm{Ci}(2z) - \gamma - \log(2z)$$

is of class $C^1(\mathbb{R})$, and it is thus bounded on finite interval of times. Thus, in $[\tau_0, \tau_1]$

$$\|L_1^d[V] - \mathcal{T}_{\tau_0}[V']\|_\infty \le C\|V'\|_\infty,$$

where the constant C depends continuously on τ_1 and vanishes in the limit $\tau_1 \to \tau_0$. Since both L_1^d and $\mathcal{T}_{\tau_0}$ are linear in V this proves also the Gateaux differentiability and its corresponding bounds. Similar results holds also for $L_1[V] - \mathcal{T}_{\tau_0}[V]$.

To analyze the order $n = 2$, one observes that

$$\begin{aligned}\left(\chi_k^{(0)}\overline{\chi}_k^2 + \chi_k^1\overline{\chi}_k^1 + \chi_k^2\overline{\chi}_k^0\right)(\tau) &= \frac{1}{k_0^3}\int_{\tau_0}^{\tau} \mathrm{d}\eta\, V(\eta)\sin(k_0(\tau-\eta))\int_{\tau_0}^{\eta}\mathrm{d}\xi\, V(\xi)\sin(k_0(\tau+\eta-2\xi)) \\ &= \frac{1}{2k_0^3}\int_{\tau_0}^{\tau}\mathrm{d}\eta\, V(\eta)\int_{\tau_0}^{\eta}\mathrm{d}\xi V(\xi)\left(\cos(2k_0(\eta-\xi)) - \cos(2k_0(\tau-\xi))\right),\end{aligned}$$

hence, for the second order, one gets

$$\begin{aligned}L_2[V](\tau) =& \frac{1}{8\pi^3}\int_{\mathbb{R}^3}\frac{\mathrm{d}\vec{k}}{2k_0^3}\int_{\tau_0}^{\tau}\mathrm{d}\eta\, V(\eta)\int_{\tau_0}^{\eta}\mathrm{d}\xi V(\xi)\left(\cos(2k_0(\eta-\xi)) - \cos(2k_0(\tau-\xi))\right), \\ L_2^d[V](\tau) =& \frac{1}{8\pi^3}\int_{\mathbb{R}^3}\frac{\mathrm{d}\vec{k}}{2k_0^3}\int_{\tau_0}^{\tau}\mathrm{d}\eta\, V(\eta)^2\cos(2k_0(\tau-\eta)) \\ &- \frac{1}{8\pi^3}\int_{\mathbb{R}^3}\frac{\mathrm{d}\vec{k}}{2k_0^3}\int_{\tau_0}^{\tau}\mathrm{d}\eta\, V(\eta)\int_{\tau_0}^{\eta}\mathrm{d}\xi V'(\xi)\cos(2k_0(\tau-\xi)),\end{aligned}$$

where the initial condition $V(\tau_0) = 0$ was used. Notice that the integral in k_0 can be computed just as in the linear case.

However, now logarithmic divergences in $\xi - \eta$ and $\xi - \tau$ for $L_2[V]$ and in $\xi - \tau$ and $\eta - \tau$ for $L_2^d[V]$ are absolutely integrable. These logarithmic divergences can be identified before taking the ϵ to 0 limit switching the order of η and $\vec{k}$ integration. Hence, in the interval $[\tau_0, \tau_1]$

$$\|L_2[V]\|_\infty \le C\|V\|_\infty^2, \qquad |\delta L_2[V, W]| \le C\|V\|_\infty\|W\|_\infty,$$

and, since $V \in D$,

$$\|L_2^d[V]\|_\infty \le C\|V\|_\infty\|V'\|_\infty, \qquad |\delta L_2^d[V, W]| \le C\|V'\|_\infty\|W'\|_\infty,$$

where C is a suitable constant which depends continuously on τ_1 and vanishes in the limit $\tau_1 \to \tau_0$.

Furthermore, for $n > 2$ it holds that

$$L_c[V] = \sum_{n\ge 3} L_n[V] = \lim_{\epsilon\to 0^+}\sum_{n\ge 3}\frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\sum_{l=0}^{n}\left(\overline{\chi_k^{n-l}}\chi_k^l\right)\mathrm{e}^{-\epsilon k}\mathrm{d}\vec{k},$$

and $L_c^d[V] = \partial_\tau L_c[V]$. From the inequality (2.26) and using that $\sum_{l=0}^n \frac{1}{l!}\frac{1}{(n-l)!} = \frac{2^n}{n!}$,

$$|L_c[V]| \le \sum_{n\ge 3}\frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\frac{1}{2k_0}\frac{2^n(\tau-\tau_0)^n}{k_0^n}\frac{1}{n!}\|V\|_\infty^n\mathrm{d}\vec{k} \le C\frac{2^2}{w_0^4}\|V\|_\infty^3\exp\left(2\frac{(\tau-\tau_0)}{w_0}\|V\|_\infty\right).$$

To bound $L_c^d[V]$, eq. (2.24) can be written in the following compact form:

$$\chi_k^{(n)} = \mathcal{R}(\chi_k^{n-1}) = \mathcal{R}^n(\chi_k^{(0)}),$$

where the operator $\mathcal{R}$ acts on a function f as $\mathcal{R}(f) = -\Delta_R(Vf)$, and Δ_R is the retarded operator defined in eq. (2.24). As $V(\tau_0) = 0$,

$$\chi_k^{(n)\prime} = -\Delta_R V' \chi_k^{n-1} - \Delta_R V \chi_k^{n-1\prime}.$$

Hence, after using recursively the previous identity, one gets an expression which depends linearly on V', that is,

$$\chi_k^{(n)\prime} = \sum_{j=0}^{n-1} \underbrace{\mathcal{R}\circ\cdots\circ\mathcal{R}}_{j} \circ \tilde{\mathcal{R}} \circ \underbrace{\mathcal{R}\circ\cdots\circ\mathcal{R}}_{n-1-j}(\chi_k^{(0)}) + \underbrace{\mathcal{R}\circ\cdots\circ\mathcal{R}}_{n}(\chi_k^{(0)\prime}),$$

where $\tilde{\mathcal{R}}(f) = -\Delta_R(V'f)$. Also, it can be written in a compact form in the following way with the help of a functional derivative which transforms $\mathcal{R}$ to $\tilde{\mathcal{R}}$, namely

$$\chi_k^{(n)\prime} = \int \mathrm{d}\eta V'(\eta) \frac{\delta \chi_k^{(n)}}{\delta V(\eta)} + \mathcal{R}^n(\chi_k^{(0)\prime}).$$

Furthermore, $\overline{\chi}_k^{(0)\prime} = -\mathrm{i}k_0 \overline{\chi}_k^{(0)}$, and $\chi_k^{(0)\prime} = \mathrm{i}k_0 \chi_k^{(0)}$, hence

$$(\overline{\chi}_k^l \chi_k^{n-l})' = \int \mathrm{d}\eta V'(\eta) \frac{\delta}{\delta V(\eta)} \overline{\chi}_k^l \chi_k^{n-l}. \tag{2.47}$$

In the estimate derived for $L_c[V]$, the bound $|\sin(k_0(\eta))/k_0| \leq 1/k_0$ was obtained without touching V; hence, one may apply the operator with the functional derivative introduced on the right hand side of (2.47) to derive an estimate for $L_c^d[V]$. In $[\tau_0, \tau_1]$,

$$\|L_c[V]\|_\infty \leq C\|V\|_\infty^3 \exp(C\|V\|_\infty), \qquad \|L_c^d[V]\|_\infty \leq C\|V\|_\infty^2 \|V'\|_\infty \exp(C\|V\|_\infty),$$

where the constant C depends continuously on τ_1 and vanishes in the limit of $\tau_1 \to \tau_0$. A similar analysis permits to get analogous estimates for the first functional derivatives

$$\|\delta L_c[V, W]\|_\infty \leq C \exp(C\|V\|_\infty)\|W\|_\infty,$$

where again the constant C depends continuously on τ_1 and vanishes in the limit of $\tau_1 \to \tau_0$. Finally, the statements of the proposition, namely the Gateaux differentiability in D with respect to the uniform norm and its bounds, can be obtained by combining the estimates for L_1, L_2, L_c, and assuming $V \in B_\delta(0)$, or by combining the estimates for L_1^d, L_2^d, L_c^d, and assuming $V' \in B_\delta(0)$. ☐

Proposition 2.2.2. *Consider a FLRW spacetime $(\mathcal{M}, g_{\mu\nu})$, whose scale factor is $a(\tau) \in C^3[\tau_0, \tau]$ with $a(\tau) > 0$, and the quasi-free state ω given in eq. (2.11) with respect to modes ζ_k, whose initial conditions (2.16) satisfy eqs. (2.42) and (2.43). Assume that Ω_k^2 given in eq. (2.12) is strictly positive in the interval $[\tau_0, \tau_1]$. The non-linear operator*

$$Q_s[V] = a^2 \left(\langle{:}\phi^2{:}\rangle_\omega - \langle{:}\phi^2{:}\rangle_{\omega^c}\right) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(|\zeta_k|^2 - |\chi_k|^2\right) \mathrm{d}\vec{k}$$

is Gateaux differentiable at V in $D^0 = \{V \in C[\tau_0, \tau_1] \mid V(\tau_0) = 0\}$, where the initial conditions for the modes χ_k are given in eq. (2.22). Similarly, the non-linear operator

$$Q_s^d[V] = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\partial_\tau |\zeta_k|^2 - \partial_\tau |\chi_k|^2 + \frac{V'(\tau_0)}{4k_0^3} \cos(2k_0(\tau - \tau_0))\right) \mathrm{d}\vec{k}$$

is Gateaux differentiable at $V' \in C[\tau_0, \tau_1]$.

Proof. Firstly, the modes ζ_k can be written as a linear combination of the modes χ_k, namely, $\zeta_k = A\chi + B\overline{\chi}_k$, where $A = A(k)$ and $B = B(k)$ are the Bogoliubov coefficients satisfying $|A|^2 - |B|^2 = 1$. Hence,

$$Q_s[V] = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\left(2|B|^2|\chi_k|^2 + A\overline{B}\chi_k\chi_k + \overline{A}B\overline{\chi}_k\overline{\chi}_k\right)\mathrm{d}\vec{k}. \tag{2.48}$$

Secondly, one shall now discuss how this expression depends on V. In particular, one shall get the properties and the form of A and B from the requirements (2.42) and (2.43), and thus the late-time control on Q_s from the known evolution of the modes χ_k discussed in proposition 2.1.1.

To analyze the form of A and B for large values of k, one notices that the initial conditions for ζ_k are chosen in such a way that eqs. (2.42) and (2.43) hold, hence both $|\zeta_k|^2 - C^{\mathcal{H}}_{\phi^2}$ and $\partial_\tau|\zeta_k|^2 - \partial_\tau C^{\mathcal{H}}_{\phi^2}$ are in $L^1(\mathbb{R}^3, \mathrm{d}\vec{k})$ at τ_0. Thus, also $\partial_\tau|\zeta_k|^2/\Omega_k$ and $\partial_\tau C^{\mathcal{H}}_{\phi^2}/\Omega_k$ are absolutely $\vec{k}$-integrable for $\tau \geq \tau_0$, because $1/\Omega_k$ is a bounded function in time, and from the definition of $C^{\mathcal{H}}_{\phi^2}$.

Furthermore, from eq. (2.43) it must exists a function $C^{\mathcal{H}}_E$ which depends on τ and k which makes $|\zeta'_k|^2 - C^{\mathcal{H}}_E$ absolutely $\vec{k}$-integrable at τ_0. Hence, also the quantity $(|\zeta'_k|^2 - C^{\mathcal{H}}_E)/\Omega_k^2$ is absolutely integrable at τ_0. This function $C^{\mathcal{H}}_E$ can be obtained arguing as for $C^{\mathcal{H}}_\varrho$, $C^{\mathcal{H}}_{\phi^2}$ and $\partial_\tau C^{\mathcal{H}}_{\phi^2}$, and has the form

$$C^{\mathcal{H}}_E(\tau, k) = \frac{k_0}{2} + \frac{V(\tau)}{4k_0} + O\left(\frac{1}{k_0^3}\right), \tag{2.49}$$

see Appendix B.

Consider now the functions

$$f_1 = \frac{|\zeta'_k|^2}{\Omega_k^2} - |\zeta_k|^2, \qquad f_2 = |\zeta_k|^2 - |\chi_k|^2 :$$

both are absolutely $\vec{k}$-integrable at τ_0, because $\frac{C^{\mathcal{H}}_E}{\Omega_k^2} - C^{\mathcal{H}}_{\phi^2}$ is in $L^1(\mathbb{R}, \mathrm{d}\vec{k})$; the same holds for $|\chi_k|^2 - C^{\mathcal{H}}_{\phi^2}$, because $(|\zeta'_k|^2 - C^{\mathcal{H}}_E)/\Omega_k^2$ and $|\zeta_k|^2 - C^{\mathcal{H}}_{\phi^2}$ are absolutely $\vec{k}$-integrable at τ_0. Also, $\frac{\partial_\tau f_2}{\Omega_k}$ is absolutely $\vec{k}$-integrable at τ_0, because $\partial_\tau C^{\mathcal{H}}_{\phi^2}/\Omega_k$ is in $L^1(\mathbb{R}^3, \mathrm{d}\vec{k})$. Therefore, evaluating f_1 and $\partial_\tau f_2/\Omega_k$ at τ_0 yields

$$f_1(\tau_0) = -\frac{2\mathrm{Re}\left(\overline{A}B\mathrm{e}^{\mathrm{i}2k_0\tau_0}\right)}{k_0}, \qquad \frac{\partial_\tau f_2(\tau_0)}{\Omega_k(\tau_0)} = \frac{2\mathrm{iIm}\left(\overline{A}B\mathrm{e}^{\mathrm{i}2k_0\tau_0}\right)}{k_0},$$

which must be both elements of $L^1(\mathbb{R}, \mathrm{d}\vec{k})$. Hence $|AB|/k_0$ is also absolutely integrable; the same holds also for $\frac{|B|^2}{k_0}$, because it can be obtained adding $f_1(\tau_0)/2$ to the absolute integrable function

$$f_2(\tau_0) = \frac{|B|^2}{k_0} + \frac{\mathrm{Re}\left(\overline{A}B\mathrm{e}^{\mathrm{i}2k_0\tau_0}\right)}{k_0}.$$

These estimates involve only initial conditions for the modes and for the scale factor, and thus they are independent of V for $\tau > \tau_0$. Furthermore, they are sufficient to obtain a bound for $Q_s[V]$ using the bounds obtained in proposition 2.1.1, namely

$$|\chi_k|^2 \leq \frac{1}{2k_0}\mathrm{e}^{\frac{2(\tau-\tau_0)\|V\|_\infty}{k_0}}, \qquad |\delta\chi_k[V,W]| \leq \frac{(\tau-\tau_0)}{\sqrt{2k_0^3}}\mathrm{e}^{\frac{(\tau-\tau_0)\|V\|_\infty}{k_0}}\|W\|_\infty.$$

Hence, from (2.48) and in any interval of time $[\tau_0, \tau]$,

$$\|Q_s[V]\|_\infty \leq C\mathrm{e}^{\frac{2(\tau-\tau_0)\|V\|_\infty}{w_0}}, \qquad \|\delta Q_s[V,W]\|_\infty \leq C\mathrm{e}^{\frac{2(\tau-\tau_0)\|V\|_\infty}{w_0}}\|W\|_\infty,$$

where w_0 equals $\Omega_k(\tau_0)$ evaluated at $k = 0$, and for a suitable constant C.

On the other hand, the last estimates obtained for A and B are not sufficient to get the desired bounds for Q_s^d. To get further control on these coefficients, one observes that

$$f_3 \doteq \partial_\tau |\zeta_k|^2 - \partial_\tau |\chi_k|^2 + \frac{V'(\tau_0)}{4k_0^3} \cos(2k_0(\tau - \tau_0))$$

is $L^1(\mathbb{R}^3, \mathrm{d}\vec{k})$ at τ_0, because the initial conditions for the state are chosen in such a way that $\partial_\tau |\zeta_k|^2 - \partial_\tau C^{\mathcal{H}}_{\phi^2}$ is absolutely k-integrable (see, e.g., eq. (2.42)), and because in the proof of proposition 2.2.1 it was proved that $\partial_\tau |\chi_k|^2 - \frac{V'(\tau_0)}{4k_0^3} \cos(2k_0(\tau - \tau_0)) - \partial_\tau C^{\mathcal{H}}_{\phi^2}$ is L^1 too (see also the remark 2.2.2). Besides, f_3 can be further expanded as

$$\begin{aligned} f_3 =& 2|B|^2 \partial_\tau \left(\overline{\chi}_k (\chi_k - \chi_k^{(0)}) + (\overline{\chi}_k - \overline{\chi}_k^{0}) \chi_k^{(0)} \right) + 4\mathrm{Re}(A\overline{B}(\chi_k - \chi_k^{(0)}) {\chi_k}') \\ &+ 4\mathrm{Re}(A\overline{B}\chi_k^{(0)} (\chi_k - \chi_k^{(0)})') + 4\mathrm{Re}(A\overline{B}\chi_k^{(0)} {\chi_k^{(0)}}') + \frac{V'(\tau_0)}{4k_0^3} \cos(2k_0(\tau - \tau_0)). \end{aligned} \tag{2.50}$$

From the previous discussion,

$$f_3(\tau_0) = 2\mathrm{Re}(A\overline{B}\mathrm{i}\mathrm{e}^{\mathrm{i}2k_0\tau_0}) + \frac{V'(\tau_0)}{4k_0^3} \tag{2.51}$$

is absolutely $\vec{k}-$integrable; hence, the imaginary part of $A\overline{B}\mathrm{e}^{\mathrm{i}2k_0\tau_0}$ equals $V'(\tau_0)/8k_0^3$ up to an absolutely $\vec{k}-$integrable function. Arguing as before, one gets also that $|\zeta_k|^2 - C^{\mathcal{H}}_{\phi^2}$ is absolutely $\vec{k}$-integrable at τ_0, and the same holds for $f_4 \doteq (|\zeta_k|^2 - C^{\mathcal{H}}_{\phi^2})/\Omega_k$. Hence,

$$f_4(\tau_0) = 2 \left(|B|^2 \frac{|{\chi_k^{(0)}}'|^2}{k_0} + \mathrm{Re}\left(A\overline{B} \frac{{\chi_k^{(0)}}'^2}{k_0} \right) \right) = \left(|B|^2 - \mathrm{Re}\left(A\overline{B}\mathrm{e}^{\mathrm{i}2k_0\tau_0} \right) \right).$$

is also an absolutely $\vec{k}-$integrable function. Since $|AB|/k_0$ is absolutely $\vec{k}-$integrable again, with $|A|^2 = 1 + |B|^2$, $|B|^2$ is also absolutely $\vec{k}-$integrable, and thus the same holds for $\mathrm{Re}\left(A\overline{B}\mathrm{e}^{\mathrm{i}2k_0\tau_0}\right)$. Therefore, one concludes that $A\overline{B}\mathrm{e}^{\mathrm{i}2k_0\tau_0}$ equals $\mathrm{i}V'(\tau_0)/8k_0^3$ up to an absolutely integrable $\vec{k}-$function. This also means that A and B are such that

$$f_5 \doteq 4\mathrm{Re}(A\overline{B}\chi_k^{(0)} {\chi_k^{(0)}}') + \frac{V'(\tau_0)}{4k_0^3} \cos(2k_0(\tau - \tau_0)) \tag{2.52}$$

is absolutely $\vec{k}-$integrable for all $\tau \geq \tau_0$. To control the integrability of f_3 at later time, one needs to evaluate the time evolutions of the modes χ_k: from eq. (2.28) of proposition 2.1.1, the first contribution in eq. (2.50) is in L^1 at any time, because $|B|^2/k_0$ is L^1. Also, both the second and the third contributions of f_3 in eq. (2.50) are elements of L^1, because $|AB|/k_0$ is L^1, $|\chi'| \leq \sqrt{k_0} C \mathrm{e}^{\|V\|_1/w_0}$, and $|\chi| \leq C\mathrm{e}^{\|V\|_1/w_0}/\sqrt{k_0}$. Finally, the contribution f_5 given in eq. (2.52) which is in the function f_3 given in eq. (2.50) is integrable. Therefore, $Q_s^d[V]$ can be rewritten as

$$\begin{aligned} Q_s^d[V] =& \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(2|B|^2 \partial_\tau |\chi_k|^2 + 4\mathrm{Re}\left(A\overline{B}\chi_k \partial_\tau \chi_k \right) + \frac{V'(\tau_0)}{4k_0^3} \cos(2k_0(\tau - \tau_0)) \right) \mathrm{d}\vec{k} \\ =& \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(2|B|^2 \partial_\tau \left(\overline{\chi_k} (\chi_k - \chi_k^{(0)}) \right) + 2|B|^2 \partial_\tau \left((\overline{\chi_k} - \overline{\chi_k^{(0)}}) \chi_k^{(0)} \right) + 4\mathrm{Re}\left(A\overline{B}\chi_k (\chi_k - \chi_k^{(0)})' \right) \right. \\ & \left. + 4\mathrm{Re}\left(A\overline{B} (\chi_k - \chi_k^{(0)}) {\chi_k^{(0)}}' \right) + 4\mathrm{Re}\left(A\overline{B}\chi_k^{(0)} {\chi_k^{(0)}}' \right) + \frac{V'(\tau_0)}{4k_0^3} \cos(2k_0(\tau - \tau_0)) \right) \mathrm{d}\vec{k}, \end{aligned}$$

where the relation $|\chi_k^{(0)}|' = 0$ was used. Recalling the estimates given in eq. (2.28), having shown the integrability of f_3 at any time in eq. (2.50), and knowing the control of χ_k and its functional derivatives, the statements of the proposition follow. $\square$

Notably, the Bogoliubov coefficients A and B introduced in the proof of the previous proposition are constructed with $a(\tau_0), a'(\tau_0), a''(\tau_0)$ and $a^{(3)}(\tau_0)$ only. This implies that the constants used in the estimates, which could depend on the initial conditions, do not contain derivatives higher than the third order.

Finally, the function

$$Q_0 = \frac{m^2a^2 + (\xi - \frac{1}{6})Ra^2}{8\pi^2} \log\left(\frac{w(\tau_0)}{a}\right) - \frac{w(\tau_0)^2}{16\pi^2} + \alpha_1 a^2 m^2 + \alpha_2 a^2 R \tag{2.53}$$

depends only on a and a'', which is differentiable if $a > 0$. Similarly, the function

$$\begin{aligned} Q_0^d = &\left(\frac{a^3H(m^2 + (\xi - \frac{1}{6})R)}{4\pi^2} + \frac{a^2(\xi - \frac{1}{6})R'}{8\pi^2}\right) \log\left(\frac{w(\tau_0)}{a}\right) - \frac{a^3H(m^2 + (\xi - \frac{1}{6})R)}{8\pi^2} \\ &+ \alpha_1 m^2 \partial_\tau(a^2) + \alpha_2 \partial_\tau(a^2 R) \end{aligned} \tag{2.54}$$

depends on a and its derivatives up to the third order, which are differentiable if $a > 0$.

2.2.3 Integration of the semiclassical Einstein equations

After discussing the regularity of the vacuum polarization, one can finally consider the semiclassical Einstein equations (1.105) in the case of FLRW spacetimes. As already pointed out in subsection 2.1.1, one needs to consider the semiclassical version of eqs. (2.5) and (2.6), where the expectation values $\langle :T_\rho{}^\rho: \rangle_\omega$ and $\langle :T_{00}: \rangle_\omega$ are used at the place of the corresponding classical quantities. These expectation values are computed in a quasi-free pure state with two-point function given in eq. (2.11), which is characterized by the initial conditions (2.16) satisfying the regularity conditions stated in eqs. (2.42) and (2.43).

Thanks to the discussions given in subsection 2.2.1 and subsection 1.3.1, the semiclassical Einstein equations on FLRW spacetimes constitute a dynamical problem for the scale factor $a(\tau)$ and for the state ω described by the following system of equations

$$\begin{cases} -R(a, a'') + 4\Lambda = 8\pi \langle :T_\rho{}^\rho: \rangle_\omega \left(a, a', a'', a^{(3)}, a^{(4)}\right), \\ G_{00}(\tau_0) - a^2\Lambda = 8\pi \langle :T_{00}: \rangle_\omega \left(a_0, a_0', a_0'', a_0^{(3)}\right), \end{cases} \tag{2.55}$$

equipped with some initial data for a and for ω. The initial conditions $\tau = \tau_0$ for the scale factor a consist of $(a(\tau_0), a'(\tau_0), a''(\tau_0), a^{(3)}(\tau_0)) = (a_0, a_0', a_0'', a_0^{(3)})$, while those for the state are given in terms of the functions Φ, E and s introduced in eq. (2.16).

In the system (2.55), $\langle :T_\rho{}^\rho: \rangle_\omega$ was written in eq. (1.124), whereas $\langle :T_{00}: \rangle_\omega$ is related to the renormalized energy density given in eq. (2.39). Notably, $\langle :T_\rho{}^\rho: \rangle_\omega$ contains both $\square R$, which depends locally on the fourth-order derivative of a, and the non-local operator $\mathcal{T}_{\tau_0}[V]$ introduced in eq. (2.46) within proposition 2.2.1, which is a fourth-order derivative contribution inside $\square \left\langle :\phi^2: \right\rangle_\omega$.

On the other hand, the second equation fulfilled at $\tau = \tau_0$ represents a constraint on the initial values for the state. As seen in section 2.2.1, $\langle :T_{00}: \rangle_\omega$ can be constructed only with the derivatives of the scale factor up to the third order using Φ, E and s, which specify the initial values for the state once the renormalization constants are fixed. Thus, one can introduce the following definition.

Definition 2.2.2. Consider a flat cosmological spacetime, whose scale factor a is characterized by the initial conditions $(a_0, a_0', a_0'', a_0^{(3)})$ fixed at τ_0 with $a_0 > 0$. The quantum state ω given in eq. (2.11) is said compatible with the initial conditions if the initial constraint given in the system (2.55)

$$H(\tau_0)^2 = \frac{8\pi}{3}\langle{:}\varrho{:}\rangle_\omega(\tau_0) + \frac{\Lambda}{3}$$

is satisfied at $\tau = \tau_0$.

In a first step, it shall be proved that it is always possible to choose a state compatible with fixed initial conditions.

Proposition 2.2.3. *Let a_0, a_0', a_0'' and $a_0^{(3)}$ be initial conditions for a and its derivatives at time $\tau = \tau_0$ chosen in such a way that $\Omega_k(\tau_0)^2$ given in eq. (2.12) is strictly positive. Let $\xi \neq 1/6$ be the coupling to the curvature . Fix the renormalization constants. It is possible to select initial conditions Φ, E, and s in eq. (2.16) that fix the quantum state ω given in eq. (2.11) in such a way that the state is sufficiently regular in the sense of definition 2.2.1 and compatible with initial conditions in the sense of definition 2.2.2.*

Proof. As shown in eq. (2.39), and in view of the form of $C_\varrho^{\mathcal{H}}$, only third derivatives of a are necessary in order to evaluate ϱ in the state ω. In particular, fix some initial conditions for the state pf the form of eq. (2.16) which are described by Φ, E, and s sufficiently regular (namely they satisfy eqs. (2.42) and (2.43)). Then, write $\zeta_k = \rho e^{i\theta}$. Hence, one gets the following real finite result

$$\begin{aligned}\langle{:}\varrho{:}\rangle_\omega(\tau_0) = &\frac{1}{(2\pi)^3 a(\tau_0)^4}\int_{\mathbb{R}^3}\left[\frac{1}{2}\left((1-6\xi)(\rho' - aH\rho)^2 + 6\xi{\rho'}^2 + (k^2 + a^2m^2)\rho^2\right) - C_\varrho^{\mathcal{H}}(\tau_0, k)\right]\mathrm{d}\vec{k}\\ &- \frac{H(\tau_0)^4}{960\pi^2} + \left(\xi - \frac{1}{6}\right)^2\frac{3H^2(\tau_0)R(\tau_0)}{8\pi^2} + \tilde\beta_1 m^4 - \tilde\beta_2 m^2 {G_0}^0(\tau_0) + (\tilde\beta_3 - \frac{\tilde\beta_4}{3}){I_0}^0(\tau_0),\end{aligned}$$

where $\rho = \sqrt{\Phi}$ and $\rho' = s\sqrt{E - \frac{1}{4\Phi}}$.

It shall be shown that $\langle{:}\varrho{:}\rangle_\omega$ can assume all values over the real line changing initial conditions for the state. It shall be discussed in some detail the case $H \neq 0$, but the other cases can be discussed similarly. The initial conditions $\tilde E, \tilde\Phi$ and $\tilde s$ for a new state $\tilde\omega$ are chosen in such a way that

$$\tilde s = s, \qquad \tilde\Phi = \Phi, \qquad \tilde E = \left(\sqrt{E - \frac{1}{4\Phi}} + \frac{C}{k^{\frac{5}{2}}}\Pi_{[p_1,p_2]}(k)\right)^2 + \frac{1}{4\Phi},$$

where C is a constant, and $\Pi_{[p_1,p_2]}$ denotes the characteristic function of the interval $[p_1, p_2]$ of the positive real line. Notice that, for every choice of the parameter p_1, p_2, the constraint

$$\tilde E - \frac{1}{4\tilde\Phi} \geq 0$$

is fulfilled. Hence, in this way,

$$\tilde\rho = \rho, \qquad \tilde\rho' = \rho' + \frac{C}{k^{\frac{5}{2}}}\Pi_{[p_1,p_2]}(k).$$

Moreover, the correction is such that

$$\begin{aligned}\langle :\varrho: \rangle_{\tilde\omega} &= \langle :\varrho: \rangle_{\omega} + \frac{1}{(2\pi)^3}\frac{1}{2a^4}\int_{\mathbb{R}^3}\left(\frac{s^2C^2}{k^5} + s\frac{2C}{k^{\frac{5}{2}}}(\rho' - (1-6\xi)aH\rho)\right)\Pi_{[p_1,p_2]}\mathrm{d}\vec{k} \\ &= \langle :\varrho: \rangle_{\omega} + \frac{1}{2\pi^2}\frac{s^2C^2}{4a^4}\left(\frac{1}{p_1^2} - \frac{1}{p_2^2}\right) + \frac{1}{(2\pi)^3}\frac{s2C}{2a^4}\int_{\mathbb{R}^3}\frac{1}{k^{\frac{5}{2}}}(\rho' - (1-6\xi)aH\rho)\Pi_{[p_1,p_2]}\mathrm{d}\vec{k} \\ &= \langle :\varrho: \rangle_{\omega} + \frac{1}{2\pi^2}\frac{s^2C^2}{4a^4}\left(\frac{1}{p_1^2} - \frac{1}{p_2^2}\right) + \frac{s2C}{2\pi^2}\frac{(6\xi-1)H}{2a^3}\log\left(\frac{p_2}{p_1}\right) \\ &+ \frac{s2C}{2\pi^2}\frac{1}{2a^4}\int_{p_1}^{p_2} O\left(\frac{1}{k^2}\right)\Pi_{[p_1,p_2]}\mathrm{d}k.\end{aligned}$$

In the last equality the following decay properties of the state was used:

$$\rho = \frac{1}{\sqrt{2k}}\left(1 + O\left(\frac{1}{k}\right)\right), \qquad \rho' = \frac{1}{\sqrt{2k}}\left(O\left(\frac{1}{k}\right)\right),$$

which hold thanks to the regularity conditions about the L^1-integrability imposed on modes ζ_k, ζ'_k at the initial time τ_0. Actually, the large-k behaviour of ρ can be obtained from the first condition in eq. (2.42), whereas the one for ρ' can be derived either from the second condition in eq. (2.42) or from eq. (2.43); in particular, the contribution proportional to $\log\left(\frac{p_2}{p_1}\right)$ follows from the leading contribution $1/\sqrt{2k}$ inside ρ. Hence, modifying p_2 and the sign of the constant C, one obtains that $\langle :\varrho: \rangle_{\tilde\omega} - \langle :\varrho: \rangle_{\omega}$, and thus $\langle :\varrho: \rangle_{\tilde\omega}$, can take all the values of the real line, because $\log(p_2/p_1)$ diverges for $p_2 \to \infty$, while the other contributions stay finite. Finally, one observes that the asymptotic behaviour of $\tilde E$ and $\tilde\Phi$ for large k equals that of E and Φ, and hence the state $\tilde\omega$ is sufficiently regular in the sense of definition 2.2.1 because this property holds for ω. □

From now on, the state ω will be considered to be fixed and chosen to be sufficiently regular according to definition 2.2.1, and compatible with the initial conditions for the scale factor a in the sense of definition 2.2.2: in this way, the energy constraint is fulfilled at τ_0.

In a second step, one has to analyze the first equation of the system (2.55) in the case of non-conformal coupling $\xi \neq 1/6$, i.e., when the higher order derivative terms $\Box R$ and $\Box\left\langle :\phi^2: \right\rangle_\omega$ cannot be avoided. To do that, one shall first rewrite the traced semiclassical Einstein equations as a system of two equations: the first one is a non-homogeneous free Klein-Gordon equation (with imaginary mass if $\xi < 1/6$) on FLRW spacetime, whereas the second one involves the vacuum polarization $\left\langle :\phi^2: \right\rangle_\omega$. To this avail, the following proposition holds.

Proposition 2.2.4. *Consider a generic spacetime (M, g), let R_{abcd}, R_{ab} and R be respectively the Riemann tensor, the Ricci tensor and the Ricci scalar of the spacetime. Over this spacetime consider a real scalar field with mass m and with coupling to the scalar curvature $\xi \neq 1/6$. Let ω be a state for this real scalar field. The traced semiclassical Einstein equations in the system (2.55) can be written as the following system of equations*

$$\begin{cases}(-\Box + M_c)F = S, \\ \left\langle :\phi^2: \right\rangle_\omega - c_\xi R = F,\end{cases} \tag{2.56}$$

where

$$c_\xi \doteq \frac{\beta_3}{3(1/6 - \xi)}, \qquad M_c \doteq -\frac{m^2}{3(1/6-\xi)}, \tag{2.57}$$

and S is a function of the derivatives of a up to the second order, which reads

$$S \doteq \frac{1}{3(\xi - 1/6)}\left(\beta_1 m^4 - \frac{\Lambda}{2\pi} + \frac{R}{8\pi} + \beta_2 m^2 R + \beta_3 M_c R + \frac{(6\xi-1)^2R^2}{1152\pi^2} + \frac{R_{abcd}R^{abcd} - R_{ab}R^{ab}}{2880\pi^2}\right).$$

Proof. The proof consists only of some algebraic manipulations of the traced semiclassical equations, with $\langle :T_\rho{}^\rho: \rangle_\omega$ given by eq. (1.123); in particular, eq. (1.124) reads

$$-R + 4\Lambda = 8\pi\bigg(-3(1/6-\xi)\Box \left\langle :\phi^2: \right\rangle_\omega - m^2 \left\langle :\phi^2: \right\rangle_\omega + \beta_3 \Box R + \beta_1 m^4 + \beta_2 m^2 R + \frac{(6\xi-1)^2 R^2}{1152\pi^2} + \frac{R_{abcd}R^{abcd} - R_{ab}R^{ab}}{2880\pi^2} \bigg).$$

Thus, eq. (2.56) follows by regrouping the state-dependent terms and isolating all the terms depending on $\Box$. Notice that all the functions $c_\xi, S(\xi, m^2, R, R_{ab}, R_{abcd})$ and M_c, whose sign depends on the value of the parameter ξ, are well-defined for $\xi \neq 1/6$. $\Box$

One shall now specialize this discussion for a FLRW spacetime. In this case, both the geometric quantities and the vacuum polarization depends only on the conformal time, whenever the state for the quantum matter is compatible with the cosmological principle, namely it is homogeneous and isotropic. Hence, both F and S are functions of τ, and eq. (2.56) is such that

$$P_c F = S, \tag{2.58}$$

where

$$P_c \doteq \frac{1}{a^3(\tau)} \left(\partial_\tau^2 + a^2(\tau) M_c - \frac{1}{6} a^2(\tau) R \right) a(\tau). \tag{2.59}$$

The second-order differential equation (2.58) can be solved by observing that P_c admits unique advanced and retarded fundamental solutions, denoted by Δ_A^c and Δ_R^c, respectively, and hence a unique solution can be written in terms of the retarded fundamental solution, after equipping eq. (2.58) with suitable initial conditions at $\tau = \tau_0$; all these observations are collected in the following proposition.

Proposition 2.2.5. *Let $a \in C^2[\tau_0, \tau]$ be a real positive function, let $h \in C[\tau_0, \tau]$ and $(f_0, f_0') \in \mathbb{R}^2$. The following problem in $C^2[\tau_0, \tau]$*

$$\begin{cases} P_c f = h, \\ (f, f')(\tau_0) = (f_0, f_0'), \end{cases} \tag{2.60}$$

where P_c given in eq. (2.59) admits a unique solution f on $C^2([\tau_0, \tau]; \mathbb{R})$ given in terms of h and the initial data. Furthermore, $\tilde{f} = af$ depends linearly on the initial data $(\tilde{f}_0, \tilde{f}_0')$, and on $\tilde{h} = a^3 h$.

The following estimate holds

$$\|\tilde{f}\|_\infty \leq \left(\|\beta\|_\infty + (\tau-\tau_0)^2 \|\tilde{h}\|_\infty \right) \exp\left((\tau-\tau_0)^2 \|\tilde{W}\|_\infty \right), \tag{2.61}$$

where

$$\tilde{W} = a^2 M_c - \frac{1}{6} a^2 R, \qquad \beta(\tau) = |\tilde{f}(\tau_0)| + (\tau-\tau_0)|\tilde{f}'(\tau_0)|.$$

Furthermore, $\tilde{f}$ depends continuously on a: denoting by $\delta\tilde{f}$ the functional derivative of f with respect to infinitesimal changes δa of a, then

$$\|\delta\tilde{f}\|_\infty \leq (\tau-\tau_0)^2 \left(\|\delta\tilde{W}\|_\infty \|\tilde{f}\|_\infty + \|\delta\tilde{h}\|_\infty \right) \exp\big((\tau-\tau_0)^2 \|\tilde{W}\|_\infty \big).$$

All these norms are finite in any $[\tau_0, \tau]$ for all finite $\tau > \tau_0$.

Proof. The problem stated in eq. (2.60) can equivalently be written as

$$\tilde{f}'' + \tilde{W}\tilde{f} = \tilde{h},$$

which is a second order linear non-homogeneous differential equations with regular coefficients. Since $a > 0$, such a problem admits thus an unique solution, and the results of lemma C.2.1 with $k = 0$ can be applied to eq. (2.60), once it is written in the form given in eq. (C.4), from which one gets eq. (2.61). From lemma C.2.1 and in particular from eq. (C.8), one also has that

$$\tilde{f} = -\int_{\tau_0}^{\tau} (\tau - \eta)\tilde{W}(\eta)\tilde{f}(\eta)\mathrm{d}\eta + \int_{\tau_0}^{\tau} (\tau - \eta)\tilde{h}(\eta)\mathrm{d}\eta + \tilde{f}_0 + (\tau - \tau_0)\tilde{f}'_0.$$

Hence,

$$\begin{aligned}|\delta\tilde{f}(\tau)| &\le (\tau - \tau_0)\int_{\tau_0}^{\tau} \left(|\delta\tilde{W}(s)||\tilde{f}(s)| + |\tilde{W}(s)||\delta\tilde{f}(s)|\right)\mathrm{d}s + (\tau - \tau_0)\int_{\tau_0}^{\tau} |\delta\tilde{h}(s)|\mathrm{d}s \\ &\le \gamma(\tau) + (\tau - \tau_0)\int_{\tau_0}^{\tau} |\tilde{W}(s)||\delta\tilde{f}(s)|\mathrm{d}s,\end{aligned}$$

where $\gamma(t) = (\tau - \tau_0)^2\left(\|\delta\tilde{W}\|_\infty\|\tilde{f}\|_\infty + \|\delta\tilde{h}\|_\infty\right)$, and by Grönwall lemma

$$|\delta\tilde{f}(\tau)| \le \gamma(\tau)\mathrm{e}^{(\tau-\tau_0)\int_{\tau_0}^{\tau}|\tilde{W}(s)|\mathrm{d}s}.$$

Thus, the remaining statements follow. □

Hence one obtains the following theorem of existence of solutions for eq. (2.56)

Theorem 2.2.1. *Consider a flat cosmological spacetime. Fix five constants τ_0, a_0, $a'_0, a''_0, a_0^{(3)}$, with $a_0 > 0$, corresponding at the initial data in τ_0 for the system (2.56), namely $a_0 = a(\tau_0), a'_0 = a'(\tau_0), a''_0 = a''(\tau_0), a_0^{(3)} = a^{(3)}(\tau_0)$. Fix the renormalization constants and let $\xi \neq 1/6$. Select a state ω with two-point function given in eq. (2.11) and characterized by eq. (2.16), which is compatible with these initial conditions, so that the energy constrain in the system (2.55) holds.*

It exists a unique F given in terms of S and the initial data, which is a solution of the traced equation given in the system (2.55), and which depends continuously on the initial data $a_0, a'_0, a''_0, a_0^{(3)}$, on the initial data for the state ω, and on a. Moreover,

$$\|\tilde{F}\|_\infty \le \left(\|\mathscr{I}_0\|_\infty + (\tau - \tau_0)^2\|\tilde{S}\|_\infty\right)\exp\left((\tau - \tau_0)^2\|\tilde{W}\|_\infty\right), \tag{2.62}$$

$$\|\delta\tilde{F}\|_\infty \le (\tau - \tau_0)^2\left(\|\delta\tilde{W}\|_\infty\|\tilde{F}\|_\infty + \|\delta\tilde{S}\|_\infty\right)\exp\left((\tau - \tau_0)^2\|\tilde{W}\|_\infty\right), \tag{2.63}$$

where $\tilde{F} = Fa$, $\tilde{S} = Sa^3$, and $\|\mathscr{I}_0\|_\infty \doteq |\tilde{F}(\tau_0)| + (\tau - \tau_0)|\tilde{F}'(\tau_0)|$ corresponds to the finite norm of $\tilde{F}(\tau)$ at the initial time τ_0 depending on the initial data of a and the state.

Then, the system of equations (2.55) reduces to the trace semiclassical equation written as

$$\left\langle :\phi^2: \right\rangle_\omega - c_\xi R = F(a, R), \tag{2.64}$$

where F is the unique solution of the system (2.56) given in terms of S, of the initial data of a, and of the state ω.

Proof. The proof starts with observing that, thanks to proposition 2.2.3, the state can be chosen to be compatible with the first Friedman equation at τ_0. The initial data on the scale factor and its first three derivatives allow to construct the corresponding initial data for F:

$$\begin{aligned}\tilde{F}(\tau_0) &= a_0\left(\left\langle :\phi^2: \right\rangle_\omega(\tau_0) - c_\xi R_0\right), \\ \tilde{F}'(\tau_0) &= a'_0\left(\left\langle :\phi^2: \right\rangle_\omega(\tau_0) - c_\xi R_0\right) + a_0\left(\partial_\tau\left\langle :\phi^2: \right\rangle_\omega(\tau_0) - c_\xi R'_0\right),\end{aligned} \tag{2.65}$$

where the expectation values $\langle :\phi^2: \rangle_\omega$ and $\partial_\tau \langle :\phi^2: \rangle_\omega$ are evaluated at $\tau = \tau_0$, respectively. These initial data depend on the modes initial data given in eq. (2.16) at $\tau = \tau_0$, and on the initial data of the geometry a_0, a_0', a_0'' and $a_0^{(3)}$. The unique solution F of the first equation in the system (2.56), which satisfies the initial conditions given in eq. (2.65), is obtained in proposition 2.2.5 together with its bounds. Thus, a partial integration of the system (2.56) yields the second equation of the system (2.64). □

Therefore, thanks to theorem 2.2.1 the problem of finding solutions of the semiclassical Einstein equations on FLRW spacetimes is reduced to the problem of finding solutions of eq. (2.64), which satisfy the desired initial conditions. Then, the existence of a unique solution of eq. (2.64), and thus of eq. (2.55), in a small interval of conformal time just after the initial time $\tau = \tau_0$ shall be proved in subsection 2.2.5.

In order to have control on the third order derivative of a, and to be able to impose the initial condition $a^{(3)}(\tau_0) = a_0^{(3)}$, one shall study the time-derivative of eq. (2.64), namely

$$\partial_\tau \left(a^2 (\langle :\phi^2: \rangle_\omega - c_\xi R - F) \right) = 0. \tag{2.66}$$

Actually, this equation is equivalent to eq. (2.64), because at τ_0 the equation without derivatives

$$\langle :\phi^2: \rangle_\omega - c_\xi R - F \big|_{\tau_0} = 0$$

holds thanks to the choice of initial condition made for F in eq. (2.65). Thus, in order to prove the existence of solutions $a(\tau)$ of eq. (2.64) which satisfy the desired initial conditions, a careful analysis of each term Q_i^d and $\mathcal{T}_{\tau_0}[V']$ inside the decomposition of the state studied in proposition 2.2.1 is necessary. Hence, the following proposition holds directly.

Proposition 2.2.6. *Fix the initial data a_0, a_0', a_0'' and $a_0^{(3)}$ for a, and assume that Ω_k^2 given in eq. (2.12) is strictly positive. Then, the semiclassical equation (2.66) can be expressed in terms of the potential (2.25), R and a as*

$$Q_0^d + \mathcal{T}_{\tau_0}[V'] + Q_f^d + Q_s^d = \partial_\tau \left(a^2 c_\xi R + a^2 F(a, R) \right), \tag{2.67}$$

where Q_0^d is given in eq. (2.53), Q_f^d and $\mathcal{T}_{\tau_0}[V']$ are introduced in proposition 2.2.1, and Q_s^d is given in proposition 2.2.2. Finally, F is given in eq. (2.64), and its properties are stated in theorem 2.2.1.

2.2.4 The unbounded operator $\mathcal{T}_{\tau_0}$, and its inversion formula

The most problematic term appearing in eq. (2.67), and containing the essence of the non-local nature of the semiclassical equations (1.105), is the operator $\mathcal{T}_{\tau_0}[V']$ defined in eq. (2.46) and applied to the derivative of the potential (2.25). This non-local term contained in the vacuum polarization depends on fourth-order derivatives of the scale factor, because its computation requires to know $V''(\eta)$ for every $\eta \in [\tau_o, \tau]$. On the one hand, it represents the source of the regularity issues found in the formulation of the semiclassical Einstein equations on cosmological spacetimes as a dynamical system [GS21]. On the other hand, this operators introduces the main difficulty of this equation, because one can prove that it is not continuous in $C([\tau_0, \tau])$ with respect to the uniform norm for any $\tau > \tau_0$.

Remark 2.2.3. Different from the conformal coupling case $\xi = 1/6$, which is governed by eq. (2.38), for arbitrary ξ the presence of a non-local term which contains third order derivatives of the scale factor $a^{(3)}$ inside $\langle :\phi^2: \rangle_\omega$, through the linear operator $\mathcal{T}_{\tau_0}[V]$ in (2.46), forbids to prove existence of solutions directly for eq. (2.64). In a similar way, the non-local term which contains fourth order derivatives of the scale factor $a^{(4)}$ inside $\partial_\tau(a^2 \langle :\phi^2: \rangle_\omega)$ through $\mathcal{T}_{\tau_0}[V']$ forbids a direct analysis of eq. (2.66).

A way to overcome the problem of the loss of derivatives of $\mathcal{T}_{\tau_0}[f]$ envisaged in Remark 2.2.3 is to study an inversion formula for $h = \mathcal{T}_{\tau_0}[f]$, and to prove the continuity of the associated inverse operator $\mathcal{T}_{\tau_0}^{-1}$. Preliminarily, up to a translation of the function $f_{\tau_0}(x) = f(x+\tau_0)$,

$$\mathcal{T}_{\tau_0}[f](x+\tau_0) = \mathcal{T}_0[f_{\tau_0}](x).$$

Thus, one can study the following operator $\mathcal{T} : C_1^\infty[0,r] \to C[0,r]$, with $r > 0$,

$$\mathcal{T}[f](x) \doteq -\frac{1}{8\pi^2}\int_{\mathbb{R}^+} f'(y)\theta(x-y)\log(x-y)\mathrm{d}y = -\frac{1}{8\pi^2}\int_0^x f'(y)\log(x-y)\mathrm{d}y \tag{2.68}$$

which equals $\mathcal{T}_0$ on $C^1[0,\tau-\tau_0]$. Clearly $\mathcal{T}$ is bounded in the C^1 sense. Indeed, since $\log x$ is integrable in $x = 0$, one finds

$$\|\mathcal{T}[f]\|_\infty \le \sup_{x\in[0,r]}\int_0^x |f'(y)|\,|\log(x-y)|\mathrm{d}y \le \|f'\|_\infty \int_0^r |\log(x-y)|\mathrm{d}y \lesssim \|f'\|_\infty,$$

where $\|X\|_\infty$ denotes the Banach norm on the space of continuous function $C[0,r]$. However, $\mathcal{T}$ is not bounded in the C^0 sense: in fact, even assuming smoothness and compact support, $\mathcal{T}[f]$ cannot be bounded by $\|f\|_\infty$.

Proposition 2.2.7. *The restriction of $\mathcal{T}$ to $C_0^\infty[0,r]$ is not bounded in the sense of $C[0,r]$.*

Proof. Consider the action of $\mathcal{T}$ on a sequence of smooth functions f_ε in the limit $\varepsilon \to 0^+$. For an arbitrary interval $[x_1,x_2] \subset (0,r)$, let

$$f_\varepsilon(x) \doteq \theta_\varepsilon(x_1 - x) - \theta_\varepsilon(x_2 - x), \quad \theta_\varepsilon(x) \doteq \int_{-\infty}^x \frac{1}{\varepsilon}\varphi\left(\frac{y}{\varepsilon}\right)\mathrm{d}y,$$

where $\varphi \in C_0^\infty[-1,1]$ is a positive mollifier (in particular, $\|\varphi\|_1 = 1$). By construction, for sufficiently small ε, one has $f_\varepsilon \in C_0^\infty[0,r]$ and $\|f_\varepsilon\|_\infty = 1$. However, for almost every x, one gets

$$\lim_{\varepsilon\to 0^+}\mathcal{T}[f_\varepsilon](x) = \begin{cases} -\log(x-x_1) + \log(x-x_2), & x > x_2, \\ -\log(x-x_1), & x_1 < x < x_2, \\ 0, & x < x_1. \end{cases}$$

Hence, for all $M > 0$ there exists $\varepsilon^* > 0$ such that $\|\mathcal{T}[f_\varepsilon]\|_\infty \ge M$ for all $\varepsilon \in (0,\varepsilon^*)$. Since $\|f_\varepsilon\|_\infty = 1$, this proves that $\mathcal{T}$ is not continuous with respect to the uniform norm. □

For this reason, $\mathcal{T}_{\tau_0}[V]$ in $\langle{:}\phi^2{:}\rangle_\omega$ and $\mathcal{T}_{\tau_0}[V']$ in $\partial_\tau(a^2\langle{:}\phi^2{:}\rangle_\omega)$ lose derivatives, and a direct analysis of eqs. (2.64) and (2.66) is not possible. A way to overcome this problem is to study an inversion formula for $h = \mathcal{T}[f]$ for functions defined on the interval $[0,r]$. Remarkably, one shall show that the inverse operator appearing in the inversion formula is more regular than $\mathcal{T}$, and hence one shall be able to employ the analogous inversion formula for $\mathcal{T}_{\tau_0}$, which is then obtained by a translation.

Proposition 2.2.8. *Consider $\mathcal{T}$ introduced in eq. (2.68). The inversion formula for $h = \mathcal{T}_0[f]$ is*

$$f(x) = f(0) + \int_0^x K(x-y)h(y)\mathrm{d}y, \tag{2.69}$$

with (locally integrable) Kernel

$$K(x) \doteq -4\pi\mathrm{i}\int_{\alpha-\mathrm{i}\infty}^{\alpha+\mathrm{i}\infty}\frac{\mathrm{e}^{sx}}{\gamma+\log s}\mathrm{d}s, \quad \alpha > \mathrm{e}^{-\gamma}, \tag{2.70}$$

where γ is the Euler-Mascheroni constant. Hence, the restriction of $\mathcal{T}$ to $D = \{f \in C^1[0,r] \mid f(0) = 0\}$ is such that $\mathcal{T} : D \to D$ and it admits a unique inverse. It is given by

$$\mathcal{T}^{-1}[h](x) = \int_0^x K(x-y)h(y)\mathrm{d}y. \tag{2.71}$$

The operator $\mathcal{T}^{-1}$ extends to a linear bounded operator on $C[0,r]$ for $r > 0$, and

$$\|\mathcal{T}^{-1}[h]\|_\infty \leq C_\infty(r)\|h\|_\infty, \tag{2.72}$$

where $C_\infty(r) > 0$ depends continuously on r and vanishes in the limit $r \to 0$.

Proof. Denoting by $\mathcal{L}\{f\}$ the Laplace transform of a bounded function $f \in C_b[0,\infty)$,

$$\mathcal{L}\{f\}(s) = \int_0^\infty \mathrm{e}^{-s\tau} f(\tau)\mathrm{d}\tau,$$

the convolution theorem[3] for the Laplace transform gives that $\mathcal{L}\{g\}\mathcal{L}\{f\} = \mathcal{L}\{g*f\}$. Furthermore, $\mathcal{L}\{f'\}(s) = s\mathcal{L}\{f\}(s) - f(0)$ and thus

$$\mathcal{L}\{\mathcal{T}[f]\}(s) = -\frac{\mathcal{L}(\log)(s)}{8\pi^2}\left(s\mathcal{L}\{f\}(s) - f(0)\right).$$

Thus, one computes

$$\mathcal{L}\{\log\}(s) = \int_0^\infty \mathrm{e}^{-st}\log t\mathrm{d}t = \int_0^\infty \mathrm{e}^{-st}\log(st)\mathrm{d}t - \int_0^\infty \mathrm{e}^{-st}\log s\mathrm{d}t = -\frac{\gamma + \log s}{s},$$

and hence one obtains that

$$\mathcal{L}\{\mathcal{T}[f]\}(s) = \frac{(\gamma + \log(s))}{8\pi^2}\left(\mathcal{L}\{f\}(s) - \frac{f(0)}{s}\right), \qquad \mathcal{L}\{f\}(s) = \frac{f(0)}{s} + \frac{8\pi^2}{\gamma + \log(s)}\mathcal{L}\{h\}(s),$$

where $h = \mathcal{T}[f]$. Hence, since K is the inverse Laplace transform of $8\pi^2(\log(s)+\gamma)^{-1}$, again by the convolution theorem of the Laplace transform eq. (2.69) is proved. By direct inspection, the restriction of $\mathcal{T}$ to D is closed in D, hence the restriction of $\mathcal{T}$ to D admits an unique inverse given in eq. (2.71). This concludes the first part of the proof.

For the second part of the proof, notice that the function $(\gamma + \log s)^{-1}$ has a simple pole at $s = \mathrm{e}^{-\gamma}$ with residue $\mathrm{e}^{-\gamma}$ and it has a branch cut for $\mathrm{Re}(s) < 0$. Furthermore, for $\mathrm{Re}(s) \in (0,\alpha)$ and $x \in \mathbb{R}$, the function $\mathrm{e}^{sx}(\gamma + \log s)^{-1}$ vanishes in the limit $\mathrm{Im}(s) \to \infty$. Hence, by the Cauchy residue theorem and after a change of variables,

$$K(x) = 8\pi^2\mathrm{e}^{\mathrm{e}^{-\gamma}x-\gamma} + 4\pi\int_{-\infty}^\infty \mathrm{e}^{\mathrm{i}kx}\frac{1}{\gamma + \log(\mathrm{i}k)}\mathrm{d}k.$$

To obtain the desired continuity, one needs to analyze

$$\mathcal{K}(x) \doteq 4\pi\int_{-\infty}^\infty \frac{\mathrm{e}^{\mathrm{i}kx}}{\gamma + \log(\mathrm{i}k)}\mathrm{d}k, \tag{2.73}$$

which is the Fourier transform of a Schwartz distribution with integral Kernel $(\gamma + \log \mathrm{i}k)^{-1}$. The desired continuity follows from the observation that $\mathcal{K}$, given in eq. (2.73), is a locally integrable

[3] Here $g * f(\tau) = \int_0^\tau g(t)f(\tau - t)\mathrm{d}t$

function on $\mathbb{R}$, which is continuous on $\mathbb{R}\setminus\{0\}$ and decays as $|x|^{-1}$ for large $|x|$. The detailed proof of the last statement can be found in the following lemma 2.2.1, whose proof descends from lemma 2.2.2 and lemma 2.2.3. Hence, thanks to the decay properties of $\mathcal{K}$ and the fact that both $\mathcal{K}$ and thus also K are absolutely integrable near 0, one obtains that $\mathcal{T}^{-1}$ extends to a linear bounded operator on $C[0,r]$ for $r>0$, and furthermore

$$\|\mathcal{T}^{-1}[h]\|_\infty \leq \|h\|_\infty \int_0^r |K(x)|\mathrm{d}x \leq C_\infty(r)\|h\|_\infty,$$

where $C_\infty(r)$ depends continuously on r and vanishes in the limit $r\to 0$. □

Before introducing the three technical lemmas used to complete the proof of proposition 2.2.8, the following observations should be made. Firstly, up to the application of a translation, analogous results of proposition 2.2.8 holds for $\mathcal{T}_{\tau_0}$ and $\mathcal{T}_{\tau_0}^{-1}$; secondly, an important property of the inversion formula (2.69) is that it respects causality, since $\mathcal{T}^{-1}$, and thus also $\mathcal{T}_{\tau_0}^{-1}$, are retarded operators. Such properties, together with the continuity shown in proposition 2.2.8, will allow to prove that a unique solution of eq. (2.66) exists in subsection 2.2.5.

In the proof of the following three lemmas, the notation $\log^2 x$ for the square of the logarithm of x, i.e., $(\log x)^2$ shall be used; furthermore, the symbol $f\lesssim h$ means that it exists a constant C such that $f\leq Ch$.

Lemma 2.2.1. *The function given in eq.* (2.73),

$$\mathcal{K}(x) = 4\pi\int_{-\infty}^{\infty}\frac{\mathrm{e}^{\mathrm{i}kx}}{\gamma+\log(\mathrm{i}k)}\mathrm{d}k,$$

is continuous for $x\neq 0$, locally integrable near 0 and bounded outside any interval containing 0.

Proof. The k-integral in eq. (2.73) can be divided into two parts, obtaining

$$\begin{aligned}\mathcal{K}(x) &= 4\pi\int_0^\infty\left(\frac{\cos(kx)+\mathrm{i}\sin(kx)}{\gamma+\log k+\mathrm{i}\pi/2}+\frac{\cos(kx)-\mathrm{i}\sin(kx)}{\gamma+\log k-\mathrm{i}\pi/2}\right)\mathrm{d}k\\ &= 8\pi\int_0^\infty\cos(kx)\frac{(\gamma+\log k)}{(\gamma+\log k)^2+\pi^2/4}\mathrm{d}k + 4\pi^2\int_0^\infty\sin(kx)\frac{1}{(\gamma+\log k)^2+\pi^2/4}\mathrm{d}k.\end{aligned}$$

Thus, the local integrability of $\mathcal{K}$ is equivalent to the local integrability of the functions I and J defined in eqs. (2.74) and (2.76), respectively, after reabsorbing the constant γ through the rescalings $k\mapsto k\mathrm{e}^{\gamma}$ and $x\mapsto x\mathrm{e}^{-\gamma}$. The statement then follows from lemma 2.2.2 and lemma 2.2.3, where the local integrability and further properties of I and J are established. □

Lemma 2.2.2. *The function*

$$I(x) \doteq \int_0^\infty\cos(kx)\frac{\log k}{\log^2 k+c}\mathrm{d}k,\qquad c>0, \tag{2.74}$$

is a continuous functions for $x\neq 0$, it is locally integrable near 0 and it decays as $|x|^{-1}$ for large $|x|$.

Proof. As the following proof can be easily generalized to arbitrary $c>0$, one can study only the case $c=1$. To prove continuity outside 0 and the decay for large values of x, we integrate by parts obtaining

$$I(x) = \int_0^\infty\frac{\sin(kx)}{x}\frac{\log^2 k-1}{k(\log^2 k+1)^2}\mathrm{d}k. \tag{2.75}$$

Hence we have that

$$|I(x)| \le \frac{1}{|x|}\int_0^\infty \frac{|\log^2 k - 1|}{k(\log^2 k+1)^2}\mathrm{d}k = \frac{1}{|x|}\int_{-\infty}^\infty \frac{|l^2-1|}{(l^2+1)^2}\mathrm{d}l = \frac{2}{|x|}$$

and continuity can be proved by the dominated convergence theorem. In order to prove the integrability near $x = 0$, one integrates by parts another time in eq. (2.75) to obtain

$$I(x) = \int_0^\infty \frac{1-\cos(kx)}{x^2}\frac{1}{k^2}\left(\frac{\log^2 k - 2\log k - 1}{(\log^2 k+1)^2} + \frac{4\log(k)(\log^2 k - 1)}{(\log^2 k+1)^3}\right)\mathrm{d}k.$$

Assume that $x \in (0,\varepsilon)$ for ε sufficiently small (the case $x < 0$ can be treated analogously). Then, after changing the variable of integration ($k \mapsto kx$), one gets

$$I(x) = \frac{1}{x}\int_0^\infty \frac{1-\cos k}{k^2}\frac{f(l)}{l^2+1}\mathrm{d}k,$$

where $l \doteq \log k - \log x$ and

$$f(l) \doteq \frac{l^2-2l-1}{l^2+1} + \frac{4l(l^2-1)}{(l^2+1)^2}$$

is a continuous bounded function. This integral can be split into two parts $I(x) = I_1(x) + I_2(x)$, where

$$I_1(x) \doteq \frac{1}{x}\int_0^{\sqrt{x}} \frac{1-\cos k}{k^2}\frac{f(l)}{l^2+1}\mathrm{d}k, \quad I_2(x) \doteq \frac{1}{x}\int_{\sqrt{x}}^\infty \frac{1-\cos k}{k^2}\frac{f(l)}{l^2+1}\mathrm{d}k,$$

so the local integrability near 0 can be discussed separately for I_1 and I_2. Since $(l^2+1)^{-1} \le 1$, $|1-\cos k| \le \frac{k^2}{2}$ and $|f(l)| \lesssim 1$,

$$|I_1(x)| \lesssim \frac{1}{x}\int_0^{\sqrt{x}} \frac{1-\cos k}{k^2}\mathrm{d}k \lesssim \frac{1}{\sqrt{x}},$$

which is integrable in $(0,\varepsilon)$. At the same time,

$$|I_2(x)| \lesssim \frac{1}{x\log^2 x}\int_{\sqrt{x}}^\infty \frac{1-\cos k}{k^2}\mathrm{d}k \le \frac{1}{x\log^2 x}\int_0^\infty \frac{1-\cos k}{k^2}\mathrm{d}k \lesssim \frac{1}{x\log^2 x},$$

using $|f(l)| \lesssim 1$ and

$$(\log k - \log x)^2 + 1 > (\log k - \log x)^2 \ge \frac{1}{4}\log^2 x$$

because $\log x < 0$ and, on the domain of k-integration, $\log k \ge \frac{1}{2}\log x$. Consequently, also I_2 is integrable in $(0,\varepsilon)$ for small ε. □

Lemma 2.2.3. *The function*

$$J(x) \doteq \int_0^\infty \sin(kx)\frac{1}{\log^2 k + c}\mathrm{d}k, \quad c > 0, \tag{2.76}$$

is a continuous functions for $x \neq 0$, it is locally integrable near 0 and it decays as $|x|^{-1}$ for large $|x|$.

Proof. The proof can be achieved similarly as made in the previous one, studying only the case $c = 1$. Integrating by parts yields

$$J(x) = \int_0^\infty \frac{1-\cos(kx)}{x} \frac{2\log k}{k(\log^2 k + 1)^2} \mathrm{d}k,$$

and thus

$$|J(x)| \le \frac{4}{|x|} \int_0^\infty \frac{|\log k|}{k(\log^2 k + 1)^2} \mathrm{d}k = \frac{4}{|x|} \int_{-\infty}^\infty \frac{|l|}{(l^2+1)^2} \mathrm{d}l = \frac{4}{|x|}.$$

Continuity of $J(x)$ for $x \neq 0$ can then be proved by the dominated convergence theorem. Finally, one has to prove the integrability near $x = 0$. For this purpose, assuming that $x \in (0, \varepsilon)$ for ε sufficiently small (the case $x < 0$ can be treated analogously), and dividing the domain of integration of $J(x)$ into $(0,1/\sqrt{x})$ and $(1/\sqrt{x}, \infty)$, $J(x)$ can be split in $J(x) = J_1(x) + J_2(x)$, with

$$J_1(x) = \int_0^{1/\sqrt{x}} \frac{1-\cos(kx)}{x} \frac{2\log k}{k(\log^2 k + 1)^2} \mathrm{d}k,$$
$$J_2(x) = \int_{1/\sqrt{x}}^\infty \frac{1-\cos(kx)}{x} \frac{2\log k}{k(\log^2 k + 1)^2} \mathrm{d}k.$$

Noting that $|1 - \cos(kx)| \le \frac{1}{2}(kx)^2$ and $\log(k)(\log^2 k + 1)^{-2} \lesssim 1$, J_1 can be estimated as

$$|J_1(x)| \lesssim \int_0^{1/\sqrt{x}} \frac{1-\cos(kx)}{kx} \mathrm{d}k \le \int_0^{1/\sqrt{x}} \frac{kx}{2} \mathrm{d}k = \frac{1}{4}.$$

At the same time, for J_2 the following estimate holds

$$|J_2(x)| \le \frac{4}{x} \int_{1/\sqrt{x}}^\infty \frac{|\log k|}{k(\log^2 k + 1)^2} \mathrm{d}k = \frac{4}{x} \int_{-\frac{1}{2}\log x}^\infty \frac{|l|}{(l^2+1)^2} \mathrm{d}l = \frac{8}{4x + x\log^2 x}.$$

Hence, we can conclude that J is integrable in $(0, \varepsilon)$ for small ε. □

2.2.5 Existence and uniqueness of local solutions

Taking into accounts the results obtained in subsection 2.2.3 and subsection 2.2.4, the existence of a unique solution of eq. (2.64), and thus of eq. (2.55), can be achieved on a small interval of conformal time just after the initial time $\tau = \tau_0$, after studying eq. (2.66) in the form presented in proposition 2.2.6.

Adopting the same strategy presented in [Pin11; PS15a], the proof consists of showing that, having fixed initial conditions for a and having chosen a state ω compatible with these initial conditions thanks to the result of proposition 2.2.3, eq. (2.64) can be viewed as a fixed point equation

$$X' = \mathcal{C}[X'], \qquad X' \in C[\tau_0, \tau_1], \tag{2.77}$$

where X can be obtained from X' by direct integration with the condition $X(\tau_0) = X_0$. In this case, X is directly related to the scale factor of the spacetime

$$X = \frac{1}{6} a^2 R = \frac{a''}{a}, \tag{2.78}$$

thus the initial conditions for X_0 and X'_0 are fixed by the initial conditions of the scale factor a

$$X_0 \doteq X(\tau_0) = \frac{a''_0}{a_0}, \qquad X'_0 \doteq X'(\tau_0) = \frac{a'''_0}{a_0} - \frac{a''_0 a'_0}{a_0^2}.$$

Moreover, $C[\tau_0, \tau_1]$ corresponds to a Banach space equipped with the uniform norm

$$\|X\|_{C[\tau_0,\tau_1]} \doteq \sup_{\tau \in [\tau_0,\tau_1]} |X(\tau)|.$$

To prove existence and uniqueness of solutions of the analyzed system, one shall show that the map $\mathcal{C}$ on $C[\tau_0, \tau_1]$ is a contraction when restricted on a suitable compact subset

$$\mathcal{B}_\delta \doteq \{X' \in C[\tau_0, \tau_1] \mid \|X' - X'_0\| \leq \delta\} \tag{2.79}$$

when $\tau_1 - \tau_0$ is sufficiently small. Thus, the existence and uniqueness of the solution descends from the application of the Banach fixed point theorem (for further details see Appendix C). The existence of this contraction map shall be provided by the continuity property of the inverse operator $\mathcal{T}_0^{-1}$ given in eq. (2.71) and proved in proposition 2.2.8.

The function X is exactly the curvature-like quantity entering the second Friedmann equation or eq. (1.124), and it is contained both in the scale factor constructed as the unique solution of

$$\begin{cases} a'' = Xa, \\ a'(\tau_0) = a'_0, \\ a(\tau_0) = a_0, \end{cases}$$

and in the potential V via the definition given in eq. (2.25)

$$V(\tau) = m^2(a^2 - a_0^2) + (6\xi - 1)(X - X_0)\,. \tag{2.80}$$

Hence, from now on both a, a', and V shall be viewed as functionals of X, and thus of X' because $X(\tau_0) = X_0$, in an interval of time $[\tau_0, \tau_1]$. On the one hand, some inequalities which guarantee the continuity for a and a' are obtained in lemma C.2.2 using Grönwall's Lemma; on the other hand, about V it holds that

$$\|V\|_\infty \leq C\,(1 + \|X - X_0\|_\infty)\,,$$

for a suitable constant C.

The first step is to rewrite eq. (2.67) in terms of the dynamic variable X', in order to obtain the explicit expression of the map $\mathcal{C}$; in this equation, the continuity of the operators involved as functional of V, and thus of X, is guaranteed by the results presented in theorem 2.2.1 and proposition 2.2.1. Then, the following lemma holds.

Lemma 2.2.4. *Given the initial data* (a_0, a'_0, X_0, X'_0)*, chosen in such a way that* $a_0 > 0$ *and* $\Omega_k^2(\tau_0)$ *in eq.* (2.12) *is strictly positive, and a state* ω *which is regular and compatible with this initial conditions, the semiclassical equation* (2.67) *can be written in the form of a fixed-point equation on* $C[\tau_0, \tau_1]$

$$X' = \mathcal{C}[X'], \tag{2.81}$$

where

$$\begin{aligned}\mathcal{C}[X'] =& X'_0 - \frac{2m^2}{(6\xi - 1)}(a[X]a'[X] - a_0 a'_0) \\ &- \frac{1}{(6\xi - 1)}\mathcal{T}_{\tau_0}^{-1}\left[[Q_0^d[X] + Q_f^d[X] + Q_s^d[X] - \left(6c_\xi X' + \partial_\tau\left(a[X]^2 F(a[X], R[X])\right)\right)\right],\end{aligned}$$

with $X[X'](\tau) = X_0 + \int_{\tau_0}^{\tau} X'(\eta)\mathrm{d}\eta$*. Each* $X' \in C[\tau_0, \tau_1]$ *determines a spacetime* $(\mathcal{M}, g[X])$ *where* $\mathcal{M} = [\tau_0, \tau_1] \times \mathbb{R}^3$ *and where* $g[X]$ *is the FLRW metric enjoying the initial conditions and constructed out of the scale factor* $a[X](\tau)$*.*

Proof. Each $X' \in C[\tau_0, \tau_1]$ determines a FLRW spacetime in the following way. First of all, X is obtained from X' by integrating in time and fixing $X(\tau_0) = X_0$. Thus, X is a functional of X'. Then, $a[X]$ is obtained from X as the unique solution of $a'' - Xa = 0$ which satisfies the initial conditions $a(\tau_0) = a_0$ and $a'(\tau_0) = a'_0$. Given X and a, V can be obtained, finally, from eq. (2.80). Thus, it is a functional of X and hence of X'.

Eqs. (2.66) and (2.67) have the form

$$\mathcal{T}_{\tau_0}[V'] = h,$$

where

$$h = -Q_0^d[X] - Q_f^d[X] - Q_s^d[X] + \left(6c_\xi X' + \partial_\tau \left(a[X]^2 F(a[X], R[X])\right)\right).$$

This equation can be inverted adapting the analysis given in proposition 2.2.8 to obtain

$$V' = V'_0 + \mathcal{T}_{\tau_0}^{-1}[h].$$

The operator $\mathcal{T}_{\tau_0}^{-1}$ equals $\mathcal{T}_0^{-1}$ given in eq. (2.71) up to a translation, and, furthermore, the continuity satisfied by $\mathcal{T}_{\tau_0}^{-1}$ coincides with the continuity of $\mathcal{T}_0^{-1}$ discussed in eq. (2.72) inside proposition 2.2.8. Finally, the proof follows after rewriting it with respect to the variable $X = \frac{a''}{a}$. □

Once the semiclassical Einstein equations are given in this fixed-point form, the following proposition holds

Proposition 2.2.9. *Fix the initial conditions for a in such a way that $a_0 > 0$ and $\Omega_k^2(\tau_0)$ given in eq.* (2.12) *is positive. Consider a state ω which is sufficiently regular and compatible with the initial conditions for a. Fix $\delta > 0$ and let $\mathcal{B}_\delta$ given in eq.* (2.79) *the closed ball in the Banach space $C[\tau_0, \tau_1]$ with finite $\tau_1 > \tau_0$, centred in $X'_c(\tau) \doteq X'_0$. For τ_1 sufficiently small, the map $\mathcal{C}$ introduced in lemma 2.2.4 with $\xi \neq 1/6$ is a contraction map on $\mathcal{B}_\delta$. Hence, there exists a unique fixed point of the equation $X' = \mathcal{C}[X']$, in $\mathcal{B}_\delta$, which represents a solution of the semiclassical Einstein equations.*

Proof. First of all, for every $X' \in \mathcal{B}_\delta$ one can assign an $X(\tau) = X_0 + \int_{\tau_0}^{\tau} X'(\eta) \mathrm{d}\eta$, and consequently a scale factor $a[X]$. Ω_k^2 given in eq. eq. (2.12) is continuous in time, because it is positive at τ_0 and it stays positive in a short interval of time. Furthermore, for $X' \in \mathcal{B}_\delta$, $|a^2 R(\tau)| \leq (\tau - \tau_0)\|X'\|_\infty$, hence if τ_1 is sufficiently small, then Ω_k^2 is positive in $[\tau_0, \tau_1]$ uniformly for $X' \in \mathcal{B}_\delta$.

The strategy of the proof is the following: $\mathcal{C}$ is a linear combination of compositions of continuous functions or functionals of a, V and X. On the one hand, a and V are Gateaux differentiable with respect to X at $X(\tau) = X_0 + \int_{\tau_0}^{\tau} X'(\eta) \mathrm{d}\eta$, and, on the other hand, their derivative satisfy the inequalities derived in lemma C.2.2; thus, all these Gateaux differential are continuous. Hence, the proof of this proposition follows from the continuity of $\mathcal{T}_{\tau_0}^{-1}$ given in proposition 2.2.8, and from observing that, if $(\tau_1 - \tau_0)$ tends to 0, then the constant $C_\infty(\tau_1 - \tau_0)$ given in eq. (2.72) tends to 0. Taking into account all of this, the thesis follows from the continuity of all the other operators, functionals or functions involved.

Some details of the proof are as follows. Consider the following constants $c_1 = -2m^2/(6\xi - 1)$ and $c_2 = (6\xi - 1)^{-1}$, then the map $\mathcal{C}$ has the form

$$X' = \mathcal{C}[X'] = X'_0 + c_1(a - a_0)a' + c_1 a_0(a' - a'_0) - c_2 \mathcal{T}_{\tau_0}^{-1}[\mathcal{F}],$$

where

$$\mathcal{F} = Q_0^d + Q_f^d + Q_s^d - \left(6c_\xi X' + \partial_\tau \left(a^2 F(a, R)\right)\right) \tag{2.82}$$

is a linear combination of continuous functionals of X. If $X \in \mathcal{B}_\delta$, then

$$\|\mathcal{C}[X'] - X'_0\|_\infty \leq |c_1|(\|a - a_0\|_\infty \|a'\|_\infty + a_0\|a' - a'_0\|_\infty) + |c_2| C_\infty(\tau_1 - \tau_0)\|\mathcal{F}\|_\infty, \tag{2.83}$$

where the estimates given in lemma C.2.2 and in proposition 2.2.8 were used. Now, for $X' \in \mathcal{B}_\delta$ it is possible to prove that $\mathcal{F}$ given in eq. (2.82) is bounded by X', because each component of $\mathcal{F}$ can be bounded using the results obtained above. Indeed, it was established in proposition 2.2.1 that Q_f^d depends continuously on V', and in proposition 2.2.2 that $\|Q_s^d\|_\infty$ can be controlled by $\|V'\|_\infty$ for V' in a suitable compact domain of $C[\tau_0, \tau_1]$, because Q_s^d is Gateaux differentiable. At the same time, Q_0^d given in eq. (2.45) is a function of a and its derivative up to the third order and of V and V'.

Also, V' depends continuously on X' with respect to the uniform topology as can be seen from eq. (2.80), and thanks to the results of lemma C.2.2. Furthermore, as established in theorem 2.2.1, F is a solution of the first equation in the system (2.56), and hence it can be controlled by X' again together with its time derivative, similarly to the results established in proposition 2.2.5. After combining all these observations, and whenever τ_1 is chosen sufficiently small, then there exists C_δ which allows to further bound the right-hand side of eq. (2.83). Hence,

$$\|\mathcal{C}[X'] - X_0'\|_\infty \leq ((\tau_1 - \tau_0) + |c_2| C_\infty(\tau_1 - \tau_0))\, C_\delta, \tag{2.84}$$

where the constant $C_\infty(\tau_1 - \tau_0)$ depends continuously on the difference $\tau_1 - \tau_0$, and it vanishes for $\tau_1 = \tau_0$. Furthermore, for $X_1, X_2 \in \mathcal{B}_\delta$,

$$\mathcal{C}[X_2'] - \mathcal{C}[X_1'] = c_1(aa'[X_2] - aa'[X_1]) - c_2 \mathcal{T}_{\tau_0}^{-1}\left[\mathcal{F}[X_2] - \mathcal{F}[X_1]\right],$$

and

$$\|\mathcal{C}[X_2'] - \mathcal{C}[X_1']\|_\infty \leq |c_1| \|aa'[X_2] - aa'[X_1]\|_\infty + |c_2| C_\infty(\tau_2 - \tau_0) \|\mathcal{F}[X_2] - \mathcal{F}[X_1]\|_\infty.$$

To prove the Lipschitz continuity of all functionals with respect to X', and hence to obtain the desired contraction property of $\mathcal{C}$ (see also section C.1), one has to evaluate the functional derivatives of $\mathcal{F}$. Considering the convex linear combination of X_1 and X_2, $X_s = (1-s)X_1 + sX_2 = X_1 + s(\delta X)$ where $\delta X = X_2 - X_1$, and using the definition of directional derivative, one obtains that

$$\mathcal{F}[X_2] - \mathcal{F}[X_1] = \int_0^1 \frac{\mathrm{d}\mathcal{F}[X_s]}{\mathrm{d}s} \mathrm{d}s = \int_0^1 \delta\mathcal{F}[X_s, \delta X] \mathrm{d}s.$$

As the space $\mathcal{B}_\delta$ is a convex space, $X_s \in \mathcal{B}_\delta$ for every s. Then, to control the functional derivative of $\mathcal{F}$ given in eq. (2.82), one has to analyze the functional derivatives of its component. Having control on how V depends on X and on a from eq. (2.80), the boundedness of the functional derivative of Q_f^d with respect to X' descends from lemma C.2.2 and from the bounds established in proposition 2.2.1. Similarly, the boundedness of Q_s^d descends from proposition 2.2.2 and that of Q_0^d directly from its definition given in eq. (2.45). Finally, the boundedness of the functional derivative of the time derivative of $a^2 F$ can be obtained by arguing as in proposition 2.2.5 (see also the explicit results stated in theorem 2.2.1).

After collecting all these observations, for $X_1, X_2 \in \mathcal{B}_\delta$ there exists a suitable constant C such that $\|\delta\mathcal{F}[X_s, \delta X]\|_\infty \leq C \|\delta X'\|_\infty$, and hence

$$\|\mathcal{F}[X_2] - \mathcal{F}[X_1]\|_\infty \leq C \|X_2' - X_1'\|_\infty.$$

Furthermore, operating in a similar way for the first contribution in the difference $\mathcal{C}[X_2'] - \mathcal{C}[X_1']$, one obtains that

$$\begin{aligned} aa'[X_2] - aa'[X_1] &= a[X_2](a'[X_2] - a'[X_1]) + (a[X_2] - a[X_1])a'[X_1] \\ &= a[X_2] \int_0^1 \mathrm{d}s \delta a'[X_s, \delta X] + a'[X_1] \int_0^1 \mathrm{d}s \delta a[X_s, \delta X], \end{aligned}$$

where δa is the functional derivative of a. Thus, using similar estimates to those of lemma C.2.2 yields

$$\|aa'[X_2] - aa'[X_1]\|_\infty \leq (\tau_1 - \tau_0)C\|X_2' - X_1'\|_\infty ,$$

where C is a suitable constant. Combining these results and using the continuity of $\mathcal{T}_{\tau_0}^{-1}$ obtained in proposition 2.2.8, then

$$\|\mathcal{C}[X_2'] - \mathcal{C}[X_1']\|_\infty \leq ((\tau_1 - \tau_0) + C_\infty(\tau_1 - \tau_0))C\|X_2' - X_1'\|_\infty \tag{2.85}$$

with respect to a suitable constant C which does not depend on $\tau_1 - \tau_0$ for $\tau_1 - \tau_0 < \epsilon$. Therefore, for $\tau_1 - \tau_0$ sufficiently small the action of $\mathcal{C}$ is internal in $\mathcal{B}_\delta$ thanks to eq. (2.84), and at the same time $\mathcal{C}$ is a contraction map thanks to eq. (2.85). □

Theorem 2.2.2. *Let $(a_0, {a'}_0, {a''}_0, a_0^{(3)})$ be some initial data for the functional equation (2.77) given at τ_0 with $a_0 > 0$ and such that $\Omega_k^2(\tau_0)$ given in eq. (2.12) is strictly positive. Consider a quasi-free state ω, which is sufficiently regular and compatible with these initial conditions. There exist a non-empty interval $[\tau_0, \tau_1]$ and a closed ball $\mathcal{B}_\delta = \{X' \in C[\tau_0, \tau_1] \mid X'(\tau_0) = X_0'\}$ of radius $\delta > 0$ such that, for sufficiently small τ_1, a unique solution to eq. (2.77) exists.*

Proof. The existence of a regular quasi-free state compatible with the initial conditions for a is established in proposition 2.2.3. On account of proposition 2.2.9, the proof is an application of the Banach fixed point theorem to the contraction map $\mathcal{C}$ on $\mathcal{B}_\delta$. □

Remark 2.2.4. The scale factor a corresponding to the unique solution obtained in theorem 2.2.2 is an element on $C^3[\tau_0, \tau_1]$, so there is not a direct control on its fourth-order derivative. Having third-order derivative of a at disposal, one can directly check the validity of the first Friedmann equation at any time in $[\tau_0, \tau_1]$, but that regularity is not sufficient to control the traced semiclassical Einstein equations (1.124) at τ larger than τ_0. For this reason, the obtained solution is only a mild (or weak) solution of the semiclassical problem.

To improve this result, namely to obtain a unique solution $a \in C^4[\tau_0, \tau_2]$ for some $\tau_0 < \tau_2 < \tau_1$, there is the need of a better control on the state. However, this could be achieved by imposing constraints on the initial conditions of the modes in eq. (2.16) which are stronger than those given in eqs. (2.42) and (2.43).

In the end, after combining the results given in proposition 2.2.3, and theorems 2.2.1, 2.2.2, a unique solution of the semiclassical Einstein equations has been found. Moreover, both the control on the vacuum polarization provided in proposition 2.2.1 and the analysis about the continuity of $\mathcal{T}_{\tau_0}^{-1}$ yield the continuity of the obtained solution with respect to the initial conditions for the scale factor; remarkably, $\mathcal{T}_{\tau_0}^{-1}$ does not depend on the initial conditions. Finally, the unique solution F obtained in theorem 2.2.1 depends continuously on its initial data, and the estimates for F allow to control how the initial data for F depend on the initial data of the scale factor.

Chapter 3

Black Hole Evaporation

"If you feel you are in a black hole, don't give up. There's a way out."

Stephen Hawking

Summary

This chapter contains the study of the evaporation of four-dimensional, spherically symmetric black holes in the framework of quantum fields in curved spacetimes, and it is based on author's works [MPRZ21; MPRZ22; Med21]. The term evaporation indicates the loss of black hole mass in time, due to the interplay with the quantum fields in the vicinity of the horizon. Because of its peculiar non-classical nature, it can be excellently described in the framework of Semiclassical Gravity, even if its full comprehension is expected to be reached by a full theory of quantum gravity, e.g., string theory or loop quantum gravity [DM00; Ash20]. This effect has also given rise to the so-called "information loss" problem, which has gained a lot of attention in the recent years, see [UW17] for a general review about this topic.

In the semiclassical picture, the mechanism of evaporation is governed by a flux of negative energy crossing the apparent horizon, which is responsible of the negative variation of the mass; moreover, it gives origin to a positive outgoing flux, which is emitted at large distances from the black hole, and which can be in principle detected in form of radiation. Both the mass shrinking and the power emission are dynamical processes, constrained by the quantum matter content outside the horizon: in this way, the presence of quantum fields determines the evolution of the black hole mass in time.

The main result of [MPRZ21], [Med21] consists of showing that the ingoing negative energy flux at the dynamical horizon, and thus evaporation, can be induced by the quantum matter trace anomaly outside the black hole horizon, whenever a suitable averaged energy inequality is satisfied, and after assuming a vacuum-like condition on the state in the past. For illustrative purposes, both the negative ingoing flux and the corresponding rate of evaporation are evaluated in the case of a null radiating star, described by the Vaidya spacetime.

This chapter is organized as follows. In section 3.1 the geometric setup of spherically symmetric black holes is presented, both in the static and in the dynamical case, see subsection 3.1.1 and subsection 3.1.2, respectively. In section 3.2, the mechanism of evaporation is conceptually discussed in the semiclassical framework, starting from the Hawking effect and its derivations (subsection 3.2.1), and then in terms of negative flux and variation of the mass (subsection 3.2.2

and subsection 3.2.3). Thus, in subsection 3.2.4 the evaporation induced by the trace anomaly of the quantum stress-energy tensor is showed in the case of massless, conformally coupled scalar fields; finally, the computation of the rate of evaporation in Vaidya spacetimes is made in subsection 3.2.5.

3.1 Spherically Symmetric Black Holes

3.1.1 The static black hole

The first part of this section is devoted to present the unique vacuum spherically symmetric solution of the Einstein equations, that is, the Schwarzschild solution, which describes a static spherical black hole of constant mass M. All the results stated here are covered by standard textbooks of General Relativity, see, e.g., [HE73; Wal84; Poi09].

Before introducing Schwarzschild spacetimes, a description of the geometry of a spherically symmetric spacetime should be introduced. A spacetime $(\mathcal{M}, g_{\mu\nu})$ is said to be spherically symmetric if the rotation group $\mathbf{SO(3)}$ acts as an isometry group on $\mathcal{M}$ in a transitive way. In this work, one shall consider spatially spherically symmetric geometry, in order to describe the exterior of spherically symmetric black holes. Assuming a central timelike worldline which is invariant under the action of the group, the group orbits which pass in the points off the central worldline are spacelike two-spheres. As the metric of spacetime is invariant under rotations, the line-element induced on each group orbit is a multiple of the canonical line-element of the unit two-sphere $\mathbb{S}^2$, which shall be denoted by

$$\mathrm{d}\Omega \doteq \mathrm{d}\theta^2 + \sin(\theta)^2 \mathrm{d}\varphi^2, \tag{3.1}$$

where $\theta \in [0, \pi)$ and $\varphi \in [0,2\pi)$. Thus, the line-element of any two-sphere reads $\mathrm{d}s^2 = r^2 \mathrm{d}\Omega$, where the radial function r is such that $r = 0$ parametrizes the central worldline. Every two-sphere is intersected at each point by a timelike half-plane of constant area radius, which is orthogonal to the group orbits, and intersects once each orbit. Then, the quotient of $\mathcal{M}$ with respect to the $\mathbf{SO(3)}$ group is a two-dimensional spacetime (Γ, γ_{ab}), with $a, b = 1,2$, normal to the two-spheres, whose boundary corresponds to one of these half-planes. Hence, $r^2 \in \mathcal{C}^\infty(\Gamma)$ measures the curvature of each sphere, and $\mathcal{A} = 4\pi r^2 \in \mathcal{C}^\infty(\Gamma)$ denotes the invariant area of each group orbit [Wal84; Chr86b; Chr91; CB08].

According to Birkhoff theorem, which states that a smooth spherically symmetric metric solution of the vacuum Einstein equations is always static, the unique static, spherically symmetric spacetime is described in coordinates (t, r) by the Schwarzschild metric

$$\mathrm{d}s^2 = -\left(1 - \frac{2M}{r}\right)\mathrm{d}t^2 + \left(1 - \frac{2M}{r}\right)^{-1}\mathrm{d}r^2 + r^2\mathrm{d}\Omega, \tag{3.2}$$

with $M \in \mathbb{R}$ (the case of vanishing mass corresponds to the flat metric). In this patch, the metric is not defined in the Schwarzschild radius $R_S = 2M$, which corresponds to a coordinate (or apparent) singularity, different from the physical singularity located in $r = 0$. Introducing the so-called "tortoise coordinate system" $(t, r^*, \theta, \phi,)$, where $r^* \doteq r + 2M\log\left(\frac{r}{2M} - 1\right)$, the metric

$$\mathrm{d}s^2 = -\left(1 - \frac{2M}{r}\right)(\mathrm{d}t^2 - \mathrm{d}r^{*2}) + r^2\mathrm{d}\Omega, \tag{3.3}$$

does not become singular at R_S, but r^* approaches $-\infty$ as r approaches R_S. Hence, the apparent singularity can be completely removed by introducing the pair of null coordinates $u = t - r^*$, $v = t + r^*$, corresponding to the advanced and retarded time, respectively. For instance, the metric can be represented in the advanced Eddington-Finkelstein coordinates (v, r):

$$\mathrm{d}s^2 = -\left(1 - \frac{2M}{r}\right)\mathrm{d}v^2 + 2\mathrm{d}v\mathrm{d}r + r^2\mathrm{d}\Omega, \tag{3.4}$$

where v parametrizes any ingoing radial null geodesic. In this parametrization, the coordinate singularity describes a null hypersurface

$$H \doteq \{p \in \mathcal{M} : \quad r - R_S = 0\}, \tag{3.5}$$

because $\ell \cdot \ell = 0$ in $r = R_S$, where $\ell^\mu = f(r)\partial^\mu H$ denotes the normal vector to H. Furthermore, it has the behaviour of a "one-way membrane", because both future-directed timelike and null curves can only cross H from the outer region $r > R_S$ to the inner region $r < R_S$ (notice that $\mathrm{d}s^2 \leq 0$ implies $\mathrm{d}r \leq 0$ in the inner region for future-directed worldlines).

After introducing the retarded time u, which, conversely, parametrizes any outgoing radial null geodesic, the Schwarzschild metric can be also parametrized in double-null coordinates (v, u) as

$$\mathrm{d}s^2 = -\left(1 - \frac{2M}{r}\right)\mathrm{d}v\mathrm{d}u + r^2\mathrm{d}\Omega, \tag{3.6}$$

where $r = r(v, u)$ is now a function of the double-null coordinates. The maximal extension $(\tilde{\mathcal{M}}, \tilde{g}_{\mu\nu})$ of the Schwarzschild eternal black hole can be obtained by constructing two new double-null coordinates $U = -\mathrm{e}^{-u/(4M)}$, $V = \mathrm{e}^{v/(4M)}$, which are the so-called Kruskal-Szekeres coordinates, in which the metric reads

$$\mathrm{d}s^2 = -\frac{32M^3}{r}\mathrm{e}^{-r/2M}\mathrm{d}V\mathrm{d}U + r^2(V, U)\mathrm{d}\Omega, \tag{3.7}$$

where $r(V, U)$ is implicitly defined by

$$UV = \left(1 - \frac{r}{2M}\right)\mathrm{e}^{r/(2M)}.$$

Now, the apparent singularity is completely removed, and outgoing and ingoing radial light rays move along curves $U =$ const. and $V =$ const., respectively. Moreover, each surface at constant r is described by an hyperboloid $UV = c$, $c \neq 0$, with $c = 1$ in the case of the physical singularity; on the other hand, the apparent singularity is located on the surface $UV = 0$. Hence, there are four regions of Kruskal spacetime: regions I $(V > 0, U < 0)$ and II $(V > 0, U > 0)$ are covered by both the Schwarzschild and Eddington-Finkelstein coordinates, while regions III $(V < 0, U < 0)$ and IV $(V < 0, U > 0)$ exist only in the maximal extension of the Schwarzschild spacetime. Moreover, the Kruskal extension $(\tilde{\mathcal{M}}, \tilde{g}_{\mu\nu})$ has both future and past null infinities $\mathscr{I}^\pm$, future and past time infinities $i^\pm$, and spacelike infinity i^0 for each region I, IV. This feature characterize, in fact, every asymptotically flat spacetime at future (*resp.* past) null infinity, such as Schwarzschild spacetimes. For a rigorous characterization of asymptotically flat spacetimes, see [Wal84; HE73; DMP17] and references therein. In this view, Kruskal coordinates picture the maximal analytic extension of a time-symmetric eternal black hole, i.e., a black hole spacetime which has always existed in the past and always will exist in the future. See Figure 3.1 for a picture of the Penrose diagram of an eternal black hole.[1]

The hypersurface given in eq. (3.5) locates the event horizon of the Schwarzschild black hole, because no physical signals can escape from H, and the inner region cannot influence the outer region (and *vice versa*). In fact, the definition of a black hole region B has a causal nature,

[1] Penrose diagrams were made in TikZ and are based on the Latex code posted in StackExchange [Sta].

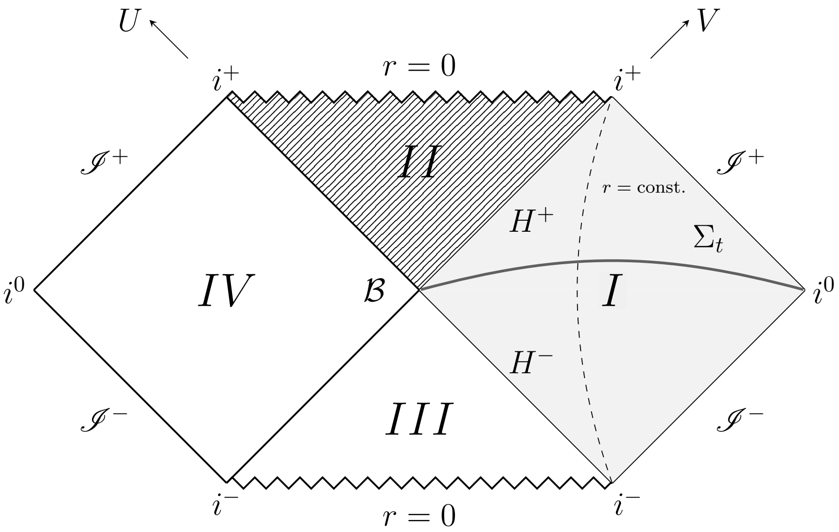

Figure 3.1: Penrose diagram of the maximally extended Schwarzschild spacetime. The event horizon H^+ separates the outer region (grey region) from the black hole region (dashed region), while Σ_t denotes a certain Cauchy surface at $t =$ const.

because B is indicated as a region of "no escape", and the event horizon H denotes its causal boundary. In the case of asymptotically flat spacetimes, this characterization of black holes can be formulated in terms of the future null infinity $\mathscr{I}^+$ as follows [Wal84; Wal95].

Definition 3.1.1. Let $(\mathcal{M}, g_{\mu\nu})$ be an asymptotically flat spacetime, then the black hole region B is the complementary of $J^-(\mathscr{I}^+)$ inside the manifold $\mathcal{M}$:

$$B \doteq \mathcal{M} \setminus J^-(\mathscr{I}^+), \tag{3.8}$$

and its boundary $H \doteq \partial B = \partial J^-(\mathscr{I}^+) \cap \mathcal{M}$ is the event horizon of the spacetime.

In the case of the Schwarzschild solution, there exists two branches of the horizon, the future and the past branch $H^\pm \subset \mathcal{M}$. They are three-dimensional null submanifolds which separate the regions $I - II$, $III - I$, and are located in $V = 0$, $U = 0$, respectively: the event horizon corresponds, actually, to H^+. The origin of this causal structure of the horizon lies in the static symmetry of the Schwarzschild spacetime and in the existence of a Killing vector

$$\xi \doteq \frac{1}{4M}(V\partial_V - U\partial_U), \tag{3.9}$$

which is a unit timelike vector at infinity. Moreover, the null surface $H = H^+ \cup H^-$ is a bifurcate Killing horizon, because the Killing vector is both tangent and normal to $H^\pm$. Furthermore, it vanishes in (0,0), i.e., on a connected two-dimensional spacelike submanifold $\mathcal{B} \subset \mathcal{M}$ called the bifurcation surface, such that $H^+ \cap H^- = \mathcal{B}$: in $\mathcal{B}$, the past and the future horizons intersect each other. From $\mathcal{B}$ the generators of the bifurcate horizon, i.e., the null light rays forming $H^\pm$, are emanated.

The Killing horizon of a Schwarzschild black hole is characterized by the surface gravity

$$\kappa_\infty^2 = -\frac{1}{2}\nabla_\mu \xi^\nu \nabla^\mu \xi^\nu \big|_{H^+}, \tag{3.10}$$

which fulfils the equation $\nabla^\mu \xi^2 = -2\kappa_\infty \xi^\mu$. The terminology "surface gravity" is motivated by following relation

$$\kappa_\infty = \lim_{r \to R_S} (Va), \tag{3.11}$$

where a is the magnitude of the acceleration along an orbit of ξ^μ, and $V = (-\xi^\mu \xi_\mu)^{1/2}$ is the redshift factor associated to ξ^μ. In this regard, κ_∞ can be interpreted as the force required at infinity to hold a unit-mass particle at rest on the event horizon [Wal84]. Since $\xi^\mu \nabla_\mu \kappa_\infty^2 = 0$ on H, κ_∞^2 is constant on each orbit of the Killing vector. Moreover, κ_∞ does not vanish on H, but $\kappa_\infty = \pm 1/(4M)$ on $H^\pm$ (the difference of sign is consequence of the different time direction of the Killing vector field, which points skew right on H^+ and skew left on H^- in Figure 3.1). Hence, H is a non-degenerate Killing horizon.

The role played by the surface gravity is crucial in the formulation of the famous four laws of black hole mechanics for stationary, axially symmetric black holes surrounded by classical matter. Here, the four laws are only stated without proofs, but a full derivation can be found in [BCH73; HE73; Wal01].

- **Zeroth law**. The surface gravity κ_∞ of a stationary black hole is constant over the event horizon H.
- **First law**. Let M, $\mathcal{A}$, and J be respectively the mass, the area of the horizon, and the angular momentum of a stationary black hole. Consider some arbitrary (infinitesimal) physical process, denoted as perturbation, which perturbs the configuration of the black hole outside the equilibrium. Then the variations of M, $\mathcal{A}$, and J at the first order in the perturbation are related by

$$\delta M = \frac{\kappa_\infty}{8\pi} \delta \mathcal{A} + \Omega \delta J, \tag{3.12}$$

  where Ω denotes the angular velocity of the rotating black hole (this term is indeed zero in the non-rotating case).
- **Second law**. If $R_{\mu\nu}\xi^\mu\xi^\nu \geq 0$ holds, then $\mathcal{A}$ does not decrease in time, i.e., $\delta\mathcal{A} \geq 0$ in eq. (3.12).
- **Third law**. It is impossible to reduce κ_∞ to zero by a finite sequence of physical operations.

3.1.2 Dynamical black holes

According to the geometric setup described at the beginning of subsection 3.1.1, any non-static, spatially spherically symmetric spacetime $(\mathcal{M}, g_{\mu\nu})$ can be represented by the warped manifold $\mathcal{M} = \Gamma \times_{r^2} \mathbb{S}^2$ endowed with the metric

$$\mathrm{d}s^2 = g_{\mu\nu}\mathrm{d}x^\mu \mathrm{d}x^\nu = \gamma_{ab}\mathrm{d}x^a \mathrm{d}x^b + r^2 \mathrm{d}\Omega, \qquad \mu,\nu = 0,\ldots,3, \quad a,b = 1,2, \tag{3.13}$$

where $\mathrm{d}\Omega$ was given in eq. (3.1). The invariant $\nabla_\mu r \nabla^\mu r$ defines the Misner-Sharp energy [MS64]

$$m \doteq \frac{r}{2}\left(1 - \nabla_\mu r \nabla^\mu r\right), \tag{3.14}$$

which describes the energy E enclosed inside the sphere of radius r at fixed time. It is a special case of the Hawking mass (1.26) for the class of spherically symmetric spacetimes, and it coincides in an asymptotically flat spacetime with the Bondi mass (1.24) at null infinity, and with the ADM mass (1.23) at spatial infinity [Hay96].

As for the Schwarzschild solution, the two-dimensional spacetime (Γ, γ_{ab}) can be expressed in several patches covering the exterior the black hole, starting from the Schwarzschild coordinates (t, r)

$$\mathrm{d}\gamma^2 = -\mathrm{e}^{2\Psi(t,r)} C(t,r)\mathrm{d}t^2 + C(t,r)^{-1}\mathrm{d}r^2, \tag{3.15}$$

where

$$C \doteq 1 - \frac{2m}{r} \tag{3.16}$$

and Ψ are smooth functions on Γ. Using, respectively, the retarded and advanced Eddington-Finkelstein coordinates u and v defined by

$$\begin{cases} \mathrm{d}v = \mathrm{d}t + J\mathrm{d}r, \\ \mathrm{d}u = \mathrm{d}t - J\mathrm{d}r, \end{cases} \qquad J \doteq \sqrt{-\frac{g_{rr}}{g_{tt}}} = e^{-\Psi}C^{-1}, \tag{3.17}$$

the metric of an evaporating black hole can be written in the advanced Eddington-Finkelstein coordinates (r, v) as

$$\mathrm{d}\gamma^2 = -\mathrm{e}^{2\Psi(v,r)}C(v,r)\mathrm{d}v^2 + 2\mathrm{e}^{\Psi(v,r)}\mathrm{d}v\mathrm{d}r. \tag{3.18}$$

Eq. (3.18) is also known as Bardeen-Vaidya metric [Bar81]. In the change of coordinate given in eq. (3.17), J denotes the Jacobian between the Schwarzschild coordinates (t, r) and the tortoise coordinates (t, r^*), which are defined by the relation $\mathrm{d}r^* = J\mathrm{d}r$. Unlike the function $C(v, r)$, which is written either in terms of topological or coordinate-invariant quantities, $\Psi(v, r)$ is subject to the parametrization freedom $v \mapsto \tilde{v}(v)$.

Since any two-dimensional metric is locally conformally flat, one can also choose to parametrize $\mathrm{d}\gamma^2$ in terms of the generalized double-null coordinates (V, U)

$$\mathrm{d}\gamma^2 = -2A(V, U)\mathrm{d}V\mathrm{d}U \tag{3.19}$$

with respect to the null normal directions ∂_V and ∂_U, employing the following local change of coordinates

$$\begin{cases} 2A\mathrm{d}U = \mathrm{e}^{2\Psi(v,r)}C(v,r)\mathrm{d}v - 2\mathrm{e}^{\Psi(v,r)}\mathrm{d}r, & \text{(3.20a)} \\ \mathrm{d}V = \mathrm{d}v. & \text{(3.20b)} \end{cases}$$

The orientation of the spacetime can also be chosen in such a way that $A(V, U) > 0$ and at spatial infinity $\partial_V r > 0$, $\partial_U r < 0$. The metric is invariant under any re-parametrization $U \mapsto \tilde{U}(U)$ and $V \mapsto \tilde{V}(V)$, where

$$\tilde{A}(\tilde{U}, \tilde{V}) = A(U, V)\left(\frac{d\tilde{U}}{dU}\right)^{-1}\left(\frac{d\tilde{V}}{dV}\right)^{-1}. \tag{3.21}$$

Thus, the future-directed null normal vector fields

$$\ell_+ \doteq A^{-1}\partial_V, \qquad \ell_- \doteq \partial_U \tag{3.22}$$

describe the outgoing and the ingoing light rays across the spheres that foliate $\mathcal{M}$, respectively. In this parametrization, the vector field ℓ_+ fulfils the geodesic equation whereas ℓ_- is an auxiliary vector; the normalization of $\ell_\pm$ is such that $g_{\mu\nu}\ell_+^\mu\ell_-^\nu = -1$.

Contrary to Schwarzschild spacetimes which model static black holes and event horizons, a general dynamical black hole is characterized by a non-constant mass and by a dynamical horizon. On the one hand, an event horizon defined in definition 3.1.1 is a global and teleological notion, because it requires the knowledge of the entire history of spacetime, which is very difficult to achieve outside the stationary symmetry. On the other hand, the dynamics of a null event horizon cannot be locally analyzed starting from the interaction with the matter environment.

To capture locally the idea of impossibility for light rays, and hence for all physical signals, of escaping from a gravitational region, one introduces the notion of trapped surface, that is fundamental, e.g., in the formulation of the singularity theorems. To this avail, one employs the definition of the expansion scalars $\theta_\pm$ associated to null geodesic congruences, see subsection 1.1.2.

Definition 3.1.2. Let $\ell_\pm$ be a pair of future-directed, affine-parametrized, null tangent vector fields associated to a set of outgoing and ingoing geodesic congruences, respectively, and let $\theta_\pm$ be the corresponding null expansion scalars. A marginally trapped surface $\mathcal{J}$ is a C^2 closed, two-dimensional spacelike hypersurface such that the two null geodesic congruences are orthogonal to $\mathcal{J}$, and converge to $\mathcal{J}$, namely $\theta_\pm \leq 0$ everywhere.

Moreover, let Σ be an (asymptotically flat) Cauchy surface which intersects the spatial infinity, then a trapped region $\mathcal{C} \subset \Sigma$ is a closed subset of Σ whose two-dimensional boundary $\partial\mathcal{C}$ is a marginally trapped surface with $\theta_+ \leq 0$. Finally, the total trapped region of Σ, denoted by $\mathcal{T}(\Sigma)$, is the union of all trapped regions on Σ, and its boundary $\partial\mathcal{T}(\Sigma)$ is called apparent horizon.

In definition 3.1.2, outgoing and ingoing means that $\ell_+^\mu n_\mu \geq 0$ and $\ell_-^\mu n_\mu \leq 0$, respectively, where n^μ is the normal vector to $\partial\mathcal{C}$ which points outwards from $\mathcal{J}$. Singularity theorems ensure that, for dynamical black holes, the apparent horizon $\partial\mathcal{T}$ lies within the event horizon, and they coincide in the stationary case, provided the classical null energy condition $T(k, k) \geq 0$ is satisfied for all null vectors k. For further details, see [HE73; Wal84].

More recently, Hayward proposed in [Hay94; Hay96; Hay98] a refinement of the terminology used in definition 3.1.2, in order to remove the dependence on the surface Σ (see also [Far15] for the definitions of apparent and trapping horizons commonly used in literature). Then, a trapping surface is defined as a compact spatial two-surface with $\theta_+\theta_- \geq 0$; it is future/past when $\theta_\pm > 0$ or $\theta_\pm < 0$, respectively, and marginal when $\theta_+ = 0$. A trapping horizon is defined as an hypersurface foliated by marginal surfaces; moreover, it is future if $\theta_- < 0$ or past if $\theta_- > 0$, outer if $\mathscr{L}_-\theta_+ < 0$ or inner if $\mathscr{L}_-\theta_+ > 0$, where $\mathscr{L}_-$ denotes the Lie derivative along ℓ_-, *cf.* section A.1.

In the special case of spherically symmetric spacetimes, the manifold $\mathcal{M}$ is foliated by spheres of radius r, which are defined to be untrapped, marginal or trapped depending on whether the dual vector $\nabla^\mu r$ is spacelike, lightlike or timelike, respectively. If $\nabla^\mu r$ is future/past-directed, then the sphere is future/past trapped: the past case is related to white holes, whereas the future one to black holes, where both outgoing and ingoing light rays are trapped into the surfaces. An hypersurface foliated by marginal spheres is called a trapping horizon and a trapping horizon is outer, degenerate or inner when $\nabla^2 r > 0$, $\nabla^2 r = 0$ or $\nabla^2 r < 0$, respectively.

Among these definitions, notions of future outer trapping horizon and dynamical horizon are important in the formulation of dynamical black holes.

Definition 3.1.3. A future outer trapping horizon is the closure of a three-dimensional surface foliated by marginal surfaces such that

$$\theta_+ = 0, \qquad \theta_- < 0, \qquad \mathscr{L}_-\theta_+ < 0 \tag{3.23}$$

hold on its two-dimensional leafs.

The first two conditions capture the fact that no outgoing ray can escape from the horizon, different from the ingoing ones which are converging therein; the third condition means that the area of the outgoing congruence is increasing just outside the horizon, and it is decreasing just inside it. If one removes the third condition, then one obtains a more generic dynamical horizon according to [AK02; AK03; AK04].

Definition 3.1.4. A dynamical horizon is the closure of a three-dimensional surface foliated by marginal surfaces such that

$$\theta_+ = 0, \qquad \theta_- < 0 \tag{3.24}$$

hold on its two-dimensional leafs.

Contrary to definitions 3.1.1 and 3.1.2, the above statements do not make any reference to the global structure of the spacetime, because they are quasi-locally and do not involve spacelike surfaces. Furthermore, contrary to the case of a static null event horizon, trapping and dynamical horizons can evolve dynamically in a process of formation or evaporation, and their evolution can be locally described in terms of the expansions of the null geodesics congruences.

In the framework of spherically symmetric black holes, the fundamental trapping horizon is the apparent horizon of the black hole, which is obtained from the expansion parameters of the congruences of outgoing/ingoing radial null geodesics, which take the form of

$$\theta_+ \doteq \frac{2}{Ar}\partial_V r, \qquad \theta_- \doteq \frac{2}{Ar}\partial_U r \tag{3.25}$$

in coordinates (V,U). Then, one states the following definition.

Definition 3.1.5. An apparent horizon of a spherically symmetric black hole is a future outer trapping dynamical horizon according to definition 3.1.3. It is located in the three-dimensional hypersurface

$$\mathcal{H} \doteq \{(p_\gamma,\Omega) \in \mathcal{M} : \quad r-2m=0\}\,. \tag{3.26}$$

From now on, the evaluation on the apparent horizon will be labelled by the subscript $\mathcal{H}$. The area of the horizon is given by

$$\mathcal{A}_{\mathcal{H}} \doteq 4\pi r_{\mathcal{H}}^2, \tag{3.27}$$

while the mass of the black hole M is defined as the Misner-Sharp energy evaluated on the horizon $r_{\mathcal{H}} \doteq 2m$

$$M \doteq m(r_{\mathcal{H}}) \overset{\mathcal{H}}{=} \frac{r_{\mathcal{H}}}{2}. \tag{3.28}$$

In coordinates (v,r) the apparent horizon is described by the line $r_{\mathcal{H}}(v)$ located in $C(v,r)=0$ (for convenience, v is rescaled in a such way that $\Psi=0$ on $\mathcal{H}$). Thus, for evaporating black holes the dynamics of the area (3.27) is fully determined by the rate at which the area shrinks

$$\dot{\mathcal{A}}_{\mathcal{H}}(v) \doteq \partial_v \mathcal{A}_{\mathcal{H}}\left(v, r_{\mathcal{H}}(v)\right), \tag{3.29}$$

while the evolution of the mass (3.28) by the rate of evaporation

$$\dot{M}(v) \doteq \partial_v M\left(v, r_{\mathcal{H}}(v)\right). \tag{3.30}$$

In arbitrary dynamical backgrounds, a global Killing field which is timelike outside the horizon is missing, so a global temporal coordinate such as the Schwarzschild time is absent. However, in spherically symmetric spacetimes a preferred notion of "time" exists due to the definition of the *Kodama vector* [Kod80]

$$K \doteq (*_\gamma \mathrm{d}r)^\sharp = A^{-1}\left(\partial_V r \partial_U - \partial_U r \partial_V\right), \tag{3.31}$$

where $*_\gamma$ is the Hodge operator on (Γ, γ_{ab}). From the definition of K, it follows straightforwardly that $K \cdot \nabla r = 0$. So, the Kodama vector is timelike on untrapped spheres, i.e., in the region outside the horizon, then it becomes lightlike on a marginal sphere, and eventually it is spacelike on trapped surfaces, i.e., in the interior of the black hole. Hence, in the outer region the Kodama covector can be made proportional to the one-form $\mathrm{d}t$, where the time coordinate t is called "Kodama time". Thus, the metric of a spherically symmetric spacetime outside the horizon is reduced to eq. (3.15) in the radial-temporal plane (t,r). Furthermore, it holds that $\|\partial_t\|^2 = \mathrm{e}^{2\Psi(t,r)}\|K\|^2$, and hence K is proportional to the timelike Killing vector ∂_t on static, spherically symmetric spacetimes. In this view, the Kodama time represents the geometrically natural choice of time for spherically symmetric black holes. However, in the time-dependent case the squared norm of K, which is equal to $|C(r,t)|$, does not coincide with the squared red-shift factor $|g_{tt}| = \mathrm{e}^{2\Psi(t,r)}C(r,t)$. For further details about the definition of the Kodama time, see [AV10].

The Kodama vector is divergenceless even if it is not a Killing field, $\nabla_\mu K^\mu = 0$, so it can be used to define the areal volume $V = 4/3\pi r^3$ and the Misner-Sharp energy (3.14) as Noether charges. Given any stress-energy tensor $T^{\mu}{}_{\nu}$, the Kodama vector defines a covariantly conserved current

$$J^{\mu}_{K} \doteq T^{\mu}{}_{\nu} K^{\nu} \tag{3.32}$$

such that

$$\nabla_{\mu} J^{\mu}_{K} = 0. \tag{3.33}$$

Hence, according to subsection 1.1.3 the following conserved charges can be given

$$V = -\int_{\Sigma} n_{\mu} K^{\mu} \mathrm{d}_h x, \tag{3.34}$$

$$m = \int_{\Sigma} n_{\mu} J^{\mu}_{K} \mathrm{d}_h x, \tag{3.35}$$

on any three-dimensional hypersurface Σ, where n_{μ} denotes the unit timelike normal vector to Σ, and $\mathrm{d}_h x = \sqrt{|\det(h)|}\mathrm{d}^3 x$ is the induced volume measure on Σ.

From the definition of K, one obtains also that

$$\mathscr{L}_K K_{\mu} = K^{\nu} \left(\nabla_{\nu} K_{\mu} - \nabla_{\mu} K_{\nu} \right) \stackrel{\mathcal{H}}{=} \pm \kappa K_{\mu}, \tag{3.36}$$

where $\mathscr{L}_K$ denotes the Lie derivative along K, and

$$\kappa \doteq \frac{1}{2} \gamma^{ab} \nabla_a \nabla_b r. \tag{3.37}$$

Hence, eq. (3.37) corresponds to the definition of the surface gravity for a dynamical black hole, and it reduces to the standard one in the case of Schwarzschild black holes (for a discussion about the different definitions of κ in literature, see [VADC11]). Actually, for asymptotically flat spacetimes such that (t, r) are the usual Minkowski coordinates, the Tolman relation holds

$$\kappa_{\infty} = \mathrm{e}^{\Psi} \sqrt{C} \kappa, \tag{3.38}$$

where C was given in eq. (3.16), and κ_{∞} is the surface gravity associated to the vector ∂_t, which coincides with the Schwarzschild surface gravity given in eq. (3.10). This relation indicates that the factor $\mathrm{e}^{-\Psi}$ measures the discrepancy between the Killing and the Kodama surface gravities at infinity; thus, it suggests that κ is the real local gravitational acceleration detected along the black hole horizon, whereas κ_{∞} can only be interpreted as the force to keep a unit-mass particle on the horizon [HDCVNZ09]. In fact, denoting by $a = \|\mathcal{L}_k k\|$ the Kodama unit acceleration, and by $k \doteq K / \|K\|$, it holds by direct inspection in the Schwarzschild patch (3.15) that

$$\kappa = \mathrm{e}^{-\Psi} a - \frac{1}{2} C \partial_r \Psi. \tag{3.39}$$

Hence, $\kappa \stackrel{\mathcal{H}}{=} a(r_{\mathcal{H}})$ because $C \stackrel{\mathcal{H}}{=} 0$ and $\Psi \stackrel{\mathcal{H}}{=} 0$, in close analogy with eq. (3.11). Furthermore, from the definition (3.37) and the geometrical requirements of marginal surfaces, a trapping horizon is outer, degenerate or inner when κ is positive, zero or negative, respectively. So, $\kappa > 0$ along an apparent horizon like $\mathcal{H}$ according to eq. (3.23), which implies also that $\partial_r m < 1/2$ in the Bardeen-Vaidya metric (3.18), where m was given in eq. (3.14).

In analogy with the static case, the four laws of black hole mechanics can be generalized at least in the spherically symmetric case to future outer trapping horizons using the definitions given in eqs. (3.31) and (3.37). They were firstly derived by Hayward in [Hay94; Hay98] (see also [Hay02]), starting from two invariants associated to the matter stress-energy tensor: the work density

$$w \doteq -\frac{1}{2} \gamma^{\mu\nu} T_{\mu\nu}, \tag{3.40}$$

where $\gamma_{\mu\nu}$ is the two-dimensional metric of the spacetime (Γ, γ_{ab}) canonically embedded into $(\mathcal{M}, g_{\mu\nu})$, and the energy flux covector

$$\psi_\mu \doteq T_{\mu\nu}\nabla^\nu r + w\nabla_\mu V. \tag{3.41}$$

For classical matter fulfilling the null energy condition, $w \geq 0$ and ψ_μ is outward achronal in untrapped regions; furthermore, ψ_μ reduces to the Bondi flux at null infinity. Moreover, these two invariants of the stress-energy tensor are related by the differential relation obtained in the following proposition.

Proposition 3.1.1. *Let K, J_K, w, and ψ_μ be respectively the Kodama vector, the Kodama conserved current, the work density, and the energy flux given in eqs. (3.31), (3.32), (3.40) and (3.41). Then, the following relation holds*

$$0 = \nabla_\mu(J_K^\mu r^2) = -K(wr^2) - *_\gamma \mathrm{d}(\psi r^2), \tag{3.42}$$

where $\psi \doteq \psi_\mu \mathrm{d}x^\mu$.

Proof. Choosing the double-null parametrization (3.19), the conservation equation (3.33) reads

$$0 = \nabla_\mu J_K^\mu = -\frac{1}{Ar^2}\left(\partial_U(r^2 J_{KV}) + \partial_V(r^2 J_{KU})\right),$$

and thus the definition of J_K stated in eq. (3.32) yields

$$\begin{aligned} 0 = \nabla_\mu J_K^\mu &= -\frac{1}{Ar^2}\left[\partial_U\left(T_{VV}r^2K^V + T_{UV}r^2K^U\right) + \partial_V\left(T_{UU}r^2K^U + T_{UV}r^2K^V\right)\right] \\ &= -\frac{1}{Ar^2}\left[\partial_U\left(-T_{VV}r^2\frac{\partial_U r}{A} + T_{UV}r^2\frac{\partial_V r}{A}\right) + \partial_V\left(T_{UU}r^2\frac{\partial_V r}{A} - T_{UV}r^2\frac{\partial_U r}{A}\right)\right]. \end{aligned}$$

Using the Einstein equations

$$\partial_V^2 r - \frac{\partial_V A}{A}\partial_V r = -\frac{r}{2}T_{VV}, \qquad \partial_U^2 r - \frac{\partial_U A}{A}\partial_U r = -\frac{r}{2}T_{UU},$$

one gets

$$0 = \nabla_\mu J_K^\mu = -\frac{1}{Ar^2}\left[\partial_U\left(\frac{T_{UV}}{A}r^2\right)\partial_V r - \partial_V\left(\frac{T_{UV}}{A}r^2\right)\partial_U r - \partial_U(T_{VV}r^2)\frac{\partial_U r}{A} + \partial_V(T_{UU}r^2)\frac{\partial_V r}{A}\right].$$

The action of the Kodama vector (3.31) on wr^2, where w was defined in eq. (3.40), yields

$$K(wr^2) = \partial_U\left(\frac{T_{UV}}{A}r^2\right)\frac{\partial_V r}{A} - \partial_V\left(\frac{T_{UV}}{A}r^2\right)\frac{\partial_U r}{A},$$

while the components of the energy flux (3.41), which read

$$\psi_V = -T_{VV}\frac{\partial_U r}{A}, \qquad \psi_U = -T_{UU}\frac{\partial_V r}{A},$$

satisfy the following relation

$$\partial_U\left(\psi_V r^2\right) - \partial_V\left(\psi_U r^2\right) = -\partial_U\left(T_{VV}r^2\right)\frac{\partial_U r}{A} + \partial_V\left(T_{UU}r^2\right)\frac{\partial_V r}{A},$$

after using the Einstein equations again. Therefore, the vanishing divergence of J_K can be also written as

$$0 = \nabla_\mu J_K^\mu = -\frac{1}{Ar^2}\left[AK(wr^2) + \partial_U\left(\psi_V r^2\right) - \partial_V\left(\psi_U r^2\right)\right].$$

Moreover, since K and ∇r are orthogonal, $(\nabla_\mu J^\mu_K) r^2 = \nabla_\mu \left(J^\mu_K r^2\right)$, and thus

$$0 = \nabla_\mu \left(J^\mu_K r^2\right) = -K(wr^2) - \frac{1}{A}\left[\partial_U \left(\psi_V r^2\right) - \partial_V \left(\psi_U r^2\right)\right].$$

Eventually, one can verify that

$$\frac{1}{A}\left[\partial_U \left(\psi_V r^2\right) - \partial_V \left(\psi_U r^2\right)\right] = *_\gamma \mathrm{d}(\psi r^2)$$

in double-null coordinates (V, U), where $\psi = \psi_\mu \mathrm{d}x^\mu$ (see also section A.1). Therefore, eq. (3.42) follows. □

Taking into account the definitions given in eqs. (3.40) and (3.41), Hayward derived the unified first law

$$\nabla_\mu m = A\psi_\mu + w\nabla_\mu V, \tag{3.43}$$

where the first term indicates the energy flux crossing the sectional area of the spherical region, while the second one corresponds the total work in the first law of thermodynamics. Furthermore, assuming the Einstein equation $w = (8\pi)^{-1} R_\theta{}^\theta$, it holds that

$$\kappa = \frac{m}{r^2} - 4\pi r w. \tag{3.44}$$

So, denoting with a prime the derivative along the horizon, i.e., $f' \doteq \mathcal{L}_z f$, where z^μ is any tangent vector to $\mathcal{H}$, Hayward proved the following dynamical laws for spherically symmetric black holes, which generalize the ones obtained in subsection 3.1.1 for stationary black holes.

- **Zeroth law**. If $w' = 0$ along a null trapping horizon $\mathcal{H}$, then $\kappa' = 0$, i.e., the trapping horizon is stationary.

- **First law**. Along a trapping horizon $\mathcal{H}$,

$$E' = \frac{\kappa}{8\pi}\mathcal{A}' + wV', \tag{3.45}$$

  where the Misner-sharp energy E coincides with the mass m given in eq. (3.14) in the spherical case (eq. (3.45) corresponds to the unified law (3.43) projected along the trapping horizon).

- **Second law**. If the null energy condition $T_{\mu\nu}k^\mu k^\nu \geq 0$ holds for any null vector k^μ, then $\mathcal{A}' \geq 0$ (the equality holds in the null case).

- **Third law**. For non-degenerate horizons, the surface gravity cannot be reduced to zero, i.e., $\kappa \nrightarrow 0$.

Notably, all these results hold in classical gravity, but they can be violated in the semiclassical formulation when quantum matter fields influence the dynamical black hole, because quantum stress-energy tensors can violate the classical energy conditions (see subsection 1.3.3). For instance, the second law does not hold in the semiclassical scenario during a process of evaporation, as shown in sections 3.2.4 and 3.2.5.

3.2 Evaporation in Semiclassical Gravity

3.2.1 Hawking effect

Historically, starting from Hawking's original works [Haw74; Haw75] evaporation in stationary spacetimes has been regarded as the appearance of thermal radiation at infinity in form of a flux of quantum particles, once a vacuum state for the matter field is taken into account in the asymptotic past. Using the formalism of canonical quantization and the geometric optics approximation to trace back in time the outgoing solution at $\mathscr{I}^+$, Hawking obtained the steady rate of emission of particles at late retarded times, i.e., when a realistic black hole is expected to have reached a stationary configuration. Given a in-quantum state ω_{in} which was a vacuum-like state at $\mathscr{I}^-$, the expectation value of the number of particles in a (late retarded time) wave packet mode emitted at $\mathscr{I}^+$ and picked at frequency $\nu > 0$ was given by

$$\langle N \rangle_{\omega_{\text{in}}} = \frac{1}{e^{\beta_H \nu} - 1}, \tag{3.46}$$

where $\beta_H \doteq 1/(k_B T_H)$ and k_B denotes the Boltzmann constant. For the explicit evaluation of eq. (3.46), see also [FNS05]. Thus, the power radiation seen at late times showed a Planck distribution depending on the so-called Hawking temperature

$$T_H = \frac{\kappa_\infty}{2\pi k_B} = \frac{1}{8\pi k_B M}, \tag{3.47}$$

where κ_∞ is the surface gravity (3.10) of the Schwarzschild spacetime. This analysis was extended later by Wald in [Wal75], who explicitly found the quantum state resulting from the particle creation effect.

The emitted radiation from the black hole at late times is quantified by the so-called Hawking luminosity

$$L_H \doteq \frac{1}{2\pi} \int_0^\infty \frac{\nu \sum_{l \geq 0} (2l+1) |D_l(\nu)|^2}{e^{2\pi\nu/\kappa_\infty} - 1} d\nu, \tag{3.48}$$

where $D_l(\nu)$ is the gravitational black hole absorption factor for an angular mode l and peak frequency ν [Can80]. Neglecting the absorption factor and assuming s-waves with $l = 0$, the value of the luminosity reads

$$L_{H,0} = \int_0^\infty \frac{\nu}{e^{2\pi\nu/\kappa_\infty} - 1} d\nu = \frac{1}{7680\pi M^2}. \tag{3.49}$$

To obtain the total luminosity L_H, Page furnished in [Pag76] an approximate value of the absorption factor $|D_l(\nu)|^2$, at low energies νM and given different values of the spin-dependent numerical coefficients k_s - *cf.* also [BFFNSZ01; FNS05; Bar17]. This value is equal to

$$L_H = \frac{4\pi}{245760\pi^2 M^2} \sum_s k_s = 4\pi M^2 \sigma_B T_H^4 \sum_s k_s, \tag{3.50}$$

where $\sigma_B = \pi^2 k_B^4/60$ is the Stefan-Boltzmann constant in the units convention $\hbar = c = 1$. For instance, in the case of a massless conformally coupled scalar field, $k_0 = 14.36$.

The correspondence between the temperature of the radiation and the surface gravity given in eq. (3.47) puts in analogy the black hole mechanics with the ordinary four laws of classical thermodynamics in a complete way (see subsection 3.1.1): if classically black holes perfectly absorb radiation, and nothing can escape from the inside, Hawking's analysis reveals that they manifest a real thermodynamical behaviour when quantum fields are interacting semiclassically with them. In light of this result, the zeroth law matches with the statement that the temperature is constant for a body at equilibrium, while the first law coincides with the first law of thermodynamics after

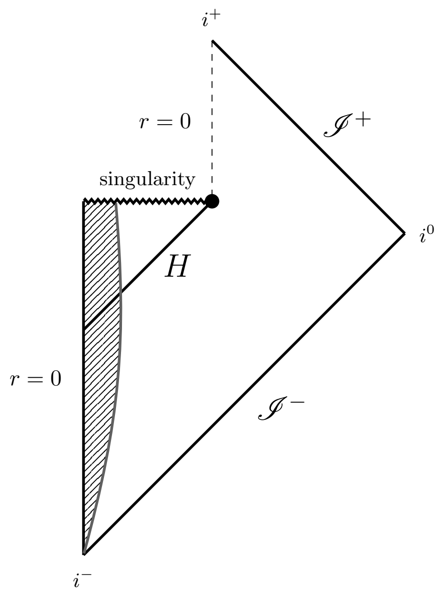

Figure 3.2: Penrose diagram of a Schwarzschild gravitational collapse followed by evaporation and leaving an empty space at the end of the evolution [Haw75; Wal95]. It represents the matter of a static star which is falling into the horizon produced by the collapsed matter in the inner region $r < R_S$, whereas the outer region $r > R_S$ is described by the Kruskal diagram of the Schwarzschild solution. At the end of evaporation, it is supposed that only empty space is left, i.e., a flat spacetime with a new regular center has formed, neglecting any back-reaction process on the spacetime geometry (the black dot represents the end of the evaporation, while the dashed line denotes the new regular centre).

identifying the entropy S of the black hole with $\mathcal{A}/4$. Hence, the second law corresponds to say that the entropy cannot decrease in time; finally, the third law states that entropy cannot be reduced to zero in any physical process, in analogy with Nernst heat theorem for the third law of thermodynamics.

Afterwards, it was shown in [FH90] that Hawking radiation with temperature given in eq. (3.47) always appears at late times in the case of a gravitational collapse which leads to a static black hole. The only assumption made in this work was that the quantum state ω is a Hadamard state approaching the ground state near the past infinity, which corresponds to say that no ingoing radiation is present at the beginning of the collapse. Following Hollands and Wald's review given in [ABIM15], Chapter 10, let f^T_{lm} be a solution of $\Box_g f = 0$ in Schwarzschild spacetime reaching $\mathscr{I}^+$ at late retarded time T, related to the spherical harmonic Y_{lm} in the angular part, with smooth compactly-supported initial data, and picked at $\nu > 0$. Then,

$$\lim_{T\to\infty} \left\langle \phi\left(f^T_{lm}\right)^* \phi\left(f^T_{lm}\right)\right\rangle_\omega = \frac{|D_l(\nu)|^2}{\mathrm{e}^{2\pi\nu/\kappa_\infty} - 1}, \tag{3.51}$$

Up to the absorption factor $D_l(\nu)$, this results coincides with the formula (3.46), i.e., the two-point correlation function given eq. (3.51) shows the same thermal nature at late times already seen in Hawking's original works. However, this computation does not contemplate any "particle creation" effect near the horizon, and it is quite general, because it does not depend on the details of the collapse and on any further geometrical approximation.

Furthermore, it reveals that the vacuum state chosen as initial condition on the matter field evolves, at late times, in a thermal state at temperature T_H. In a Schwarzschild spacetime, this state corresponds to the Unruh state $\omega_{\mathcal{U}}$, which was originally introduced in the mode decomposition formalism [Unr76; Can80], and then rigorously constructed as globally Hadamard in [DMP11] (see also [DMP17]). The Unruh state plays the right role of quantum state where the evaporation of static black holes can be studied: different from other states, such as the Boulware state and the Hartle-Hawking state, it respects both the time-translational invariance and the isometries of $\mathbb{S}^2$, it is a vacuum state in the asymptotic past $\mathscr{I}^-$, it is regular on the event horizon, and finally it contains Hawking radiation at future infinity $\mathscr{I}^+$.

There is another way to derive Hawking radiation, which differs both from Hawking's original result and from Fredenhagen-Haag's approach: it allows to obtain the Hawking temperature (3.47) purely as a local property of the event horizon, without referring to any asymptotic effect at large distances, or at late times, from the black hole. This derivation was made by Moretti and Pinamonti in [MP12], and was inspired by a previous paper due to Parikh and Wilczek - *cf.* [PW00]. In this work, Parikh and Wilczek showed that the tunnelling probability of a pair of particle-antiparticle across the event horizon had a characteristic thermal form $\mathrm{e}^{-\beta_H E}$ at the lowest order in the energy E, where β_H is the inverse Hawking temperature. On the other hand, Moretti and Pinamonti showed that the same thermal behaviour can be recovered by analysing the scaling limit property of the quantum state ω in a small region $\mathcal{O} \subset \mathcal{M}$ containing a bifurcate Killing horizon. Such a quantum state has to satisfy a weaker version of the Hadamard condition near the horizon, namely its two-point function must have the form

$$\omega_2(x, x') = \lim_{\epsilon \to 0^+} \frac{U(x, x')}{\sigma_\epsilon(x, x')} + z_\epsilon(x, x'), \tag{3.52}$$

where $z_\epsilon(x, x')$ is a distribution which is less singular than σ_ϵ^{-1} (in this view, the Unruh state fulfils this singular behaviour as Hadamard state, for instance). Moreover, they consider two compactly-supported functions f, f' such that the supports of f_λ and f'_λ lie respectively in $J^+(H) \cap \mathcal{O}$ and $J^-(H) \cap \mathcal{O}$, with $f_\lambda(V, U, \theta, x_3, x_4) = \lambda^{-1} f(\lambda^{-1} V, U, x_3, x_4)$ for $\lambda > 0$ in the Kruskal coordinates adapted to the horizon. Thus, they proved that the tunnelling probability through the horizon is

$$\lim_{\lambda \to 0^+} |\, \langle \phi(f_\lambda)^* \phi(f'_\lambda) \rangle_\omega \,|^2 \propto E_0^2 \mathrm{e}^{-\beta_H E_0}, \tag{3.53}$$

after taking into account some wave packets peaked around a certain value E_0, in agreement with Parikh and Wilczek's paper.

In more recent years, the same thermodynamic correspondence between the four laws of thermodynamics and the laws of black hole dynamics, which holds for stationary black holes, has been also proven for spherically symmetric backgrounds. As before, such a correspondence is inspired by interpreting the surface gravity as local temperature of the apparent horizon, and the very same value given in eq. (3.47) holds even in the dynamical case, with κ_∞ replaced by the Kodama surface gravity given in eq. (3.37). However, in the dynamical case both the temperature $T_{\mathcal{H}}$ of the apparent horizon and its relative thermodynamic inverse $\beta_{\mathcal{H}}$, which respectively read

$$T_{\mathcal{H}} \doteq \frac{\kappa}{2\pi}, \qquad \beta_{\mathcal{H}} \doteq \frac{1}{k_B T_{\mathcal{H}}}, \tag{3.54}$$

are non-constant functions, but they can vary during the dynamical evolution of $\mathcal{H}$. Once the relations given in eq. (3.54) is established, the area of the horizon $\mathcal{A}_{\mathcal{H}}$ corresponds to the dynamical entropy of the black hole, that is, the Wald-Kodama entropy [AH99; HMA99]

$$S_{\mathcal{H}} \doteq \frac{1}{4} \mathcal{A}_{\mathcal{H}}. \tag{3.55}$$

Different from the stationary case, the derivation of eqs. (3.54) and (3.55) has been obtained only by local analysis near the horizon, since it is very challenging to compute the expected Hawking radiation at late times in the case of dynamical black holes. Actually, both a derivation of the Hawking radiation and a generalization of the results obtained by Fredenhagen and Haag are still absent for spherically symmetric black holes. On the one hand, in [DCNVZZ07; HDCVNZ09] the temperature (3.54) is obtained by generalized Parikh and Wilczek's result in the case of dynamical horizons and for one-particle excitations. On the other hand, in [KPV21] the results obtained in [MP12] for Killing horizons are generalized to apparent horizons, and a relation between the relative entropy of coherent states and the area of the horizon which recalls eq. (3.55) is given in the scaling limit approach. For a derivation of the entropy-area law using the definition of relative entropy between quantum coherent states, see [D'A21].

3.2.2 Negative flux and evaporation

As stated by Hawking in [Haw75], and thereafter by Unruh in [Unr77], the origin of the radiation which appears far from the black hole has to be searched in the vicinity of the horizon, where a corresponding flux of negative energy has flown down into the black hole to compensate the energy carried at infinity. Indeed, the mechanism of evaporation can be fully described in the semiclassical scenario by a negative ingoing flux, which is responsible of both the shrink of the horizon area and the loss of black hole mass given in eqs. (3.27) and (3.28). This negative flux on the horizon shall be denoted by T_{VV} in double-null coordinates (3.19), or equivalently by T_{vv} using the Bardeen-Vaidya metric (3.18): in fact, it holds that $T_{vv} = T_{VV}$ on $\mathcal{H}$, according to the parametrizations given in eqs. (3.18) and (3.19), respectively. So, the evolution of the apparent horizon can be analyzed from a local point by studying the interplay between $\mathcal{H}$ and T_{VV}, assuming the (semiclassical) Einstein equations as the only dynamical equations governing such an interplay, and without referring to any expected thermal radiation emitted at infinity.

To see this, assume that the matter content is fully described by a generic stress-energy tensor $T_{\mu\nu}$. According to the definition of trapping horizon, the local dynamics of $\mathcal{H}$ can be related to the evolution of the expansion parameter θ_+ given in eq. (3.25) along an outgoing null geodesic. Denoting with $\mathrm{d}/\mathrm{d}\lambda = \mathcal{L}_+ = \ell_+^\mu \nabla_\mu$ the directional derivative along ℓ_+, the equation $G_{VV} = 8\pi T_{VV}$ reads

$$\frac{\mathrm{d}\theta_+}{\mathrm{d}\lambda} = -\frac{1}{2}\theta_+^2 - 8\pi T_{\mu\nu}\ell_+^\mu \ell_+^\nu, \tag{3.56}$$

which represents the Raychaudhuri equation (1.15) for the null affine-parametrized outgoing geodesics congruence,. If the stress-energy tensor is associated to classical matter, the null energy condition $T_{\mu\nu}k^\mu k^\nu \geq 0$ holds for any null vector k^μ and hence $\mathrm{d}\theta_+/\mathrm{d}\lambda \leq 0$. Thus, assuming the initial condition $\theta_+(V_0) = 2/(Ar) > 0$ at the beginning of the collapse, there must exist a region where $\theta_+ = 0$ for $V > V_0$, namely that a trapped surface has formed during the gravitational collapse. On the other hand, when evaluated on the apparent horizon, where $\theta_+ = 0$, eq. (3.56) reduces to

$$\frac{\mathrm{d}\theta_+}{\mathrm{d}\lambda} \overset{\mathcal{H}}{=} -8\pi \frac{T_{VV}(r_{\mathcal{H}})}{A^2}, \tag{3.57}$$

namely the evolution of the apparent horizon is directly related to the ingoing energy flux T_{VV} evaluated on $\mathcal{H}$. If such a component has a quantum nature, then it can violates the classical null energy condition, and hence if T_{VV} is negative on the horizon, it happens that $\mathrm{d}\theta_+/\mathrm{d}\lambda > 0$. Therefore, in this case, the trapped surface formed during the collapse tends to disappear, namely it evaporates.

This process of evaporation of the horizon makes manifest both as a loss of the black hole mass defined in eq. (3.28) and as a shrink of the area of the horizon given in eq. (3.27). To describe it in a local way, one shall introduce the following definition.

Definition 3.2.1. Given an apparent horizon defined in eq. (3.26), a portion of apparent horizon $\delta\mathcal{H}$ is the one-dimensional submanifold $\delta\mathcal{H} \subseteq \pi_\gamma(\mathcal{H})$, where $\pi_\gamma : \Gamma \times \mathbb{S}^2 \to \Gamma$ denotes the natural projection on the two-dimensional spacetime (Γ, γ_{ab}). On $\delta\mathcal{H}$, there is defined the variation of mass of the black hole mass

$$\Delta M \doteq \int_{\delta\mathcal{H}} \mathrm{d}m, \tag{3.58}$$

and the surface area element

$$\sqrt{\mathcal{A}_{\delta\mathcal{H}}} \doteq \int_{\delta\mathcal{H}} \mathrm{d}\sqrt{\mathcal{A}_{\mathcal{H}}}. \tag{3.59}$$

In the Bardeen-Vaidya metric given in eq. (3.18), $\delta\mathcal{H}$ is parametrized by a curve enclosed between two arbitrary points $(v_P, r_{\mathcal{H}}(v_P))$ and $(v_Q, r_{\mathcal{H}}(v_Q))$ in the (v, r) plane. On $\mathcal{H}$, the relation $\mathrm{d}r = (1 - 2\partial_r m)^{-1} 2\partial_v m \mathrm{d}v$ holds, and hence eq. (3.57) becomes a dynamical law for the rate $\dot{M}$ defined in eq. (3.30), using that $\Psi(v, r_{\mathcal{H}}) = 0$. Thus, both eq. (3.57) and $G_{vv} r^2 \overset{\mathcal{H}}{=} 8\pi T_{vv} r^2$ read as

$$\dot{M}(v) = \mathcal{A}_{\mathcal{H}}(v) T_{vv}(v, r_{\mathcal{H}}(v)), \tag{3.60}$$

where $\mathcal{A}_{\mathcal{H}}$ was given in eq. (3.27). Then, taking into account the surface gravity (3.37) on $\mathcal{H}$,

$$\Delta M = \int_{v_P}^{v_Q} \frac{\dot{M}}{4M\kappa} \mathrm{d}v = 4\pi \int_{v_P}^{v_Q} \frac{M}{\kappa} T_{vv}(r_{\mathcal{H}}) \mathrm{d}v. \tag{3.61}$$

Since $\kappa \overset{\mathcal{H}}{>} 0$ and $T_{vv} \overset{\mathcal{H}}{=} T_{VV}$, both the rate of evaporation (3.30) and the variation of the mass (3.58) are negative when $T_{VV}(r_{\mathcal{H}}) < 0$. The relation between the rate of evaporation given in eq. (3.30) and the rate of shrink of the area given in eq. (3.29) reads

$$\dot{\mathcal{A}}_{\mathcal{H}}(v) = \frac{8\pi}{\kappa} \dot{M}(v), \tag{3.62}$$

after differentiating the relation $C(v, r) = 0$ with respect to v, where C was defined in eq. (3.16), and hence employing the definition of κ (3.37) in coordinates (v, r). Plugging this relation inside ΔM, the following Riemann Penrose inequality (1.27) for $\delta\mathcal{H}$ holds:

$$\Delta M = \frac{\sqrt{\mathcal{A}_{\delta\mathcal{H}}}}{\sqrt{16\pi}}, \tag{3.63}$$

where both ΔM and $\sqrt{\mathcal{A}_{\delta\mathcal{H}}}$ were given in definition 3.2.1. Moreover, given the vector $n_{\mathcal{H}} \doteq g^{\mu\nu} \partial_\nu \mathcal{H} \partial_\mu$ normal to the apparent horizon in the (v, r) plane, then

$$g_{\mu\nu} n^\mu_{\mathcal{H}} n^\nu_{\mathcal{H}} \overset{\mathcal{H}}{=} -16 M \kappa \dot{M}. \tag{3.64}$$

So, if $\Delta M < 0$ then $\dot{M} < 0$ and $n_{\mathcal{H}}$ is spacelike, hence $\mathcal{H}$ is a timelike surface, namely the corresponding black hole is evaporating.

The common view regarding the local effect of evaporation as a quantum emission of radiation at future infinity is justified by the static symmetry of Schwarzschild spacetimes, which allows to put in directly correspondence the negative ingoing flux on the event horizon with the positive outgoing flux detected at infinity in form of black hole luminosity (3.48), when a quantum state such as the Unruh state is employed (see [FR93]). Thus, the relation between the evaporating mass and the radiation at infinity is obtained by equating, instant by instant, the rate of evaporation with the value of the luminosity at infinity, assuming a very slow variation of the mass in time compared with the mass M of the black hole. In this approximation, also called adiabatic or quasi-static, one neglects how the back-reaction of the quantum matter field is dynamically changing the spacetime geometry. All these statements are summarized in the following proposition [Can80].

Proposition 3.2.1. *In a Schwarzschild spacetime consider the Unruh state $\omega_{\mathfrak{U}}$, which is regular on the horizon, it is a vacuum in the asymptotic past, and it respects both the time-translational invariance and the spherical symmetry of the spacetime. Let*

$$F \doteq - \langle :T_{\mu\nu}: \rangle_{\mathfrak{U}} \, u^\nu n^\nu \tag{3.65}$$

be the energy flux evaluated in $\omega_{\mathfrak{U}}$, where $u^\mu = (1,0,0,0)$ denotes the timelike four-velocity, and n^μ the spacelike unit normal vector such that $n \cdot u = 0$. Then, it holds that

$$\frac{\dot{M}(v)}{4\pi} = \lim_{r \to R_S} \left(\langle :T_{VV}: \rangle_{\mathfrak{U}} \, r^2 \right) = - \lim_{r \to \infty} \left(\langle :T_{uu}: \rangle_{\mathfrak{U}} \, r^2 \right) = - \frac{L_H}{4\pi}, \tag{3.66}$$

in the adiabatic approximation, where $R_S = 2M$ and $L_H \doteq -4\pi r^2 F$ is the positive luminosity of the black hole (3.48) detected in $\omega_{\mathfrak{U}}$.

Proof. Consider the Schwarzschild metric described both in tortoise coordinates (t, r^*, θ, ϕ) and in double-null coordinates (v, u, θ, ϕ), (V, U, θ, ϕ), *cf.* eqs. (3.3), (3.6) and (3.7). It is straightforward to check that

$$\langle :T_{tr^*}: \rangle_{\mathfrak{U}} = \langle :T_{vv}: \rangle_{\mathfrak{U}} - \langle :T_{uu}: \rangle_{\mathfrak{U}} \,, \tag{3.67}$$

where $\left\langle :T^{tr^*}: \right\rangle_\omega$ is only function of r with the choice of $\omega_{\mathfrak{U}}$.

Thanks to the static symmetry of the spacetime, $\partial_t \langle :T_{tt}: \rangle_{\mathfrak{U}} = 0$, and the conservation equation $\nabla^\mu \langle :T_{\mu\nu}: \rangle_{\mathfrak{U}} = 0$ in the temporal component implies that

$$\langle :T_{tr^*}: \rangle_{\mathfrak{U}} = \frac{C}{4\pi r^2}, \tag{3.68}$$

where $C \in \mathbb{R}$. In eq. (3.68), all the additional contributions inside eq. (1.119) vanish because the metric (3.3) fulfils both $g_{tr^*} = 0$ and $R_{\mu\nu} = 0$, and hence $G_{tr^*} = I_{tr^*} = J_{tr^*} = 0$.

As $\omega_{\mathfrak{U}}$ is regular on the horizon, $\langle :T_{UU}: \rangle_{\mathfrak{U}}$ is finite on the horizon, and hence in the retarded Eddington-Finkelstein coordinates $\langle :T_{uu}: \rangle_{\mathfrak{U}} = \kappa^2 U^2 \langle :T_{UU}: \rangle_{\mathfrak{U}} = 0$, because $U = 0$ in H^+. Therefore, $\langle :T_{tr^*}: \rangle_{\mathfrak{U}} = \langle :T_{vv}: \rangle_{\mathfrak{U}}$ on H^+, and hence

$$\lim_{r \to R_S} \left(\langle :T_{vv}: \rangle_{\mathfrak{U}} \, r^2 \right) = \lim_{r \to R_S} \left(r^2 \langle :T_{tr^*}: \rangle_{\mathfrak{U}} \right) = \lim_{r \to \infty} \left(r^2 \langle :T_{tr^*}: \rangle_{\mathfrak{U}} \right), \tag{3.69}$$

where $R_S = 2M$, and the last equality holds because $r^2 \langle :T_{tr^*}: \rangle_{\mathfrak{U}}$ is a conserved quantity in the spacetime. Furthermore, $\langle :T_{vv}: \rangle_{\mathfrak{U}} \, r^2 = \langle :T_{VV}: \rangle_{\mathfrak{U}} \, r^2$ on the horizon, while it vanishes at infinity assuming a vacuum state $\omega_{\mathfrak{U}}$ in the asymptotic past. Finally, using eq. (3.67) at large r,

$$\lim_{r \to R_S} \left(\langle :T_{VV}: \rangle_{\mathfrak{U}} \, r^2 \right) = - \lim_{r \to \infty} \left(\langle :T_{uu}: \rangle_{\mathfrak{U}} \, r^2 \right) = -C. \tag{3.70}$$

The constant C is obtained from the definition of the flux given in eq. (3.65), which yields $F = - \langle :T_{tr^*}: \rangle_{\mathfrak{U}}$ up to a normalization factor. Thus, $C = L_H$ after reabsorbing that factor in the definition of C, and hence eq. (3.66) holds in the adiabatic approximation after using eq. (3.60). □

It should be stressed, actually, that eq. (3.66) loses meaning outside the adiabatic approximation, since the rate $\dot{M}(v)$ always vanishes in case of constant mass. The following statement, in fact, holds:

Proposition 3.2.2. *The Schwarzschild spacetime (3.2) with constant mass M is not a solution of the semiclassical Einstein equations, namely any eternal black hole can be never in equilibrium with the back-reaction of a quantum matter field in the semiclassical scenario.*

3.2.3 Constraining the mass from the outside

The direct correspondence given in Eq. (3.66) between the ingoing negative flux and the positive outgoing flux holds in Schwarzschild spacetime thanks to the existence of a global Killing field which is timelike outside the event horizon, but it is missing in arbitrary dynamical backgrounds. In this case, the mechanism of evaporation and the following emission of power radiated should be dealt separately only as causally related processes: on one hand, evaporation is a local effect affecting the horizon and induced by the negative ingoing flux; on the other hand, the expected Hawking radiation is associated to the positive outgoing flux emitted to infinity, and it depends globally on the entire history of spacetime.

Moreover, the adiabatic approximation is unable to describe evaporations when the spacetime is treated with its full dynamics, since it does not give informations about the evolution of the apparent horizon. In this respect, the Penrose diagram shown in Figure 3.2 should be modified in case of dynamical backgrounds outside that approximation, because the dynamics of the horizon depends sharply on the negative flux $\langle :T_{VV}:\rangle_\omega$, and the causal structure of the spacetime may be significantly modified in the back-reaction process. Conversely, a semiclassical model of evaporation should necessarily rely on the semiclassical Einstein equations (1.105) to study the variation of the mass $M(v)$ induced by the back-reaction of the quantum matter content, without further assumptions.

In the absence of further symmetries, and without a suitable (Hadamard) state which was a vacuum state in the past, it is very challenging to evaluate, or at least to estimate, the negative energy flux across the horizon. However, it turns out that some constraints for $T_{VV}(r_{\mathcal{H}})$, and thus for ΔM, can be given in terms of the matter stress-energy tensor evaluated in the causal past and outside the black hole horizon. This result implies that the behaviour of the mass can be obtained by studying the influence of the matter field outside $\mathcal{H}$, without directly evaluating $T_{VV}(r_{\mathcal{H}})$. For instance, it will be shown in section 3.2.4 that some components of the stress-energy tensor can be constrained outside the black hole horizon by the trace anomaly, forcing ΔM to be negative.

To obtain such constraints, one shall apply the divergence theorem (Stokes' theorem) - *cf.* section A.2 - to both the Kodama current (3.32) and the following radial current

$$J_r^\mu \doteq T^{\mu\nu}\nabla_\nu r, \tag{3.71}$$

which is constructed in such a way that the corresponding flux across $\delta\mathcal{H}\times\mathbb{S}^2$ coincides with $4\pi\Delta M$. More precisely, one considers

$$J_r^\mu = J_1^\mu + J_2^\nu = T^{U\mu}\partial_U r + T^{V\mu}\partial_V r, \tag{3.72}$$
$$J_K^\mu = J_1^\mu - J_2^\nu = T^{U\mu}\partial_U r - T^{V\mu}\partial_V r. \tag{3.73}$$

From eq. (3.33), $\nabla_\mu J_1^\mu = \nabla_\mu J_2^\mu$ and $\nabla_\mu J_1^\mu = \frac{1}{2}\nabla_\mu J_r^\mu$; furthermore, $J_2 = 0$ on the horizon because $\partial_V r = 0$ on $\mathcal{H}$, hence the flux across $\delta\mathcal{H}\times\mathbb{S}^2$ of J_r and J_K coincide. Finally, a direct analysis of this flux shows that the flux across $\delta\mathcal{H}\times\mathbb{S}^2$ of both J_r and J_K coincides (up to a factor 4π) with ΔM given in eq. (3.58).

The domain over which the divergence theorem is applied to obtain ΔM is actually spherically symmetric and it has the form $\mathrm{D}\times\mathbb{S}^2$, where D is a suitable portion of Γ. To define D more precisely, consider

$$S_0 \doteq \{(V,U,\theta,\varphi)\in\mathcal{M} \mid V = V_0,\ U = U_0\}, \tag{3.74}$$
$$S_1 \doteq \{(V,U,\theta,\varphi)\in\mathcal{M} \mid V = V_1,\ U = U_0\}, \tag{3.75}$$

where U_0, V_0 and $V_1 > V_0$ are chosen such that both S_0 and S_1 lie outside the apparent horizon $\mathcal{H}$ and in such a way that $(V_1, U_2)\times\mathbb{S}^2$ is contained on $\mathcal{H}$ for some U_2. Consider now $\delta\mathcal{H}\times\mathbb{S}^2$

the portion of $\mathcal{H}$ which intersects $J^+(S_0) \cap (\mathcal{M} \setminus I(S_1))$, and denote by $P_{\mathcal{H}} = (V_1, U_2)$ and $Q_{\mathcal{H}} = (V_0, U_1)$ the points which define $\delta\mathcal{H}$ in the (V, U) plane. The domain $\mathrm{D} \times \mathbb{S}^2$ is then obtained by considering the portion of $J^+(S_0) \cap (\mathcal{M} \setminus I(S_1))$ which lies outside the apparent horizon $\mathcal{H}$. If $\mathcal{H}$ is spacelike or null,

$$\mathrm{D} \times \mathbb{S}^2 \doteq J^+(S_0) \cap J^-(\delta\mathcal{H} \times \mathbb{S}^2), \tag{3.76}$$

while, if $\mathcal{H}$ is timelike,

$$\mathrm{D} \times \mathbb{S}^2 \doteq J^+(S_0) \cap O, \tag{3.77}$$

where O is the portion of $J^-(\delta\mathcal{H} \times \mathbb{S}^2)$ which lies outside the horizon. With these definitions, $\rho_0, \delta_0, \gamma \in \partial D$ denote the curves in the (V, U) plane between (V_0, U_1) and (V_0, U_0), (V_0, U_0) and (V_1, U_0), (V_1, U_0) and (V_1, U_2), respectively. See Figure 3.3 for a representation of D.

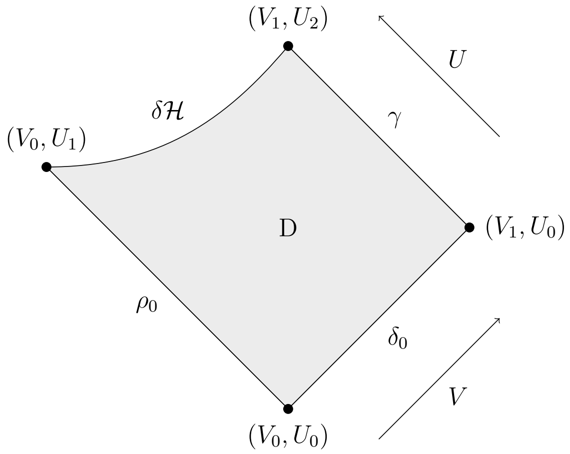

Figure 3.3: Picture of the domain of integration D given a spacelike portion $\delta\mathcal{H}$ of the apparent horizon. In this case, $\mathrm{D} \times \mathbb{S}^2 = J^+((V_0, U_0) \times \mathbb{S}^2) \cap J^-(\delta\mathcal{H} \times \mathbb{S}^2)$, with $U_2 < U_1$. The initial data are posed on the curves ρ_0 and δ_0 of the boundary $\partial\mathrm{D}$ (*copyright by S. Roncallo*).

Thus, we have the following proposition.

Proposition 3.2.3. *Consider the spherically symmetric spacetime* (3.19) *and a stress-energy tensor $T_{\mu\nu}$ which respects the spherical symmetry and which satisfies the following initial conditions at the boundary of $J^+(S_0)$, where S_0 is given in eq.* (3.74)*:*

$$T_{\mu\nu}(p) = 0, \qquad p \in \partial J^+(S_0). \tag{3.78}$$

Consider the domain D introduced in eq. (3.76) *or in eq.* (3.77)*, where the disjoint components of ∂D are denoted by $\delta\mathcal{H}$, ρ_0, δ_0, γ, and where $P_{\mathcal{H}}$ and $Q_{\mathcal{H}}$ are the extreme points of $\delta\mathcal{H}$ as explained above (see also Figure 3.3). Then the variation of the mass* (3.58) *is given in terms of the current J_r defined in eq.* (3.72) *as*

$$\Delta M = -\left(\mathcal{S} + \mathcal{W}\right), \tag{3.79}$$

where

$$\mathcal{S} \doteq 2\pi \int_D (\nabla_\mu J^\mu_r) \mathrm{d}\mathcal{V}_D, \tag{3.80}$$

$$\mathcal{W} \doteq 4\pi \int_\gamma \frac{T_{UV} r^2}{A} (-\partial_U r) \mathrm{d}U, \tag{3.81}$$

and $\mathrm{d}\mathcal{V}_D \doteq Ar^2\mathrm{d}V\wedge\mathrm{d}U$ *denotes the volume form on* D *in the* (V,U) *plane. In particular, according to eqs.* (3.79) *to* (3.81)*,* $\mathcal{S}$ *is the matter source inside the domain* D*, whereas* $\mathcal{W}$ *is related to the component of* $T_{\mu\nu}$ *that is associated to the work done by the matter given in eq.* (3.40) *when evaluated on* $\mathcal{H}$*, in view of Hayward's first law* (3.45)*. Moreover, applying the divergence theorem to the current* J_K *and comparing the result with eq.* (3.79) *yield* $\mathcal{R}=\mathcal{S}$*, where*

$$\mathcal{R} \doteq 4\pi \int_\gamma \frac{T_{UU}r^2}{A}\partial_V r \mathrm{d}U \tag{3.82}$$

is related to the outgoing energy flux T_{UU} *across* γ*.*

Proof. Using that $T^{UV} = A^{-2}T_{UV}$ and $T^{UU} = A^{-2}T_{VV}$ we can relate the current J_1 defined in eq. (3.72) to the variation of the mass (3.58) computed along the line enclosed between $(V_0,U_1),(V_1,U_2)\in\delta\mathcal{H}$ in the (V,U) plane (see Figure 3.3). In (V,U) coordinates, the derivatives of the Misner-Sharp energy (3.14) read

$$\begin{cases} \partial_V m = \dfrac{4\pi r^2}{A}\left(T_{UV}\partial_V r - T_{VV}\partial_U r\right), & (3.83a) \\ \partial_U m = \dfrac{4\pi r^2}{A}\left(T_{UV}\partial_U r - T_{UU}\partial_V r\right). & (3.83b) \end{cases}$$

Evaluating eqs. (3.83a) and (3.83b) on $\partial_V r \overset{\mathcal{H}}{=} 0$, we obtain that

$$\Delta M = 4\pi\int_{\delta\mathcal{H}} r^2(-\partial_U r)\left(\frac{T_{VV}}{A}\mathrm{d}V - \frac{T_{VU}}{A}\right)\mathrm{d}U = 4\pi\int_{\delta\mathcal{H}} Ar^2\left(J_1^V\mathrm{d}U - J_1^U\mathrm{d}V\right). \tag{3.84}$$

Eq. (3.79) can be obtained by applying the divergence theorem (Stokes' theorem) to the current J_1 on the domain $\mathrm{D}\times\mathbb{S}^2$. Using the spherical symmetry to integrate out the angular variables (φ,θ), we obtain that

$$-\int_D\left(\nabla_\mu J_1^\mu\right)\mathrm{d}\mathcal{V}_\mathrm{D} = \int_{\delta\mathcal{H}}\left(J_1^V Ar^2\mathrm{d}U - J_1^U Ar^2\mathrm{d}V\right) + \int_{\rho_0} J_1^V Ar^2\mathrm{d}U + \int_{\delta_0} J_1^U Ar^2\mathrm{d}V - \int_\gamma J_1^V Ar^2\mathrm{d}U.$$

With the choice of the initial conditions (3.78), both the integrals along ρ_0 and δ_0 vanish. By substitution of eq. (3.84) at the place of the integral over $\delta\mathcal{H}$, we get

$$-\int_\mathrm{D}\left(\nabla_\mu J_1^\mu\right)\mathrm{d}\mathcal{V}_\mathrm{D} = \frac{\Delta M}{4\pi} - \int_{U_0}^{U_2} Ar^2 J_1^V\mathrm{d}U.$$

Thus, eq. (3.79) is obtained by employing the definition $J_1 = (J_r - J_K)/2$, where J_r and J_K are given in eqs. (3.72) and (3.73), and by using that $\nabla_\mu J_1^\mu = \frac{1}{2}\nabla_\mu J_r^\mu$, since $\nabla_\mu J_K^\mu = 0$ everywhere. □

Corollary 3.2.1. *In dynamical backgrounds such that* $\mathcal{W}=0$*, where* $\mathcal{W}$ *was defined in eq.* (3.81)*,*

$$\Delta M = -\mathcal{R}. \tag{3.85}$$

This corollary, which follows trivially from proposition 3.2.3, shows that in the quantum case the variation of the mass is related to the outgoing flux $\langle{:}T_{UU}{:}\rangle_\omega$ across γ, which can interpreted as Hawking radiation sourced by $\mathcal{S}$ and emitted from the evaporating black hole to infinity. In this view, the relation (3.85) generalizes eq. (3.66) to more general non-static, spherically symmetric black holes outside the adiabatic approximation, in which $\mathcal{R}$ plays the role of dynamical luminosity of the black hole. Moreover, in this case $\Delta M < 0$ implies that $\mathcal{R} > 0$.

However, this is only a very special case of evaporation, due to the features of spacetimes with vanishing $\mathcal{W}$: actually, proposition 3.2.3 reveals that the signs of ΔM and $\mathcal{R}$ are not, in general, directly related as in eq. (3.85); on the contrary, it may happen that $\Delta M < 0$ even if $\mathcal{R} = 0$ for spacetimes in which $\mathcal{W}$ does not vanish, for instance.

3.2.4 Evaporation induced by the trace anomaly

In the previous subsection, eq. (3.79) showed that the ingoing energy flux T_{VV} on the horizon together with ΔM are constrained by the matter content outside and in the causal past of the horizon, encoded in the source $\mathcal{S}$ and in the flux $\mathcal{W}$ given in eqs. (3.80) and (3.81) on the domain $\mathrm{D} \times \mathbb{S}^2$. In this section, it is shown that a negative ingoing flux on the horizon, and thus the mechanism of evaporation, can be obtained considering the non-vanishing trace anomaly (1.120) of a quantum stress-energy tensor $\langle :T_{\mu\nu}: \rangle_\omega$, associated to a massless, conformally coupled scalar field ϕ.

It is already known that the evaporation of a black hole, viewed as emission of Hawking radiation at infinity, can be ascribed to the presence of such an anomalous trace in the vicinity of the horizon - *cf.* [DFU76; CF77; CV14]. However, such analysis are often provided after making some approximations on the spacetime, such as the adiabatic or the geometric optics approximation, which reduce the problem to a two-dimensional analysis, see also [Bal84; BB89]. On the contrary, a full semiclassical approach to study the evaporation sourced by the trace anomaly should only rely on the semiclassical Einstein equations in four dimensions, without making further assumptions or referring to asymptotic effects which need global informations about the spacetime.

On the other hand, it is also known that the trace anomaly is not sufficient to ensure evaporation, but another condition has to be imposed on the spacetime geometry (see also [Eme19]): indeed, in spherically symmetric spacetimes parametrized by the metric given in eq. (3.19) the angular component

$$\left\langle :T_\theta{}^\theta: \right\rangle_\omega = -\left\langle :T_U{}^U: \right\rangle_\omega + \frac{1}{2}\left\langle :T_\rho{}^\rho: \right\rangle_\omega = \frac{\langle :T_{UV}: \rangle_\omega}{A} + \frac{1}{2}\left\langle :T_\rho{}^\rho: \right\rangle_\omega \tag{3.86}$$

is completely determined by $\langle :T_\rho{}^\rho: \rangle_\omega$ only once $\langle :T_{UV}: \rangle_\omega$ is known (or *vice versa*). In this work, it is assumed a suitable averaged quantum energy condition on the UV-component of the stress-energy tensor outside the horizon, in which the smearing function $f(V,U)$ is a smooth exponential which decreases along the V-direction, and it is supported in the outer region. The role of $f(V,U)$ is to tame those terms inside the trace which do not contribute to a negative variation of the mass (3.58). More precisely, the following theorem holds.

Theorem 3.2.1. *Consider a free quantum massless, conformally coupled scalar field ϕ propagating on a spherically symmetric dynamical background, whose metric, expressed according to eq. (3.19), solves the semiclassical Einstein equations (1.105) for a quantum state ω. Suppose that ω is such that it makes the initial conditions stated in eq. (3.78) valid for the quantum stress-energy tensor $\langle :T_{\mu\nu}: \rangle_\omega$. Let*

$$f(V,U) \doteq f_0(V) \exp(-8\pi\lambda\beta(V,U)), \tag{3.87}$$

where $\beta(V,U)$ is any solution of $\partial_U \beta(V,U) = \frac{2}{r}\partial_V r R_U{}^V$, and $f_0(V) = \exp\{-k(V-V_0)\}$, for any $V \geq V_0$, is an exponentially decreasing function with a sufficiently large $k > 0$. Let ΔM be given by eq. (3.58). If

$$\int_{U_0}^{U_{\mathcal{H}}} \frac{\langle :T_{UV}: \rangle_\omega r^2}{A} f(V,U) A \mathrm{d}U \geq 0 \tag{3.88}$$

in the domain $D \times \mathbb{S}^2$ defined in eqs. (3.76) and (3.77), for any $V \in [V_0, V_1]$, (i.e., the integral in the left-hand side of the inequality is taken along any ingoing radial null curve connecting the initial point (V, U_0) and $(V, U_{\mathcal{H}}) \in \delta\mathcal{H}$), then, $\Delta M < 0$, namely the evaporation occurs along $\delta\mathcal{H}$.

For a qualitative behaviour of $f(V,U)$ in some special cases, see Figure 3.4[2].

[2]Both the definition of the quantum energy condition given in eq. (3.88) and the final part of the proof of theorem 3.2.1 were slightly modified in [MPRZ22] from the original version published in [MPRZ21].

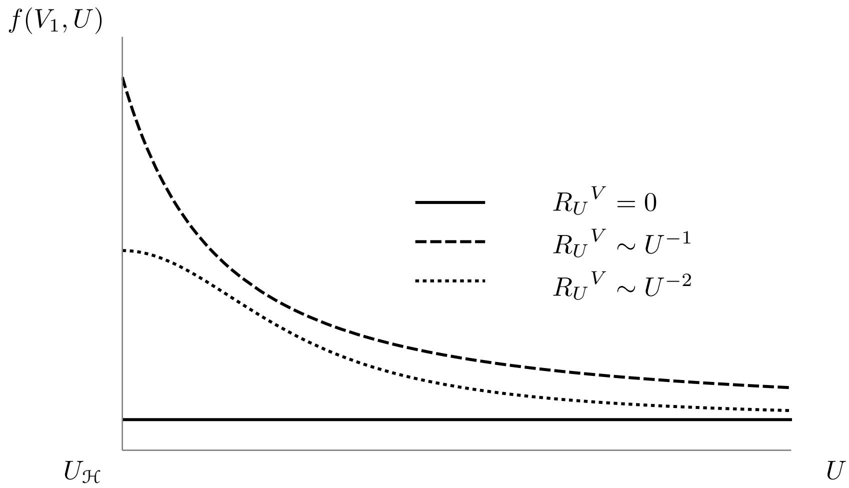

Figure 3.4: Plots of the qualitative behaviour of the smearing function $f(V,U)$ (3.87) at fixed $V = V_1$ for special choices of spacetime geometries. In the Schwarzschild and in the Vaidya spacetimes ($R_\theta{}^\theta = R_U{}^V = 0$), f is trivially a positive constant. In spacetimes where $R_\theta{}^\theta = 0$ which are asymptotically flat (i.e., $\partial_V r/r$ decays as U^{-1} and $R_U{}^V$ at least as U^{-1} for large U), f is bounded and greater than a strictly positive constant, and it approaches that constant for large U. In this respect, f is similar to the sampling functions entering usual quantum averaged weak energy conditions (see, e.g., [FF20]).

Proof. The proof consists of applying the divergence theorem (Stokes' theorem) on the domain $\mathrm{D} \times \mathbb{S}^2$ to a quantum current $\tilde{J}$ depending on $\langle :T_{\mu\nu}: \rangle_\omega$, which is a weighted version of J_1 given in eqs. (3.72) and (3.73). The weight is given in terms of a strictly positive function $f(V,U)$ which will be fixed later. Let

$$\tilde{J}_\mu \doteq \xi^\nu \langle :T_{\nu\mu}: \rangle_\omega \,, \qquad \xi^\nu = f(V,U)(\partial_V)^\nu$$

be the weighted current, and

$$\Delta_h M \doteq \int_{\delta\mathcal{H}} h \mathrm{d}m \tag{3.89}$$

the weighted variation of the mass with respect to the function

$$h(V,U) \doteq \frac{f(V,U)A(V,U)}{-\partial_U r(V,U)}. \tag{3.90}$$

The divergence of $\tilde{J}$ is related to the variation of the weighted mass (3.89) by the following equation:

$$\Delta_h M = -4\pi \int_D \nabla_\mu \tilde{J}^\mu \mathrm{d}\mathcal{V}_D - 4\pi \int_{U_0}^{U_2} \frac{\langle :T_{UV}: \rangle_\omega}{A} f A r^2 \mathrm{d}U, \tag{3.91}$$

where

$$\Delta_h M = 4\pi \int_{\delta\mathcal{H}} r^2 \left(\tilde{J}_V \mathrm{d}V - \tilde{J}_U \mathrm{d}U\right). \tag{3.92}$$

Eq. (3.91) can be obtained similarly to what already done in the proof of proposition 3.2.3 for the current J_1, namely by applying the divergence theorem (Stokes' theorem) to the weighted current $\tilde{J}_\mu$ on the domain $\mathrm{D} \times \mathbb{S}^2$, under the assumptions of 3.2.3 for the domain D and imposing the initial conditions (3.78) on $\langle :T_{\mu\nu}: \rangle_\omega$.

Using the conservation equation $\nabla^\mu \langle :T_{\mu\nu}: \rangle_\omega = 0$, the relation (3.86), and the semiclassical equations $A^{-1} \langle :T_{UV}: \rangle_\omega = R_\theta{}^\theta/(8\pi)$, $A^{-1} \langle :T_{VV}: \rangle_\omega = -R_V{}^U/(8\pi)$,

$$\nabla \cdot \tilde{J} = \frac{1}{8\pi}\left[-\left(-R_V{}^U \partial_U f + R_\theta{}^\theta \partial_V f\right) + f\left(-R_\theta{}^\theta \frac{\partial_V A}{A} + 2R_\theta{}^\theta \frac{\partial_V r}{r} + 8\pi \langle :T_\rho{}^\rho: \rangle_\omega \frac{\partial_V r}{r}\right)\right].$$

Here, $\langle :T_\rho{}^\rho: \rangle_\omega$ is a geometric quantity given in terms of the trace anomaly in eq. (1.120). Inside $\langle :T_\rho{}^\rho: \rangle_\omega$ there is a positive contribution which can be isolated, after computing explicitly the product

$$C_{\alpha\beta}{}^{\gamma\delta} C_{\gamma\delta}{}^{\alpha\beta} = \left(R + \frac{12\kappa}{r}\right)^2 = 4\left(R_U{}^U + R_\theta{}^\theta + \frac{6\kappa}{r}\right)^2$$

and the difference

$$R_\mu{}^\nu R_\nu{}^\mu - \frac{1}{3}R^2 = 2R_V{}^U R_U{}^V + \frac{2}{3}\left((R_U{}^U)^2 + \left(R_\theta{}^\theta\right)^2\right) - \frac{8}{3}R_\theta{}^\theta R_U{}^U.$$

Hence, the anomaly can be rewritten as

$$\langle :T_\rho{}^\rho: \rangle_\omega = \lambda\left(4\left(R_U{}^U + R_\theta{}^\theta + \frac{6\kappa}{r}\right)^2 + \frac{2}{3}\left((R_U{}^U)^2 + \left(R_\theta{}^\theta\right)^2\right) + 2R_V{}^U R_U{}^V - \frac{8}{3}R_U{}^U R_\theta{}^\theta\right),$$

where the first two terms are manifestly positive. Plugging this expression inside eq. (3.91) yields

$$\begin{aligned}\Delta_h M = &-4\pi\lambda \int_{\mathrm{D}} \left(4\left(R_U{}^U + R_\theta{}^\theta + \frac{6\kappa}{r}\right)^2 + \left((R_U{}^U)^2 + \left(R_\theta{}^\theta\right)^2\right)\right)\frac{\partial_V r}{r} f \mathrm{d}\mathcal{V}_{\mathrm{D}} \\ &- 4\pi \int_{\mathrm{D}} \left(-\frac{\partial_V f}{f} + \partial_V \log\left(A^{-1}r^2\right) - \lambda\frac{64\pi}{3}R_U{}^U\frac{\partial_V r}{r}\right)\frac{R_\theta{}^\theta}{8\pi} f \mathrm{d}\mathcal{V}_{\mathrm{D}} \\ &- 4\pi \int_{\mathrm{D}} \left(+\frac{\partial_U f}{f} + 8\pi\lambda\frac{2\partial_V r}{r}R_U{}^V\right)\frac{R_V{}^U}{8\pi} f \mathrm{d}\mathcal{V}_{\mathrm{D}} - 4\pi\int_{U_0}^{U_2} \frac{\langle :T_{UV}: \rangle_\omega r^2}{A} f(V_1, U) A \mathrm{d}U.\end{aligned} \tag{3.93}$$

Since D is a normal domain, e.g., with respect to the V-axis for any $\mathcal{F}(V,U) \in \mathcal{C}^\infty(\mathcal{M})$, it holds that

$$\int_{\mathrm{D}} \mathcal{F}(V,U)\mathrm{d}\mathcal{V}_D = \int_{V_0}^{V_1} \mathrm{d}V \int_{U_0}^{U_{\mathcal{H}}(V)} \mathcal{F}(V,U)Ar^2 \mathrm{d}U, \tag{3.94}$$

where $U_{\mathcal{H}}(V)$ is the solution of $2r(V,U) - m(V,U) = 0$.

The goal is to prove now that $\Delta_h M$ is strictly negative using eq. (3.93) and a strictly positive sampling function $f(V,U)$, whose role is to tame the effects of all terms inside (3.93) which do not give a negative contribution to $\Delta_h M$: in particular, $f(V,U)$ is such that all these unwanted terms vanish in D. Let $\beta(V,U)$ be any fixed primitive function of

$$\partial_U \beta(V,U) = \frac{2}{r}\partial_V r R_U{}^V,$$

then the U-derivative of f is fixed in such a way to cancel the volume integral whose integrand is proportional to $R_V{}^U$, namely it must be a solution of the equation

$$\left(\frac{\partial_U f}{f} + 8\pi\lambda\frac{2\partial_V r}{r}R_U{}^V\right) = 0.$$

Hence, the sampling function (3.87) is got, with $f_0(V)$ as integration constant. Plugging this function $f(V,U)$ in the contributions of eq. (3.93) yields

$$\begin{aligned}\Delta_h M = &-4\pi\int_{V_0}^{V_1} f_0(V)\,(\gamma_3(V) + \gamma_1(V))\mathrm{d}V + 4\pi\int_{V_0}^{V_1} \partial_V f_0(V)\,\gamma_2(V)\mathrm{d}V \\ &- 4\pi\int_{U_0}^{U_2} \frac{\langle :T_{UV}: \rangle_\omega r^2}{A} f(V_1, U) A \mathrm{d}U,\end{aligned} \tag{3.95}$$

where

$$\gamma_1(V) = \frac{1}{8\pi}\int_{U_0}^{U_{\mathcal{H}}} R_\theta{}^\theta \left(\partial_V \log(A^{-1}r^2) + 8\pi\lambda\left(-\frac{8}{3}R_U{}^U\frac{\partial_V r}{r} + \partial_V\beta(V,\tilde{U})\right)\right)\frac{f}{f_0}Ar^2\mathrm{d}\tilde{U},$$

$$\gamma_2(V) = \frac{1}{8\pi}\int_{U_0}^{U_{\mathcal{H}}} R_\theta{}^\theta \frac{f}{f_0}Ar^2\mathrm{d}\tilde{U},$$

and γ_3 is

$$\gamma_3(V) = \lambda\int_{U_0}^{U_{\mathcal{H}}(V)}\left(4\left(R_U{}^U + R_\theta{}^\theta + \frac{6\kappa}{r}\right)^2 + \frac{2}{3}\left((R_U{}^U)^2 + (R_\theta{}^\theta)^2\right)\right)\frac{\partial_V r}{r}\frac{f}{f_0}Ar^2\mathrm{d}\tilde{U}.$$

To prove that $\Delta_h M$ is strictly negative, the three contributions given by the three integrals on the right hand side of eq. (3.95) are analyzed separately. Since $\partial_V r > 0$ outside the horizon, γ_3 can be controlled as follows:

$$\gamma_3(V) \geq \frac{144}{13}\lambda\int_{U_0}^{U_{\mathcal{H}}(V)}\kappa^2\frac{\partial_V r}{r}\frac{f}{f_0}A\mathrm{d}U,$$

where the lower bound depending on κ^2 is obtained by minimizing the quadratic form in $R_\theta{}^\theta$ and $R_U{}^U$ displayed in the parenthesis inside the integrand, and hence observing that the minimum depends only on κ^2/r^2. From the behaviour on the apparent horizon of the expansion parameters of the ingoing and outgoing radial null geodesics given in eq. (3.23), and according to the definition of κ given in (3.37), κ is strictly positive on the apparent horizon, and by continuity it stays positive also near the horizon. Thus, $\gamma_3(V)$ is strictly positive for $V \in [V_0, V_1]$.

Moreover, the initial conditions given on the hypersurface ρ_0 which is part of ∂D imply that $R_\theta{}^\theta = A^{-1}\langle{:}T_{UV}{:}\rangle_\omega = 0$ on ρ_0, and hence $\gamma_1(V_0) = \gamma_2(V_0) = 0$. Then, $\gamma_1 + \gamma_3$ is strictly positive for $V = V_0$, and by continuity it stays strictly positive also for V near V_0. Therefore, we may find a constant $\delta > 0$ such that $f_0(\gamma_3 + \gamma_1)$ is strictly positive on $[V_0, V_0 + \delta]$. If k in f_0 is sufficiently large, the integral of $f_0(\gamma_3 + \gamma_1)$ over $[V_0, V_1]$ is dominated by the contribution on $[V_0, V_0 + \delta]$. Hence, the first contribution in the right-hand side of eq. (3.95) containing $\gamma_3 + \gamma_1$ is strictly negative for that choice of k.

Furthermore, the term containing γ_2 in $\Delta_h M$ in eq. (3.95) is nonpositive, because $\partial_V f_0 < 0$ on $[V_0, V_1]$, and $\gamma_2(V) \geq 0$ for all $V \in [V_0, V_1]$ according to the hypothesis stated in eq. (3.88).

Finally, the condition (3.88) also implies that the last integral appearing in $\Delta_h M$ in eq. (3.95), which is computed for $V \in V_1$ and supported in $[U_0, U_2]$, gives a negative (or vanishing) contribution to $\Delta_h M$.

Taking into account all this and with this choice of $f(V,U)$, $h(V,U)$ given in eq. (3.90) is also positive and smooth. Hence, it is bounded from below in $\delta\mathcal{H}$, so $0 > \Delta_h M \geq C\Delta M$, where $C > 0$, and the proof of the theorem holds. □

At this stage, some remarks can be made about the formulation of Theorem 3.2.1: they are listed below.

Remark 3.2.1. In the result obtained in theorem 3.2.1, the quantum trace anomaly indeed drives the evaporation of the spherical black hole, because in the case of classical free matter field the initial conditions (3.78) would imply that the stress-energy tensor vanishes on $\partial\mathrm{D} \times \mathbb{S}^2$. Thus, eq. (3.88) would hold trivially, and hence $\Delta M = 0$, namely $\delta\mathcal{H}$ would be stable under the influence of the matter field. Moreover, the quantum averaged energy condition stated in the inequality (3.88) is compatible with the thermodynamic interpretation of w given by Hayward in eq. (3.40) as the work done by the matter on the horizon, which is expected to be positive at least on its average. If such a condition holds, the weighted version of the flux $\mathcal{R}$ defined in eq. (3.82) is also positive, namely the averaged outgoing flux is positive, in agreement with the interpretation of $\mathcal{R}$ as Hawking radiation.

Remark 3.2.2. It may be possible to reformulate the equation for $\Delta_h M$, so that the condition stated in eq. (3.88) can be replaced by the following quantum energy inequality

$$\int_{\mathrm{D}} \frac{\langle :T_{UV}: \rangle_\omega \, r^2}{A} g(V, U) \mathrm{d}\mathcal{V}_D \geq 0, \tag{3.96}$$

where

$$g(V, U) \doteq \partial_V f_0(V) \exp(-8\pi\lambda\beta(V, U)),$$

is the new exponential sampling function, and D is the domain given in eqs. (3.76) and (3.77) (that integral corresponds, actually, to the second contribution in eq. (3.95) proportional to γ_2). In this case, f_0 can be chosen to satisfy $\partial_V f_0(V) < 0$ on D, and can be constructed in order to approach sufficiently fast the hypersurface ρ_0 where $\langle :T_{UV}: \rangle_\omega = 0$ (in the extremal case, $g(V)$ can diverge as $V \to V_0$). Furthermore, the boundary condition $f_0(V_1) = 0$ can be assumed, so that $\langle :T_{UV}: \rangle_\omega$ vanishes also on γ, and hence even the third contribution in eq. (3.95). Under all these assumptions, the proof of theorem 3.2.1 holds again.

However, unlike before, the averaged quantum energy condition stated as in eq. (3.96) can be better studied in the framework of quantum energy conditions, thanks to theorem 1.3.1 and the inequality (1.126) formulated in subsection 1.3.3. Moreover, one of the hypersurfaces composing ∂D can be replaced by a timelike integral curve σ_K of the Kodama vector K: as discussed in subsection 3.1.2, K is indeed timelike outside $\mathcal{H}$, and the normal vector to σ_K corresponds to the gradient ∇r, because $K \cdot \nabla r = 0$ in this region. Therefore, the timelike hypersurface σ_K always exists outside $\mathcal{H}$.

Remark 3.2.3. It is expected that the averaged condition (3.88) can be formulated in more general terms and for a larger class of smooth functions $f(V, U)$, once a sufficiently well-behaved state ω has been chosen on spherically symmetric spacetimes. Unfortunately, the lack of control on the evolution of a quantum state ω which was a vacuum in the past, namely satisfying eq. (3.78), prevents to formulate explicitly a general quantum energy condition compatible with all the previous statements. An explicit expression for $\langle :T_{UV}: \rangle_\omega$ evaluated in Hadamard states on spherically symmetric spacetimes has been obtained in [Jan22] in the case of Vaidya spacetimes (see subsection 3.2.5), assuming $m(v)$ proportional to $\Theta(v - v_0)$, with $v_0 \in \mathbb{R}$. This expectation value is pointwise positive near the horizon, but becomes negative part dominates for large r[3]. Then, the inequality (3.96) is expected to be fulfilled in this case by choosing a suitable positive sampling function picked near $\mathcal{H}$, which decay to zero sufficiently fast for large r, or alternatively by constructing a flattened region D (a thin strip, for instance) closed to the portion of horizon $\delta\mathcal{H}$.

Moreover, such a condition can be fulfilled at least in an approximate way in the causal past: actually, classical solutions are approximately valid in Semiclassical Gravity, because quantum corrections are small outside the horizon. In this approximation, eq. (3.88) is satisfied - even pointwise - in the most realistic spherically symmetric models of collapse, where the classical matter sourcing the background fulfils the dominant energy condition $A^{-1}T_{UV} \geq 0$. As examples, one can think at the Lemaître-Tolman-Bondi models like the Oppenheimer-Snyder solution, where the collapse is driven by an (in)homogeneous spherical cloud of dust at zero pressure satisfying the weak energy condition, see, e.g., [GP09] and references therein. Furthermore, in Christodoulou's

[3] The author is grateful to D. Janssen to point out his result.

works about the collapse in the case of matter described by a classical scalar field [Chr86a; Chr86b; Chr91] the collapsing matter is described by a classical massless scalar field ϕ that is invariant under rotations and having stress-energy tensor given by $T_{\mu\nu} = \partial_\mu \phi \partial_\nu \phi - \frac{1}{2} g_{\mu\nu} \partial_\rho \phi \partial^\rho \phi$. Hence, $T_{UV} = 0$ and the dominant energy condition holds again.

An immediate generalization of the foregoing argument may be carried out by extending the analysis to arbitrary massless conformally coupled fields, after modifying the coefficient λ given in eq. (1.121). In the general case, the four-dimensional anomalous trace given in eq. (1.120) reads

$$\langle :T_\rho{}^\rho: \rangle_\omega^{(\mathrm{an})} = b_F F + b_G G, \tag{3.97}$$

where $F = C_{\alpha\beta\gamma\delta} C^{\alpha\beta\gamma\delta}$ is the square of the Weyl tensor, $G = R_{\mu\nu\rho\sigma} R^{\mu\nu\rho\sigma} - 4 R_{\mu\nu} R^{\mu\nu} + R^2$ is the Euler density and b_F, b_G are coefficients depending on the numbers of particles n_s of spin s. For the explicit values of b_F and b_G, see, e.g., [BD82]. Arguably, a generalization of the Theorem 3.2.1 can be obtained for arbitrary fields after choosing properly the coefficients inside $\langle :T_\rho{}^\rho: \rangle_\omega$.

3.2.5 An illustrative example: Vaidya spacetimes

There is a special dynamical background which is approximately solution of the semiclassical Einstein equations, where one can evaluate explicitly the rate of evaporation induced by the trace anomaly: it is the Vaidya spacetime, which describes the geometry outside a null radiating star made by infalling dust. In Bardeen-Vaidya parametrization (3.18), the spacetime is described by the line element

$$\mathrm{d}s^2 = -C_{\mathrm{Va}}(v,r)\mathrm{d}v^2 + 2\mathrm{d}v\mathrm{d}r + r^2 \mathrm{d}\Omega, \tag{3.98}$$

where $C_{\mathrm{Va}}(v,r) = 1 - 2M(v)/r$ depends on the time-dependent mass of the star. This metric solves the Einstein equations through a stress-energy tensor of the form

$$T_{\mu\nu} = \frac{\dot{M}(v)}{4\pi r^2} n_\mu n_\nu, \tag{3.99}$$

where $\dot{M}$ was defined in eq. (3.30) and $n_\mu = -\partial_\mu v$ denotes the future-directed tangent vector to ingoing null geodesics. The event horizon of this spacetime is determined by the following ordinary differential equation

$$\frac{\mathrm{d}r}{\mathrm{d}v} = \frac{1}{2} C_{\mathrm{Va}}(v,r), \tag{3.100}$$

whereas the apparent horizon (3.26) is identified by the expansion parameters

$$\theta_+ = \frac{2C_{\mathrm{Va}}}{r}, \qquad \theta_- = -\frac{2}{r}, \tag{3.101}$$

and hence located on the surface $r - 2M(v) = 0$; finally, the surface gravity (3.37) reads $\kappa(v) = 1/(4M(v))$. For further details about this special spacetime, see, e.g., [GP09; Bla21] and references therein. In this case, the semiclassical regime identified by $R_{\mu\nu\rho\sigma} R^{\mu\nu\rho\sigma} \ll m_P^4$ is always satisfied when $M/m_P \gg (3/4)^{1/4} \simeq 0.93$, where m_P is the Planck mass, which holds for astrophysical masses, e.g., $M_\odot / m_P \simeq 10^{38}$ for a solar mass $M_\odot$.

In the Vaidya spacetime, the trace anomaly (1.120) reads

$$\langle :T_\rho{}^\rho: \rangle_\omega = 48\lambda \frac{M(v)^2}{r^6}, \tag{3.102}$$

where λ is the coefficient (1.121), and the rate of evaporation can be computed directly from eq. (3.60), after evaluating the negative ingoing flux $\langle :T_{VV}: \rangle_\omega$ on $\mathcal{H}$. To obtain $\langle :T_{VV}: \rangle_\omega$, one employs eq. (3.79) or, alternatively, the conservation equation $\nabla^\mu \langle :T_{\mu V}: \rangle_\omega = 0$, which yields

$$-\frac{1}{Ar^2} \partial_U \left(\langle :T_{VV}: \rangle_\omega r^2 \right) - \frac{1}{r^2} \partial_V \left(A^{-1} \langle :T_{UV}: \rangle_\omega r^2 \right) - 2 \left\langle :T_\theta{}^\theta: \right\rangle_\omega \frac{\partial_V r}{r} = 0,$$

where $\left\langle :T_\theta{}^\theta: \right\rangle_\omega$ was given in eq. (3.86).

On the other hand, it is very challenging, in principle, to evaluate the renormalized component $\langle :T_{UV}: \rangle_\omega$ on a state which is a vacuum state in the past. Furthermore, contrary to its classical counterpart, such a component is expected not to vanish in a generic quantum state ω (see, e.g., [DFU76] for the two-dimensional case); namely, a Vaidya spacetime is not expected to be a full solution of the semiclassical equations. Here, to perform the computation one shall assume for simplicity that there exists a quantum state ω in which $\langle :T_{UV}: \rangle_\omega = 0$ and which makes Vaidya spacetime a semiclassical solution outside the horizon. With this assumption, the ingoing flux fulfils the following differential equation in (v, r) coordinates

$$\partial_r(\langle :T_{VV}: \rangle_\omega r^2) = 24\lambda M(v)^2 \left(\frac{1}{r^5} - \frac{2M(v)}{r^6} \right).$$

Integrating in $(r_{\mathcal{H}}, \infty)$, imposing the initial condition $\langle :T_{VV}: \rangle_\omega r^2 \to 0$ when $r \to \infty$, and changing sign, the ingoing flux reads

$$\langle :T_{VV}: \rangle_\omega r^2 \stackrel{\mathcal{H}}{=} -24\lambda M^2 \int_{r_{\mathcal{H}}}^{+\infty} \left(\frac{1}{r^5} - \frac{2M(v)}{r^6} \right) \mathrm{d}r = -\frac{3\lambda}{40M(v)^2}. \tag{3.103}$$

Hence, the rate of evaporation obtained from eq. (3.60) is

$$\dot{M}(v) = -\frac{3\pi\lambda}{10M(v)^2} = -\frac{1}{9600\pi M(v)^2}. \tag{3.104}$$

It should be stressed that the analytical result given in (3.104) differs in the numerical coefficient from the values of luminosity given in eqs. (3.49) and (3.50). This is due to the evaluation of the negative flux obtained in eq. (3.103), which takes into account the backreaction of the quantum field from $\mathscr{I}^-$ to $\mathcal{H}$, outside the quasi-static limit and in the approximation of $\langle :T_{UV}: \rangle_\omega = 0$.

Eq. (3.104) is an ordinary differential equation with respect to v and it can be integrated by separation of variables, yielding the evaporation law

$$M^3(v) = M_0^3 - \frac{9\pi\lambda}{10}(v - v_0), \tag{3.105}$$

where $M_0 \doteq M(v_0)$ is the total mass at the initial time v_0. Thus, the evaporation process is completed in the advanced time interval $\Delta v \doteq v - v_0 = 3200\pi M_0^3$. Moreover, according to eq. (3.62), the negative rate (3.104) induces also a negative rate of shrink of the area of the horizon, which can be computed explicitly. Hence, a negative variation of the entropy (3.55) holds, namely

$$\frac{\mathrm{d}S_{\mathcal{H}}(v)}{\mathrm{d}v} = -\frac{12\pi^2\lambda}{5M(v)} = -\frac{1}{1200M(v)}, \tag{3.106}$$

which is dimensionally compatible with the results presented, e.g., in [Pag13] and in the references therein.

Remark 3.2.4. In the same approximations as before, one could equivalently assume in the conservation equation that there exists a quantum state ω such that the $\theta\theta$-component of the stress-energy tensor vanishes, thus obtaining $\langle :T_{UV}: \rangle_\omega$ using the relation for the trace given in eq. (3.86). However, in this case one would obtain a different expression for the ingoing flux:

$$\langle :T_{VV}: \rangle_\omega r^2 \stackrel{\mathcal{H}}{=} \frac{6\lambda}{M(v)^2} \left(\frac{\dot{M}(v)}{3} - \frac{1}{40} \right), \tag{3.107}$$

and thus a different equation for $\dot{M}(v)$:

$$\left(1 - \frac{\lambda}{M^2}\right)\dot{M}(v) = -\frac{3\lambda}{40M^2(v)}. \tag{3.108}$$

Actually, this equation reduces to eq. (3.104) in the limit of $\lambda \ll M^2$, which indeed holds for astrophysical black holes. In fact, this evaluation confirms that Vaidya spacetimes are not exact solutions of the semiclassical Einstein equations.

Chapter 4

Linearized Semiclassical Theories of Gravity

> *"Within the context of Semiclassical Gravity [...], it is not necessarily logically inconsistent to consider the full effect of the higher derivative terms in the theory."*
>
> *Wai-Mo Suen*

Summary

The content of this chapter is based on author's paper [MP22], which aims to investigate the issue of stability of solutions of the semiclassical Einstein equations in the linearized regime, that is, at the linear order in the interaction. In a physical viewpoint, this is a key problem in the analysis of semiclassical Einstein equations, because proving stability would mean showing that semiclassical theories of gravity are able to describe the dynamics of a quantum system interacting with curvature in a an effective regime, i.e., when quantum gravity effects can be neglected.

A question of well-posedness of semiclassical theories arises because of the presence of higher order derivative of the metric in the dynamical equations, due to the back-reaction of the quantum matter field upon the spacetime geometry encoded in the quantum stress-energy tensor (see subsection 1.3.1). As seen in the cosmological case, *cf.* section 2.2, the presence of both non-local quantum contributions and higher order derivatives makes it difficult to find semiclassical solutions, even in the local case. Thus, understanding when such solutions are also stable for large times turns to be a further more complicated task to pursue.

The main result obtained in [MP22] consists in proving that, if the quantum field driving the back-reaction is massive, then the stability of background solutions can be restored at the linear order, after assuming some sufficient (but not necessary) conditions on the parameters of the theory. This result is achieved for spatially compact perturbations, i.e., perturbations over the background geometry that are not arbitrarily dispersed in space, as expected for physically reasonable anisotropies. On the other hand, removing the assumption of massive quantum fields seems to give rise also to unstable runaway solutions, namely solutions of exponential form which arbitrarily grow in time, and thus which destabilize the background configuration. This conclusion is, actually, in accordance with other results present in the literature about semiclassical theories of gravity, see, e.g., [Hor80; Jor87; Kay81]. The linearized semiclassical system investigated in this

chapter is a toy model, consisting of a quantum scalar field in interaction with a second classical scalar field playing the role of a classical background. The equations governing the dynamics of linear perturbations around simple exact solutions of this toy model are analyzed by constructing the corresponding retarded fundamental solutions, and thus by discussing the associated initial-value problem. Under the assumptions stated before, it is proved that linear perturbations with compact spatial support decay polynomially in time for large times, thus indicating stability of the underlying semiclassical solution.

This chapter is organized as follows. In section 4.1 a discussion about the history of runaway solution in semiclassical theory of gravity is addressed (see subsection 4.1.1), and a superficial approach to the ideas of Stochastic Gravity as extension of Semiclassical Gravity is followed in subsection 4.1.2. In section 4.2 the stability results of the chapter about linearized semiclassical theories of gravity are presented, based on author's publication. The description of the toy model employed to investigate the issue, the construction of the vacuum polarization associated to the toy model, and the main statements of the chapter are gathered in subsection 4.2.1, subsection 4.2.2, and subsection 4.2.3, respectively. Finally, in subsection 4.2.4 a promising extension of the previous results to the cosmological case is explained, with particular emphasizes on the application of the Einstein-Langevin equations to model a stable semiclassical early Universe at large times.

4.1 Are Spacetimes Unstable in Semiclassical Gravity?

4.1.1 The issue of runaway solutions

A generic feature which makes manifest in effective field theories involving back-reaction, not only of gravity, is the appearance of higher-order time derivatives in the dynamical equations. In the case of Semiclassical Gravity, the semiclassical Einstein equations (1.105) become fourth-order differential equations in the coefficient of the metrics, when arbitrary couplings with the curvature are involved, as discussed in subsection 1.3.1 and subsection 1.3.2. Hence, there is a shared idea in gravitational and quantum communities about Semiclassical Gravity and higher-order theories of gravity that such approximated models of non-classical gravity contain unavoidably non-physical solutions, due to the effective nature of their formulations (see [Sue92; FW96] for a discussion about the self-consistency of Semiclassical Gravity).

In the framework of linearized semiclassical theories around fixed backgrounds, they usually refer to this class of solutions as "runaway solutions", which consist of solutions of the linearized system around some background which grow exponentially in time. In the perturbative viewpoint, the consequences for physical systems which admit runaway solutions are quite catastrophic, because exponentially growing perturbations become dominant over the stable background solutions at large times. Therefore, it can no longer be assumed that the overall system remains stable in time. In this picture, furthermore, the full solution of the system acquires a very different form from the chosen background, and at the same time it is expected to be very sensitive to the chosen initial conditions.

A first example in which the issue about pathological solutions arising from effective field theories appears is the Abraham-Lorentz-Dirac equation, which describes the motion of a non-relativistic charged particle influenced by both an external field and the electromagnetic field produced by itself [FW96; Poi99; Jac98]. Denoting with $\vec{E}(t,\vec{x})$ the external field, the equation of motion of the particle reads

$$\ddot{\vec{x}} = \frac{q}{m}\vec{E}(t,\vec{x}) + \tau\dddot{\vec{x}},$$

where q is the electric charge, m is the mass, and $\tau = 2q^2/(3m^3c^3)$ is the timescale associated to the radiation reaction force $\vec{F} = m\tau\dot{\vec{a}}$.

This equation captures the dynamics of the particle in a certain regime of validity $\tau^* \gg \tau$, where τ^* denotes the timescale over which the acceleration changes. Furthermore, it shares similar conceptual features of the semiclassical equations, because it describes the back-reaction of the radiation emitted upon the particle itself. Thus, it involves a higher-order derivative term depending on τ, which is responsible of the appearance of runaway solutions for large times. Indeed, assuming a compactly-supported external field $\vec{E}(t, \vec{x})$, the general solution can be written as

$$\vec{a} = \mathrm{e}^{t/\tau} \left(\vec{a}_0 - \frac{q}{m\tau} \int_{-\infty}^{t} \vec{E}(s, \vec{x}) \mathrm{e}^{-s/\tau} \mathrm{d}s \right) , \tag{4.1}$$

where $\vec{a}_0 \doteq \vec{a}(t_0)$ denotes the further initial condition of the initial-value problem. Eq. (4.1) displays a class of runaway solutions for large times of the form $\dddot{\vec{x}} \sim \exp(t/\tau)$, in particular outside the regime of validity of the equation, i.e., when $\tau^* \sim \tau$. In this respect, Ostrogradsky's theorem merits a remark, because it states that a classical Lagrangian containing higher-order derivatives leads to an Hamiltonian which is linear in the canonical momentum, thus providing unstable configurations of the system (for some references about this theorem and its applications in higher-order theories of gravity, see [Woo07; Woo15]), A way to remove this class of physical solutions is to choose suitable initial data such that the space of solutions is reduced to the classical case. However, some phenomena of pre-acceleration appear in this procedure, in which the acceleration at time t depends on the external field evaluated at future times $t' > t$, thus violating causality. For further details, see also [Yag06]. Therefore, the validity of this equation is often put in doubt, just as in the case of the semiclassical equations.

The first papers which investigated the issue of runaway solution in the framework of Semiclassical Gravity are due to Horowitz and Wald [HW78; Hor80], in which they argued that the presence of higher-order derivative terms in the semiclassical equations gave rise to exponentially growing solutions at timescales closed to the Planck scale, i.e., in a regime where the semiclassical approximation fails. They came to this conclusion by linearising the semiclassical equations around fixed background geometries, thus indicating that the chosen backgrounds are unstable within this context. Remarkably, such runaway solutions seem to arise even in flat spacetime, viewed as trivial solution of the semiclassical Einstein equations. Namely, Minkowski spacetime appears to be unstable in Semiclassical Gravity (see also [Kay81; Yam82; Jor87; Sue89; MW20]).

In [Hor80], Horowitz studied the weak-field limit of the semiclassical Einstein equations (1.105), taking into account a linear small perturbation $\gamma_{\mu\nu}$ having compact support over the flat background $\eta_{\mu\nu}$, and a massless quantum field which drives the back-reaction upon the background. Thus, he obtained the following linearized semiclassical Einstein equations

$$\dot{G}_{\mu\nu} = 8\pi \langle 0 | \dot{T}_{\mu\nu} | 0 \rangle , \tag{4.2}$$

where the dot denotes the linearized form of the corresponding tensor. In particular, a quantum Maxwell field interacting with the weak gravitational field was considered as matter field entering the right-hand sides of eq. (4.2). On the one hand, it was shown that this semiclassical theory admits well-behaved solutions satisfying $\dot{G}_{\mu\nu} = 0$; on the other hand, unstable runaway solutions, which are homogeneous in space and exponentially grow in time, appeared closed to a certain critical length scale. Afterwards, in [RD81] similar conclusions were obtained in the case of massive quantum fields, stating that stability could be retained only by admitting masses well above the Planck mass. Finally, the analysis led by Horowitz was extended in [FW96], in order to comprise both first-order perturbations having a well-behaved spatial Fourier transforms, namely spatially compact perturbations which decay sufficiently fast to infinity, and a non-vanishing incoming quantum state as source of perturbations. As before, it was argued that linearized semiclassical theory of gravity may lead to the appearance of unphysical runaway solutions at this order in perturbation theory, and hence to the instability of the vacuum state on the flat spacetime under the influence of quantum matter fields in the semiclassical picture.

For the sake of the completeness on this discussion, it is necessary to remember that a prescription of reduction of order was proposed in [Sim91; PS93; FW96] to eliminate runaway unstable solutions. This method is based on truncating perturbatively the equations of motion up to a certain order of derivatives, in such a way that no higher-order derivatives in time may appear in the resulting dynamics. Thus, the time derivative of the previous truncated equation is derived one more time, and hence the obtained higher-order derivative is substituted in the original equation. In this way, the final equation contains no derivative term of higher order anymore, and thus it can be equivalently solved as a classical differential equation, without worrying about the arising of unphysical solutions at large times.

Before concluding with the discussion about runaway solutions, it should be pointed out that a first proposal of renormalization scheme of semiclassical theories was given in [RDKK80] by means of a toy model, which shares, in fact, the same conceptual features of a semiclassical theory of gravity. It has been proposed in this paper that a consistent renormalized theory may be achieved by fixing the renormalization constants appearing in the regularized quantum stress-energy tensor of the matter field. In this way, unphysical solutions may be discarded from the equation by suitable choices of these renormalization freedoms, as expected in the standard approach to renormalized quantum theories. Similar ideas shall be employed in section 4.2 to show the stability of linearized semiclassical theories of gravity.

4.1.2 Bird's-eye view on Stochastic Gravity

A further formulation of semiclassical theories of gravity developed by Hu and Verdaguer in the nineties is constituted by the so-called Stochastic Semiclassical Gravity, or more simply Stochastic Gravity, in which the semiclassical Einstein equations (1.105) are replaced by new Einstein-Langevin equations. All the details about the formulation of this theory can be found in the recent monograph [HV20], containing also authors' original references (the idea presented here can be found specially in Chapter 10). The aim of this subsection is, actually, to point out briefly some ideas inferred from Stochastic Gravity, which may be useful for the discussion made in subsection 4.2.4.

Whereas the semiclassical Einstein equations aim to evaluate the back-reaction of the quantum matter field through the expectation value of quantum stress-energy tensor, the goal of the Einstein-Langevin equations is to incorporate also the fluctuations induced by the quantum stress-energy tensor on the spacetime geometry, adding a Gaussian white noise inside the semiclassical model. More precisely, its correlation distribution has a specific Kernel, which is modelled by a bitensor constructed from the two-point correlation of $T_{\mu\nu}$. Namely, it is defined as

$$N_{\mu\nu\rho'\sigma'}(x,y) \doteq \frac{1}{2}\left\langle\{:t_{\mu\nu}:(x), :t_{\rho'\sigma'}:(y)\}\right\rangle_\omega$$

in the notations for bitensors presented in subsection 1.2.3. Here, brackets denote the anti-commutator $\{f,g\} \doteq fg + gf$, while

$$t_{\mu\nu} \doteq :T_{\mu\nu}: - \left\langle :T_{\mu\nu}:\right\rangle_\omega \mathbb{I}$$

is evaluated on a sufficiently regular (possibly Hadamard) state which renormalizes $:T_{\mu\nu}:$. Once the Gaussian white noise has been introduced, a new classical Gaussian stochastic field $\tau_{\mu\nu}(x)$ can enter the semiclassical equations, as dissipative source term which encodes the fluctuations of the spacetime metric induced by the quantum source. Since any Gaussian noise is fully characterized by its second stochastic moment, $\tau_{\mu\nu}(x)$ is well-defined by the following properties

$$\left\langle\tau_{\mu\nu}(x)\right\rangle_s = 0, \qquad \left\langle\tau_{\mu\nu}(x)\tau_{\rho'\sigma'}(y)\right\rangle_s = N_{\mu\nu\rho'\sigma'}(x,y),$$

where expectation values are in the sense of a statistical averaged. By construction, $\tau_{\mu\nu}$ is covariantly conserved on the background geometry, i.e., $\nabla^\mu \tau_{\mu\nu} = 0$, and, furthermore, it is traceless for conformally-coupled fields ($g^{\mu\nu}\tau_{\mu\nu} = 0$), so no further contributions to the trace anomaly (1.120) appear in the semiclassical equations.

Based on these statements, the Einstein-Langevin equations are ready to be formulated as follows. Assume that the spacetime metric can be decomposed into a background contribution $g^{(0)}_{\mu\nu}$ and a perturbation $h_{\mu\nu}$ over the background, which is sourced by $\tau_{\mu\nu}$ in the back-reaction process. Suppose also that the background metric fulfils the semiclassical Einstein equations at the zeroth-order, i.e., in the absence of perturbations. Then, the Einstein-Langevin equations read as

$$G^{(1)}_{\mu\nu}\left[g^{(0)}_{\mu\nu} + h_{\mu\nu}\right] + \Lambda\left(g^{(0)}_{\mu\nu} + h_{\mu\nu}\right) = 8\pi G \left\langle :T_{\mu\nu}: \right\rangle^{(1)}_{\omega} \left[g^{(0)}_{\mu\nu} + h_{\mu\nu}\right] + \tau_{\mu\nu}\left[g^{(0)}_{\mu\nu}\right]. \tag{4.3}$$

Here, the superscript (1) indicates the linearization of the corresponding tensor with respect to $h_{\mu\nu}$. Thus, both the linearized Einstein tensors and stress-energy tensor depend on both the background and the perturbation metrics, whereas the induced fluctuations of the metric encoded in $\tau_{\mu\nu}$ depend only on the background. On the one hand, these equations correspond to the linearization of eqs. (1.105), with the addiction of the cosmological constant Λ and of the classical stochastic tensor $\tau_{\mu\nu}$. On the other hand, they represent the dynamical equations for the perturbation, because the background was fixed at the zeroth-order as solution of the unperturbed semiclassical Einstein equations (1.105).

The validity of semiclassical theories, and their relations to runaway solutions, has been also investigated in Stochastic Gravity by studying the linear response of the stochastic perturbation $\langle h_{\mu\nu}\rangle_s$ on the background metric (see also [AMPM02; AMPM03]). As previously said, the purpose of this subsection is not to provide details about the related works: they can be easily found in the references cited before, actually. Furthermore, they are mainly based on a reduction of order procedure, which is not in author's interest to deepen at this stage. On the contrary, it is essential to underline briefly the motivations behind the validity criterion proposed in this framework.

As pointed out in [Pin11] for the cosmological scenario, the variance of the renormalized quantum stress-energy tensor is always divergent in the semiclassical formulation. For instance, the expectation value of $:\phi^2:$ has divergent fluctuations even if evaluated in a Hadamard state, as one can infer from eq. (1.87), in which $H^2_{0+}(x, x')$ diverges in the coinciding point limit. As shown in this reference, a possible solution to overcome this issue is to smear the variance of $\phi^2(f)$ with a suitable $f \in \mathcal{D}(\mathcal{M})$, and thus proving that it vanishes in a certain limit of large spatial support of f, *cf.* [Pin11], Theorem 5.2.

Another way to investigate the role of fluctuations in the semiclassical picture is to consider the matter-gravity induced fluctuations in the semiclassical equations directly, in order to formulate a full theory of back-reaction in a self-consistent way. An interesting approach to study quantum fluctuations was introduced in [PS15b; DM14], in which curvature fluctuations induced by the quantum stress-energy tensor are evaluated by interpreting the Einstein tensor as a stochastic field, just as the matter counterpart. In this viewpoint, perturbations of the background spacetime are specified by the n-points correlation functions associated to the stochastic Einstein tensor, which are equated to the n-points correlation functions of the quantum stress-energy tensor in the semiclassical Einstein equations (1.105).

On the other hand, in the framework of Stochastic Gravity the induced fluctuations on the spacetime enter directly the semiclassical equations as stochastic source, and the back-reaction effects of the fluctuations to the background metric are included through the addition of the Gaussian white noise. Hence, a solution of Semiclassical Gravity is valid when it results stable under the influence of the metric perturbations induced by the fluctuations of the stress-energy tensor, which enter eq. (4.3) through $\tau_{\mu\nu}$. Therefore, in this stochastic viewpoint, the addition of a classical source to the semiclassical Einstein equations is necessary both for self-consistency and to obtain stable semiclassical perturbations on fixed backgrounds. This is the very relevant statement for the scopes of this work, and thus it shall be recalled in subsection 4.2.4 at the end of this chapter.

However, it should be stressed that some approximations on the probability distribution associated to the quantum stress-energy tensor are present both in eqs. (1.105) and in eqs. (4.3), because the cumulative fluctuations at higher orders are always neglected. Therefore, the need to have small stochastic fluctuations is required in both semiclassical models. In this respect, even Stochastic Gravity remains an effective theory for the description of the interplay between matter and gravity.

4.2 Stability of Linearized Semiclassical Gravity

4.2.1 The semiclassical toy model

Taking inspiration from similar models studied in [RDKK80; JAMS20], the investigation of a semiclassical toy model is proposed in this chapter, consisting of the interplay between a quantum scalar field ϕ and another classical background scalar field ψ in the Minkowski spacetime $(\mathcal{M}, \eta_{\mu\nu})$. The goal is to understand the well-posedness of an initial-value problem of the semiclassical Einstein equations (1.105) for global stable solutions in time[1].

The equations of motion governing the corresponding free theory are assumed to be

$$\begin{cases} \Box\phi - m^2\phi = \lambda\psi\phi, & (4.4a) \\ g_2\Box\psi - g_1\psi = \lambda_1\phi^2 - \lambda_2\Box\phi^2, & (4.4b) \end{cases}$$

where $g_1, g_2, \lambda, \lambda_1, \lambda_2$ denote the real coupling constants of the theory. Although the choice $\lambda_2 = 0$ implies that the system descends from a Lagrangian of two scalar fields, no further constraints on the coupling constants are imposed, in order to describe as many semiclassical theories as possible. Actually, there is sufficient freedom in the definition of the coupling constants to fix $\lambda_2 = 1$ in the non-vanishing case. However, keeping $\lambda_2 \neq 1$ allows to eqs. (4.4a) and (4.4b) to mimic precisely the traced semiclassical Einstein equations (1.124), as discussed in subsection 4.2.4.

The first equation (4.4a) represents the equation of motion of a linear, Klein-Gordon like quantum massive field ϕ, with mass m and external potential $\lambda\psi$, whose quantization is performed according to subsection 1.2.2. In light of the quantum nature of ϕ, eq. (4.4b) can be interpreted in the semiclassical approximation by taking the expectation values of ϕ^2 in a suitable quantum state ω on the CCR algebra $\mathcal{A}(\mathcal{M}, \eta_{\mu\nu})$. In this way, $\langle :\phi^2: \rangle_\omega$ reads as the vacuum polarization of ϕ in ω. Therefore, the semiclassical system corresponding to eqs. (4.4a) and (4.4b) turns out to be

$$\begin{cases} \Box\phi - m^2\phi = \lambda\psi\phi, \\ g_2\Box\psi - g_1\psi = \lambda_1 \langle :\phi^2: \rangle_\omega - \lambda_2\Box \langle :\phi^2: \rangle_\omega . \end{cases} \tag{4.5}$$

The linearization of this system around fixed classical solutions of eq. (4.5) labelled by (ψ_0, ω) is realized as follows. The classical scalar field is decomposed into the background contribution ψ_0 plus a perturbation ψ_1, so that

$$\psi = \psi_0 + \psi_1.$$

[1] Unlike the previous chapters, the convention on $\hbar \neq 1$ shall be restored both here and in the following sections, to highlight the quantum contributions in the semiclassical equations.

Then, in a first step, the quantization of ϕ is performed on the fixed background ψ_0 by constructing the CCR *-algebra $\mathcal{A}(\mathcal{M}, \eta_{\mu\nu})$ equipped with the canonical commutation relations emerging from to the zeroth-order equation

$$\Box\phi - m^2\phi - \lambda\psi_0\phi = 0. \tag{4.6}$$

Furthermore, both the quantum state ω and the background field ψ_0 satisfy the semiclassical equation, namely the second equation in the system given in eq. (4.5), which thus represents a constraint for the couple (ψ_0, ω). The vacuum polarization on this background theory is then obtained by a Hadamard point-splitting regularization (1.86), which yields

$$\left\langle :\phi^2: \right\rangle_\omega^{(\mathrm{bac})}(x) = \hbar \lim_{x' \to x} \left(\Delta_{+,\omega}(x', x) - H_{0^+}(x', x)\right) + cm^2 + c\lambda\psi_0(x), \tag{4.7}$$

where $\Delta_{+,\omega}$ is the two-point function of the state ω, H_{0^+} is the Hadamard parametrix (1.57), and $c \in \mathbb{R}$ is the renormalization constant associated to the Wick observable $:\phi^2:$ (see subsection 1.2.5).

In the second step, the influence of the perturbation ψ_1 on ϕ is analyzed by means of perturbation theory (see subsection 1.2.5), taking into account both the interacting Lagrangian

$$\mathcal{L}_I \doteq -\frac{\lambda}{2}\psi_1\phi^2 \tag{4.8}$$

and the Bogoliubov map (1.99) constructed from the smeared interacting action

$$V \doteq \int_U \mathcal{L}_I(x) f(x) \mathrm{d}^4x = -\frac{\lambda}{2}\int_U \phi^2(x)\psi_1(x) f(x)\mathrm{d}^4x.$$

This interacting action is located in the spacetime subregion $U \subset \mathcal{M}$ and depends on a smooth cut-off $f \in \mathcal{D}(\mathcal{M})$, which will be eventually removed in the adiabatic limit $f \to 1$ as $U \to \mathcal{M}$.

From eq. (1.100), the perturbative expansion of the interacting vacuum polarization induced by the Lagrangian (4.8) reads at the linear order in V as

$$\left\langle :\phi^2: \right\rangle_\omega = \left\langle :\phi^2: \right\rangle_\omega^{(\mathrm{bac})} + \left\langle :\phi^2: \right\rangle_\omega^{(\mathrm{lin})} + \dots.$$

where

$$\left\langle :\phi^2: \right\rangle_\omega^{(\mathrm{bac})} \doteq \omega(\phi^2), \qquad \left\langle :\phi^2: \right\rangle_\omega^{(\mathrm{lin})} \doteq \frac{i}{\hbar}\left(\omega(T\left(V\phi^2\right)) - \omega(V\phi^2)\right). \tag{4.9}$$

Finally, the linearization procedure consists of studying the semiclassical theory described by the system of equations given in eq. (4.5), where interacting vacuum polarization is approximated by truncating at first order the formal power series in the interaction Lagrangian (4.8) occurring in the map R_V defined in eq. (1.99). On the other hand, the state for the interacting quantum theory is constructed by means of the state satisfying eq. (4.6) on the linear quantum theory, i.e., on $\mathcal{A}(\mathcal{M}, \eta_{\mu\nu})$, and it is fixed once and forever, no matter the form of the linear perturbation ψ_1.

Hence, on the one hand the background theory is described by (ψ_0, ω), in which both ψ_0 and ω satisfy the semiclassical equation

$$g_2\Box\psi_0 - g_1\psi_0 = (\lambda_1 - \lambda_2\Box)\left\langle :\phi^2: \right\rangle_\omega^{(\mathrm{bac})}. \tag{4.10}$$

On the other hand, the linear perturbation theory of the background is described by the classical field ψ_1, which fulfils the following linearized semiclassical equation

$$g_2\Box\psi_1 - g_1\psi_1 = (\lambda_1 - \lambda_2\Box)\left\langle :\phi^2: \right\rangle_\omega^{(\mathrm{lin})}, \tag{4.11}$$

where $\left\langle :\phi^2: \right\rangle_\omega^{(\mathrm{lin})}$ was constructed in eq. (4.9). Eq. (4.11) is the only equation which constrains the dynamics at the linear order, and it must be seen as the real dynamical equation for the linear perturbation ψ_1.

4.2.2 Free and interacting vacuum polarizations

After laying the groundwork for the perturbative formulation of the interacting semiclassical toy model, the goal is to show that perturbations ψ_1 over (ψ_0, ω) which solve eq. (4.5) decay for large time at linear order in perturbation theory, and for proper choices of the coupling constants of the model. To achieve this result, it is essential to assume compactly-supported initial data on the fields, and to consider perturbations around the background solution which have spatial compact support, in order to avoid the class of exponentially growing solutions discussed in section 4.2.

Before discussing the linearization form of the interacting vacuum polarization, some details on the chosen background solution (ψ_0, ω) should be discussed. For the sake of simplicity, the background ψ_0 can be assumed constant, so that the zeroth-order free vacuum polarization in ω acquires the following constant expectation value

$$\omega(\phi^2) = \left\langle :\phi^2: \right\rangle_\omega^{(\mathrm{bac})} = -\frac{g_1}{\lambda_1}\psi_0, \qquad \psi_0 \in \mathbb{R}. \tag{4.12}$$

In view of the renormalization freedom expressed by the constant c in eq. (4.7), the previous equation is always satisfied on $(\mathcal{M}, \eta_{\mu\nu})$ by choosing a translational invariant state, for any choice of $\psi_0 \in \mathbb{R}$. Besides, a choice of constant background external field ψ_0 implies only a mass renormalization of the quantum field, in the end, that is,

$$m_\lambda^2 \doteq m^2 + \lambda\psi_0 = m^2 - \lambda\frac{\lambda_1}{g_1}\left\langle :\phi^2: \right\rangle_\omega^{(\mathrm{bac})}. \tag{4.13}$$

The constraint $m_\lambda^2 \geq 0$ necessary to obtain a physical reference state always holds for sufficiently small λ_1/g_1, and it holds trivially in the case of vanishing expectation value of the Wick square. Furthermore, a suitable choice of the renormalization constant c in eq. (4.7) allows to set $\left\langle :\phi^2: \right\rangle_\omega^{(\mathrm{bac})} = 0$.

To simply further the analysis, and in view of the above argument, the choice of the Minkowski vacuum state, whose two-point function was given in eq. (1.52), is sufficient to carry out the stability analysis. In the viewpoint of the toy model, the zeroth-order theory chosen in this way corresponds to select Minkowski spacetime as background metric in a realistic semiclassical theory of gravity. However, other choices of quantum states on $(\mathcal{M}, \eta_{\mu\nu})$ such as the KMS thermal state, whose two-point function was given in eq. (1.81), do not alter significantly our analysis. In this last case, the renormalized mass (4.13) is associated to the thermal mass

$$\left\langle :\phi^2: \right\rangle_\beta = \frac{m_\beta^2}{2} \doteq \frac{1}{2\pi^2\beta^2}\mathcal{E}(\beta m), \qquad \mathcal{E}(x) = \int_x^\infty \frac{\sqrt{z^2 - x^2}}{e^z - 1}\mathrm{d}z, \tag{4.14}$$

where $\beta = 1/(k_B T)$ is the inverse of the temperature of the field.

After discussing the zeroth-order contribution, the next step consists of constructing the linearized interacting vacuum polarization entering the semiclassical equation (4.11), using the Bogoliubov map (1.99) and the representation of ϕ^2_{int} given in eq. (1.100) truncated at the linear order. Then, the linearized contribution defined in eq. (4.9) reads in the adiabatic limit $f \to 1$ as

$$\left\langle :\phi^2: \right\rangle_\omega^{(\mathrm{lin})} = -i\hbar\lambda \int_{\mathcal{M}} \left(\Delta_{F,\omega}^2(y - x) - \Delta_{+,\omega}^2(y - x)\right)\psi_1(y)\mathrm{d}y, \tag{4.15}$$

where $\Delta_{F,\omega}(y, x) = \hbar^{-1}\left\langle :T\left(\phi(y)\phi(x)\right):\right\rangle_\omega$ and $\Delta_{+,\omega}(y, x) = \hbar^{-1}\left\langle :\phi(y)\phi(x): \right\rangle_\omega$ are the Feynman propagator and the two-point function associated to ω, respectively. The expectation value given in eq. (4.15) can also be expressed in terms of propagators related to the Minkowski vacuum state, after evaluating

$$\Delta_{F,\omega}^2 - \Delta_{+,\omega}^2 = \Delta_F^2 - \Delta_+^2 + i2\Delta_A W,$$

where $\Delta_F(x,x') = \hbar^{-1}\langle 0|T(\phi(x)\phi(x'))|0\rangle$, $\Delta_+(x,x') = \hbar^{-1}\langle 0|\phi(x)\phi(x')|0\rangle$, Δ_A is the advanced propagator, and $W \doteq \Delta_{+,\omega} - \Delta_+$. A diagrammatic representation of the propagators in the integrand at the right-hand side of eq. (4.15) is given in Figure 4.1.

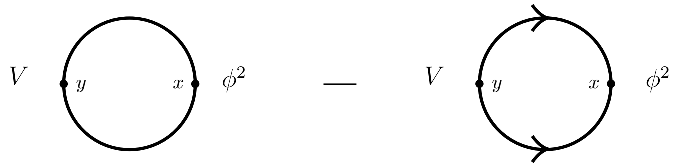

Figure 4.1: Picture of the one-loop contribution $T\left(V\phi^2\right) - V\phi^2$ at the linear order in $\hbar$. The propagator $\Delta_F(y-x)$ is represented by a non-oriented line because it is symmetric in the exchange of $x \leftrightarrow y$, while the two-point function $\Delta_+(y-x)$ by an arrow from y to x [GHP16].

Thus, the right-hand side of eq. (4.15) can be evaluated by using the Källén-Lehmann spectral representations of Δ_+^n and Δ_F^n given in eqs. (1.74) and (1.94), respectively, which yield

$$-i\left(\Delta_F^2(x) - \Delta_+^2(x)\right) = (\Box + a)\int_{4m^2}^{\infty} \mathrm{d}M^2 \frac{\varrho(M^2)}{M^2+a}\Delta_A(x, M^2), \tag{4.16}$$

where

$$\varrho(M^2) = \frac{1}{16\pi^2}\sqrt{1 - \frac{4m^2}{M^2}}$$

is the spectral density given in eq. (1.75) for $n = 2$, the constant $a > -4m^2$ encodes the renormalization freedom present in the construction of $\Delta_F^2(x)$, and $\Delta_A(x, M^2)$ is the advanced propagator of the Klein-Gordon field of mass M. Thus, eq. (4.15) can be written at the linear order outside $x = 0$ as

$$\left\langle :\phi^2: \right\rangle_\omega^{(\mathrm{lin})} = \hbar\lambda\,(\mathcal{K}_a + \mathcal{W})\,(\psi_1), \tag{4.17}$$

and it depends on the operator $\mathcal{K}_a : \mathcal{D}(\mathcal{M}) \to C^\infty(\mathcal{M})$ having regularized integral Kernel

$$\mathcal{K}_a(x-y) \doteq \int_{4m^2}^{\infty} \mathrm{d}M^2 \varrho(M^2)\frac{1}{M^2+a}(\Box + a)\Delta_R(x-y, M^2). \tag{4.18}$$

Here, the d'Alembert operator is taken in the distributional sense as in eq. (4.16). It is essential to stress also that $\mathcal{K}_a(x-y)$ has a retarded internal structure, because it depends on the retarded propagator $\Delta_R(\cdot, M^2)$ associated to the Klein Gordon equation with mass M, whose spatial Fourier Kernel reads as

$$\tilde{\Delta}_R(t, \vec{p}, M^2) = -\frac{\sin(\omega_0 t)}{\omega_0}\Theta(t), \qquad \omega_0 = \sqrt{|\vec{p}|^2 + M^2}, \tag{4.19}$$

cf. eq. (1.42). On the other hand, the integral Kernel of the state-dependent operator $\mathcal{W} : \mathcal{D}(\mathcal{M}) \to C^\infty(\mathcal{M})$ is equal to the pointwise multiplication of the advanced propagator with the smooth part of the two-point function W, i.e., $\mathcal{W} \doteq 2\Delta_A W$.

After choosing the Minkowski vacuum as reference state, both W and $\mathcal{W}$ vanish, because the smooth function $\mathcal{W}_+(x,x')$ obtained in eq. (1.53) and associated to the Minkowski vacuum two-point function vanishes in the coinciding limit. Thus, the linearized expectation value of the Wick square given in eq. (4.17) simplifies as

$$\left\langle :\phi^2: \right\rangle_0^{(\mathrm{lin})} = \hbar\lambda\,\mathcal{K}_a(\psi_1). \tag{4.20}$$

For later purposes, the evolution of $\left\langle :\phi^2: \right\rangle_0^{(\mathrm{lin})}$ in time under the influence of ψ_1 must be taken in control: to this end, the following proposition contains a detailed study of the Kernel given in eq. (4.18) in the Fourier domain.

Proposition 4.2.1. *Let $\psi_1 \in \mathcal{S}(\mathcal{M})$ be a Schwartz function on $\mathcal{M}$, and let $\hat{\psi}_1$ be its Fourier transform. Then the Fourier transform of the linearized expectation value of the Wick square given in eq. (4.20) can be written as*

$$\mathcal{F}\left\{\langle:\phi^2:\rangle_0^{(\mathrm{lin})}\right\}(p_0,\vec{p}) = \lim_{\epsilon\to 0^+} \frac{\lambda\hbar}{16\pi^2} F_a(-(p_0-i\epsilon)^2+|\vec{p}|^2)\hat{\psi}_1(p_0,\vec{p}), \tag{4.21}$$

given for strictly positive mass $m>0$ and for $a>-4m^2$. The function $F_a(z)$ admits the following integral representation:

$$F_a(z) = \int_{4m^2}^{\infty}\sqrt{1-\frac{4m^2}{M^2}}\left(\frac{1}{M^2+a}-\frac{1}{M^2+z}\right)\mathrm{d}M^2, \tag{4.22}$$

and it has the following properties:

a) *$F_a(z)$ is an analytic for $z\in\mathbb{C}\setminus(-\infty,-4m^2]$ and continuous for $z=-4m^2$;*

b) *the domain $F_a(z)$ has a branch cut on $z\in(-\infty,-4m^2)$ because there the imaginary part is discontinuous (the real part is continuous but not differentiable);*

c) *$F_a(a)=0$;*

d) *$F_a(s)$ is real for $s\in\left[-4m^2,\infty\right)$, it is strictly increasing for $s\in\left[-4m^2,\infty\right)$, and it diverges for large $|s|$;*

e) *The imaginary part of F_a admits the following integral representation:*

$$\mathrm{Im}(F_a(z)) = \mathrm{Im}(z)\int_{4m^2}^{\infty}\sqrt{1-\frac{4m^2}{M^2}}\left(\frac{1}{|M^2+z|^2}\right)\mathrm{d}M^2,$$

it is strictly positive for $\mathrm{Im}(z)>0$, and strictly negative for $\mathrm{Im}(z)<0$. Furthermore, it vanishes for $z\in(-4m^2,\infty)$, and it is discontinuous on $z\in(-\infty,-4m^2)$ (the absolute value is finite).

Finally, for $z\notin(-\infty,0)$ and $a>0$, $F_a(z)$ takes the form

$$F_a(z) = 2\sqrt{\frac{z+4m^2}{z}}\log\left(\frac{\sqrt{z+4m^2}+\sqrt{z}}{2m}\right) - 2\sqrt{\frac{a+4m^2}{a}}\log\left(\frac{\sqrt{a+4m^2}+\sqrt{a}}{2m}\right). \tag{4.23}$$

The qualitative behaviour of $\mathrm{Re}(F_a(z))$ and of $|\mathrm{Im}(F_a(z))|$ for $z\in(-4m^2,\infty)$ is plotted in Figure 4.2.

Proof. Using the definition of $\mathcal{K}_a$ in eq. (4.18) and the Fourier transform of the distribution Δ_R given in eq. (1.41), then taking the Fourier transform on both sides of eq. (4.20), and eventually applying the convolution theorem to $\mathcal{K}_a(\psi_1)$, the Fourier transform of the interacting vacuum polarization yields

$$\mathcal{F}\left\{\langle:\phi^2:\rangle_0^{(\mathrm{lin})}\right\}(p_0,\vec{p}) = \lim_{\epsilon\to 0^+}\lambda\hbar\int_{4m^2}^{\infty}\mathrm{d}M^2\varrho_2(M^2)\frac{1}{M^2+a}\frac{1}{-(p_0-i\epsilon)^2+|\vec{p}|^2+M^2}\left(-p_0^2+|\vec{p}|^2-a\right)\hat{\psi}(p_0,\vec{p}),$$

where $\hat{\psi}_1(p_0,\vec{p})\in\mathcal{S}(\mathcal{M})$. Then, the first part of the thesis follows after recalling the form of $\varrho_2(M^2)=\frac{1}{16\pi^2}\sqrt{1-\frac{4m^2}{M^2}}$ and the definition of $F_a(z)$.

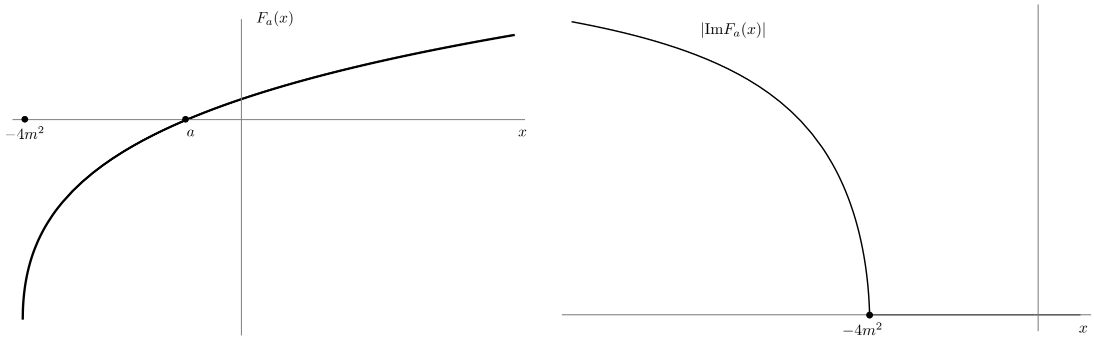

Figure 4.2: The first graph contains the qualitative behaviours of $F_a(x)$ for $x \in (-4m^2, \infty)$ with $-4m^2 < a < 0$. The second graph is the qualitative behavior of $|\mathrm{Im}F_a(x)|$.

The list of properties of $F_a(z)$ can be inferred directly from its integral representation. To check the validity of the representation of $F_a(z)$ given in eq. (4.23), consider

$$A_a(z) \doteq \frac{1}{a-z}\left(2\sqrt{\frac{z+4m^2}{z}}\log\left(\frac{\sqrt{z+4m^2}+\sqrt{z}}{2m}\right) - 2\sqrt{\frac{a+4m^2}{a}}\log\left(\frac{\sqrt{a+4m^2}+\sqrt{a}}{2m}\right)\right).$$

From the expression of F_a given in eq. (4.23), $F_a(-p_0^2+|\vec{p}|^2) = (p_0^2-|\vec{p}|^2+a)A_a(-p_0^2+|\vec{p}|^2)$. Then, take inverse Fourier transform in time of $A_a(-p_0^2+|\vec{p}|^2)$, that is,

$$\tilde{\mathcal{A}}(t,\vec{p}) \doteq \lim_{\epsilon\to 0^+}\frac{1}{2\pi}\int_{-\infty}^{\infty} A(-(p_0-i\epsilon)^2+|\vec{p}|^2)\mathrm{e}^{ip_0t}\mathrm{d}p_0.$$

The integrand in $\tilde{\mathcal{A}}$ has two branch cuts for $(p_0-i\epsilon)^2 > (|\vec{p}|^2+4m^2)$ located in the upper half complex plane and it is analytic outside the two branch cuts (it has no poles); furthermore, $|A(-(w-i\epsilon)^2+|\vec{p}|^2)|$ for $w\in\mathbb{C}$ vanishes in the limit $|w|\to\infty$. Hence, that inverse Fourier transform can be obtained by standard results of complex analysis, such as Cauchy residue theorem and Jordan's lemma. In particular, as $A(-(w-i\epsilon)^2+|\vec{p}|^2)$ is analytic in the lower half plane, $\tilde{\mathcal{A}}=0$ for $t<0$. If $t>0$, only the two branch cuts matter in the evaluation of the integral over the real line which gives $\tilde{\mathcal{A}}$. So, the contributions due to the two branch cuts for $t>0$ can be combined to give

$$\tilde{\mathcal{A}}(t,\vec{p}) = \lim_{\epsilon\to 0^+}\frac{1}{2\pi}\int_{\sqrt{|\vec{p}|^2+4m^2}}^{\infty}\left(A(-w^2+|\vec{p}|^2+i\epsilon)-A(-w^2+|\vec{p}|^2-i\epsilon)\right)\left(\mathrm{e}^{iwt}-\mathrm{e}^{-iwt}\right)\mathrm{d}w.$$

Changing variable of integration to $M^2 = w^2-|\vec{p}|^2$ and computing the discontinuity of the function

$$\mathfrak{L}(z) \doteq \log\left(\frac{\sqrt{z+4m^2}+\sqrt{z}}{2m}\right)$$

along its cut, which reads

$$\lim_{\epsilon\to 0^+}\mathfrak{L}(x+i\epsilon)-\mathfrak{L}(x-i\epsilon) = i\pi, \tag{4.24}$$

one obtains for $t>0$ that

$$\tilde{\mathcal{A}}(t,\vec{p}) = \frac{i2\pi}{2\pi}\int_{4m^2}^{\infty}\frac{1}{M^2+a}\left(\sqrt{1-\frac{4m^2}{M^2}}\right)\frac{\left(e^{i\omega_0t}-e^{-i\omega_0t}\right)}{2\omega_0}\mathrm{d}M^2,$$

where $\omega_0 = \sqrt{|\vec{p}|^2 + M^2}$. So

$$\mathcal{A}(x) = \int_{4m^2}^{\infty} \frac{1}{M^2 + a} \left(\sqrt{1 - \frac{4m^2}{M^2}} \right) \Delta_R(x, M^2) \mathrm{d}M^2,$$

and hence $(\Box + a)\mathcal{A}$ is equal to $\mathcal{K}_a$ up to a factor given in eq. (4.18). Therefore, the expression of $F_a(z)$ given in eq. (4.22) follows, thus proving that it coincides with eq. (4.23). $\square$

Remark 4.2.1. In the limit of vanishing mass $m^2 = 0$ and for $-p_0^2 + |\vec{p}|^2 > 0$, the function $F_a(-p_0^2 + |\vec{p}|^2)$ given in eq. (4.22) reduces to

$$F_a(-p_0^2 + |\vec{p}|^2) = \log\left(\frac{-p_0^2 + |\vec{p}|^2}{a} \right). \tag{4.25}$$

This logarithmic behaviour is similar to the case studied in [Hor80] for the linearized semiclassical Einstein equations in the weak-field limit of gravity, after considering massless quantum fields (see also [HH81; FW96]).

4.2.3 Stability of linearized solutions

Evaluating the linearized semiclassical equation (4.11) yields

$$(g_2\Box - g_1)\psi_1(x) = (\lambda_1 - \lambda_2\Box) \left\langle :\phi^2: \right\rangle_0^{(\mathrm{lin})}(x), \tag{4.26}$$

where the non-local state-dependent contribution $\left\langle :\phi^2: \right\rangle_0^{(\mathrm{lin})}$ defined in eq. (4.20) was constructed in terms of the linear operator $\mathcal{K}_a$ introduced in eq. (4.20), and it was studied in proposition 4.2.1 in momentum space.

Eq. (4.26) is a linear equation in the perturbation field ψ_1, whose character depends strictly on the parameters $(a, g_1, g_2, \lambda, \lambda_1, \lambda_2)$. To highlight its mathematical structure, it can be also rewritten in the following form:

$$\hbar\lambda P_\lambda \mathcal{K}_a(\psi_1)(x) + P_g\psi_1(x) = 0, \tag{4.27}$$

where $P_\lambda \doteq \lambda_2\Box - \lambda_1$, and $P_g \doteq g_2\Box - g_1$.

Because of the presence of a second d'Alembert operator, which appears inside $\left\langle :\phi^2: \right\rangle_0^{(\mathrm{lin})}$ through eq. (4.18), eq. (4.26) contains fourth-order derivatives in ψ_1. Thus, it is similar to the semiclassical equations which usually appear in semiclassical theories of gravity, and it manifests the same conceptual issues already known in Semiclassical Gravity as higher-order theory of gravity, see section 4.1 and subsection 4.2.4.

Instead of analyzing eq. (4.27) directly, it is convenient to study the corresponding linear equation equipped with a compactly-supported smooth source term, namely

$$\hbar\lambda P_\lambda \mathcal{K}_a(\psi_1)(x) + P_g\psi_1(x) = f(x), \tag{4.28}$$

where $\mathcal{K}_a$ is the linear operator introduced in eq. (4.17), and $f \in \mathcal{D}(\mathcal{M})$.

The strategy of this section is as follows. In a first step, it shall be shown that this equation manifests an hyperbolic nature, and its retarded fundamental solutions shall be constructed as an operator $D_R : C_0^\infty(\mathcal{M}) \to C^\infty(\mathcal{M})$, in analogy with the fundamental solutions of the Klein-Gordon operator P - *cf.* subsection 1.2.1. Then, it shall be proved that past compact solutions of the form $\psi_1 = D_R(f)$ decay as $1/t^{3/2}$ for large times t thanks to the regularity properties of D_R, hence getting the stability of the corresponding backgrounds against perturbation sourced by f.

Afterwards, in a second step, smooth spatially compact solutions of the homogeneous equation (4.27) shall be studied, in order to obtain the corresponding solutions of eq. (4.11). To determine uniquely a solution in the future and in the past of t_0, eq. (4.27) shall be equipped with suitable initial conditions at $t_0 = 0$, i.e., smooth compactly-supported initial data of the form

$$\psi_1^{(j)}(0, \vec{x}) = \varphi^j(\vec{x})$$

for $j \in \{0{,}1\}$ or $j \in \{0{,}1{,}2{,}3\}$, with $\varphi^j \in \mathcal{D}(\mathbb{R}^3)$. It shall be proved that the number of initial conditions necessary to determine a spatially compact solution depends on the choice of the parameters: in some cases, four initial conditions have to be imposed, while, in other cases, only two initial conditions are sufficient to obtain a solution. Finally, there are also cases where no solution exists. Eventually, it shall be shown that there exist wide ranges of values of $(a, g_1, g_2, \lambda, \lambda_1, \lambda_2)$ such that solutions of eq. (4.27) with compactly-supported initial data decay faster than $1/t^{3/2}$ for large times. Therefore, the stability of the linearized back-reacted system can be restored even in this case.

The first step consists of showing that eq. (4.26) manifests an hyperbolic nature once it is written as eq. (4.27), because past compact solutions of eq. (4.28) respect causality. This result is achieved in the following proposition.

Proposition 4.2.2. *Consider the equation* (4.28) *sourced by* $f \in \mathcal{D}(\mathcal{M})$ *in the form*

$$\hbar\lambda P_\lambda \mathcal{K}_a(\psi_1)(x) + P_g\psi_1(x) = f(x).$$

Set $\lambda_2 \neq 0$ *and* $g_2 \neq 0$. *Let* ψ_1 *be a past compact solution of eq.* (4.28)*, then*

$$\psi_1 = \Delta_{R,\lambda} f - \hbar\lambda\mathcal{K}_a(\psi_1) - \Delta_{R,\lambda}(P_g - P_\lambda)\psi_1 \tag{4.29}$$

where $\Delta_{R,\lambda}$ *is the retarded fundamental solution of* $P_\lambda \Delta_{R,\lambda} = \mathbb{I}$. *Moreover,* ψ_1 *respects causality, namely* $supp\psi_1 \subset J^+(suppf)$.

Proof. Assuming a past compact solution ψ_1 by hypothesis, the retarded operator associated to P_λ applied on both sides of eq. (4.28) yields

$$\hbar\lambda\mathcal{K}_a(\psi_1) + \Delta_{R,\lambda} P_g \psi_1 = \Delta_{R,\lambda} f.$$

Using the definition of fundamental solution $(\Delta_{R,\lambda} \circ P_\lambda)\psi_1 = \psi_1$, this equation can be written also as

$$\hbar\lambda\mathcal{K}_a(\psi_1) + \Delta_{R,\lambda}(P_g - P_\lambda)\psi_1 + \psi_1 = \Delta_{R,\lambda} f,$$

and hence as

$$\psi_1 = \Delta_{R,\lambda} f - \hbar\lambda\mathcal{K}_a(\psi_1) - \Delta_{R,\lambda}(P_g - P_\lambda)\psi_1,$$

thus yielding eq. (4.29). Notice that both $\Delta_{R,\lambda}$ and $\Delta_{R,\lambda}(P_g - P_\lambda)$ have the retarded property, i.e., $\text{supp}(\Delta_{R,\lambda} f) \subset J^+(\text{supp} f)$ and $\text{supp}(\Delta_{R,\lambda}(P_g - P_\lambda) f) \subset J^+(\text{supp} f)$. Similarly, $\mathcal{K}_a$ satisfies also the retarded property, because it is an integral of retarded operators by construction. So, the form of every solution ψ_1 cannot be influenced by any modification of ψ_1 or f outside of $J^-(x)$.

To prove that $\psi_1(x) = 0$ for $x \notin J^+(\text{supp} f)$, eq. (4.29) can be iterated to write the solution ψ_1 as

$$\psi_1 = \sum_{n \geq 0} \psi_{1,n},$$

where $\psi_{1,0} = \Delta_{R,\lambda} f$, and $\psi_{1,n+1} \doteq \lambda\mathcal{K}_a(\psi_{1_n}) - \Delta_{R,\lambda}(P_g - P_\lambda)\psi_{1,n} = \mathcal{O}(\psi_{1,n})$. Hence,

$$\psi_1 = \sum_{n \geq 0} \mathcal{O}^n(\Delta_{R,\lambda} f).$$

If $\text{supp} f \cap J^-(x) = \emptyset$, each term in the series used to compute $\psi_1(x)$ vanishes, and hence the series converges to $\psi_1(x) = 0$. ☐

The constraints on the parameters λ_2 and g_2 given by hypothesis in proposition 4.2.2 can be easily removed adapting the first part of the proof. For example, if $g_2 = 0$, there is no need to add $P_\lambda \Delta_{R,\lambda}$ in the right hand side of eq. (4.29). On the other hand, if $\lambda_2 = 0$, then the proof starts with getting an analogous of eq. (4.29) after applying the retarded operator $\Delta_{R,g}$ at the place of $\Delta_{R,\lambda}$ on both sides of eq. (4.28). Finally, if both $\lambda_2 = 0$ and g_2 vanish, then there is no need of applying any retarded operator to eq. (4.28).

The analysis proceeds with studying the retarded fundamental solution of eq. (4.28), in order to understand the form of its solutions. From the results of proposition 4.2.2, which states that past compact solutions of (4.28) are causal, the analysis of fundamental solutions can be performed in the Fourier domain, because the spatial Fourier transform can be always applied on compactly-supported functions. Hence,

$$-\left((\lambda_1 + \lambda_2(-p_0^2 + |\vec{p}|^2))\frac{\lambda\hbar}{16\pi^2}F_a(-(p_0 - i0^+)^2 + |\vec{p}|^2) + g_2(-p_0^2 + |\vec{p}|^2) + g_1\right)\hat{\psi}(p_0,\vec{p}) = \hat{f}(p_0,\vec{p}), \tag{4.30}$$

where $f \in \mathcal{D}(\mathcal{M})$. Eq. (4.28) can be equivalently written in a more compact form as

$$S(-(p_0 - i0^+)^2 + |\vec{p}|^2)\hat{\psi}(p_0,\vec{p}) = \hat{f}(p_0,\vec{p}),$$

where

$$S(z) \doteq -(\lambda_1 + \lambda_2 z)\frac{\lambda\hbar}{16\pi^2}F_a(z) - (g_1 + g_2 z). \tag{4.31}$$

In order to obtain the retarded fundamental solutions associated to the Kernel $S(z)$, one needs preliminarily the set of points in the complex plain in which $S(z)$ vanishes. Denoting this set by $\mathcal{S}$, then the characterization of elements in $\mathcal{S}$ can be obtained by setting some conditions on the parameters $(a, g_1, g_2, \lambda, \lambda_1, \lambda_2)$, such that this set contains only real elements, and, furthermore, it includes only negative elements in further special cases. Notably, the following constraint shall be imposed on the parameters:

$$g_2\lambda_1 - \lambda_2 g_1 \geq 0. \tag{4.32}$$

This characterization is studied in the following proposition.

Proposition 4.2.3. *Let $\mathcal{S} \subset \mathbb{C}$ be set of zeros of $S(z)$ given in eq. (4.31). Fix the parameters in such a way that $g_2\lambda_1 - \lambda_2 g_1 \geq 0$, $\lambda > 0$, $-4m^2 < a$. Then, two cases are distinguishable:*

- *a) if $\lambda_2 \neq 0$, $g_2\lambda_1/\lambda_2 = -g_1$, and $\lambda_1/\lambda_2 \leq 4m^2$, then $\mathcal{S} \subset (-4m^2, \infty) \cup \{-\lambda_1/\lambda_2\} \subset \mathbb{C}$;*
- *b) $\mathcal{S} \subset (-4m^2, \infty) \subset \mathbb{R} \subset \mathbb{C}$ otherwise.*

Furthermore, $\mathcal{S}$ contains one, two or no elements depending on the parameters $(a, g_1, g_2, \lambda, \lambda_1, \lambda_2)$.

Proof. Consider the equation $S(z) = 0$ written in the following form:

$$(\lambda_1 + \lambda_2 z)\frac{\lambda\hbar}{16\pi^2}F_a(z) = -(g_1 + g_2 z). \tag{4.33}$$

To prove that the solution set is of the form stated in item a) and b), the proof proceeds as follows. After multiplying both sides of the equation by $(\lambda_1 + \lambda_2\overline{z})$, taking the imaginary part yields the following equation:

$$|\lambda_1 + \lambda_2 z|^2 \mathrm{Im}\left(\frac{\lambda\hbar}{16\pi^2}F_a(z)\right) = -(g_2\lambda_1 - \lambda_2 g_1)\mathrm{Im}(z),$$

where the global sign of right-hand side depends only on $\mathrm{Im}(z)$, because the inequality (4.32) holds by hypothesis. In particular, for strictly positive $\mathrm{Im}(z)$ the right-hand side is negative, while the left-hand side is strictly positive thanks to item e) of proposition 4.2.1. Similarly, for strictly negative $\mathrm{Im}(z)$ the right-hand side is positive, while the left-hand side is strictly negative.

Moreover, as $\mathrm{Im}(F_a(x))$ is not 0 also for $x < -4m^2$ (see Figure 4.2), the only possible solutions of eq. (4.33) need to be searched within $(-4m^2, \infty) \cup \{-\lambda_1/\lambda_2\}$, when $\lambda_2 \neq 0$, or in $(-4m^2, \infty)$, otherwise. Furthermore, if both $\lambda_2 \neq 0$ and $z = -\lambda_1/\lambda_2 \leq -4m^2$, then the left-hand side of eq. (4.33) vanishes, whereas the right hand side vanishes only when $g_2\lambda_1/\lambda_2 = -g_1$.

Solved the imaginary equation, the analysis is reduced to study the following real equation:

$$(\lambda_1 + \lambda_2 s)\frac{\lambda\hbar}{16\pi^2}F_a(s) = -(g_1 + g_2 s), \qquad s \in (-4m^2, \infty) \cup \{-\lambda_1/\lambda_2\}. \tag{4.34}$$

The properties of the function $F_a(s)$ for $s \in (-4m^2, \infty) \subset \mathbb{R}$ are listed in proposition 4.2.1, and the plot of this function is reported in Fig 4.2. So, depending on the choice of parameters, there are cases where either one or two positive solutions of this equation exist, and there are cases where only one or two negative solutions exist. It is also possible to find cases where one positive and one negative solution exists. Finally, there are cases where no solutions exists at all. □

Taking into account all the previous statements, the explicit form of the retarded fundamental solution of eq. (4.28) can be now obtained, and hence the main result of the section holds, that is, past compact solutions decay to zero for sufficiently large times, as expected for a perturbation over a stable background.

Theorem 4.2.1. *Consider the semiclassical equation with a source term $f \in C_0^\infty(\mathcal{M})$ given in eq. (4.28) in the form*

$$\hbar\lambda P_\lambda \mathcal{K}_a(\psi_1)(x) + P_g\psi_1(x) = f(x).$$

Fix as non-vanishing constants at least one of the two g_i, and at least one of the λ_i, assume that the inequality $g_2\lambda_1 - \lambda_2 g_1 \geq 0$ holds, and set $-4m^2 < a < 0$. Suppose that the set $\mathcal{S}$ defined in proposition 4.2.3 contains only real negative elements. Then, the Fourier transform of the retarded fundamental solution D_R of eq. (4.28) reads

$$\hat{D}_R(p_0, \mathbf{p}) = \frac{1}{S(-(p_0 - i0^+)^2 + |\mathbf{p}|^2)},$$

where $S(z)$ was defined in eq. (4.31). Hence,

$$D_R(x) = -\sum_{s\in\mathcal{S}} \frac{1}{S'(s)}\Delta_R(x,s) - \frac{\lambda\hbar}{16\pi^2}\int_{4m^2}^{\infty}\sqrt{1-\frac{4m^2}{M^2}}\frac{(\lambda_2 M^2 - \lambda_1)}{|S(-M)|^2}\Delta_R(x, M^2)\mathrm{d}M^2, \tag{4.35}$$

where the elements of $\mathcal{S}$ are the zeros of $S(s)$, with $s \in (-4m^2, \infty) \cup \{-\lambda_1/\lambda_2\}$. The retarded fundamental solution D_R is a linear operator which maps smooth compactly-supported functions to smooth functions, and each solution ψ_1 of eq. (4.28) with past compact support can be expressed as

$$\psi_1 = D_R(f). \tag{4.36}$$

Thus, $\psi_1(t, \vec{x})$ decays as $1/t^{3/2}$ for large t for $\lambda_2 \neq 0$.

Proof. Having established the causal property of past compact solutions in proposition 4.2.2, it convenient to analyze eq. (4.28) in the Fourier domain. Using the results given in proposition 4.2.1, it reads

$$S(-(p_0 - i0^+)^2 + |\vec{p}|^2)\hat{\psi}(p_0, \vec{p}) = \hat{f}(p_0, \vec{p}),$$

where the multiplicative operator S was defined in eq. (4.31). Thus, the Fourier transform of the retarded operator D_R yields

$$\hat{D}_R(p_0, \vec{p}) = \frac{1}{S(-(p_0 - i0^+)^2 + |\vec{p}|^2)}, \tag{4.37}$$

and hence its Fourier inverse transform

$$\tilde{D}_R(t, \mathbf{p}) = \lim_{\epsilon \to 0^+} \lim_{R \to \infty} \frac{1}{2\pi} \int_{-R}^{R} \frac{1}{S(-(z - i\epsilon)^2 + |\mathbf{p}|^2)} \mathrm{e}^{itz} \mathrm{d}z$$

can be evaluated by means of standard methods of complex analysis. In view of the properties of the function $F_a(z)$ given in eq. (4.22), the function $h(z) \doteq 1/S(-(z - i\epsilon)^2 + |\vec{p}|^2)$ is defined in $\mathbb{C} \setminus \{\{z - i\epsilon \leq -\sqrt{|\mathbf{p}|^2 + 4m^2}\} \cup \{z - i\epsilon \geq \sqrt{|\mathbf{p}|^2 + 4m^2}\}\}$. For $|z| > R$, it holds that $|h(z)| < l(|z|)$, where the function $l(r)$ vanishes in the limit of large positive r, because, in the worse case, $1/S(-z^2 + |\mathbf{p}|^2)$ is dominated by $c/F_a(-z^2 + |\mathbf{p}|^2)$ for large $|z|$, for some constant c, and $|F_a(-z^2 + |\mathbf{p}|^2)|$ grows as $\log|z|$ for large $|z|$. Therefore, the contour γ can be closed in the upper or lower plane, according to the sign of t, with a semicircle which does not contribute to the integral in the limit $R \to \infty$.

The function $1/S(-(z - i\epsilon)^2 + |\mathbf{p}|^2)$ has two poles for each zero s of S. Assuming negative $s \in \mathcal{S}$ by hypothesis, then the poles are located on the line $\mathrm{Im}(z) = i\epsilon$, and correspond to the complex numbers

$$z = i\epsilon \pm \sqrt{|\mathbf{p}| - s}.$$

Furthermore, the function $1/S(-(z - i\epsilon)^2 + |\mathbf{p}|^2)$ has two branch cuts located at $z = x + i\epsilon$, where $x^2 \geq |\vec{p}|^2 + 4m^2$. Thus, $1/S$ is analytic in the lower half plane, and hence $\tilde{D}_R = 0$, after closing the contour in the lower half plane for $t < 0$.

On the other hand, if $t > 0$, then the contour γ is closed in the upper half plane, and hence the contributions due to both the poles and the branch cuts need to be taken into account. In this case, after deforming the previous contour γ to a new $\tilde{\gamma}$ in such a way to avoid both the poles and the branch cuts, then the result of the contour integral over $\tilde{\gamma}$ vanishes. Therefore, the only two non-vanishing contributions in $\tilde{D}_R$, denoted by $\tilde{O}$ and $\tilde{C}$, are due to the poles and the branch cuts, respectively.

The contribution due to the poles can be directly evaluated using the Cauchy residue theorem, which yields

$$\tilde{O}(t, \vec{p}) = -\frac{2\pi i}{2\pi} \sum_{s \in \mathcal{S}} \frac{1}{S'(s)} \left(\frac{\mathrm{e}^{iw_s t} - \mathrm{e}^{-iw_s t}}{2w_s} \right) = \sum_{s \in \mathcal{S}} \frac{1}{S'(s)} \frac{\sin(w_s t)}{w_s},$$

where $w_s \doteq \sqrt{|\vec{p}|^2 - s}$. Hence, in view of eq. (4.19),

$$O(x) = -\sum_{s \in \mathcal{S}} \frac{1}{S'(s)} \Delta_R(x, s). \tag{4.38}$$

The contribution due to the branch cuts can be combined in the following form

$$\tilde{C}(t, \vec{p}) = \lim_{\epsilon \to 0^+} \frac{1}{2\pi} \int_{\sqrt{|\vec{p}|^2 + 4m^2}}^{\infty} \left[\frac{1}{S(-p_0^2 + |\vec{p}|^2 + i\epsilon)} - \frac{1}{S(-p_0^2 + |\vec{p}|^2 - i\epsilon)} \right] \left(e^{ip_0 t} - e^{-ip_0 t} \right) \mathrm{d}p_0.$$

Thus, recalling eq. (4.19) again, it can be written in the position domain as

$$C(x) = \lim_{\epsilon \to 0^+} \frac{-i}{2\pi} \int_{4m^2}^{\infty} \left[\frac{1}{S(-M^2 + i\epsilon)} - \frac{1}{S(-M^2 - i\epsilon)} \right] \Delta_R(x, M^2) \mathrm{d}M^2.$$

The discontinuity in the two branch cuts is only due to the imaginary part of $F_a(z)$ - *cf.* eq. (4.24). So,

$$C(x) = -\frac{\lambda\hbar}{16\pi^2} \int_{4m^2}^{\infty} \sqrt{1 - \frac{4m^2}{M^2}} \frac{(\lambda_2 M^2 - \lambda_1)}{|(\lambda_2 M^2 - \lambda_1) \frac{\lambda\hbar}{16\pi^2} F_a(-M^2) + (g_2 M^2 - g_1)|^2} \Delta_R(x, M^2) \mathrm{d}M^2, \tag{4.39}$$

thus getting eq. (4.35) by combining eqs. (4.38) and (4.39). Note that the integral over M^2 in eq. (4.39) can be always performed, even when both λ_2 and g_2 vanish, because $\hat{\Delta}_R$ and $1/|F_a(-M)|^2$ decay as $1/M^2$ and $1/|\log(M)|^2$ for large M, respectively.

Finally, the decay of $\psi_1 = D_R(f)$ for large t descends straightforwardly from lemma C.3.1 applied to $D_R(f)$, which implies that $\Delta_R(f,-s)$ decays as $1/t^{3/2}$ for large t, with $s \leq 0$. Therefore, the contribution $O(f)$ due the poles given in eq. (4.38) has the desired time decay property. The same results holds also for the contribution $C(f)$ due to the branch cuts given in eq. (4.39), because for $\lambda_2 \neq 0$ the function $M^2/|S(-M^2)|$ is integrable in $\mathrm{d}M^2$, and, furthermore, f is smooth and compactly-supported in time, so its time Fourier transform is a Schwartz function. □

Remark 4.2.2. From the form of the Kernel of D_R obtained in eq. (4.35), a generic past compact solution $\psi_1 = D_R(f)$ defined in eq. (4.36) can be decomposed into two parts:

$$\psi_1(x) = \psi_1^O(x) + \psi_1^C(x),$$

where $\psi_1^O = -\sum_{s\in\mathcal{S}} \frac{1}{S'(s)}\Delta_R(f,s)$ denotes the contribution due to the poles of $1/S$, while ψ_1^C is the contribution due the branch cuts. Actually, while there is a chance to determine ψ_1^O by means of a finite number of initial conditions given at some time t_1 in the future of supp$f$, it is expected that ψ_1^C cannot be determined by a finite number of initial conditions, because the integration of M^2 is over uncountably many points.

In spite of this fact, the homogeneous equation (4.27) may still, in some cases, give origin to a well-posed initial-value problem, in which unique spatially compact solutions can be found. In fact, the contribution due the branch cuts cannot enter the construction of the solutions of the homogeneous equation on the whole space, because the Kernel of the multiplicative operator T, which acts on $\mathcal{S}(\mathbb{R}^4)$ and is defined as

$$T(z) \doteq \frac{S(z)}{\prod_{s\in\mathcal{S}}(z-s)}, \qquad z = -(p_0 - i\epsilon)^2 + |\vec{p}|^2, \tag{4.40}$$

does not contain non-vanishing elements. Thus, $T(z)$ is invertible, and hence it disappears from the equation $S(z)\hat{\psi}_1 = 0$. Therefore, only contributions due to the poles can give origin to non-trivial solutions of the homogeneous equation (4.27).

Remark 4.2.3. The decay rate of the smooth past compact solutions ψ_1 proved in theorem 4.2.1 is the same which was obtained by means of Strichartz estimates for real, massive quantum scalar fields in four-dimensional Minkowski spacetime [Str77][2]. Actually, this behaviour is justified by the form of the fourth-order differential equation (4.28), which is composed of massive Klein-Gordon like operators on $(\mathcal{M}, \eta_{\mu\nu})$. Thus, the fundamental solutions are still a combination of Klein-Gordon like fundamental solutions, and hence the past compact solutions given in eq. (4.36) inherit the same late-time behaviour estimated for real Klein-Gordon fields.

Eventually, solutions of the linearized semiclassical equation without source (4.28) can be discussed according to the previous results on past compactly-supported solutions.

Theorem 4.2.2. *Consider the semiclassical equation* (4.26) *written as*

$$(g_2\Box - g_1)\psi_1(x) = (\lambda_1 - \lambda_2\Box)\left\langle :\phi^2: \right\rangle_0^{(\mathrm{lin})}(x).$$

Fix as non-vanishing constants at least one of the two parameters g_1, g_2, and at least one of the two couplings λ_1, λ_2. Assume that the inequality $g_2\lambda_1 - \lambda_2 g_1 \geq 0$ holds, and set $-4m^2 < a < 0$.

[2] The author would thank C. Dappiaggi for indicating him this reference.

Let $\mathcal{S} \subset (-4m^2, \infty) \cup \{-\lambda_1/\lambda_2\} \subset \mathbb{R}$ be the set of zeros of $S(z)$ given in eq. (4.31). As discussed in proposition 4.2.3, $\mathcal{S}$ contains one, two or no elements depending on the parameters $(a, g_1, g_2, \lambda, \lambda_1, \lambda_2)$. If $\mathcal{S} = \emptyset$, then eq. (4.26) admits no solutions. If $\mathcal{S} \neq \emptyset$, then the spatial Fourier transform of a smooth solution $\psi_1(t, \vec{x})$ of eq. (4.26) with spatial compact support is of the form

$$\tilde{\psi}_1(t, \vec{p}) = \sum_{s\in\mathcal{S}} \left(C_+^s(\vec{p})\mathrm{e}^{+it\sqrt{|\vec{p}|^2-s}} + C_-^s(\vec{p})\mathrm{e}^{-it\sqrt{|\vec{p}|^2-s}} \right).$$

Moreover, if $\mathcal{S}$ contains only negative elements, then each solution ψ_1 of eq. (4.26) is uniquely fixed by the initial values at $t = 0$, namely

$$\psi_1^{(j)}(0, \vec{x}) = \varphi^j(\vec{x}), \qquad j \in \{0, \dots, 2|\mathcal{S}|\},$$

where $|\mathcal{S}|$ is the cardinality of $\mathcal{S}$, and $\varphi^j \in C_0^\infty(\mathbb{R}^3)$. Finally, $\psi_1(t, \vec{x})$ decays for large time at least as $1/t^{3/2}$ in this case.

Proof. Eq. (4.26) can be analyzed in the Fourier domain, as before. Using the results given in proposition 4.2.1, it reads

$$\left((\lambda_1 + \lambda_2(-p_0^2 + |\vec{p}|^2)) \frac{\lambda\hbar}{16\pi^2} F_a(-(p_0 - i0^+)^2 + |\vec{p}|^2) + (g_2(-p_0^2 + |\vec{p}|^2) + g_1) \right) \hat{\psi}_1(p_0, \vec{p}) = 0. \tag{4.41}$$

Let $\tilde{\psi}(t, \vec{p})$ be the spatial Fourier transform of a generic solution $\psi_1(t, \vec{x})$ of the form given in eq. (4.36). Then, it is a linear combination of $\mathrm{e}^{ip_0^j t}$ with $z = -{p_0^j}^2 + |\vec{p}|^2 \in \mathcal{S}$, where $\mathcal{S}$ is the set of points of the complex plain in which the function S given in eq. (4.31) vanishes, namely in which eq. (4.33) holds. Moreover, according to proposition 4.2.3, $\mathcal{S}$ must be contained either in $(-4m^2, \infty) \subset \mathbb{C}$, or in $(-4m^2, \infty) \cup \{-\lambda_1/\lambda_2\} \subset \mathbb{C}$ for $\lambda_2 \neq 0$, $g_2\lambda_1/\lambda_2 = -g_1$, and $\lambda_1/\lambda_2 \leq 4m^2$.

According to the number of negative solutions of eq. (4.26), the explicit form of $\psi_1(t, \vec{x})$ reads as follows. If $\mathcal{S}$ contains only one negative solution $x = -\tilde{n}$, with $\tilde{n} \geq 0$, then any solution $\psi_1(t, \vec{x})$ having smooth compactly-supported initial data at $t = 0$ is of the form

$$\psi_1(t, \vec{x}) = \int_{\mathbb{R}^3} \left(C_+(\vec{p})\mathrm{e}^{iw_{\tilde{n}}t} + C_-(\vec{p})\mathrm{e}^{-iw_{\tilde{n}}t} \right) \mathrm{e}^{i\vec{p}\cdot\vec{x}} \mathrm{d}\vec{p},$$

where $w_{\tilde{n}}(\vec{p}) = \sqrt{|\vec{p}|^2 + \tilde{n}}$, and $C_\pm$ are obtained from $(\hat{\varphi}^0(\vec{p}), \hat{\varphi}^1(\vec{p}))$ by solving

$$\begin{pmatrix} \hat{\varphi}^0 \\ \hat{\varphi}^1 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ iw_{\tilde{n}} & -iw_{\tilde{n}} \end{pmatrix} \begin{pmatrix} C_+ \\ C_- \end{pmatrix},$$

which yields

$$\begin{pmatrix} C_+ \\ C_- \end{pmatrix} = \frac{i}{2w_{\tilde{n}}} \begin{pmatrix} -iw_{\tilde{n}} & -1 \\ -iw_{\tilde{n}} & 1 \end{pmatrix} \begin{pmatrix} \hat{\varphi}^0 \\ \hat{\varphi}^1 \end{pmatrix},$$

namely

$$C_+(\vec{p}) = \hat{\varphi}^0(\vec{p}) - \frac{i}{2w_{\tilde{n}}}\hat{\varphi}^1(\vec{p}), \qquad C_-(\vec{p}) = \hat{\varphi}^0(\vec{p}) + \frac{i}{2w_{\tilde{n}}}\hat{\varphi}^1(\vec{p}).$$

Thus, the desired decay of $\psi(t, \vec{x})$ for large t follows from lemma C.3.1.

On the contrary, if $\mathcal{S}$ contains only two distinct negative elements, then four initial data are needed to fix any solution $\psi_1(t, \vec{x})$. Denoting with $s_1 = -n_1$ and $s_2 = -n_2$ the two distinct elements of $\mathcal{S}$, with $n_i \geq 0$, the linearized solution of the semiclassical equation (4.26) is a combination of two solutions of the Klein Gordon equation with different square masses n_i. In this case, the solution $\psi_1(t,\vec{x})$ with smooth compactly-supported initial data $(\varphi^0(\vec{x}),\varphi^1(\vec{x}),\varphi^2(\vec{x}),\varphi^3(\vec{x}))$ at $t=0$ is of the form

$$\psi_1(t,\vec{x}) = \int_{\mathbb{R}^3}\left(C^1_+(\vec{p})\mathrm{e}^{iw_1 t} + C^1_-(\vec{p})\mathrm{e}^{-iw_1 t}\right)\mathrm{e}^{i\vec{p}\cdot\vec{x}}\mathrm{d}\vec{p} + \int_{\mathbb{R}^3}\left(C^2_+(\vec{p})\mathrm{e}^{iw_2 t} + C^2_-(\vec{p})\mathrm{e}^{-iw_2 t}\right)\mathrm{e}^{i\vec{p}\cdot\vec{x}}\mathrm{d}\vec{p},$$

where $w_i(\vec{p}) = \sqrt{|\vec{p}|^2 + n_i}$, and $C^i_\pm(\vec{p})$ are obtained from $(\hat{\varphi}^0(\vec{p}),\hat{\varphi}^1(\vec{p}),\hat{\varphi}^2(\vec{p}),\hat{\varphi}^3(\vec{p}))$ by solving

$$\begin{pmatrix}\hat{\varphi}^0\\ \hat{\varphi}^1\\ \hat{\varphi}^2\\ \hat{\varphi}^3\end{pmatrix} = \begin{pmatrix}1 & 1 & 1 & 1\\ iw_1 & -iw_1 & iw_2 & -iw_2\\ -w_1^2 & -w_1^2 & -w_2^2 & -w_2^2\\ -iw_1^3 & +iw_1^3 & -iw_2^3 & +iw_2^3\end{pmatrix}\begin{pmatrix}C^1_+\\ C^1_-\\ C^2_+\\ C^2_-\end{pmatrix}.$$

The determinant of that matrix is equal to $-4(n_1-n_2)^2 w_1 w_2$, and hence $C^i_\pm(\vec{p})$ can be written as linear combinations of $(\hat{\varphi}^0(\vec{p}),\hat{\varphi}^1(\vec{p}),\hat{\varphi}^2(\vec{p}),\hat{\varphi}^3(\vec{p}))$, i.e.,

$$\begin{pmatrix}C^1_+\\ C^1_-\\ C^2_+\\ C^2_-\end{pmatrix} = \frac{1}{2(n_1-n_2)}\begin{pmatrix}-w_2^2 & i\frac{w_2^2}{w_1} & -1 & \frac{i}{w_1}\\ -w_2^2 & -i\frac{w_2^2}{w_1} & -1 & -\frac{i}{w_1}\\ w_1^2 & -i\frac{w_1^2}{w_2} & 1 & -\frac{i}{w_2}\\ w_1^2 & i\frac{w_1^2}{w_2} & 1 & \frac{i}{w_2}\end{pmatrix}\begin{pmatrix}\hat{\varphi}^0\\ \hat{\varphi}^1\\ \hat{\varphi}^2\\ \hat{\varphi}^3\end{pmatrix}.$$

Notice that these coefficients have either w_1 or w_2 in the denominator, in the worse case. Therefore, the desired decay of $\psi(t,\vec{x})$ for large t is obtained by applying Lemma C.3.1 as before.

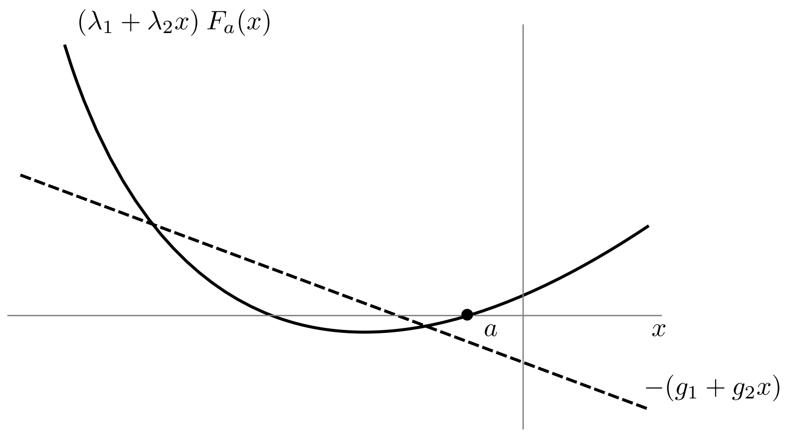

Figure 4.3: Plots of the qualitative behaviours of $(\lambda_1+\lambda_2 x)(\frac{\lambda\hbar}{16\pi^2})F_a(x)$ and $(g_1+g_2 x)$ in $\left[-4m^2,\infty\right)$, where the constants are such that $g_i>0$, $\lambda_i>0$, and $-4m^2 < -\frac{\lambda_1}{\lambda_2} < -\frac{g_1}{g_2} < a < 0$.

□

The previous theorem establishes that, if the space of solutions of eq. (4.34) contains only negative elements, then all solutions of the linearized semiclassical equation (4.26) with compactly-supported initial values decay at large times. In the following corollary, certain sufficient (but not necessary) conditions are identified on the parameters $(a,g_1,g_2,\lambda,\lambda_1,\lambda_2)$ which ensure such a behavior.

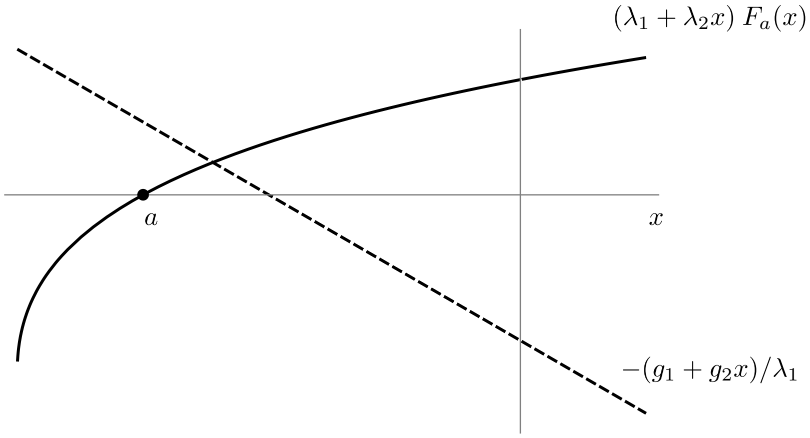

Figure 4.4: Plots of the qualitative behaviours of $F_a(x)$ and $(g_1 + g_2 x)/\lambda_1$ in $\left[-4m^2, \infty\right)$, where the constant are such that $g_i > 0$, $\lambda_2 = 0$, $\lambda_1 > 0$, $\frac{\lambda\hbar}{16\pi^2} F_a(-4m^2) < -(g_1 - g_2 4m^2)/\lambda_1$, and $\frac{\lambda\hbar}{16\pi^2} F_a(0) > -g_1/\lambda_1$.

Corollary 4.2.1. *Under the hypotheses of theorem 4.2.2, the space of solutions of eq. (4.34) contains only negative elements if the following sufficient conditions on $(a, g_1, g_2, \lambda, \lambda_1, \lambda_2)$ hold:*

a) If $\lambda_2 = 0$, $\frac{g_2}{\lambda_1} \geq 0$, if $-\frac{g_1}{\lambda_1} \leq \frac{\lambda\hbar}{16\pi^2} F_a(0)$, and $\frac{\lambda\hbar}{16\pi^2} F_a(-4m^2) \leq -\frac{g_1}{\lambda_1} + 4m^2 \frac{g_2}{\lambda_1}$, then $\mathcal{S}$ contains only one negative solutions.

b) If $-\lambda_1/\lambda_2 < -g_1/g_2 < a < 0$, then $\mathcal{S}$ contains only negative solutions, and $|\mathcal{S}|$ is either 1 or 2.

c) If $-4m^2 < -\lambda_1/\lambda_2 < a < 0$, $g_2 > 0$ and $0 \leq -\frac{g_1}{\lambda_1} \leq \frac{\lambda\hbar}{16\pi^2} F_a(0)$, then $\mathcal{S}$ contains only negative solutions, and $|\mathcal{S}|$ is either 1 or 2.

If these conditions hold, then the corresponding solutions of eq. (4.26) with compact spatial support decay at least as $1/t^{3/2}$ at large times.

Proof. a) Case $\lambda_2 = 0$, $\frac{g_2}{\lambda_1} \geq 0$. Eq. (4.34) takes the form

$$\frac{\lambda\hbar}{16\pi^2} F_a(x) = -\left(\frac{g_1}{\lambda_1} + \frac{g_2}{\lambda_1} x\right), \qquad x \in (-4m^2, +\infty).$$

The real part of that equation has now a positive solution if $-\frac{g_1}{\lambda_1} > \frac{\lambda\hbar}{16\pi^2} F_a(0)$. From the plot displayed in Figure 4.4, one infers that a single negative solution appears if $-\frac{g_1}{\lambda_1} \leq \frac{\lambda\hbar}{16\pi^2} F_a(0)$ and $\frac{\lambda\hbar}{16\pi^2} F_a(-4m^2) \leq -\frac{g_1}{\lambda_1} + 4m^2 \frac{g_2}{\lambda_1}$, while no solutions exist otherwise.

b) Case $a < 0$, $-\lambda_1/\lambda_2 \leq -g_1/g_2 \leq a < 0$. From the plot displayed in Figure 4.3, it is found that all the possible solutions are negative, and in particular either one or two solutions exist.

c) Case $-\lambda_1/\lambda_2 < a < 0$ and $0 \leq -\frac{g_1}{\lambda_1} \leq \frac{\lambda\hbar}{16\pi^2} F_a(0)$. This case is similar to the one displayed in Figure 4.3, but now the line $-g_2 x + g_1$ intercepts the vertical line between $y = 0$ and $y = \frac{\lambda\hbar}{16\pi^2} F_a(0)$. Hence, all the possible solutions are negative, and there is always at least one solution.

Finally, the proof follows by applying the results of theorem 4.2.2. □

To summarize, it was shown that the desired decay as $1/t^{3/2}$ for large time t of the solutions of the linearized Einstein equation (4.26) with compact spatial support holds if and only if the zeros of S defined in eq. (4.31) are all contained in the negative real axis. In this case, perturbations become negligible with respect to the background solution, thus indicating the stability of the background. On the contrary, if some zeros were located in the positive real axis, then unstable runaway solutions would destabilize the background configuration. Finally, if no zeros are present in S, then eq. (4.26) does not admit solutions, but its counterpart with source given in eq. (4.28) still has non vanishing past compact solutions which decay in time, due to the contribution given by the source through the branch cuts.

Remark 4.2.4. According to the results presented in proposition 4.2.3, every solution of eq. (4.34) is located in the positive real axis whenever the quantum field ϕ is massless, i.e., when $m = 0$, even if the inequality (4.32) holds (recalling that $F_a(z)$ is reduced to eq. (4.25) in the massless case). For this reason, it may be expected that any stability result cannot be achieved for massless fields, at least when homogeneous equations are taken into account, even if compactly-supported initial data are selected.

This observation is in accordance with the stability issue established in [Hor80], where it was shown that exponentially growing runaway solutions appear when the back-reaction of a quantum Maxwell field interacting with a weak gravitational field is taken into account in the framework of Semiclassical Gravity.

4.2.4 Applications to cosmological spacetimes

The analysis employed in the toy model presented in eqs. (4.4a) and (4.4b) can be used to guess the behaviour of the linearized solutions of the semiclassical Einstein equations (1.105) in cosmological spacetimes, where the quantum matter is modelled by a massive scalar field ϕ, while the geometry is described by the metric $g_{\mu\nu}$ of a flat Friedmann-Lemaître-Robertson-Walker spacetime - *cf.* chapter 2. As already discussed in subsection 2.2.3, the back-reaction of the matter field can be evaluated by the traced semiclassical equations (1.124), taking into account the form of the trace $\langle :T_\rho{}^\rho: \rangle_\omega$ obtained in eq. (1.123).

According to the perturbative approach explained in subsection 4.2.1, the linearization of the traced semiclassical equations is derived by analyzing a linear perturbation of this cosmological system around a spacetime which is a solution of the semiclassical Einstein equations. The interaction between matter content and geometrical curvature is described by the smeared interacting action

$$V_R = -\frac{\xi}{2} \int_{\mathcal{M}} R(x)\phi^2(x) f(x) \mathrm{d}_g x, \qquad f \in \mathcal{D}(\mathcal{M}),$$

which corresponds to the coupling-to-curvature part in the Klein-Gordon action (1.28). In this viewpoint, the quantum matter field is not fully free anymore, but it is interpreted as an interacting Klein-Gordon field influenced by the spacetime curvature through the external potential $\delta V_R/\delta\phi = -\xi\phi R$. Moreover, the Ricci scalar curvature plays the role of the classical field ψ in light of the correspondence between toy model and cosmological system.

Actually, this different approach, in which the total Lagrangian is split in a free and interacting part, is equivalent to study exactly the entire Klein-Gordon action according to the principle of Perturbative Agreement [HW05; DHP18]: it states that any result of a perturbative model must coincide with that obtained in an exact formulation, whenever an arbitrary quadratic contributions in the interacting Lagrangian is taken into account.

For the sake of simplicity, a background solution having vanishing curvature can be chosen at a first stage of this analysis. For example, the Minkowski spacetime, which is trivially a solution of the semiclassical Einstein equations by setting the vacuum as reference state. With this assumption, a formal correspondence arises between the linearization of eq. (1.123) and the linearized semiclassical equation (4.26), after regarding the linearized Ricci scalar as the perturbative external field ψ_1 over a vanishing background $\psi_0 = 0$. In this respect, the cosmological constant Λ is a zeroth-order contribution which can be assumed to vanish, whereas the trace anomaly given in eq. (1.120) is at least quadratic in the components of the Riemann curvature tensor $R_{\mu\nu\rho\sigma}$, and thus it is negligible at the linear order in R.

Taking into account all of this and restoring the Newton constant G, eq. (1.124) takes the form of the linearized semiclassical equation (4.26) through the following correspondence between the cosmological parameters and the set of constants $(g_1, g_2, \lambda, \lambda_1, \lambda_2)$:

$$g_1 = -\frac{1}{8\pi G}, \qquad g_2 = \gamma, \qquad \lambda = \xi, \qquad \lambda_1 = m^2, \qquad \lambda_2 = 3\left(\xi - \frac{1}{6}\right), \tag{4.42}$$

where γ is the renormalization constant associated to $\Box_g R$ in $\langle :T_\rho{}^\rho: \rangle_\omega$. In the cosmological framework, g_1 turns to be a fixed negative parameter (in Planck's units, $\hbar = 1$ and $(8\pi G)^{-1} = m_P^2/8\pi$, where m_P is the Planck mass), while, on the other hand, λ can be fixed to be strictly positive and different from 1/6 by assuming non-minimally and non-conformally coupled fields, i.e, $\xi \neq 0, 1/6$; hence, $\lambda_2 \neq 0$. On the contrary, both g_2 and λ_2 are free parameters of the semiclassical theory, whose signs can be chosen such that the inequality (4.32) holds, i.e.,

$$\gamma \frac{m^2}{m_P^2} \geq -\frac{3}{8\pi}\left(\xi - \frac{1}{6}\right), \qquad \gamma \in \mathbb{R}. \tag{4.43}$$

Remark 4.2.5. The formal analogy between the results obtained for the toy model and the analysis performed in cosmological spacetimes is further enforced by analyzing the internal structure of the linearized vacuum polarization expressed via the Kernel $\mathcal{K}_a$ in eq. (4.17). It can be shown that the following non-local retarded operator

$$\mathcal{T}_\Omega[f](t) = -\frac{1}{8\pi^2}\int_0^t \log(\Omega(t-s))\hat{\hat{f}}(s, \vec{p})\, \mathrm{d}s, \qquad \Omega \doteq \sqrt{|\vec{p}|^2 + 4m^2}, \tag{4.44}$$

acting on ψ_1 is hidden inside $\left\langle :\phi^2: \right\rangle_\omega^{(\mathrm{lin})}$. It corresponds exactly to the same unbounded operator found in cosmological spacetimes, *cf.* eq. (2.46), and hence it manifests the same conceptual issues of the unbounded operator $\mathcal{T}[f]$ studied in the cosmological chapter. Remarkably, it does not depend on the choice of the free Hadamard state ω, because it is contained in the one-loop contribution (4.16), namely in $\mathcal{K}_a$, and thus it is independent of the choice of W in eq. (4.17). Furthermore, $\mathcal{T}_\Omega[f]$ is also invertible according to the results of subsection 2.2.4, i.e., it shares the same property of the multiplicative operator $T(z)$ defined in eq. (4.40).

This formal analogy does not surprise, in fact, because the same singularity structure is shared by any vacuum polarization in both flat and curved spacetimes, whenever it is considered a class of states whose two-point function is locally of Hadamard form (see subsection 1.2.3).

Based on these statements, it should be quite straightforward to prove that the semiclassical equation (4.11) admits local solutions in small interval of time $[t_0, t_1]$, $t_1 > t_0$, using the same ideas presented in section 2.2 for the cosmological case.

Under these assumptions, there are choices of the parameters (m^2, ξ, γ, a) for which the cosmological version of eq. (4.34) admits only negative solutions. For example, corollary 4.2.1 can be applied by choosing $\xi > 1/6$, $\gamma > 0$, $a > -4m^2$, and sufficiently large m^2, so that only negative solutions exist. Namely, in these cases solutions of the cosmological linearized semiclassical Einstein equations written as in the traced form given in (1.124) with spatial compact support decay to zero for large times, thus showing the stability of the chosen background.

On the other hand, one may expect that too large values of m^2, even beyond the Planck scale m_P, would be physically unacceptable for quantum fields describing elementary particles.

In this view, the result is similar to the one obtained in [RD81] for massive quantum scalar fields in flat spacetime. Firstly, the conditions stated here are only sufficient, so other cases in which stable solutions cannot be a priori excluded, for different choices of the parameters (m^2, ξ, γ, a). Secondly, and most importantly, it is expected that the linearized perturbations in a more realistic cosmological model should be sourced by $f \in \mathcal{D}(\mathcal{M})$ localized somewhere in the past, modelling some anisotropic or stochastic fluctuations at microscopic levels. This is exaclty the case of the Einstein-Langevin equations (4.3), in which the classical source is modelled by the stochastic tensor $\tau_{\mu\nu}$, and whose trace is expected to not vanish for arbitrary non-conformally coupled fields, i.e., when $\xi \neq 1/6$ (see [HV20], Chapter 5). In this picture, the stochastic source in the past drives the fluctuations of the gravitational field, firstly. Then, it gives origin to the external perturbation which enters the cosmological linearized semiclassical Einstein equations as external source in a self-consistence way, as discussed in subsection 4.1.2.

In this model with an external source, the cosmological counterpart of the linearized semiclassical equation (4.28) should be taken into account, with parameters $g_1, g_2, \lambda, \lambda_1, \lambda_2$ fixed as in eq. (4.42) and satisfying the inequality (4.43). Under these assumptions, and based on the results shown in theorem 4.2.1 and remark 4.2.2, the linearized curvature solution R depends on both the contributions due to the poles and the branch cuts of $S(z)$. However, the contribution arising from poles are not present for several, apparently more physically acceptable values of the parameters (m^2, ξ, γ, a). For example, for sufficiently large ratio m_P^2/m^2, and fixing

$$0 < \xi < 1/6, \qquad \gamma > 0, \qquad a > -4m^2,$$

then the condition (4.43) holds. Therefore, with this choice of parameters, the past compact linearized solution induced by a smooth compactly supported source f has no poles contribution, and hence it decays at zero for large times according to the results stated in theorem 4.2.1.

Conclusions

Both a synopsis of the main results obtained in this Ph.D thesis and some future outlooks are given in this section. The main results can be essentially split into three categories, linked to each other by the study of semiclassical Einstein equations in curved spacetimes. Unfortunately, the initial goal of extending the analysis performed in the Master thesis about Operator Product Expansion did not lead to novel results, but it cannot be excluded that such a research may be developed again in the future.

In the first part of the activity, the study of semiclassical Einstein equations was addressed in cosmological spacetimes in the framework of inflationary Cosmology, in order to analyze the back-reaction induced by a quantum scalar field on the background geometry, described by a Friedmann-LeMaître-Robertson-Walker spacetime. For arbitrary coupling with the curvature scalar, this massive quantum field induces a non-classical dynamics on the spacetime, in which higher-order derivatives of the metric appear up to the fourth order. Furthermore, the presence of a linear unbounded operator in the state-dependent contribution forbids to solve the semiclassical equation directly, and hence recursive methods to approximate a solution do not converge.

However, it was shown that the semiclassical equations can be rewritten in a new, non-standard form, through the application of an inversion formula for that unbounded operator, whose inverse is a more regular operator that the starting one. Thanks to this procedure, the proof of local existence and uniqueness of the solution of the semiclassical Einstein equation can be then obtained, and an initial-value formulation can be now locally formulated in Cosmology.

In the second part of the activity, the semiclassical methods were applied in Black Hole Physics to investigate the issue of black hole evaporation in spherically symmetric spacetimes. In this class of backgrounds, fundamental physics notions as mass and surface gravity are at disposal thanks to the spherical symmetry, and the spherical singularity which characterizes these dynamical black holes is covered by an apparent horizon. Within this context, it is relevant to study the mechanism of evaporation, in which the black hole mass can decrease in time under the influence of a quantum matter field located in the vicinity of the horizon. In particular, it was shown that the negative ingoing energy flux driving the loss of black hole mass can be sourced by the quantum trace anomaly outside the black hole horizon, with the assumption of some physically reasonable conditions, and in the case of massless, conformally-coupled scalar fields.

Finally, the issue about global stable solutions of the semiclassical Einstein equations was treated in the last part of the activity. This problem was analyzed by using a semiclassical toy model in flat spacetime, consisting of a quantum scalar field in interaction with a second classical scalar field, which plays the role of the classical background. This model mimics formally the evolution of a free massive quantum scalar field induced by the semiclassical Einstein equations in cosmological spacetimes, after interpreting the classical scalar field as the scalar curvature of the spacetime.

The perturbative equation which governs the dynamics of the linearized perturbations is a fourth-order differential equation, and thus it manifests the same conceptual issues already known in Semiclassical Gravity. Hence, this toy model aims to answer the question about the existence of runways solutions, which seem to appear in semiclassical theories of gravity in form of exponentially growing functions in time. If these unphysical solutions are present, then the background solution cannot be assumed to be stable anymore, even in the case of the flat spacetime.

On the contrary, it was proved that runaway solutions can be always avoided in this toy model, whenever the quantum scalar is massive, and spatially compact perturbations are taken into account. If both these assumptions hold, then there are several choices of the renormalization parameters such that perturbations decay to zero for large times, thus recovering stability of the back-reacted system.

All these three subjects can be extended in the future by further analysis and new insights. For more discussions about the backreaction problem in Semiclassical (stochastic) Gravity in the contexts of Cosmology and black hole evaporation, see also [HV20] and references therein.

The novel aspect of the work investigated in the Black Hole Physics framework was to consider the evolution of the black hole in a fully semiclassical model and from a local point of view. On the one hand, no global processes were taken into account to analysis the interplay between quantum matter and geometry, such as the expected Hawking radiation emitted at late times. On the other hand, no further approximations usually provided in literature were made, such as the adiabatic one. Moreover, it was emphasized that evaporation is strictly related to the influence of the negative ingoing flux on the horizon, which shrinks the area of the black hole. Therefore, it should not be confused with the emission of thermal radiation at infinity, even if these two mechanisms are clearly causally related. To highlight further this argument, both the negative ingoing flux and the corresponding rate of evaporation were evaluated for null radiating black holes, and thus they were compared to the standard results obtained for static black holes.

This study represents only a first step towards the formulation of a semiclassical model of evaporation for dynamical black holes, which takes into account the back-reaction of the quantum matter fields on the spacetime geometry in a self-consistent way. Actually, it is expected that a complete answer to the question about the final state of black hole evaporation should be given in a full theory of quantum gravity, i.e., when microscopic effects of gravity enter the game. However, some important topics of physical interest can be investigated in the semiclassical picture starting from the ideas developed in this work, despite the unavoidable limitations of such a formulation.

Firstly, the results obtained here could be extended to more general quantum fields beyond the massless, conformally-coupled case, i.e., when the state-dependent contributions inside the traced semiclassical equations appear, such as the vacuum polarization. In fact, evaluating the renormalized quantum stress-energy tensor in black hole geometries is a difficult task when performed outside the static limit and without adiabatic approximations, even due to the lack of a quantum state. In this direction, a joint work with E. A. Kontou and N. Pinamonti is focusing on the analysis of evaporation in spherically symmetric backgrounds by means of quantum energy inequalities assumed on the renormalized stress-energy tensor. This work is currently under development.

Secondly, it may be very interesting to evaluate explicitly the expected thermal radiation emitted during evaporation, and hence comparing the results with the ones already obtained in the adiabatic approximation for the Schwarzschild spacetime, see [Bar81; Bal84; Yor85; BB89; Mas95]. Hence, the ultimate result should be to include the backreaction of the (expected) thermal radiation emitted at late times upon the black hole geometry using the semiclassical Einstein equations. This study is crucial to understand how such thermal effects modify the evolution of the dynamical spacetime, and thus to formulate a full model of black hole evaporation. Again, all these problems appears problematic to be tackled, at least without a suitable quantum matter state which is able to yield a renormalized stress-energy tensor. In fact, no semiclassical solutions including Hawking radiation in four-dimensional dynamical black holes exist to date.

This solution including backreaction is actually available only in the two-dimensional case for Callen-Giddings-Harvey-Strominger (CGHS) black holes [APR11a; APR11b].

In the cosmological framework, the analysis performed in this work shows that an initial-value problem for the semiclassical Einstein equations can be formulated in the local case, after rewriting them in a new, non-standard form. Furthermore, the analysis performed in this work allows to furnish a way to approximate local solutions using recursive approaches, and hence computing them by means of numerical methods. This is a physically relevant result in Cosmology, because showing that semiclassical equations admit solutions is clearly essential to evaluate the backreaction effects upon the cosmological geometry in a self-consistent way.

Indeed, our current understanding of the early Universe relies largely on the backreaction effects of quantum matter fields upon the spacetime geometry. In particular, the semiclassical description provides a coherent framework where investigating the evolution of the inflationary Universe, which is usually modelled by a Friedmann-LeMaître-Robertson-Walker spacetime affected by small gravitational perturbations [LNSZ76; HP78]. These perturbations may be viewed as the result of backreaction effects of the quantum fluctuations induced by the matter fields, and hence their evolution should be described by scale factors which are solutions of the semiclassical Einstein equations. In a more phenomenological viewpoint, it is expected, furthermore, that those perturbations may have sourced the inhomogeneities which have given rise to the seeds of structure formation observed today. Finally, according to the analysis made in [Hac10; DHMP10; Hac16], the semiclassical description offers a natural explanation of the origin of the observed dark energy, because the dynamics induced by quantum fields displays the same features of the cosmological constant in the Friedmann equations.

Taking into account the issue of backreaction of cosmological perturbations, a physically significant problem which may tackled in the future is the formulation of a theory of cosmological perturbations in the semiclassical picture. To date, no derivations of this theory in Semiclassical Gravity are present, which improve the original results obtained by using the classical Einstein equations in General Relativity. For some references about the formalism of the theory of cosmological perturbations, see [MFB92; Bra04; Hay14]. To this avail, it is expected that a semiclassical version of this theory relies on the semiclassical Einstein equations, in which the renormalized quantum stress-energy encodes the backreaction of the quantum matter which should give origin to the perturbations of the cosmological metric. Therefore, a first step of this analysis may be to evaluate the semiclassical corrections to the equation of motions associated to the metric perturbations, e.g., in the scalar case. Classically, scalar perturbations are quantized in terms of gauge-invariant variable, the so-called Mukhanov-Sasaki variable, which describes a conformally-coupled scalar field with a time-dependent effective mass [Muk85; Muk88; MFB92].

Eventually, the analysis performed here in perturbative linearized Semiclassical Gravity has indicated a possible way to achieve stability in several linearized semiclassical theories of gravity. More generally, a full comprehension of the long-time behaviour of the semiclassical Einstein equations is currently absent, for arbitrary quantum matter fields. In particular, it is not clear how both the non-local state-dependent contributions and the higher-order derivative terms can influence the dynamics of the underline geometry, and if unstable solutions caused by these contributions may spoil the evolution at large times. However, the semiclassical toy model presented in this monograph seems to give a positive answer to the issue of stability of Minkowski spacetime in Semiclassical Gravity, at least in the linearized regime. This analysis would be handed in striking contrast with the state of art of semiclassical theories, which seems to predict unavoidably instabilities in the semiclassical picture. Actually, author's opinion is that the issue of runaways solutions lies not so much in the weakness of the semiclassical theories, but the fact that a full understanding of their formulation has not been achieved yet.

Moreover, the same toy model promises to give new insights about the evolution of the early Universe in inflationary Cosmology. In this viewpoint, a more in-depth study of the stability of the semiclassical (stochastic) equations in cosmological spacetimes deserves further attention, because it may help to establish the behaviour of the scale factor of the Universe at large times. In fact, on the part of the author there is the hope that further new results may be achieved in this direction, starting from what has been found in this Ph.D activity.

Appendix A

Differentiation and Integration on Manifolds

A.1 Differentiation of Vectors and Forms

In this appendix, some standard results about differentiation and integration on manifolds are listed, mostly based on the references [Wal84; Sch80; Poi09; Fra11; Car19].

The fundamental notion of derivation in curved manifolds $\mathcal{M}$ is encoded in the covariant differentiation, which generalizes the action of the usual partial derivative in flat spacetime independently of coordinates. In this monograph, ∇_μ shall denote the covariant derivative associated to the Levi-Civita connection, as the unique torsion-free and metric compatible connection on $(\mathcal{M}, g_{\mu\nu})$, evaluated in a certain coordinate charts (U, φ). Hence, its action on a certain tensor field T shall be denoted by $\nabla_{;\mu_1\ldots\mu_n} T = \nabla_{\mu_1} \cdots \nabla_{\mu_n} T$. By means of the covariant derivative, both the divergence of a vector field

$$\nabla_\rho V^\rho = \frac{1}{\sqrt{|\det(g)|}} \partial_\sigma (V^\sigma \sqrt{|\det(g)|}), \qquad V \in T_p\mathcal{M} \tag{A.1}$$

and the covariant directional derivative of T along a curve can be evaluated in the spacetime. In particular, given a curve γ parametrized in coordinates by $x^\mu(\lambda)$ and identified by the tangent vector $u^\mu = \mathrm{d}x^\mu/\mathrm{d}\lambda$, the directional derivative is denoted as

$$\mathcal{L}_u \doteq u^\rho \nabla_\rho. \tag{A.2}$$

If $\mathcal{L}_u T = 0$, then T is said to be parallel transported along the curve. Thus, a geodesic is defined as a curve along which its tangent vector is parallel-transported, namely it satisfies the geodesic equation $\mathcal{L}_u u^\mu = 0$; this last equation is invariant under an affine transformation $\lambda \mapsto a\lambda + b$, $a, b \in \mathbb{R}$.

Another relevant type of derivation is the Lie derivative, which describes how a tensor field changes along the manifold $\mathcal{M}$ under diffeomorphisms. Given a one-parameter group of diffeomorphisms ϕ_t generated by the vector field $K \in T_p\mathcal{M}$, the rate of change of a tensor T under this flow of the diffeomorphism is given by the Lie derivative

$$\mathscr{L}_K T \doteq \lim_{t\to 0} \frac{1}{t} \left(\phi^*_{-t} T - T\right), \tag{A.3}$$

where $\phi^* f \doteq f \circ \phi$ denotes the pullback of f by ϕ, and the tensors in eq. (A.3) are all evaluated in $p \in \mathcal{M}$. If ϕ_t is a one-parameter group of isometries preserving the metric tensor, i.e., such that $\phi_t^* g = g$, then $\mathscr{L}_K g = 0$, and hence K is a Killing vector field (for further details, see [Wal84]).

In order to address the procedure of integration on curved manifolds, it is essential to introduce the notion of exterior derivative acting on differential forms.

Definition A.1.1. A differential p-form is a totally antisymmetric tensor of type $(0, p)$

$$\omega_{\mu_1\ldots\mu_p} \doteq \omega_{[\mu_1\ldots\mu_p]} \in \Lambda^p(\mathcal{M}),$$

where $\Lambda^p(\mathcal{M})$ is the vector space of all antisymmetric p-forms over a manifold $\mathcal{M}$, and $[\mu_1\ldots\mu_p]$ denotes the antisymmetric combination of tensors respect to indices $\mu_1\ldots\mu_p$. With respect to the natural basis $\{\mathrm{d}x^{\mu_i}\}_i$ of $\Lambda^p(\mathcal{M})$, labelled by $i = 1,\ldots p$,

$$\omega = \omega_{[\mu_1\ldots\mu_p]}\mathrm{d}x^{[\mu_1} \otimes \cdots \otimes \mathrm{d}x^{\mu_p]}.$$

Given $A, B \in \Lambda^p(\mathcal{M})$, one can always construct a $(p+q)$-form using a linear and associative map $\wedge : \Lambda^p(\mathcal{M}) \times \Lambda^q(\mathcal{M}) \to \Lambda^{p+q}(\mathcal{M})$ such that $A \wedge B = (-1)^{pq} B \wedge A$. This map is the exterior product $A \wedge B$:

$$A \wedge B = (A \wedge B)_{\mu_1\ldots\mu_{p+q}}\mathrm{d}x^{[\mu_1} \otimes \cdots \otimes \mathrm{d}x^{\mu_p} \otimes \mathrm{d}x^{\mu_{p+1}} \otimes \cdots \otimes \mathrm{d}x^{\mu_{p+q}]}, \tag{A.4}$$

whose components are

$$(A \wedge B)_{\mu_1\ldots\mu_{p+q}} \doteq \frac{(p+q)!}{p!q!} A_{[\mu_1\ldots\mu_p} B_{\mu_{p+1}\ldots\mu_{p+q}]}. \tag{A.5}$$

Thus, a wedge product always vanishes if some index μ_i appears twice, and hence every antisymmetric p-form can be also expressed as

$$\omega = \frac{1}{p!}\omega_{\mu_1\ldots\mu_p}\mathrm{d}x^{\mu_1} \wedge \cdots \wedge \mathrm{d}x^{\mu_p}. \tag{A.6}$$

A derivation preserving the antisymmetric nature of forms is the exterior derivative

$$\begin{aligned} &\mathrm{d} : \Lambda^p(\mathcal{M}) \to \Lambda^{p+1}(\mathcal{M}) \\ &\mathrm{d}\omega \doteq \mathrm{d}\omega_{\mu_1\ldots\mu_p} \wedge \mathrm{d}x^{\mu_1} \wedge \cdots \wedge \mathrm{d}x^{\mu_p} = \frac{1}{p!}\partial_\nu\omega_{\mu_1\ldots\mu_p}\mathrm{d}x^\nu \wedge \mathrm{d}x^{\mu_1} \wedge \cdots \wedge \mathrm{d}x^{\mu_p}, \end{aligned} \tag{A.7}$$

where $\partial_\nu\omega_{\mu_1\ldots\mu_p} \doteq \partial_{[\nu}\omega_{\mu_1\ldots\mu_p]}$. As anti-derivative operator, it fulfils a modified version of the Leibniz rule $\mathrm{d}(A \wedge B) = \mathrm{d}A \wedge B + (-1)^p A \wedge \mathrm{d}B$. In component-basis representation the exterior derivative reads

$$(\mathrm{d}\omega)_{\mu_1\ldots\mu_p,\nu} = (p+1)\partial_{[\nu}\omega_{\mu_1\ldots\mu_{p+1}]}. \tag{A.8}$$

A p-form $\omega \in \Lambda^p(\mathcal{M})$ is said to be closed if $\mathrm{d}\omega = 0$, and exact if $\omega = \mathrm{d}\eta$ for some $(p-1)$-form $\eta \in \Lambda^{p-1}(\mathcal{M})$. An exact form is always closed because $\mathrm{d}^2 = \mathrm{d} \circ \mathrm{d} = 0$, but the converse is not generally true. A criterion for the converse implication is furnished by the so-called Poincaré lemma [Nak03].

Theorem A.1.1. *Let $U \subset \mathcal{M}$ be a coordinate neighbourhood which is contractible to a point $p \in \mathcal{M}$, i.e., there exists a map $F : U \times I \to \mathbb{R}$, $I = [0,1]$, such that*

$$F(x,0) = x, \qquad F(x,1) = p$$

for all $x \in U$ (heuristically, it means that U can be shrunk to p within itself). Then any closed p-form $\omega \in \Lambda^p(U)$ is locally exact, namely there exists some $(p-1)$-form $\eta \in \Lambda^{p-1}(U)$ such that $\omega = \mathrm{d}\eta$ in U.

In physical applications, the exterior derivative has the fundamental property of defining all the derivative operators constructed from the differential operator ∇. For instance, the gradient $\mathrm{d}f = \partial_\nu f dx^\nu$ is the exterior derivative of a 0-form, while the curl of a vector field $\nabla \wedge V$, $V = (v^1, \dots, v^n) \in \mathbb{R}^n$ is the exterior derivative $\mathrm{d}\omega$ of the dual vector $\omega = g(V, \cdot)$.

The second fundamental operation on forms is the so-called Hodge duality: given a n-dimensional manifold $\mathcal{M}$, the Hodge star operator $\star$ is the map

$$\begin{aligned} \star : \Lambda^p(\mathcal{M}) &\to \Lambda^{n-p}(\mathcal{M}) \\ (\star\omega)_{\mu_{p+1}\cdots\mu_n} &\doteq \frac{1}{p!}\omega^{\mu_1\cdots\mu_p}\epsilon_{\mu_1\cdots\mu_{p+1}\cdots\mu_n}, \end{aligned} \tag{A.9}$$

where ϵ is the Levi-Civita pseudo-tensor

$$\epsilon_{\mu_1,\cdots\mu_n} \doteq \sqrt{|\det(g)|}\varepsilon_{\mu_1,\cdots\mu_n}, \qquad \epsilon^{\mu_1,\cdots\mu_n} = \frac{\mathrm{sgn}(g)}{\sqrt{|\det(g)|}}\varepsilon^{\mu_1,\cdots\mu_n}, \tag{A.10}$$

constructed from the Levi-Civita symbol

$$\varepsilon_{\mu_1,\cdots\mu_n} \doteq \begin{cases} +1 & \text{for even permutation of } 1\dots n, \\ -1 & \text{for odd permutation of } 1\dots n, \\ 0 & \text{otherwise.} \end{cases} \tag{A.11}$$

The idea of "duality" descends from the property that applying the transformation twice one gets back to the original space: in case of the Hodge star operator $\star(\star\omega)_{\mu_1\dots\mu_p} = (-1)^{s+p(n-p)}\omega_{\mu_1\dots\mu_p}$. Note that ϵ is a pseudo-tensor because ε is a tensor density, like the determinant of the metric $g = |g_{\mu\nu}|$, with unit weight, and it changes sign under parity; hence, it contains intrinsically the orientation of the spacetime.

A.2 Integration and Stokes' Theorem

Differential forms appear also in the framework of integration on n-dimensional manifolds $\mathcal{M}$, because the antisymmetric property of n-forms is essential to obtain an oriented n-dimensional volume element of an open region $\mathcal{V} \subset \mathcal{M}$. To this aim, the combination of the wedge product and the Levi-Civita tensor given in eqs. (A.4) and (A.10), respectively, provides a natural notion of volume element, namely

$$\epsilon \doteq \frac{1}{n!}\sqrt{|\det(g)|}\varepsilon_{\mu_1,\dots\mu_n}\mathrm{d}x^{\mu_1} \wedge \cdots \wedge \dots \mathrm{d}x^{\mu_n}, \tag{A.12}$$

where the normalization factor $(n!)^{-1}$ is such that

$$\epsilon^{\mu_1,\cdots\mu_n}\epsilon_{\mu_1,\dots\mu_n} = (-1)^s n!,$$

with s the number of minus signs in the eigenvalues of the metric (for examples, $s = 0$ in the Riemannian case and $s = 1$ in the Lorentzian case). Thus,

$$\begin{aligned} \epsilon &= \epsilon_{\mu_1\dots\mu_n}\mathrm{d}x^{\mu_1} \otimes \cdots \otimes \mathrm{d}x^{\mu_n} = \frac{1}{n!}\epsilon_{\mu_1\dots\mu_n}\mathrm{d}x^{\mu_1} \wedge \cdots \wedge \mathrm{d}x^{\mu_n} \\ &= \frac{1}{n!}\sqrt{|\det(g)|}\varepsilon_{\mu_1\dots\mu_n}dx^{\mu_1} \wedge \cdots \wedge \mathrm{d}x^{\mu_n} = \sqrt{|\det(g)|}\mathrm{d}x^0 \wedge \cdots \wedge \mathrm{d}x^{n-1}, \end{aligned}$$

where, in the last step, the factor $(n!)^{-1}$ was reabsorbed in the new wedge product to take care of the overcounting inside $\varepsilon_{\mu_1\dots\mu_n}\mathrm{d}x^{\mu_1} \wedge \cdots \wedge \mathrm{d}x^{\mu_n}$, due to the sum over permutations of the indices.

Hence, the element ϵ acquires the real meaning of infinitesimal volume, because it identifies the following integral measure on a n-dimensional (finite) domain $\mathcal{V}$

$$\mu(\mathcal{V}) = \int_{\mathcal{V}} \mathrm{d}\mu \doteq \int_{\mathcal{V}} \sqrt{|\det(g)|}\, \mathrm{d}x^0 \cdots \mathrm{d}x^{n-1} = \int_{\mathcal{V}} \mathrm{d}_g x, \qquad \mathrm{d}\mu(\mathcal{V}) = \mathrm{d}_g x, \tag{A.13}$$

which takes naturally into account the orientation of $\mathcal{V}$. In the end, the integral over $\mathcal{V}$ can be viewed as a map from $\Lambda^p(\mathcal{M})$ to $\mathbb{R}$, where the volume element $\mathrm{d}^n x$ on $\mathbb{R}^n$ is an antisymmetric tensor density constructed through wedge products as $\mathrm{d}^n x = \mathrm{d}x^0 \wedge \cdots \wedge dx^{n-1} \in \Lambda^p(\mathcal{M})$.

This point of view leads to one of the most powerful theorems in differential geometry, that is, Stokes' theorem [Wal84]:

Theorem A.2.1. *Let $\mathcal{V}$ be a n-dimensional region with boundary $\partial\mathcal{V}$, and ω an $(n-1)$-form on $\mathcal{M}$. Then,*

$$\int_{\mathcal{V}} \mathrm{d}\omega = \int_{\partial\mathcal{V}} \omega. \tag{A.14}$$

Eq. (A.14) can be also expressed in terms of the Hodge star dual (A.9) of a n-form θ. On the one hand, denoting with $p = n-1$,

$$\omega = \star\theta, \qquad \omega_{\mu_1\ldots\mu_p} = (\star\theta)_{\mu_1\ldots\mu_p} = \epsilon_{\nu\mu_1\ldots\mu_p}\theta^\nu,$$

and, on the other hand,

$$(\mathrm{d}\omega)_{\lambda\mu_1,\ldots,\mu_p} = (p+1)\nabla_{[\lambda}\epsilon_{\nu\mu_1\ldots\mu_p]}\theta^\nu = n\, \epsilon_{[\nu\mu_1\ldots\mu_p}\nabla_{\lambda]}\theta^\nu,$$

which yields

$$\star(\mathrm{d}\omega) = \frac{n}{n!}\epsilon^{\lambda\mu_1\ldots\mu_p}\epsilon_{[\nu\mu_1\ldots\mu_p}\nabla_{\lambda]}\theta^\nu = (-1)^s\nabla_\nu\theta^\nu.$$

Finally, as $\star(\star f) = (-1)^s f$ for duality of scalars, it holds that

$$\mathrm{d}\omega = \star\nabla_\nu\theta^\nu = \epsilon\nabla_\nu\theta^\nu, \tag{A.15}$$

since $\epsilon = \star 1$ by definition of the volume element. Therefore, the divergence of a vector always corresponds to the exterior derivative of an $(n-1)$-form. Hence, Stokes' theorem can be rewritten as

$$\int_{\mathcal{V}} \epsilon\, \nabla_\nu\theta^\nu = \int_{\partial\mathcal{V}} \epsilon_{\nu\mu_1\ldots\mu_p}\theta^\nu, \tag{A.16}$$

or, equivalently,

$$\int_{\mathcal{V}} \epsilon\, \nabla_\nu\theta^\nu = \int_{\partial\mathcal{V}} \epsilon_{\nu\mu_1\ldots\mu_p}\theta^\nu, \tag{A.17}$$

where ϵ and $\epsilon_{\nu\mu_1\ldots\mu_p}$ were defined in eqs. (A.10) and (A.12), respectively.

Stokes' theorem involves integration on the boundary of the volume region, which can be characterized as a $(n-1)$-submanifold $\Sigma \subset \mathcal{M}$, that is, an hypersurface in the spacetime. Any spacelike, timelike, or null hypersurface is always selected by a constraint on the coordinates $\Phi(x^\mu) = 0$, and hence it is labelled by its gradient $\partial_\mu\Phi$, which is always normal to the surface. Thus, the unit normal vector associated to Σ can be always obtained by normalizing the vector $X^\mu = g^{\mu\nu}\partial_\nu\Phi$, i.e.,

$$n^\mu = \frac{\sigma X^\mu}{\sqrt{|g^{\nu\rho}X_\nu X_\rho|}}, \tag{A.18}$$

where $\sigma = n^\mu n_\mu = \pm$ if Σ is timelike or spacelike, respectively. In the null case, eq. (A.18) is not defined, and the normal vector $k^\mu = -g^{\mu\nu}\partial_\nu\Phi$ is both tangent and normal to Σ. Hence, k^μ fulfils the geodesic equation

$$\mathcal{L}_k k^\mu = \kappa k^\mu, \tag{A.19}$$

where the constant κ is called surface gravity. In fact, the null integral curves $x(\lambda)$ of $k^\mu = \frac{\mathrm{d}x^\mu}{\mathrm{d}\lambda}$ are the generators of the null hypersurface, while κ measures how the chosen parametrization with respect to λ is not affine: given an affine-parametrized normal vector field ℓ^μ, such that $k^\mu = f\ell^\mu$ for some scalar function f, then

$$\kappa = k^\nu \partial_\nu \log(f). \tag{A.20}$$

Everytime a hypersurface Σ is given, there exists a preferred coordinate system on a manifold which is naturally adapted to Σ, that is, $\{z, y^1, \dots, y^{n-1}\}$, where z is the affine parameter related to n^μ such that $(\partial_z)^\mu = n^\mu$. In this coordinate system called Gaussian normal coordinates, the metric can be parametrized as

$$ds^2 = \sigma dz^2 + h_{ij} dy^i dy^j \qquad i = 1, \dots, n-1, \tag{A.21}$$

where $\sigma = g(\partial_z, \partial_z) = n^\mu n_\mu$, and $h_{ij} \doteq (\phi^* g)_{ij} = g(\partial_i, \partial_j)$ is the induced metric, i.e., the restricted metric to the submanifold Σ, associated to the line element $\mathrm{d}s^2_\Sigma = h_{ij}\mathrm{d}y^i\mathrm{d}y^j$ (in the null case, the intrinsic coordinates system has to be adapted to the generators of the null hypersurface). Furthermore, in Gaussian normal coordinates,

$$\epsilon = \sqrt{|\det(h)|}\mathrm{d}z \wedge \mathrm{d}y^1 \wedge \cdots \wedge \mathrm{d}y^{n-1} = \mathrm{d}z \wedge \hat{\epsilon},$$

where $\sqrt{|\det(g)|} = \sqrt{|\det(h)|}$ in these coordinates, and $\hat{\epsilon} = \sqrt{|\det(h)|}\mathrm{d}^{n-1}y = \mathrm{d}_y h$ is the volume element on the submanifold Σ.

Based on all those statements, Stokes' theorem reduces to the divergence theorem (or Gauss' integral theorem) in a finite region $\mathcal{V} \subset \mathcal{M}$, after denoting with n^μ the unit normal vector to the hypersurface $\Sigma = \partial\mathcal{V}$. For instance, in the case of a spacelike hypersurface Σ_z defined by $z = const$, with $n^\mu = (1,0,\dots,0)$, the following relation

$$\epsilon_{\nu\mu_1\dots\mu_{n-1}}\theta^\nu = (n_\nu\theta^\nu)\hat{\epsilon}_{\mu_1\dots\mu_{n-1}}$$

shows that the $(n-1)$-form $\epsilon_{\nu\mu_1\dots\mu_{n-1}}\theta^\nu$ can be integrated on the boundary with respect to the induced volume element $\hat{\epsilon}$. Thus, viewing θ^ν as a vector field, eq. (A.17) can be written in term of the divergence of θ^μ as

$$\int_{\mathcal{V}} \nabla_\nu \theta^\nu \mathrm{d}_g x = \int_\Sigma n_\nu \theta^\nu \mathrm{d}_h y. \tag{A.22}$$

Namely, the standard n-dimensional divergence theorem is recovered in curved manifolds.

Appendix B

Regularization Scheme in Cosmological Spacetimes

B.1 Generalized Adiabatic Point-splitting

In this appendix a review of the steps to obtain the expression of those renormalized Wick observables which enter the cosmological semiclassical problem described by the system (2.55), namely $\langle :\phi^2: \rangle_\omega$, $\langle :\partial_0\phi\partial_0\phi: \rangle_\omega$ and $\langle :\varrho: \rangle_\omega$. To this aim, one needs to choose sufficiently regular states ω whose two-point functions satisfy the definition 2.2.1, and hence to evaluate the coefficients $C^{\mathcal{H}}_{\phi^2}$, $C^{\mathcal{H}}_{\varrho}$, and $C^{\mathcal{H}}_{E}(\tau, k)$ given in eqs. (2.41) and (2.49), respectively.

The regularization scheme presented here was fully developed in [SV08; Deg13] (see also [Sie15]), and it takes inspiration from the adiabatic point-splitting regularization provided in [PF74; Bun80]. In this procedure, the adiabatic bidistribution constructed with adiabatic modes of order N ($\zeta_k^{(N)}, \partial_\tau \zeta_k^{(N)}$) is subtracted from the two-point function of the homogeneous and isotropic pure state (2.11), instead of the Hadamard singularity. Moreover, the order N is determined by the composite operator that must be regularized: for instance, in the case of $:\phi^2:$ zeroth-order modes are sufficient, whereas at least fourth-order modes are needed to regularize $:\varrho:$. Thanks to the regularity features of adiabatic states, which are Hadamard for infinite N, the two regularization prescriptions are local and covariant, and hence they can only differ by local curvature tensors of the spacetime. Another equivalent point-splitting procedure to renormalize Wick observables in cosmological spacetimes can be found in [GS21].

A generalized version of the adiabatic point-splitting regularization was studied in [Sch10; Deg13][1], which aims to obtain the state-dependent part of expectation values of the fields and its derivatives, instead of subtracting the adiabatic modes directly. The strategy of this "momentum-space" renormalization is to perform the regularization procedure in momentum space, using equivalent subtractions which share the same $\vec{k}$-asymptotic behaviours of the truncated Hadamard

[1] To be compatible with the conventions adopted in these original papers, a slightly different definition of the the Hadamard parametrix (1.57) shall be used, such that there is a prefactor $(2\pi)^{-2}$ in front of $h_{0^+}(x', x)$, $\sigma(x', x)$ is defined as the signed squared geodesic, and $L = \sqrt{2}\lambda$ is the Hadamard length scale.

parametrix (1.60). To this aim, the form of H_N is necessary to compute the Hadamard point-splitting formula (1.86) in FLRW spacetimes, that is,

$$\langle :(\mathfrak{D}_1\phi)\,(\mathfrak{D}_2\phi):\rangle_\omega = \lim_{x'\to x}\mathfrak{D}_1\mathfrak{D}_2'\left[\frac{1}{(2\pi)^3 a(\tau')a(\tau)}\int_{\mathbb{R}^3} d\vec{k}\,\left(\overline{\zeta}_k(\tau')\zeta_k(\tau)-\hat{\mathcal{H}}_N(\tau',\tau,k)\right)\mathrm{e}^{i\vec{k}\cdot(\vec{x}'-\vec{x})}\right], \tag{B.1}$$

where $\hat{\mathcal{H}}_N(\tau,\tau',k) \doteq a(\tau)a'(\tau)\hat{H}_N(\tau,\tau',k)$. Notice that the spatial Fourier transform can be taken straightforwardly, because the (truncated) Hadamard parametrix is spatially isotropic and homogeneous, i.e., $H_{0^+}(\tau',\vec{x}',\tau,\vec{x}) = \tilde{H}_{0^+}(\tau,\tau',r)$, $r \doteq \|\vec{x}'-\vec{x}\|$. Actually, in FLRW spacetimes it is sufficient to take the truncated Hadamard parametrix $\mathcal{H}_1$ in the point-splitting procedure, because the restriction to the diagonal $x = x'$ of a first order bi-differential operator applied to $\mathcal{H}-\mathcal{H}_N$ vanishes for $n \geq 1$. Moreover, using the equation of motion, the second-order derivatives can be replaced by higher-order spatial derivatives, so, at the end of this analysis, the expressions for the truncated Hadamard parametrix of order 1 $\mathcal{H}_1$ are sufficient to perform the point-splitting (for further details, see [Sch10]). Therefore, one needs to evaluate the following coinciding limits in Synge's brackets (1.54):

$$[\mathcal{H}_1]\,,\qquad [\partial_\tau\mathcal{H}_1] \doteq \left[\mathcal{H}_1^{(\tau)}\right],\qquad [\partial_{\tau\tau'}\mathcal{H}_1] \doteq \left[\mathcal{H}_1^{(\tau\tau')}\right],\qquad [\triangle\mathcal{H}_1] \doteq [\mathcal{H}_1^{(\triangle)}],$$

where $\triangle \doteq \partial_{rr} + (2/r)\partial_r$, $r \doteq \|\vec{x}'-\vec{x}\|$. According to the references [Sch10; Deg13], the strategy to perform this adiabatic-like regularization reads as follows.

- **First step**. Evaluate the singular distributions $\lim_{\varepsilon\to 0^+}\sigma_\varepsilon^{-1}$ and $\lim_{\varepsilon\to 0^+}\log(\sigma_\varepsilon)$ inside $\mathcal{H}_1$ in the position space. Note that the point-splitting procedure can be applied to the symmetric parts of the distributions involved, because the antisymmetric part is always proportional to the causal propagator of the theory. Thus, one can prove the following lemma ([Sch10], Section 2.2.2).

  Lemma B.1.1. *Denoting with $\sigma_+(\tau',\vec{x}',\tau,\vec{x}) = \tilde{\sigma}_+(\tau',\tau,\|\vec{x}'-\vec{x}\|)$, the symmetrized distribution $\left[(\tilde{\sigma}_+)^{-1}\right]^s : \mathcal{D}(I_\tau\times I_\tau\times\mathbb{R}^3)\to\mathbb{C}$ can be written as*

  $$\left[(\tilde{\sigma}_+)^{-1}\right]^s(f) = \int_{I_\tau'}\int_{I_\tau}\tilde{\sigma}_{\Delta\tau}^{-1}\left(\frac{f(\tau',\tau,\cdot)}{\tilde{q}(\tau',\tau,\|\cdot\|)}\right)a^4(\tau')a^4(\tau)\mathrm{d}\tau'\mathrm{d}\tau,$$

  where $[\tilde{q}]_\tau = a^2$, $\Delta\tau \doteq \tau'-\tau$, and the function $\Delta\tau \mapsto \tilde{\sigma}_{\Delta\tau}^{-1}(h)$ is such that

  $$\begin{aligned}\tilde{\sigma}_{\Delta\tau}^{-1}(h)\lceil_{\Delta\tau=0} &= \lim_{\varepsilon\to 0^+}\int_{\mathbb{R}^3}\frac{h(\vec{x})}{\vec{x}^2+\varepsilon^2}\mathrm{d}\vec{x} \doteq \frac{1}{r_+^2}(h),\\ \partial_{\Delta\tau}\left(\tilde{\sigma}_{\Delta\tau}^{-1}(h)\right)\lceil_{\Delta\tau=0} &= 0,\\ \partial_{\Delta\tau\Delta\tau}\left(\tilde{\sigma}_{\Delta\tau}^{-1}(h)\right)\lceil_{\Delta\tau=0} &= \lim_{\varepsilon\to 0^+}\int_{\mathbb{R}^3}\frac{\triangle h(\vec{x})}{\vec{x}^2+\varepsilon^2}\mathrm{d}\vec{x} \doteq \frac{2}{r_+^4}(h),\end{aligned} \tag{B.2}$$

  for fixed $h\in\mathcal{D}(\mathbb{R}^3)$. In a similar way, the symmetrized distribution $[\log(\tilde{\sigma}_+)]^s : \mathcal{D}(I_\tau\times I_\tau\times\mathbb{R}^3)\to\mathbb{C}$ can be written as

  $$\begin{aligned}[\log(\tilde{\sigma}_+)]^s(f) = &\int_{I_\tau'}\int_{I_\tau}\log(\tilde{q}(\tau',\tau,\|\vec{x}\|))f(\tau',\tau,\vec{x})a^4(\tau')a^4(\tau)\mathrm{d}\tau'\mathrm{d}\tau\mathrm{d}\vec{x}\\ &+\int_{I_\tau'}\int_{I_\tau}\tilde{lo}_{\Delta\tau}\left(f(\tau',\tau,\cdot)\right)a^4(\tau')a^4(\tau)\mathrm{d}\tau'\mathrm{d}\tau,\end{aligned}$$

where the function $\Delta\tau \mapsto \tilde{lo}_0(h)$ *is such that*

$$\tilde{lo}_{\Delta\tau}(h)\restriction_{\Delta\tau=0} = \int_{\mathbb{R}^3} \log(\vec{x}^2) h(\vec{x}) \mathrm{d}\vec{x}, \tag{B.3}$$

$$\partial_{\Delta\tau}\left(\tilde{lo}_{\Delta\tau}(h)\right)\restriction_{\Delta\tau=0} = 0, \tag{B.4}$$

$$\partial_{\Delta\tau\Delta\tau}\left(\tilde{lo}_{\Delta\tau}(h)\right)\restriction_{\Delta\tau=0} = -2 \lim_{\varepsilon\to 0^+} \int_{\mathbb{R}^3} \frac{h(\vec{x})}{\vec{x}^2+\varepsilon^2} = -\frac{2}{r_+^2}(h). \tag{B.5}$$

- **Second step**. Evaluate the Hadamard recursion relations in cosmological spacetimes, using the property that FLRW is conformally related to the flat spacetime in conformal coordinates, and thus obtaining the coinciding-point limits of $\mathcal{H}$ in spatial coordinates. Preliminarily, one computes the coinciding-point limits of the Hadamard coefficients v_0 and v_1 with respect to the Hadamard length scale L, which read

$$[v_0] = \frac{L^2}{4}W, \qquad [\partial_\tau v_0] = \frac{L^2}{8}W',$$
$$\left[\partial_\tau^2 v_0\right] = \frac{L^2}{12}W'', \qquad [v_1] = \frac{L^4}{32}\left(\frac{W''}{3} + W^2\right),$$

where $W(\tau) = w(\tau)^2$, with $w(\tau)$ given in eq. (2.40). Then, the coinciding-point limits of the Hadamard parametrix are evaluated at the first order in the position space, and yield

$$[\mathcal{H}_1] = \frac{1}{4\pi^2 a^2}\left\{\frac{1}{r_+^2} + [v_0]\,\tilde{\mathrm{lo}}_0 + R_{\mathcal{H}_k}(\tau)\right\}, \tag{B.6}$$

$$[\mathcal{H}_1^{(\triangle)}] = \frac{1}{4\pi^2 a^2}\left\{\frac{2}{r_+^4} + \frac{2\,[v_0]}{r_+^2} + [v_1]\,\tilde{\mathrm{lo}}_0 + R^{(\triangle)}_{\mathcal{H}_k}(\tau)\right\}, \tag{B.7}$$

$$[\mathcal{H}_1^{(\tau)}] = \frac{1}{4\pi^2 a^2}\left\{[\partial_\tau v_0]\,\tilde{\mathrm{lo}}_0 + R^{(\tau)}_{\mathcal{H}_k}(\tau)\right\}, \tag{B.8}$$

$$[\mathcal{H}_1^{(\tau\tau')}] = \frac{1}{4\pi^2 a^2}\left\{-\frac{2}{r_+^4} + \frac{1}{2}\left[\partial_\tau^2 v_0\right]\tilde{\mathrm{lo}}_0 + \frac{2\,[v_0]}{r_+^2} + 2\,[v_1]\,\tilde{\mathrm{lo}}_0 + R^{(\tau\tau')}_{\mathcal{H}_k}(\tau)\right\}, \tag{B.9}$$

where

$$\tilde{\mathrm{lo}}_0 \doteq 4\pi \int_0^\infty r^2 \log\left(\frac{r^2}{L^2}\right) h(r)\mathrm{d}r. \tag{B.10}$$

The local rest functions $R^{(\cdot)}_{\mathcal{H}_k}(\tau)$ taken in the coinciding limit $\tau' \to \tau$ are constructed from the Hadamard parametrix, and hence they depend only on the geometry of the spacetime; for their explicit forms, see [Sch10], Section 5.3.2.[2]

- **Third step**. Rewrite the distributions r_+^{-2}, r_+^{-4}, and $\tilde{\mathrm{lo}}_0$ as modes integrals in the momentum space, in order to be subtracted from the two-point function. From [Sch10], Lemma 5.6, the following distributional inverse Fourier transforms hold

$$\mathcal{F}^{-1}_{\vec{x}}\{k_+\} = -\frac{1}{\pi^2 r_+^4}, \qquad \mathcal{F}^{-1}_{\vec{x}}\left\{k_+^{-1}\right\} = \frac{1}{2\pi^2 r_+^2}, \qquad \mathcal{F}^{-1}_{\vec{x}}\left\{k_+^{-3}\right\} = -\frac{1}{2\pi^2}\tilde{\mathrm{lo}}_0.$$

[2]It may be of great helpful using a computer algebra system to perform all these computations. Inside the rest functions, contributions containing the Digamma function, and hence the Euler-Mascheroni constant γ, can be always dropped by a suitable rescale of the Hadamard length scale.

where k_+^z denote the homogeneous distributions introduced, e.g., in [GS21], Section A.1. The last Fourier transform can be also regularized by adding a Heaviside function of the form $\Theta(k-\mu^2)$, where $\mu > 0$ is a cut-off proportional to L^{-1}. Since $\Theta(k-\mu^2)/k^3 - 1/k(k^2+\mu^2) \in L^1(\mathbb{R}, \vec{k})$, it can be further written as

$$\mathcal{F}_{\vec{x}}^{-1}\left\{\frac{1}{k(k^2+\mu^2)}\right\} = -\frac{1}{2\pi^2}\tilde{\log}_0,$$

up to a logarithmic rest depending on μ. Then, one employs a function $\Omega : \mathbb{R}^+ \to \mathbb{R}$ which shares the same $\vec{k}$-asymptotic behaviour of the above distributions in the momentum space, in order to obtain an adiabatic-like regularization prescription. In particular, one chooses a sum of the form $\sum_{n\geq 0} c_n \Omega_n(k)$, where

$$\Omega_n : k \mapsto \frac{1}{(k^2+A)^{n+\frac{1}{2}}}, \tag{B.11}$$

with $A > 0$ - *cf.* [Sch10], Section 5.3.6. To obtain an adiabatic-like regularization, one may set $A = W(\tau_0)$, where $W(\tau_0) = a_0^2\left(m^2 + \left(\xi - \frac{1}{6}\right)R_0\right)$ can be always chosen positive by fixing properly the initial data at $\tau = \tau_0$. Hence,

$$k^2 + A = k_0^2 = k^2 + a_0^2 m^2 + \left(\xi - \frac{1}{6}\right) R_0 a_0^2.$$

B.2 Examples of Renormalized Expectation Values

The expectation value of the Wick square $:\phi^2:$ is obtained from eq. (B.6) using a quantum state whose finite part is only continuous function of time, such as the conformal vacuum or the zero-th order adiabatic state (see also [EG11]). The Hadamard coefficient (B.6) evaluated in momentum space reads

$$\left[\hat{\mathcal{H}}_1\right] = \frac{1}{a^2}\left\{\frac{1}{2k} - \frac{W}{k(k^2+\mu^2)} + \frac{W}{8\pi^2}\log(a) + \frac{R}{288\pi^2}\right\}.$$

Thus, its singular behaviour can be compared with the adiabatic coefficient $C_{\phi^2}^{\mathcal{H}}(\tau,k)$ given in eq. (2.41) to obtain a finite expression of $\langle :\phi^2: \rangle_\omega$: fixing $\mu^2 = \mathrm{e}^2/4$, one finds that

$$C_{\phi^2}^{\mathcal{H}}(\tau,k) - \frac{1}{2k} + \frac{W(\tau)}{k(k^2+\mu^2)} = \frac{1}{2k_0} - \frac{V(\tau)}{4k_0^3} - \frac{1}{2k} + \frac{W(\tau)}{k(k^2+\mu^2)} \in L^1(\mathbb{R}, k^2 dk),$$

in particular

$$\int_{\mathbb{R}^3} \frac{\mathrm{d}\vec{k}}{4\pi}\left(\frac{1}{2k_0} - \frac{V(\tau)}{4k_0^3} - \frac{1}{2k} + \frac{W(\tau)}{k(k^2+\mu^2)}\right) = \frac{1}{4\pi}\left(\frac{W(\tau_0)}{8} - W(\tau)\log(W(\tau_0))\right).$$

Note that the second term in the rest function can be dropped by choosing $\mu^2 = W(\tau_0)\mathrm{e}^2/4$. Hence, from eq. (B.1) with $\mathfrak{D}_1 = \mathfrak{D}_2' = \mathbb{I}$, and recalling that $W(\tau) = w(\tau)^2$,

$$a^2\langle :\phi^2: \rangle_\omega = \frac{1}{(2\pi^3)}\int_{\mathbb{R}^3}\left(|\chi_k|^2 - C_{\phi^2}^{\mathcal{H}}(\tau,k)\right) + \frac{1}{(2\pi^3)}\int_{\mathbb{R}^3}\left(C_{\phi^2}^{\mathcal{H}}(\tau,k) - \frac{1}{2k} + \frac{W}{k(k^2+\mu^2)}\right) d\vec{k} \tag{B.12}$$

$$+\frac{W}{8\pi^2}\log(a) + \frac{R}{288\pi^2} = \frac{1}{(2\pi^3)}\int_{\mathbb{R}^3}\left(|\chi_k|^2 - C_{\phi^2}^{\mathcal{H}}(\tau,k)\right) + Q_0, \tag{B.13}$$

where Q_0 was given by eq. (2.53). As the contribution proportional to R can be absorbed in the renormalization freedoms of $:\phi^2:$, one finally obtains the expression for $\left\langle :\phi^2: \right\rangle_\omega$ given in eq. (2.39).

The renormalization of $\langle :\partial_0\phi\partial_0\phi: \rangle_\omega$ can be achieved similarly to the vacuum polarization, starting from the Hadamard coefficient (B.9), whose singular part reads in the momentum space as

$$[\hat{\mathcal{H}}_1^{(\tau\tau')}] = \frac{1}{a^2}\left\{\frac{k}{2} + \frac{W}{4k} - \frac{W^2 + W''}{16k(k^2+\mu^2)}\right\}$$

such that $|\zeta_k'|^2 - [\mathcal{H}^{(\tau,\tau')}] \in L^1(\mathbb{R}, \vec{k})$ (the explicit form of the rest function $R_{\mathcal{H}_k}^{(\tau\tau')}(\tau)$ is irrelevant for the scopes of this evaluation). Fixing $\mu^2 = W(\tau_0)\mathrm{e}^2/4$ to optimize the rest function, that singular part can be replaced by the coefficient $C_E^{\mathcal{H}}(\tau, k)$ defined in eq. (2.49):

$$C_E^{\mathcal{H}}(\tau, k) = \frac{k_0}{2} + \frac{V(\tau)}{4k_0} - \frac{V''(\tau) + V(\tau)^2}{16k_0^3}, \tag{B.14}$$

since

$$\begin{aligned}\int_{\mathbb{R}^3} \frac{\mathrm{d}\vec{k}}{4\pi}\left(\frac{k_0}{2} + \frac{V(\tau)}{4k_0} - \frac{V''(\tau)+V(\tau)^2}{16k_0^3} - \frac{k}{2} - \frac{W(\tau)}{4k} + \frac{W(\tau)^2 + W''(\tau)}{16k(k^2+\mu^2)}\right)\\ = \frac{W(\tau_0)}{16}\left(\frac{W(\tau_0)}{4} - W(\tau)\right),\end{aligned}$$

namely $C_E^{\mathcal{H}}(\tau, k) - [\mathcal{H}^{(\tau,\tau')}] \in L^1(\mathbb{R}, \vec{k})$. In this difference, no time derivatives of order higher than two appear in the rest function. On the other hand, the contribution proportional to k_0^3, which depends on the fourth-order derivative of $a(\tau)$, can be neglected from $C_E^{\mathcal{H}}(\tau, k)$ in the evaluations made in proposition 2.2.2, because one needs to compute $(|\zeta_k'|^2 - C_E^{\mathcal{H}})/\Omega_k^2$, and hence only singularities up to k_0^{-1} must be subtracted.

The regularized energy density operator $:\varrho:$ is obtained starting from the 00-component of the quantum stress-energy tensor (1.108) and taking the second-order modes, provided that no time derivatives of order higher than fourth appear. The computation of $\varrho \doteq T_{\mu\nu}e_0^\mu e_0^\nu$, where $e_0^\mu = \partial_t = a^{-1}\partial_\tau$, yields

$$\varrho = (1-2\xi)\partial_0\phi\partial_0\phi - 2\xi(\partial_0\partial_0\phi)\phi + 2\xi\mathcal{H}_a\partial_0\phi + 3\xi\mathcal{H}_a^2\phi^2 + \tag{B.15}$$

$$2\xi\left((\partial_0^2 - \triangle)\phi + 2\mathcal{H}_a\partial_0\phi\right)\phi + \left(2\xi - \frac{1}{2}\right)(\partial_0\phi\partial_0\phi - h^{ij}\partial_i\phi\partial_j\phi) + \frac{1}{2}a^2m^2, \tag{B.16}$$

where $\mathcal{H}_a \doteq a'/a$, and h^{ij} denotes the induced spatial metric associated to FLRW spacetimes (2.3). In this computation, the following relations were used:

$$\nabla_0\nabla_0\phi = (\partial_0^2 - \mathcal{H}_a\partial_0)\phi, \qquad \nabla^\rho\phi\nabla_\rho\phi = -a^{-2}\left(\partial_0\phi\partial_0\phi - h^{ij}\partial_i\phi\partial_j\phi\right),$$
$$G_{00} = 3\mathcal{H}_a^2, \qquad \nabla_\rho\nabla^\rho\phi = -a^{-2}\left(\partial_0^2 - \triangle + \frac{2a'}{a}\partial_0\right)\phi.$$

As the expectation value $\langle :\varrho: \rangle_\omega$ in a quantum state ω represents a distribution of matter, it can be defined on a three-dimensional volume $\mathcal{V}$ as [Bun80]

$$\langle :T_{00}: \rangle_\omega \doteq \frac{\left\langle \int_{\mathcal{V}} d^3\vec{x}\sqrt{h}\, :T_{00}: \right\rangle_\omega}{\left\langle \int_{\mathcal{V}} d^3\vec{x}\sqrt{h} \right\rangle_\omega}. \tag{B.17}$$

Assuming that $\langle :T_{00}: \rangle_\omega$ decays rapidly for a sufficiently large $\mathcal{V}$, the spatial term $h^{ij}\partial_i\phi\partial_j\phi$ leads to

$$\int d^3\vec{x}\sqrt{h}\, h^{ij}\partial_i\phi\partial_j\phi = \int d^3\vec{x}\sqrt{h}\,\nabla_i\left(\phi'\partial^i\phi\right) - \int d^3\vec{x}\sqrt{h}\,\phi\triangle\phi,$$

where the first terms can be converted to a surface term which vanishes in this large-volume limit. Thus, the expression of the renormalized expectation value of the energy density finally reads as

$$\left\langle :T_{00}\left(\bar{\phi},\phi\right): \right\rangle_\omega = \frac{1}{2}\left\langle :\partial_0\bar{\phi}\partial_0\phi: \right\rangle_\omega + 6\xi\mathcal{H}_a\left\langle :(\partial_0\bar{\phi})\phi: \right\rangle_\omega - \frac{1}{2}\left\langle :\bar{\phi}\triangle\phi: \right\rangle_\omega + \frac{1}{2}\left(6\xi\mathcal{H}_a^2 + a^2m^2\right)\left\langle :\phi^2: \right\rangle_\omega . \tag{B.18}$$

To obtain the expression of the unrenormalized energy density per modes given in eq. (2.31), it is sufficient to replace ϕ with ζ_k/a in eq. (B.18), where ζ_k are the modes associated to a homogeneous and isotropic pure state (2.11), after symmetrized the contributions proportional to $\left\langle :(\partial_0\bar{\phi})\phi: \right\rangle_\omega$ and $\left\langle :\bar{\phi}\triangle\phi: \right\rangle_\omega$. Thus, according to the Hadamard point-splitting regularization (B.1) and the definition of the quantum stress-energy tensor given in eq. (1.119), the corresponding expectation value of the renormalized Wick operator gets

$$\begin{aligned}\langle :\varrho: \rangle_\omega = {} & \lim_{x'\to x}\mathcal{R}(x',x)\left[\frac{1}{(2\pi)^3 a(\tau')a(\tau)}\int_{\mathbb{R}^3} d\vec{k}\,\left(\overline{\zeta}_k(\tau')\zeta_k(\tau) - \hat{\mathcal{H}}_1(\tau',\tau,k)\right)\mathrm{e}^{i\vec{k}\cdot(\vec{x}'-\vec{x})}\right] \\ & - \frac{1}{4\pi^2}[v_1] + C_{00},\end{aligned} \tag{B.19}$$

where

$$\mathcal{R}(x',x) \doteq \frac{1}{2a^2}\left(\partial_{\tau'}\partial_\tau + 12\xi\mathcal{H}_a\partial_{\tau'} - \triangle + 6\xi\mathcal{H}_a^2 + a^2m^2\right), \tag{B.20}$$

is the differential operator related to $:\varrho:$. Here, both the renormalization freedom

$$C_{00} = -c_1m^4 + 3c_2m^2H^2 + \left(c_3 + \frac{c_4}{3}\right)I_{00}, \qquad I_{00} = 18\dot{H}^2 - 36\ddot{H}H - 108\dot{H}H^2, \tag{B.21}$$

and the coefficient of the trace anomaly given in eq. (1.66)

$$\begin{aligned}[v_1] = {} & \frac{m^4}{8} - \frac{1}{60}\left(\dot{H}H^2 + H^4\right) + \frac{1}{24}\left(\frac{1}{5} - \xi\right)\left(\dddot{H} + 6\ddot{H}H + 4\dot{H}^2 + 12\dot{H}H^2\right) \\ & + \frac{1}{8}(6\xi-1)^2\left(\dot{H}^2 + 4\dot{H}H^2 + 4H^4\right) + \frac{1}{4}(6\xi-1)m^2(\dot{H} + 2H^2)\end{aligned} \tag{B.22}$$

are expressed in cosmological time t.

After some (long) computations which combine the expressions of the Hadamard coefficients given in eqs. (B.6) to (B.9) and the corresponding rest functions, the expression of $\langle :\varrho: \rangle_\omega$ evaluated in a homogeneous and isotropic pure state becomes

$$\begin{aligned}\langle :\varrho: \rangle_\omega = {} & \frac{1}{(2\pi)^3a^4}\int_{\mathbb{R}^3}\left(\frac{|\zeta_k'|^2}{2} + \left(k^2 + a^2m^2 - (6\xi-1)\,a^2H^2\right)\frac{|\zeta_k|^2}{2} + aH\,(6\xi-1)\,2\mathrm{Re}(\overline{\zeta}_k\zeta_k')\right. \\ & \left. - C_\varrho^{\mathcal{H}}(\tau,k)\right)\mathrm{d}\vec{k} + R_{\mathcal{H}_k}^{\varrho}(\tau) - \frac{1}{4\pi^2}[v_1] + C_{00},\end{aligned} \tag{B.23}$$

where $C_\varrho^{\mathcal{H}}(\tau,k)$ was given in eq. (2.41), and

$$R_{\mathcal{H}_k}^{\varrho}(\tau) - \frac{1}{4\pi^2}[v_1] = \frac{1}{96\pi^2}\left\{-\frac{H^4}{10} + \frac{m^2}{3}(36\xi-5)G_{00} - \frac{1}{180}\left(60\xi-11\right)I_{00} + (6\xi-1)^2H^2R\right\}. \tag{B.24}$$

Here, the cut-off scale a^2/L^2 was chosen to regularize the logarithmic distribution (B.10), after dropping a contribution $\mathrm{e}^{2\gamma-2}$ through a rescaling of L; also, the factor a^2 allows to remove a contribution proportional to $\log(a)$ from the rest function. The formula for $\langle{:}\varrho{:}\rangle_\omega$ written in eq. (2.39) is finally obtained after reabsorbing the contributions proportional to the renormalization freedoms inside a new redefinition of C_{00}. Notably, in eq. (B.24) the higher-order derivatives terms coming from $R^{\varrho}_{\mathcal{H}_k}(\tau)$ are exactly cancelled by the ones contained in the trace anomaly, as expected from proposition 2.1.2. Actually, without the choice of the regularization scale μ inside $C^{\mathcal{H}}_{\varrho}(\tau, k)$, eq. (B.24) acquires an additional term of the form

$$\left[R^{\varrho}_{\mathcal{H}_k}(\tau) - \frac{1}{4\pi^2}[v_1]\right]_{\mu^2 = \frac{e^{2\gamma-2}a^2}{2\lambda^2}} - \left[R^{\varrho}_{\mathcal{H}_k}(\tau) - \frac{1}{4\pi^2}[v_1]\right]_{\mu^2=0}$$
$$= \frac{1}{4\pi^2}\left(\frac{m^4}{16} + \frac{m^2}{18}(6\xi-1)G_{00} - \frac{1}{288}a^2(6\xi-1)^2 I_{00}\right)\left(2 - 2\gamma + \log\left(\frac{a^2}{2\lambda^2}\right)\right),$$

and thus eq. (7.13) in [Sie15], Section 7.3.2 is regained (see also [Hac16], Section 3.2.3).

Appendix C

Auxiliary results from Mathematical Analysis

C.1 Functional Derivatives and Fixed-point Theorem

The proof of local existence and uniqueness of cosmological solutions of the semiclassical Einstein equations performed in chapter 2 employed the Banach fixed-point theorem and the notion of contraction on Banach spaces. Here, some results shall be reviewed, according to the definitions and the nomenclatures followed in the Appendix A of [PS15a], which are mostly inferred from [Ham82].

Definition C.1.1. A seminorm on a vector space F is a real-valued function $\| \, \| : F \to \mathbb{R}$ such that $\forall f, g \in F$ and $c \in \mathbb{R}$

1. $\|f\| \geq 0$,
2. $\|f + g\| \leq \|f\| + \|g\|$,
3. $\|cf\| = |c| \cdot \|f\|$.

A collection of seminorms $\{\| \, \|_n : n \in \mathbb{N}\}$ defines a unique topology such that the sequence $f_i \to f$ if and only if $\|f - f_i\|_n \to 0$ for all $n \in \mathbb{N}$. Thus, the vector space is locally convex topological whenever a collection of seminorms arises, and it is metrizable if and only if the collection is also a sequence, i.e., it is countable. The vector space is Hausdorff if and only if $f = 0$ when $\|f\|_n = 0$ for all n.

Definition C.1.2. A Fréchet space is a complete Hausdorff metrizable locally convex topological vector space

Definition C.1.3. Given $f \in F$ on a Fréchet space F, if $f = 0$ whenever $\|f\| = 0$, then $\| \, \|$ is a norm. If the collection of seminorms of F contains only one norm, then F is a Banach space. In this case, the Banach space $(F, \| \, \|)$ is complete with respect to $\| \, \|$, i.e., every Cauchy sequence f_i such that $\|f - f_i\| \to 0$ converges in F.

An example of Banach space which has been used in chapter 2 is the space $C^N[a, b]$ of N-differentiable functions, $0 \leq N \leq \infty$, equipped with the (uniform) norm

$$\|f\|_N = \sum_{j=0}^{N} \sup_{x \in [a,b]} |D^j f(x)|.$$

The case $N = 0$ has been employed in the cosmological problem referring to the scale factor $a(\tau)$ as a continuous function in a small interval of time $[\tau_0, \tau_1]$.

On Fréchet spaces, and hence on Banach spaces $\mathcal{D}$, a notion of directional derivative, also named as Gateaux derivative, can be posed; if the derivative involves functionals $F : \mathcal{D} \to \mathbb{R}$, it is also called functional derivative.

Definition C.1.4. Let $\mathcal{F}$ and $\mathcal{G}$ be Fréchet (Banach) spaces, $\mathcal{D} \subset \mathcal{F}$, and $F : \mathcal{D} \to \mathcal{F}$ a continuous non-linear map. The Gateaux differential of F at $V \in \mathcal{D}$ in the direction $W \in \mathcal{D}$ is defined as the map

$$
\begin{aligned}
&\delta F : \mathcal{D} \times \mathcal{D} \to G \\
&\delta F[V, W] \doteq \lim_{\epsilon \to 0^+} \frac{F[V + \epsilon W] - F[V]}{\epsilon},
\end{aligned}
\tag{C.1}
$$

where the limit $\epsilon \to 0^+$ is taken with respect to the norm topology of $\mathcal{D}$. Moreover, the functional $F : \mathcal{D} \to \mathbb{R}$ is said to be Gateaux differentiable in V, and the map (C.1) is called Gateaux derivative of F in V, if the functional derivative at V exists for every direction $W \in \mathcal{D}$, and, furthermore, $\delta F[V, W]$ is linear and continuous in W.

The Gateaux derivative fulfils all the properties of ordinary derivatives, such as linearity, continuity, the fundamental theorem of calculus, and the chain rule to evaluate composition of functionals. Let F be a functional which depends on V through another functional $A[V]$ having functional dependence on V, i.e., $F[V] = \tilde{F}[A[V]]$, then the functional derivative of F in $W = \delta V$ reads

$$
\begin{aligned}
\delta F[V, \delta V] &= \lim_{\epsilon \to 0^+} \frac{\tilde{F}[A[V + \epsilon \delta V]] - \tilde{F}[A[V]]}{\epsilon} \\
&= \lim_{\epsilon \to 0^+} \frac{\tilde{F}[A[V] + \epsilon \delta A[V, \delta V]] - \tilde{F}[A[V]]}{\epsilon} = \delta \tilde{F}[A, \delta A[V, \delta V]].
\end{aligned}
$$

Thus, assuming that both $\tilde{F}$ and A are Gateaux differentiable, namely there exists two positive constants C_1 and C_2 which do not depend on A and V such that

$$
|\delta \tilde{F}[A, B]| \leq C_1 \|B\|, \qquad \|\delta A[V, W]\| \leq C_2 \|W\|.
$$

then $|\delta F[V, \delta V]| \leq C_1 C_2 \|\delta V\|$, and hence the Lipschitz continuity is obtained. For further properties of the directional derivative, see [Ham82], Part I.3.

The Gateaux differentiability is essential to prove the locally Lipschitz continuity of functionals on Fréchet and Banach spaces.

Proposition C.1.1. *Let $F : \mathcal{D} \to \mathbb{R}$ be a functional on the Fréchet (Banach) space $(\mathcal{D}, \| \, \|)$ whose functional derivative $\delta F[V, W]$ depends continuously on W uniformly in V, namely*

$$
\|\delta F[V, W]\| \leq C \|W\|
$$

for some $C \geq 0$ which does not depend on V. Then, F is locally Lipschitz continuous on $\mathcal{D}$, i.e., for every neighborhood $U \subset \mathcal{D}$ of $V_0 \in U$ there exists a constant $C \geq 0$ called Lipschitz constant such that, for all $V_1, V_2 \in U$,

$$
|F[V_1] - F[V_2]| \leq C \|V_1 - V_2\|. \tag{C.2}
$$

In the case of a composite functional $F[V] = \tilde{F}[A[V]]$, where both $\tilde{F}$ and A are Gateaux differentiable with Lipschitz constants C_1 and C_2, respectively,

$$
|F[V_1] - F[V_2]| \leq C_1 C_2 \|V_1 - V_2\|. \tag{C.3}
$$

Proof. The proof follows directly from the property of functional derivatives $\delta F[V,W]$, which are linear in W and satisfies the fundamental theorem of calculus in $U \subset \mathcal{D}$, namely

$$F[V_1]-F[V_2]=\int_0^1 \frac{\mathrm{d}}{\mathrm{d}\epsilon}F[V_2+\epsilon(V_1-V_2)]\mathrm{d}\epsilon=\int_0^1 \delta F[\epsilon V_1+(1-\epsilon)V_2, V_1-V_2]\mathrm{d}\epsilon$$

for $V_1, V_2 \in U$. Taking the norm on both sides and assuming the Gateaux differentiability of F,

$$\|F[V_1]-F[V_2]\| \le \int_0^1 \|\delta F[\epsilon V_1+(1-\epsilon)V_2, V_1-V_2]\|\mathrm{d}\epsilon \le C\|V_1-V_2\|,$$

where C is the supremum of $\|\delta F[V,W]\|$, and eq. (C.2) follows. The same proof can be applied also in the case of composite functionals $F[V]=\tilde{F}[A[V]]$, thus getting eq. (C.3). □

The notion of contraction is strictly related to the value of the Lipschitz constant associated to a Lipschitzian functional F in the Banach space $(X, \| \, \|)$, because F is said to be a contraction if and only if F satisfies eq. (C.2) with $C<1$. The main property of contractions in complete metric spaces consists of satisfying Banach's contraction principle, which leads to Banach's fixed-point theorem.

Theorem C.1.1. *Let $(X, \| \, \|)$ be a complete metric space and let $F: X \to X$ be a contraction with Lipschitzian constant C. Then F admits a unique fixed point $u=F(u)$ in X. Furthermore, denoting with $F^n(x)$, $n \ge 0$, the iterative action of F on x such that $F^0=x$, $F^{n+1}(x)=F\left(F^n(x)\right)$, for any $x \in X$*

$$\lim_{n\to\infty} F^n(x)=u,$$

with

$$\|F^n(x)-u\| \le \frac{C^n}{1-C}\|F(x)-x\|.$$

Banach fixed-point theorem is useful in practice to prove that (functional) equations of the form $x=F(x)$ admits locally a unique solution in a compact set U like a one-dimensional closed interval, since such a solution corresponds to the unique fixed-point of the contraction map F; notably, it is necessary that F is also an internal operator in U to obtain this result, i.e. $F(U) \subset U$, otherwise the proof cannot hold. On the contrary, if F satisfies such requirements, then the following theorem can be formulated, using as compact set a closed ball.

Theorem C.1.2. *Let $(X, \| \, \|)$ be a complete metric space and let*

$$B(x_0,r)=\{x \in X : \|x-x_0\| < r\}$$

be the ball of radius $r>0$ centered in $x_0 \in X$. Assume that $F: B(x_0,r) \to X$ is a contraction with Lipschitzian constant C and, moreover, $\|F(x_0)-x_0\| < (1-C)r$, namely F is internal in $B(x_0,r)$. Then F has a unique fixed point in $B(x_0,r)$.

The proofs of both the theorems can be found, e.g., in [AMO01], Chapter 1.

C.2 Grönwall's Lemma

In the study of wave equations in curved spacetimes, it is not uncommon to run into a second-order differential initial-value problem for the solution $f \in C^n[\tau_0,\infty)$, with $n \ge 2$, of the form

$$\begin{cases} f''+(k^2+W)f=h, \\ (f(\tau_0), f'(\tau_0))=(f_0,f_0'), \end{cases} \tag{C.4}$$

where k is some constant, W and h are known functions in $C^n[\tau_0,\infty)$ and where f_0, f_0' are suitable constants expressing initial conditions for f at τ_0. Thus, it is often convenient to obtain some estimates on the behaviour of f, in order to keep its evolution in time under control. To this aim, the so-called Grönwall's Lemma allows to obtain some bounds on a function f which satisfies a certain differential inequality [Gro19; AM01]

Theorem C.2.1. *Let $I = [\tau_0,\infty) \subset \mathbb{R}$, $\tau_0 \in I$, and $\alpha, \beta, u : I \to \mathbb{R}^+$ some non-negative, continuous function in I. If*

$$u(\tau) \leq \alpha(\tau) + \int_{\tau_0}^{\tau} \beta(\eta)u(\eta)\mathrm{d}\eta \tag{C.5}$$

for all $\tau \in I$, then

$$u(\tau) \leq \alpha(\tau) \exp \int_{\tau_0}^{\tau} \alpha(\eta)\beta(\eta) \exp\left(\int_{\eta}^{\tau} \beta(\sigma)\mathrm{d}\sigma\right)\mathrm{d}\eta \tag{C.6}$$

for all $\tau \in I$. If, in addition, α is a non decreasing function on I, then

$$u(\tau) \leq \alpha(\tau) \exp \int_{\tau_0}^{\tau} \beta(\eta)\mathrm{d}\eta \tag{C.7}$$

for all $\tau \in I$.

Proof. Let be $v(\tau) \doteq \int_{\tau_0}^{\tau} \beta(\eta)u(\eta)\mathrm{d}\eta$, $v(\tau_0) = 0$, then it follows from eq. (C.5) that

$$\partial_\tau v(\tau) = \beta(\tau)u(\tau) \leq \alpha(\tau)\beta(\tau) + \beta(\tau)v(\tau).$$

After multiplying for $\gamma \doteq \exp(-v)$, one obtains the inequality $\partial_\tau(v\gamma) \leq \alpha\beta\gamma$, and hence $v \leq (1/\gamma)\int_{\tau_0}^{\tau} \alpha\beta\gamma\mathrm{d}\eta$. So,

$$u(\tau) \leq \alpha(\tau) + v(\tau) \leq \alpha(\tau) + \int_{\tau_0}^{\tau} \alpha(\eta)\beta(\eta) \exp\left(\int_{\eta}^{\tau} \beta(\sigma)\mathrm{d}\sigma\right)\mathrm{d}\eta$$

which is the first claimed estimate for u. Thus, if α is also a monotone increasing function in I, then $\alpha(\eta) \leq \alpha(\tau)$, and hence

$$\begin{aligned} u(\tau) &\leq \alpha(\tau)\left(1 + \int_{\tau_0}^{\tau} \beta(\eta) \exp\left(\int_{\eta}^{\tau} \beta(\sigma)\mathrm{d}\sigma\right)\mathrm{d}\eta\right) = \alpha(\tau)\left(1 - \exp\left(\int_{\eta}^{\tau} \beta(\sigma)\mathrm{d}\sigma\right)\Big|_{\tau_0}^{\tau}\right) \\ &\leq \alpha(\tau) \exp\left(\int_{\tau_0}^{\tau} \beta(\eta)\mathrm{d}\eta\right), \end{aligned}$$

which concludes the proof. □

Thus, some useful properties of the solution of eq. (C.4) can be derive in the next lemmas: these estimates will be essential in section 2.2 to prove existence and uniqueness of solutions of the semiclassical Einstein equations in cosmological spacetimes.

Lemma C.2.1. *Let $f \in C^n[\tau_0,\infty)$ be the unique solution of (C.4). Hence, for $k \geq 0$*

$$f = -\Delta_R^k * (Wf) + \Delta_R^0 * h + f_0 \cos(k(\tau - \tau_0)) + f_0' \frac{\sin(k(\tau - \tau_0))}{k}, \tag{C.8}$$

where $\Delta_R^k(\tau) = \frac{\sin(k\tau)}{k}\theta(\tau)$ for $k \geq 0$ is the retarded fundamental solutions of $\mathrm{d}^2/\mathrm{d}\tau^2 + k^2$ and in particular at $k = 0$ $\Delta_R^0(\tau) = \tau\theta(\tau)$. Furthermore, the convolution $*$ is computed on the interval $[\tau_0,\infty)$. Then, the following estimate holds for $k \geq 0$, $\tau \geq \tau_0$:

$$|f(\tau)| \leq \left(|f_0| + (\tau - \tau_0)|f_0'| + (\tau - \tau_0)^2\|h\|_\infty\right) \exp\left((\tau - \tau_0)^2\|W\|_\infty\right). \tag{C.9}$$

Furthermore, for $k > 0$ we have for $\tau \geq \tau_0$

$$|f(\tau)| \leq \left(|f_0| + \frac{1}{k}|f_0'| + \frac{1}{k}\int_{\tau_0}^{\tau} |h(\eta)|\mathrm{d}\eta\right) \exp\left(\frac{1}{k}\int_{\tau_0}^{\tau} |W|\mathrm{d}\eta\right). \tag{C.10}$$

Proof. Equation (C.8) can be obtained by computing the convolution of both sides of (C.4) with Δ_R^k on $[\tau_0, \infty)$ and integrating by parts a couple of times. Applying Grönwall lemma, from equation (C.8) one gets for $\tau \geq \tau_0$

$$|f(\tau)| \leq (\tau - \tau_0)\int_{\tau_0}^{\tau} |W(\eta)f(\eta)|\mathrm{d}\eta + (\tau - \tau_0)\int_{\tau_0}^{\tau} |h(\eta)|\mathrm{d}\eta + |f_0| + |f_0'|(\tau - \tau_0),$$

or for $k > 0$

$$|f(\tau)| = \frac{1}{k}\int_{\tau_0}^{\tau} |W(\eta)f(\eta)|\mathrm{d}\eta + \frac{1}{k}\int_{\tau_0}^{\tau} |h(\eta)|\mathrm{d}\eta + |f_0| + \frac{1}{k}|f_0'|,$$

hence by Grönwall lemma the desired estimate for $|f(\tau)|$ stated in (C.9) and in (C.10) follows. □

Lemma C.2.2. *Let $a \in C^2[\tau_0, \tau_1]$ be the unique solution of $a'' = Xa$ with $a'(\tau_0) = a_0'$ and $a(\tau_0) = a_0$ with $X \in C^1[\tau_0, \tau_1]$. Then the following inequalities hold:*

$$\|a - a_0\|_\infty \leq (\tau_1 - \tau_0)\left(|a_0'| + |a_0|\frac{(\tau_1 - \tau_0)}{2}\|X\|_\infty\right) \exp\left(\frac{(\tau_1 - \tau_0)^2}{2}\|X\|_\infty\right),$$

$$\|a' - a_0'\|_\infty \leq \frac{(\tau_1 - \tau_0)^2}{2}\left(a_0\|X\|_\infty + \|a\|_\infty\|X'\|_\infty\right) \exp\left(\frac{(\tau_1 - \tau_0)^2}{2}\|X\|_\infty\right),$$

$$\|\delta a\|_\infty \leq \frac{(\tau_1 - \tau_0)^2}{2}\|a\|_\infty \exp\left(\frac{(\tau_1 - \tau_0)^2}{2}\|X\|_\infty\right)\|\delta X\|_\infty,$$

$$\|\delta a'\|_\infty \leq \frac{(\tau_1 - \tau_0)^2}{2}\left(\|(a\delta X)'\|_\infty + \|X'\delta a\|_\infty\right) \exp\left(\frac{(\tau_1 - \tau_0)^2}{2}\|X\|_\infty\right),$$

where $\delta a[X, \delta X]$ denotes the functional derivatives with respect to infinitesimal changes $\delta X \in C^1[\tau_0, \tau_1]$ and where the uniform norms are computed on the interval (τ_0, τ_1).

Proof. From Lemma (C.2.1) applied to the equation $a'' = Xa$, namely for $k = 0$, the retarded fundamental solution reads $\Delta_R(\tau) = \tau\theta(\tau)$, hence from (C.8) one gets

$$a(\tau) = a_0 + (\tau - \tau_0)a_0' + \int_{\tau_0}^{\tau} (\tau - \eta)X(\eta)a(\eta)\mathrm{d}\eta. \tag{C.11}$$

Then,

$$|a - a_0| \leq (\tau - \tau_0)|a_0'| + \int_{\tau_0}^{\tau} (\tau - \eta)|X(\eta)||a(\eta) - a_0|\mathrm{d}\eta + |a_0|\frac{|(\tau - \tau_0)|^2}{2}\|X\|_\infty.$$

Grönwall inequality gives the first inequality. The bound for the first derivative can be obtained in a similar way starting from the first derivative of equation (C.11)

$$a'(\tau) - a_0' = \int_{\tau_0}^{\tau} (\tau - \eta)\left(X(\eta)a_0 + X'(\eta)a(\eta)\right)\mathrm{d}\eta + \int_{\tau_0}^{\tau} (\tau - \eta)X(\eta)(a'(\eta) - a_0')\mathrm{d}\eta,$$

then writing the corresponding local inequality and finally applying again Grönwall inequality. The inequalities for the functional derivatives are obtained computing the first functional derivatives of (C.11), which read

$$\delta a = \int_{\tau_0}^{\tau} (\tau - \eta)\left(\delta X(\eta)a(\eta) + X(\eta)\delta a(\eta)\right)\mathrm{d}\eta,$$

$$\delta a' = \int_{\tau_0}^{\tau} (\tau - \eta)\left((\delta X(\eta)a(\eta))' + X'(\eta)\delta a(\eta) + X(\eta)\delta a'(\eta)\right)\mathrm{d}\eta.$$

Eventually, we the desired results is got after operating as before. □

C.3 Large-time Decay

This appendix contains a proof of the Lemma which establishes the decay at large times of certain functions expressed in the Fourier domain. This result is essential to achieve the main statements presented in subsection 4.2.3 about the stability of linearized semiclassical solutions. The main ideas of this proof are already presented in literature, and they can be found, e.g., in [BB02].

Lemma C.3.1. *Let $\tilde{f} \in \mathcal{S}(\mathbb{R}^3)$ be a Schwartz function, and consider its spherical average*

$$f(p) = \frac{1}{4\pi} \int \tilde{f}(\vec{p}) \mathrm{d}\Omega,$$

where $p \doteq |\vec{p}|$ and $\mathrm{d}\Omega$ denotes the standard measure on the two-dimensional surface of the unit sphere. Consider

$$W(t) = \int_0^\infty f(p) \frac{\mathrm{e}^{i\omega t}}{\omega} p^2 \mathrm{d}p, \qquad \omega = \sqrt{p^2 + m^2},$$

then $W(t)$ decays for large times as $t^{-3/2}$ if $m > 0$, and as t^{-2} if $m = 0$.

Proof. Consider, in a first step, the massless case $m = 0$, i.e., $\omega = p$. Then,

$$W(t) = \int_0^\infty f(p) \mathrm{e}^{ipt} p \mathrm{d}p = \frac{1}{(it)^2} \int_0^\infty f(p) p \partial_p^2 \mathrm{e}^{ipt} \mathrm{d}p.$$

After integrating by parts twice, and using the rapid decay of $f \in \mathcal{S}(\mathbb{R}^3)$,

$$W(t) = \frac{f(0)}{(it)^2} + \frac{f(0)}{(it)^2} \int_0^\infty \partial_p^2 (p f(p)) \mathrm{e}^{ipt} \mathrm{d}p, \tag{C.12}$$

where $\partial_p^2(pf(p)) \in L^1(\mathbb{R}^+)$ because $f(p)$, together with its derivatives, is of rapid decrease. Hence, by Riemann-Lebesgue lemma

$$\lim_{t \to \infty} \int_0^\infty \partial_p^2 (p f(p)) \mathrm{e}^{ipt} \mathrm{d}p = 0,$$

which implies that the second contribution in eq. (C.12) vanishes more rapidly than $1/t^2$ for large times.

Similar ideas are followed to prove the decaying behaviour in the massive case $m > 0$. After changing variable of integration

$$p = \sqrt{\frac{y}{t}\left(\frac{y}{t} + 2m\right)},$$

the starting integral reads

$$W(t) = \frac{\mathrm{e}^{imt}}{t^{3/2}} \int_0^\infty f\left(\sqrt{\frac{y}{t}\left(\frac{y}{t} + 2m\right)}\right) \mathrm{e}^{iy} \sqrt{\frac{y}{t} + 2m} \sqrt{y} \mathrm{d}y.$$

The evaluation of this integral is performed by inserting an ϵ regulator, and thus by dividing the integral in two parts,

$$W(t) = \frac{e^{imt}}{t^{3/2}} f(0) \sqrt{2m} \lim_{\epsilon \to 0^+} \int_0^\infty \mathrm{e}^{iy - \epsilon y} \sqrt{y} \mathrm{d}y + \frac{\mathrm{e}^{imt}}{t^{3/2}} \lim_{\epsilon \to 0^+} \int_0^\infty \left(g\left(\frac{y}{t}\right) - g(0)\right) \mathrm{e}^{iy - \epsilon y} \sqrt{y} \mathrm{d}y,$$

where $g(y) = \sqrt{y+2m} f(\sqrt{y(y+2m)})$. On one side, the first contribution tends to a constant as $\epsilon \to 0$, because

$$\lim_{\epsilon\to 0^+} \int_0^\infty \mathrm{e}^{iy-\epsilon y} \sqrt{y} \mathrm{d}y = \frac{\sqrt{\pi}}{2(-i)^{3/2}}.$$

On the other side, it can be shown that the second contribution decays faster then $1/t^{3/2}$. To prove it, consider the following integral

$$A \doteq \lim_{\epsilon\to 0^+} \int_0^\infty \left(g(\frac{y}{t}) - g(0) \right) \mathrm{e}^{iy} \mathrm{e}^{-\epsilon y} \sqrt{y} \mathrm{d}y,$$

which is equal to

$$A = \lim_{\epsilon\to 0^+} \frac{1}{(i-\epsilon)^2} \int_0^\infty \sqrt{y} \left(g\left(\frac{y}{t}\right) - g(0) \right) \partial_y^2 \left(\mathrm{e}^{iy-\epsilon y} - 1 \right) \mathrm{d}y.$$

After integrating by parts twice, and in view of the decay properties of g and its derivatives for large arguments,

$$A = \lim_{\epsilon\to 0^+} \frac{1}{(i-\epsilon)^2} \int_0^\infty \partial_y^2 \sqrt{y} \left(g\left(\frac{y}{t}\right) - g(0) \right) \left(\mathrm{e}^{iy-\epsilon y} - 1 \right) \mathrm{d}y.$$

Thus, after defining for $0 < \delta < 1/2$

$$h_\delta(x) \doteq (x)^{3/2-\delta} \, \partial_x^2 \left(\sqrt{x} \, (g(x) - g(0)) \right),$$

the above integral reads

$$A = \lim_{\epsilon\to 0^+} \frac{1}{(i-\epsilon)^2} \frac{1}{t^\delta} \int_0^\infty h_\delta\left(\frac{y}{t}\right) \frac{\left(\mathrm{e}^{iy-\epsilon y} - 1\right)}{y^{3/2-\delta}} \mathrm{d}y.$$

In this representation, $h_\delta(x)$ is a bounded function, because the difference $g(x) - g(0)$ vanishes as $x \to 0$, and g decays faster to 0 for large x. Therefore,

$$|A| \leq \lim_{\epsilon\to 0^+} \frac{C}{t^\delta} \int_0^\infty \left| \frac{\left(\mathrm{e}^{iy-\epsilon y} - 1\right)}{y^{3/2-\delta}} \right| \mathrm{d}y.$$

for a suitable constant C. Since C is uniform in ϵ and $0 < \delta < 1/2$, the limit as $\epsilon \to 0$ can be taken before computing the integral by applying the dominated convergence theorem, and yields the following bound

$$|A| \leq \frac{\tilde{C}}{t^\delta}.$$

This last result concludes the proof.

□

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