Probing of Singular Geometries in the Functional Schrödinger Formulation of Quantum Field Theory

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Contents

Zusammenfassung

Die vorliegende Dissertation befasst sich mit der Definition möglicher Konsistenzkriterien für Quantenfeldtheorien auf allgemeinen Raumzeiten. Obwohl vergleichbare Vollständigkeitsbedingungen für den klassischen, geometrischen und quantenmechanischen Kontext bereits existieren, wurden sie bisher kaum für feldtheoretische Anwendungen in Betracht gezogen. Die Schrödinger Formulierung der Quantenfeldtheorie ermöglicht die Evolution von Quantenfeldern in enger Anlehnung an bestehende quantenmechanische Konzepte zu betrachten. Insbesondere beschäftigt sich diese Arbeit mit der Anwendung auf Raumzeiten welche klassisch als singulär gelten und der Frage inwiefern sich die klassische Singularität auf die Quantenevolution auswirkt.

Für ein bestimmtes Beispiel wurde gezeigt, dass die quantenmechanische Beschreibung die klassisch singulären Effekte abmildern kann. Basierend auf der Arbeit von Belinskii, Khalatnikov und Lifschitz, welche verallgemeinerte Kasner Raumzeiten als allgemeinstes Beispiel raumartig singulärer Raumzeiten nahelegen, zeigen wir daher deren Quantenvollständigkeit. Darüberhinaus diskutieren wir, dass solche Raumzeiten über einen natürlichen Destabilisierungsmechanismus verfügen, welcher einen Übergang zu isotropen Raumzeiten ermöglicht, was sie zu natürlichen Kandidaten für mögliche präinflationäre Kosmologien macht.

Die übliche Form der Schrödinger Gleichung erfordert die explizite Abtrennung der Zeitrichtung, was Sie für Anwendungen im Kontext der allgemeinen Relativitätstheorie eher unhandlich macht. Wir nutzen die Definition des Zeitflusses durch achronale Mengen und nutzen die sogenannte Null-Reduktion, um die funktionale Schrödinger Evolution auch auf nicht global hyperbolischen Raumzeiten zu ermöglichen. Als Beispiel einer konkreten Anwendung betrachten wir Gravitationswellen-Hintergründe sowohl im Brinkmann als auch im Einstein Rosen Patch. Wir zeigen, dass bezüglich des Brinkmann Beobachters Konfigurationen mit nicht leerem Gravitationsgedächtnis auf eine Menge mit Maßnull fokussiert werden. Abschließend kommentieren wir, auf welche Weise Rückwirkungen in diesem Kontext behandelt werden könnten.

Zu guter Letzt legen wir numerische Methoden dar, welche zur Anwendung gebracht werden können, um die unweigerlich auftretenden Gaußschen Pfadintegrale der obigen Rechnungen in komplizierteren Szenarien zu lösen. Als Beispiel wenden wir diese Methoden auf den Vakuumzerfall eines Skalarfeldes in de Sitter an, um die darin auftauchende Funktionaldeterminante erstmals numerisch zu bestimmen.

Abstract

This thesis deals with possible consistency criteria for quantum field theory on general manifolds. While there are many existing criteria for the completeness of motion in the classical, geometrical and quantum mechanical context, it was only until recently that similar methods were applied to quantum field theory in curved space-time. Making use of the functional Schrördinger formulation of quantum field theory it is possible to analyze the evolution of test fields in very close analogy to the quantum mechanical case. The main aim of this thesis is to study these aspects of quantum field theory in the vicinity of space-times points that would be considered singular in the sense of the Hawking Penrose theorems, and to investigate in what way the classically singular background configuration influences the quantum mechanical evolution.

While it has been shown for a specific case that the quantum evolution may ameliorate the singular nature of the theory, we wish to investigate a more general setting. To this end we consider generalized Kasner universes as the work of Belinskii, Khalatnikov and Lifschitz suggests that this is the most general setup for the occurrence of space-like singularities. It is also discussed how these space-times exhibit a natural decay mechanism towards more isotropic solutions, making them a prime candidate for a possible pre-inflationary phase.

In its standard formulation the Schrödinger formulation requires the explicit separation of a time direction, a feature not well suited to general relativity. Exploiting the fact that a more physical definition of time flow can be given in terms of achronal sets, we adapt the dual null foliation of space-times to the functional Schrödinger picture, to allow for the treatment of geometries that are not globally hyperbolic. As an example we consider the famous plane wave space-times in both the Brinkmann and Einstein Rosen patches. Our analysis concludes that Einstein-Rosen space-times support exclusively configurations with non-empty gravitational memory that are focussed to a set of measure zero in the focal plane with respect to a Brinkmann observer. To conclude, we provide a rough framework to estimate the qualitative influence of back-reactions on these results.

Finally, many of the calculations above require the evaluation of Gaussian path integrals, amounting to the evaluation of functional determinants. We discuss how this can be achieved numerically, and as a proof of concept provide a novel calculation of the false vacuum decay rate in a de Sitter space-time.

1. Introduction

Since it was conceived by Einstein in 1915, it was clear that the general theory of relativity admits solutions which are of singular nature. Since the beginning, the existence of these space-time singularities has confounded physicists, as their physical significance was, and to a certain extent still is, unclear. Classically, physical observables and the invariants of the curvature tensor diverge in the vicinity of a singularity, and it thus appears foolish to further trust the theory in this regime. The question of what to make of these singularities from a physical perspective has thus drawn much attention for the past decades. In principle, there seem to be two distinct logical possibilities to console the appearance of singularities within the framework of Einsteins theory with the physical reality we observe today. The first and perhaps most prevalent rests on the fact that, being a classical theory, general relativity cannot be fundamental. Thus the appearance of singularities may only signal the breakdown of an approximation to the "true" underlying quantum theory of gravity. One would then expect this fundamental theory of gravity to be void of such singularities. Unfortunately, owing to its perturbative non-renormalizability, no quantum theory of gravity is available to date, and there seems little chance to give a definitive verdict on the question whether such a theory remedies the existence of singularities in the near future.

The second logical possibility lies in the realization that a classical singularity must not be observable and therefore must not bear any physical significance per se. In fact, one is easily tempted to simply equate the physical space-time with the semi Riemannian manifold that is used to model it, within the scope of general relativity. In its barest form the physical space-time is a set of events that satisfy certain causal relations between them. While the description in terms of manifolds has proven very fruitful, they themselves are not observable and thus physical. In this sense the physically relevant question is whether singularities necessarily lead to un-physical predictions. If, by some mechanism, singularities are shielded from physically observable consequences, their existence must not rule out the viability of space-time models. The situation is then comparable to an electron moving in a coulomb potential. Albeit the potential diverges in the limit $r \to 0$, there is no physical state that can realize this configuration as the probability to find the electron at the origin is strictly zero for all hydrogen wave functions. This perspective offers the advantage that it can be studied without the necessity of a quantum theory of gravity, and the conclusions drawn should be independent of the completion that such a theory may eventually have to offer.

For a long time the celebrated Singularity theorems by Hawking and Penrose were the premier way through which the nature of singular solutions to the Einstein equations was understood. While they give a set of general criteria guaranteeing the emergence of a singularity, in their basic form they do not offer any interpretation of the physical consequences. As it is clear that any truly physical measurement will be fundamentally quantum in nature, it seems natural to look for a way of qualifying space-time models at least at the semi-classical level. To this end, the minimal requirement that has to be met is for the space-time to admit a "sensible" evolution of quantum fields, even close to the singularity. In this spirit the notion of quantum completeness was introduced in the context of quantum field theory in curved space-time [1]. It provides such a criterion within the context of the semi-classical approximation, and hence allows for a way to discriminate between space-times where the classical singularity becomes a problem for the feasibility of quantum field theory, and those where it has no bearing on the evolution of quantum fields. In adhering to the semi-classical treatment of gravity it is possible to circumvent the issues posed by the quantization thereof and yet remain on the same footing as the original theorems, that too do not account for any flexibility in the background.

In the present thesis we will be mainly concerned with the application of this concept to examples of immediate physical importance. In the first three chapters we review the concepts necessary for the application of these ideas to general space-times. We illustrate how they naturally generalize notions that are already well established in both classical and quantum physics. In the fourth chapter, which is based largely on the authors publication [2], we discuss the generalized Kasner space-time as a precursor to inflationary cosmologies, which suffer from both quantum and geodesic incompleteness. We present the author's contribution in establishing that these pre-inflationary scenarios are in fact quantum complete both for free and interacting theories and that the existence of the initial singularity does not spoil the evolution of quantum fields. We also present the work of Belinskii, Khalathnikov and Lifschitz to show that the conclusions drawn from the Kasner example are in some sense universal to space-like singularities.

In the next chapter we present the general Hamiltonian theory of null foliations with the intent to generalize the aforementioned concepts to non-globally hyperbolic space-times. In the subsequent chapter we introduce an important representative of this class of space-times; the plane wave metric. We construct the proper generalization of the Schrödinger formulation of quantum field theory for general null foliations and then apply it to the specific example of a gravitational shock wave to establish quantum completeness on this backgrounds. Unlike in the Kasner case the classical singularity remains relevant for the quantum theory here, and a treatment of the ensuing back-reactions is included. This chapter is based largely on the authors publication [3]

We close with an introduction to the possibility of the numerical investigation of the Schrödinger wave functional in curved space-times. As a proof of concept we present a similar calculation in the context of false vacuum decay. The author's contribution to the calculation of the fully renormalized functional determinant appearing in the vacuum decay rate in a fixed de Sitter universe is presented, and the possibility of the adaption of the Gel'fand Yaglom techniques to the Schrödinger case is briefly discussed. The results of this Chapter are largely a subset of those found in the authors publication [79], which is in preparation at the time of submission of this thesis.

2. Schrödinger Representation of Quantum Field Theory in Minkowski Space

Historically, the formulation of quantum field theory has been based largely on the Heisenberg formulation of quantum mechanics. The Schrödinger approach to quantum field theory, despite being known for essentially the same amount of time, has taken a back seat in many applications. Undoubtedly this is mainly due to technical reasons as it is somewhat unwieldy, particularly in its handling of scattering problems, which make up the largest part of the early developments in quantum field theory. It was only later that it received more attention, initially from Jackiw, Guth and others [4, 5] due to its better handling of certain aspects of problems in curved space-times. After all, quantum field theory is more than just a theory of the s-matrix and the Schrödinger approach seems more suited to a variety of questions we shall treat in detail later. Even recently, there has been a surge in interest for the Schrödinger approach, particularly in cosmological applications. Nonetheless, as many readers will not be familiar with the Schrödinger quantization of fields, we begin by introducing the approach and setting the notation for the rest of this thesis. Most of this section is known and well understood; however due to its exotic nature, there are many caveats about the Schrödinger approach to quantum field theory that are not readily found, even within the specialized literature. In fact, to the best of the author's knowledge, there is no "standard" treatment of Schrödinger field theory and most books with a somewhat general scope skip its discussion altogether, the only exception we are aware of being the book by Hatfield [6]. In the following, we give a brief review of the quantization of fields in the Schrödinger formalism. We begin with the derivation of the Schrödinger equation for a quantum field.

The Schrödinger Equation of a Quantum Field

To begin with, we concentrate on the treatment of scalar fields, for they already exhibit most of the features that we are interested in. Following the general physical intuition that a quantum field is nothing more than an infinite collection of Harmonic Oscillators, we consider the Hamiltonian of N such oscillators.

$$H = \frac{1}{2}\sum_{i=1}^{N} p_j^2 + \frac{1}{2}\sum_{i,j=1}^{N} \omega_{ij} q_i q_j. \tag{2.1}$$

For a quantum field the index i is promoted to a continuous label $\mathbf{x}$, attaching, loosely speaking, an oscillator to every point in space. It is clear that in the limit $N \to \infty$ the summations must be replaced by integrals, whilst functions are promoted to functionals. In the position representation of ordinary quantum mechanics, we represent the momentum operator by an ordinary derivative, while the position operator is purely a multiplicative function. It is clear therefore that in our analogy we must replace the derivative by a functional derivative, while we replace the position function with the field itself:

$$\hat{p} \mapsto -i\frac{\delta}{\delta\phi(\mathbf{x})} =: \pi(\mathbf{x}), \quad \hat{q} \mapsto \phi(\mathbf{x}). \tag{2.2}$$

Note that in a slight abuse of notation, we will omit the hat on the field operators, it will be clear from the context whether we refer to $\phi(\mathbf{x})$ as an operator or as a function in the sense above. If we make these replacements in (2.1), we find that the Hamiltonian becomes a functional operator. Moreover, postulating a space of functionals $\Psi[\phi;t]$, on which this operator may act, we can in principle write down a Schrödinger-type equation

$$i\frac{\partial}{\partial t}\Psi[\phi;t] = \left[-\frac{1}{2}\int d^3\mathbf{x}\frac{\delta^2}{\delta\phi(\mathbf{x})^2} + \frac{1}{2}\int d^3\mathbf{x}d^3\mathbf{y}\phi(\mathbf{x})K(\mathbf{x},\mathbf{y})\phi(\mathbf{y})\right]\Psi[\phi;t]. \tag{2.3}$$

The form of the kernel K will be dictated by requiring relativistic invariance [7]. In quantum mechanics we associate the physical states of the system with the wave functions that are eigenfunctions of the Hamiltonian. Their time-evolution is the given by the corresponding Schrödinger equation. Likewise we conclude here that the physical state of the system will given by the functional solutions to (2.3). As such the wave-functionals are explicitly time-dependent and we are working in the analog of the Schrödinger representation of quantum mechanics.

2.1. Schrödinger Equation for Scalar Fields

After this short heuristic justification let us consider the general quantization procedure for a scalar field theory. We start from the Lagrangian density of the free field

$$\mathcal{L} = \frac{1}{2}\left(\partial_\mu\phi(\mathbf{x})\partial^\mu\phi(\mathbf{x}) - m^2\phi^2(\mathbf{x})\right). \tag{2.4}$$

The Hamiltonian is derived as usual by means of a Legendre transformation. The canonical momentum variable associated with the field ϕ is found to be

$$\pi(\mathbf{x}) = \frac{\partial\mathcal{L}}{\partial\dot{\phi}} = \dot{\phi}, \tag{2.5}$$

from which we obtain the Hamiltonian

$$H = \frac{1}{2}\int d^3\mathbf{x}\left(\pi^2(\mathbf{x}) + |\nabla\phi(\mathbf{x})|^2 + m^2\phi^2(\mathbf{x})\right). \tag{2.6}$$

As in the previous example we must now find a representation of the operators spanning the algebra of observables in terms of the fields therein. We must also insist that this representation is compatible with the canonical commutation relations (CCR). Fortunately, the replacements in the initial example do just that by virtue of the properties of functional derivatives

$$[\pi(\mathbf{x}),\phi(\mathbf{y})] = -i\delta(\mathbf{x}-\mathbf{y}), \quad [\pi(\mathbf{x}),\pi(\mathbf{y})] = [\phi(\mathbf{x}),\phi(\mathbf{y})] = 0. \tag{2.7}$$

Again, insertion into (2.6) gives us the functional Hamiltonian

$$H = \frac{1}{2}\int d^3\mathbf{x}\left(-\frac{\delta^2}{\delta\phi(\mathbf{x})^2} + |\nabla\phi(\mathbf{x})|^2 + m^2\phi^2(\mathbf{x})\right). \tag{2.8}$$

The usual approach is now to formulate the abstract Schrödinger equation for a quantum state $|\Psi\rangle$,

$$i\partial_t|\Psi\rangle = H|\Psi\rangle \tag{2.9}$$

in terms of the Hamiltonian (2.8), to obtain a functional differential equation for the wave functional in the position representation

$$\Psi[\phi,t] := \langle\phi|\Psi\rangle. \tag{2.10}$$

2.2. States

2.2.1. Formal Construction

From the close analogy to the quantum mechanical formulation of wave functions, it is clear that we expect the space of admissible functionals to be a generalization of the L^2-space of wave functions that usually constitutes our Hilbert space. Since the Schrödinger picture is employed less often, little is written about its formal construction. The reason for this is most likely the close analogy to the standard wave-mechanics that comprises a large part of any undergraduate quantum mechanics curriculum. While it is certainly helpful to exploit this analogy to gain some intuition at first sight, it fails, or at least becomes decreasingly transparent, as one tries to apply it to more involved concepts even though they may still be understood completely in the quantum mechanical case. These obstacles may be placed into two categories, technical and conceptual. Naturally, considering non-trivial backgrounds introduces a multitude of technical difficulties that need not be addressed in the textbook presentation of quantum mechanics. However, these technical aspects do not spoil the analogy, for they would lead to complications in quantum mechanics already [1]. Instead, it is the underlying Hilbert-space that changes subtly in nature. As issues of the first type do not feature prominently in the formal construction to

[1] As soon as one decides, for example, to investigate the quantum mechanics of a particle on a sphere, instead of the usual flat product $\mathbb{R}\times\mathbb{R}^2$, one is required to view the wave function not as a function but as section on a appropriate bundle

follow, we will discuss the general case right away. The only appreciable difference to the flat case will be the appearance of some factors of the metric determinant, owed to our choice of embedding. We return to the special case of a flat space-time in the next section. Most of the following discussion is also found in [2].

To begin with we are equipped with a space-time and its metric $(\mathcal{M}, g)$. It is of course one of the great features of the formulation of general relativity that it forces the abandonment of separate notions of time and space, merging them into a single entity. To define time-evolution in the sense of quantum mechanics however, we must select a time-like direction that is everywhere well-defined. We must hence restrict $\mathcal{M}$ to be globally hyperbolic. This allows us to choose a time function t and a vector field v on $\mathcal{M}$ such that surfaces $(\Sigma_t)_{t\in I\subset\mathbb{R}}$ of constant time are Cauchy hypersurfaces and such that $\nabla_v t = -1$. The interval I must not necessarily cover the entire real line; in fact, it usually will only be some finite interval that encompasses the relevant events. We may therefore view the spacetime as a product $\mathbb{R}\times\Sigma_t$, at least locally. A field configuration is some map $\phi : \mathcal{M} \to \mathbb{K}$, where the field $\mathbb{K}$ is assumed to be either $\mathbb{R}$ or $\mathbb{C}$ for simplicity. Next, one introduces a space of all possible instantaneous field configurations, which we shall henceforth denote by $\mathcal{C}(\Sigma_t)$ and is simply obtained by a restriction to maps $\phi : \Sigma_t \to \mathbb{K}$. We complete the configuration space to a formal measure space $(\mathcal{C}(\Sigma_t), \mathscr{D}\phi)$, by equipping it with the functional measure $\mathscr{D}\phi$. From here on the construction is of course purely formal, as the existence of said measure has yet to be shown. We continue to construct the $\mathbb{K}$-vector space of measurable wave functionals $\Psi_t : \mathcal{C}(\Sigma_t) \to \mathbb{K}$, whose modulus is square integrable. In analogy to quantum mechanics we denote this space as $\mathcal{L}^2(\mathcal{C}(\Sigma_t))$. On this functional version of the $\mathcal{L}^2$-space we have the usual seminorm

$$||\Psi_t||^2 := \int_{\mathcal{C}(\Sigma_t)} \mathscr{D}\phi |\Psi_t[\phi]|^2. \tag{2.11}$$

This norm is only positive semidefinite since there may be field configurations in $\mathcal{C}(\Sigma_t)$ that are zero $\mathscr{D}\phi$-almost everywhere but not strictly zero. We thus further group this space into a space of representatives of equivalence classes. We begin by defining the following subspace of $\mathcal{L}^2\big(\mathcal{C}(\Sigma_t)\big)$:

$$\mathcal{N}\big(\mathcal{C}(\Sigma_t), \mathscr{D}\phi\big) := \big\{\Psi_t \in \mathcal{L}^2\big(\mathcal{C}(\Sigma_t)\big) : \Psi_t[\phi] = 0 \ \mathscr{D}\phi - \text{almost everwhere}\big\}. \tag{2.12}$$

Now obviously $||\cdot||$ will be a norm on the quotient space

$$L^2\big(\mathcal{C}(\Sigma_t), \mathscr{D}\phi\big) := \mathcal{L}^2\big(\mathcal{C}(\Sigma_t)\big)/\mathcal{N}\big(\mathcal{C}(\Sigma_t), \mathscr{D}\phi\big), \tag{2.13}$$

as $||\Psi_t|| = 0$ implies $\Psi_t \equiv 0$. One would now like to interpret $|\Psi_t[\phi]|^2$ as a probability density in the usual sense. Thus, if $\mathcal{U}$ is a measurable subset of $\mathcal{C}(\Sigma_t)$ and $\lambda_{\mathcal{U}}$ the indicator functional corresponding to $\mathcal{U}$, then $||\lambda_{\mathcal{U}}\Psi_t||^2$ corresponds to the probability for the field configuration on the constant time slice Σ_t to be given by some $\phi \in \mathcal{U}$. As is the case in ordinary quan-

tum mechanics, one requires that the functionals $|\Psi_t|^2$ remain normalizable for $t \in I$ to uphold the probabilistic interpretation of the theory. However, unlike in most quantum mechanical problems we will see that the stricter condition $||\Psi_t|| = 1$ cannot be satisfied for all $t \in I$ in non-trivial backgrounds, as we shall discuss in depth later. In contrast to the Heisenberg approach, a state $|\Psi\rangle$ is now represented by a wavefunctional $\Psi[\phi]$, where $\phi(\mathbf{x})$ is now a c-number field on the surface Σ_t. Operators on this space are represented by functional kernels and do not carry explicit time-dependence i.e.

$$|\tilde{\Psi}\rangle = \hat{O}|\Psi\rangle \to \tilde{\Psi}[\phi] = \int \mathscr{D}\phi\, \hat{O}[\phi,\varphi]\Psi[\varphi]. \tag{2.14}$$

In particular, the field operators $\hat{\Phi}[f]$ are now implemented by the appropriate operator multiplication, as we choose the corresponding kernel to be diagonal. More precisely, we define the action of the field operator $\hat{\Phi}[f]$ by the multiplication with $\phi[f]$, where f is some smearing function with compact support on Σ_t such that the expectation value $\langle\Psi|\hat{\Phi}[f]|\Psi\rangle$ is well-defined. As we wish to find an analogue of quantum mechanics on the space defined, we must impose the canonical commutation relations. This fixes the form of the canonical momentum field operator to be of the form of a functional derivative

$$\pi(\mathbf{x}) = -i\frac{1}{\sqrt{g_{\Sigma_t}}}\frac{\delta}{\delta\phi} \tag{2.15}$$

along the direction of f.

2.2.2. The Ground State

Returning to the Minkowski case, we conclude that the space of physical states will be comprised of solutions to the functional Schrödinger equation which are normalizable in the sense defined above. Furthermore, as we are interested in the energy eigenstates of the system we turn to the time-independent Schrödinger equation in search of a potential ground state

$$\frac{1}{2}\int d^3\mathbf{x}\left(-\frac{\delta^2}{\delta\phi(\mathbf{x})^2} + |\nabla\phi(\mathbf{x})|^2 + m^2\phi^2(\mathbf{x})\right)\Psi[\phi] = E\Psi[\phi]. \tag{2.16}$$

The solutions to (2.16) will take the form of Gaussian functionals, as one might guess bearing in mind the form of the ground state for the harmonic oscillator in quantum mechanics. It can also be seen from a simple power counting argument [6]. We therefore make the Ansatz

$$\Psi[\phi] = \mathcal{N}\exp\left(-\frac{1}{2}\int d^3\mathbf{x}d^3\mathbf{y}\ \phi(\mathbf{x})K(\mathbf{x},\mathbf{y})\phi(\mathbf{y})\right). \tag{2.17}$$

As we will ultimately be interested in the normalizability of functionals, we choose only the Ansatz decaying exponentially. Theoretically, an oscillatory Ansatz would also provide a solution to (2.16), albeit at the cost of making E imaginary. In this case, a Wick rotation would lead

to an Eucledian action. While this approach ist often followed, we will not pursue it here. In principle, both the normalization constant $\mathcal{N}$ and the integration kernel K may depend on time explicitly. However, as we are only interested in the time-independent part of the Schrödinger equation for now, we will suppress this dependency so as not to clutter up notation. It will become important later however. Inserting this Ansatz into the Schrödinger equation (2.16) we can separate the field-dependent and field-independent parts. For the former we obtain

$$\int d^3\mathbf{x}\; K(\mathbf{x},\mathbf{x}) = E, \tag{2.18}$$

coming from the double functional differentiation on the exponential factor. For the field dependent part we obtain a term stemming from the product rule as well as one from the non-functional part of the Hamiltonian

$$\int d^3\mathbf{x}\, d^3\mathbf{y}\, d^3\mathbf{z}\; \phi(\mathbf{x})K(\mathbf{x},\mathbf{z})K(\mathbf{z},\mathbf{y})\phi(\mathbf{y}) = \frac{1}{4}\int d^3\mathbf{x}\; \phi(\mathbf{x})(-\nabla^2+m^2)\phi(\mathbf{x}). \tag{2.19}$$

Given that our initial Lagrangian was completely translation invariant, we expect this property to be respected by the integration kernel $K(\mathbf{x},\mathbf{y}) = K(\mathbf{x}-\mathbf{y})$. Moreover, usually translation invariance indicates that it will be useful to pass into a momentum-space description in order to reduce the problem to an algebraic one. Defining therefore the Fourier transform

$$f(\mathbf{x}) = \int \frac{d^3k}{(2\pi)^3} f(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{2.20}$$

applying it to the above and solving for the kernel, we obtain

$$K(\mathbf{k}) = \pm\frac{1}{2}\sqrt{\mathbf{k}^2+m^2}, \tag{2.21}$$

in which we immediately recognize the dispersion relation in Minkowski space, and therefore set $K(\mathbf{k}) = \frac{1}{2}\omega_k$, choosing the positive sign in order to ensure normalizability. With this in hand we can now solve the field-independent part of the stationary Schrödinger equation to see

$$E = \frac{1}{2}\int d^3\mathbf{k}\; \omega_k \delta^3(0). \tag{2.22}$$

As expected, the energy is given by the dispersion relation. The divergent factor of $\delta^3(0)$ comes from the infinite volume of space and thus constitutes an IR-divergence that was to be expected. It can usually be safely removed with the use of a cut-off.

A posteriori we can see that the suppression of time-dependence was justified, as neither the dispersion relation nor the integral measures are time-dependent in Minkowski space. This will change in dynamical space-times as the dispersion, and therefore the kernel acquire an explicit time-dependence. None the less the normalization of this state is still formally infinite. This can be seen very straightforwardly by considering the Gaussian integral resulting from the Ansatz

(2.17)

$$||\Psi||_2 = \int \mathscr{D}\phi \Psi[\phi]^* \Psi[\phi] \sim \frac{1}{\sqrt{\mathrm{Det}\, K}}. \tag{2.23}$$

Although we will not be concerned with them here, it is interesting to note that in the fermionic case the result will be directly proportional to the square root of the determinant $||\Psi||_2 \sim \sqrt{\mathrm{Det}\, K}$. As we have seen, the kernel has eigenvalues of ω_k and thus the ground state normalization is simply proportional to the infinite product of harmonic oscillators. This result is to be expected as we have outlined that a quantum field can be thought of as just that: an infinite set of harmonic oscillators. The remaining product over the momenta k is clearly UV-divergent and must be regularized to obtain a sensible result.

ζ-Regularization

There are in principle many ways of achieving a regularization of the determinant. The computation of functional determinants arises often in quantum field theories, and there are consequently a multitude of procedures for this, both numerical and analytic. The most straightforward way of arriving at a finite result is a simple hard UV cut-off. Often this approach, despite its lack of elegance, is enough to derive qualitative results. Numerical approaches make use of the Gelfand Yaglom theorem or use Green function techniques and will be discussed later in more detail. An elegant and relatively simple analytical approach is offered by the use of ζ-function analytical continuations. To see how this pertains to the case above we discuss the regularization of a massless one-dimensional field here, in close analogy to [7]. The generalization to higher dimensions is trivial, while the inclusion of a mass term simply introduces technical complications that do not change the overall picture. In this case the operator constituting the kernel is simply $K \sim -\nabla_x^2$. To proceed, we must choose boundary conditions. As we have to regulate the infinite volume factor that appears in the energy anyway, it seems natural to choose Dirichlet conditions for a box of length L. The eigenfunctions are thus given by

$$\varphi_n(x) = \sin\left(\frac{\pi n x}{L}\right) \tag{2.24}$$

with eigenvalues

$$\lambda_n = \frac{\pi^2 n^2}{L^2}. \tag{2.25}$$

The sought-after determinant will be given by the infinite product

$$\mathrm{Det} - \nabla_x^2 = \prod_n^\infty \frac{\pi^2 n^2}{L^2}. \tag{2.26}$$

To make sense of this, we define the generalized ζ-function

$$\zeta_{-\nabla^2}(s) := \sum_n \lambda_n^{-s}. \tag{2.27}$$

Using the properties of the logarithm, this can be related to the determinant through

$$\frac{\mathrm{d}}{\mathrm{d}s}\sum_n \exp(-s\ln(\lambda_n)) = -\sum_n \exp(-s\ln(\lambda_n))\ln(\lambda_n) \stackrel{s\to 0}{=} -\sum_n \ln(\lambda_n). \tag{2.28}$$

Thus,

$$\ln\left(\mathrm{Det}-\nabla_x^2\right) = -\frac{\mathrm{d}}{\mathrm{d}s}\zeta_{-\nabla^2}(s)\bigg|_{s=0}. \tag{2.29}$$

It is easily seen that the ζ-function in question can be given in terms of the normal Riemann ζ-function $\zeta_R(s)$:

$$\zeta_{-\nabla^2}(s) = \left(\frac{L}{\pi}\right)^{2s}\zeta_R(2s), \tag{2.30}$$

and therefore we may exploit its properties to derive the final result

$$\mathrm{Det}\,K = \ln(2L). \tag{2.31}$$

Again, this result is time-independent and we may choose our normalization constant to exactly cancel the functional part, thereby fixing the norm of the Minkowski ground state to one.

2.2.3. Excitations

To make contact with the usual Fock space interpretation of quantum field theory, we proceed to construct excited states from the ground state found above. In fact, the ground state as described above can in this sense be defined as the state of minimal excitations. In static space-times, the connection to the energy eigenvalue of equation (2.16) can be used to relate this to a state of minimal energy. For dynamical space-times this is more complicated, as the best that can be done is to study the instantaneous eigenstates of the Hamiltonian. Even at the flat level the construction is subtle as there is some ambiguity concerning the choice of the annihilation operator, defined by the usual relation

$$a\,|0\rangle = 0. \tag{2.32}$$

To achieve this, many authors define the following annihilation operator

$$a(\mathbf{x}) = i\pi(\mathbf{x}) + \int d^3\mathbf{y}\; K(\mathbf{x},\mathbf{y})\phi(\mathbf{y}), \tag{2.33}$$

and a corresponding creation operator. While this does annihilate the vacuum, this choice is problematic, as it does not give rise to the proper commutation relation

$$[a(\mathbf{x}), a^\dagger(\mathbf{y})] = 2\mathrm{Re}K(\mathbf{x},\mathbf{y}). \tag{2.34}$$

This can easily be seen from direct computation and the canonical commutation relation

$$[\pi(\mathbf{x}), \phi(\mathbf{y})] = i\delta(\mathbf{x}-\mathbf{y}). \tag{2.35}$$

It is not clear what this non-standard choice of commutation relation implies, but it seems problematic especially from the point of view of Lorentz invariance. Furthermore, it is not clear at this stage of how to determine the adjoint since this may only be done formally at best. For example, simply changing the sign of the second term in (2.33) will also generate a state proportional to the first excited state when applied to the vacuum, altering the commutation relation (2.34) to be complex in general. In order to steer clear of these problems, we adopt a different convention similar to the one used by [8] defining the annihilation operator as

$$a(\mathbf{x}) := \frac{1}{\sqrt{2}} \int d^3\mathbf{y}\ i\pi(\mathbf{x}) K(\mathbf{x},\mathbf{y})^{-1/2} + K(\mathbf{x},\mathbf{y})^{1/2} \phi(\mathbf{y}). \tag{2.36}$$

Here we have adopted a matrix notation for the Kernel such that

$$\int d^3\mathbf{z}\ K(\mathbf{x},\mathbf{z})^{-1/2} K(\mathbf{z},\mathbf{y}) = K(\mathbf{x},\mathbf{y})^{1/2}. \tag{2.37}$$

While this might seem strange at first sight, it can be directly shown (for example for the K determined above) that this property is indeed satisfied for most well-behaved functions K. Since the ultra-local operator above annihilates the vacuum, the next step is to endow it with the functional information needed in this context. In order to achieve this lift to the functional level, we define the functional generalization as

$$a_\lambda := \int d^3\mathbf{y}\ a(\mathbf{y}) \varphi^*_\lambda(\mathbf{y}), \tag{2.38}$$

where the function φ_λ is any solution to the equations of motion

$$(\Delta - m^2)\varphi_\lambda = \alpha_\lambda \varphi_\lambda \tag{2.39}$$

and the λ is a placeholder for all information labeling this solution such as momentum or, in more general cases, spin etc.. By construction this operator will satisfy the properties of an annihilation operator with respect to the vacuum functional defined above

$$a_\lambda \Psi[\phi] = 0. \tag{2.40}$$

In order to proceed with a minimal weight construction of the Fock space of excited states, we must now identify the appropriate creation operator, such that the canonical commutation relations are satisfied. The simplest guess is to use the adjoint of the expressions derived so far. This is a slight abuse of notation, as we do not give a well-defined definition of the functional "adjoint"; this would require a careful study of the domains of the functional operators involved and is beyond the purview of this discussion. We can however proceed formally and in close

analogy to the well known finite-dimensional case

$$a^\dagger(\mathbf{x}) := \frac{1}{\sqrt{2}} \int d^3\mathbf{y} \; -i\pi^\dagger(\mathbf{x}) K^*(\mathbf{x},\mathbf{y})^{-1/2} + K^*(\mathbf{x},\mathbf{y})^{1/2} \phi(\mathbf{y}), \tag{2.41}$$

and

$$a^\dagger_\lambda := \int d^3\mathbf{y} \; a^\dagger(\mathbf{y}) \varphi_\lambda(\mathbf{y}). \tag{2.42}$$

We have included a complex conjugation on the kernel K here, despite the fact that the kernel will be strictly real in Minkowski space. We have seen that the kernel is essentially given by the dispersion relation on the underlying space-time manifold, and can therefore already anticipate that the kernel will not remain purely real for general geometries, which will cause some ambiguity in the choice of creation operators as we will discuss later. The definitions given above reproduce the expected commutation relations, by virtue of the canonical relations satisfied by ϕ and π

$$[a(\mathbf{x}), a^\dagger(\mathbf{y})] = \delta(\mathbf{x}-\mathbf{y}). \tag{2.43}$$

Therefore, making use of the completeness and orthonormality of the mode solutions we obtain

$$[a_\lambda(\mathbf{x}), a^\dagger_\gamma(\mathbf{y})] = \delta_{\lambda\gamma}\delta(\mathbf{x}-\mathbf{y}) \tag{2.44}$$

Excitations can now be built in the usual way by repeated application of the functional creation operator, the interpretation being a state that contains a corresponding number of excitations

$$\Psi^{(N)}_{\lambda_1\cdots\lambda_N}[\phi] := \prod_{i=1}^{N} a^\dagger_{\lambda_i} \Psi^{(0)}[\phi]. \tag{2.45}$$

It is interesting to note that the on-shell information only enters at the level of the excited states through (2.39). This is not surprising of course, as we expect the perturbative vacuum (as a state devoid of excitations) not to depend on kinematical information.

Inequivalence of Fock Spaces

To close our discussion of excited states, we want to highlight an observation first made by Jackiw [9]. Unlike in the quantum mechanical case, the wave functionals that make up the perturbative Fock space do not span the entire functional space. This is very much in contrast to the usual case, where the eigenfunctions of the Hamiltonian span the entire L^2-space. Therefore, any square-integrable function may be expanded in any particular set of eigenfunctions belonging to a self-adjoint operator on our Hilbert space. This is not true for the generalized L^2-space of wave functionals we have constructed. We can see this by considering two different kernels K_1 and K_2, determining the ground states arising from the quantization of two Hamiltonians H_1 and H_2, respectively. The overlap between these two respective ground states will be given in

terms of a path integral

$$\int \mathscr{D}\phi \Psi^{(1)*}[\phi]\Psi^{(2)}[\phi] \sim \exp -\frac{V}{2}\int_p \ln \frac{1}{2}\left(\sqrt{\frac{\omega_1(p)}{\omega_2(p)}}+\sqrt{\frac{\omega_2(p)}{\omega_1(p)}}\right). \tag{2.46}$$

Again, the left hand side exhibits an infrared infinity as the volume tends towards infinity. However, even when ignoring this the integrand will still diverge in p unless the two dispersions approach each other very rapidly for large momenta. We can thus conclude that the Fock-spaces spanned by the two respective vacua will be orthogonal within the functional L^2-space. This is so, since the overlap above will appear in every inner product between arbitrarily excited states. The functional space can therefore host an infinity of inequivalent and mutually orthogonal Fock-spaces. It is important to note that this is in fact one of the main strengths of the Schrödinger formalism, when representing transformations in terms of the operator kernels, we do not need to pre-select a specific Fock-space.

This is especially interesting for applications on curved space-times, as here the inequivalence of the particle concept that stems from the choice of physically different vacua is one of the most puzzling problems one faces. Often times the appropriate selection of an in- or outgoing vacuum cannot be uniquely achieved, and hence the interpretation of results is made much more difficult. The Schrödinger formalism does not suffer from this in quite the same way and is consequently ideally suited to the study of phenomena in curved spaces. This is not to say of course that it does not suffer from the ill-defined concept of a particle. If one attempts to resolve the excitations, the results will explicitly depend on the choice of the kernel entering the ground state functional. However, in the study of transformation groups this choice does not enter.

Relation to Green Functions

In order to conclude this introduction we will close by showing the relationship between the quantities involved in the Schrödinger quantization and the more familiar ones of the Green-function based approach of the Heisenberg picture. To do so, we compute the propagator for the free scalar field. By definition it is given through the two point function

$$\langle 0|\,\phi(\mathbf{x})\phi(\mathbf{y})\,|0\rangle\,\theta(t-t_0) = \theta(t-t_0)\int \mathscr{D}\phi\ \phi(\mathbf{x})\phi(\mathbf{y})\Psi[\phi]^*\Psi[\phi]. \tag{2.47}$$

Passing to the Fourier transform we see that the Gaussian integral on the right hand side reduces to

$$\int \mathscr{D}\phi\ \phi(\mathbf{k})\phi(\mathbf{p})\exp\left(-\int \frac{d^3\mathbf{q}}{(2\pi)^3}\ \phi(\mathbf{q})K(\mathbf{q})\phi(-\mathbf{q})\right)\theta(t-t_0) \propto \frac{(2\pi)^3}{\omega_k}\delta(\mathbf{p}-\mathbf{k})\theta(t-t_0), \tag{2.48}$$

due to the fact that only even moments give a non-vanishing result. Therefore, we may evaluate one of the Fourier integrals trivially and are left with the familiar expression

$$\langle 0|\,\phi(\mathbf{x})\phi(\mathbf{y})\,|0\rangle\,\theta(t-t_0) = \int \frac{d^3\mathbf{q}}{(2\pi)^3}\frac{1}{2\omega_k}e^{-i\mathbf{q}\cdot(\mathbf{x}-\mathbf{y})}\theta(t-t_0), \tag{2.49}$$

where from we see that the Feynman propagator comes out precisely as it should

$$i\Delta_F = \int \frac{d^3\mathbf{q}}{(2\pi)^3}\frac{1}{2\omega_k}\left(e^{-i\mathbf{q}\cdot(\mathbf{x}-\mathbf{y})}\theta(t-t_0) + e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{y})}\theta(t_0-t)\right). \tag{2.50}$$

This result is very useful as it shows that the kernel K may, in a loose sense, be thought of as the inverse of the propagator, which is particularly useful when considering its scaling in less transparent scenarios. A direct application of this correspondence will prove to be unnecessary in most practical cases however.

3. Schrödinger Representation in Curved Space-times

3.1. Schrödinger Equation In General Backgrounds

As we have introduced the wave-functional as an analogue to the wave function on the more general functional space of field configurations in Minkowski space, we may now proceed to explicitly construct it for a more general class of space-times. The first and possibly most serious obstacle to overcome is the lack of manifest covariance in the formulation of Schrödinger quantum field theory. This is an inheritance from the Schrödinger equation itself, as it seems to make a distinction between time and space. This imbalance between space and time is of course only spurious, and it is well known, that an appropriate choice of the kernel $K(\mathbf{x},\mathbf{y})$ in the Schrödinger equation renders the entire expression relativistically invariant. The fact that this is not obvious often presents a challenge to the interpretation of results. This privation is possibly the reason why the Schrödinger picture has received less attention, compared to its Heisenberg counterpart. In order to keep things as simple as possible, we will therefore restrict the discussion to globally hyperbolic space-times for now. These space-times possess a Cauchy surface; thus, it is always possible to find a description of space-time in terms of a stack of spatial hypersurfaces and a vector field orthogonal to them. This restriction facilitates the application of the formalism developed in the Minkowski section, as we can identify the time direction with the said vector and treat the remaining dimensions as spatial. Carefully ensuring relativistic invariance throughout, one can therefore work with the resulting wave-functionals as one would in flat space. It is possible to drop the requirement of global hyperbolicity as we shall prove in a later chapter.

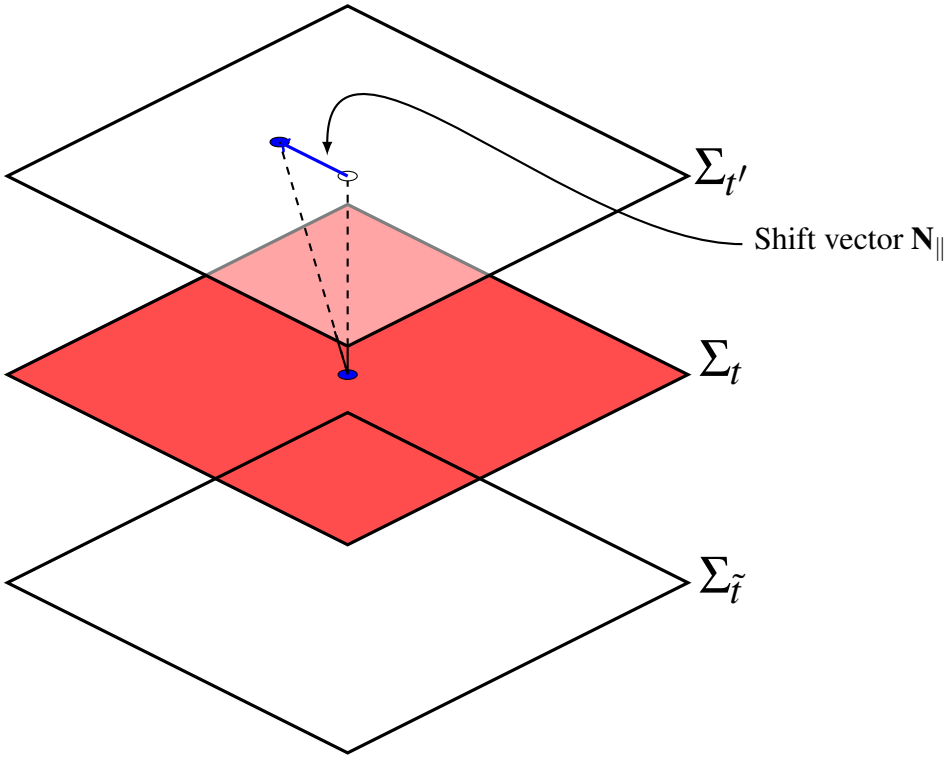
3.1.1. Foliation

To cast the metric into a form most useful for the task at hand we perform the famous ADM split [10] for the general Lorenzian, hyperbolic space-time $(\mathcal{M},g)$.

Definition. *A space-time $(\mathcal{M},g)$ is called **globally hyperbolic** if it possesses a global Cauchy surface Σ.*

The restriction to globally hyperblic space-times is particularly useful for our purposes as it allows us to exploit the fact that any such manifold has the topology $\mathbb{R}\times\Sigma$, and therefore $\mathcal{M}$

may be foliated by a one-parameter family of smooth Cauchy surfaces Σ_t [11, 12].



Given that we wish to identify the time direction with the direction orthogonal to these surfaces, and hence define time-evolution as a map from one such surface to another, we will only consider constant-time hypersurfaces Σ_t. Given such a Σ_t, we choose the normal vector $\mathbf{n}$ such that $g(\mathbf{n},\mathbf{n}) = -1$, where the sign is in principle arbitrary but chosen here to be negative to ensure that the resulting time vector field is future directed. In the following and throughout this thesis, we will always choose greek indices to run over the entire dimension of the manifold $\alpha,\beta,\ldots \in (0,1,\cdots,d)$, while latin indices will always denote spatial directions $a,b,\ldots \in (1,2,\cdots d)$. With this we may define a projector onto the spatial hypersurface Σ_t for every $\mathbf{v} \in Vec(\mathcal{M})$ as

$$P^{\|}(\mathbf{v}) := \mathbf{v} + g(\mathbf{v},\mathbf{n})\mathbf{n} \tag{3.1}$$

while the obvious projector along the time-like direction is

$$P^{\perp}(\mathbf{v}) := g(\mathbf{v},\mathbf{n})\mathbf{n}. \tag{3.2}$$

Using the above definitions, we can decompose any vector $T \in Vec(\mathcal{M})$ with $\nabla_T x^0 = 1$ as

$$T = N_{\perp}\mathbf{n} + \mathbf{N}_{\|}. \tag{3.3}$$

Subsequently, we may decompose any one-form as

$$dx^{\mu} = x^{\mu}_{,t}\,dt + x^{\mu}_{,a}\,dx^a = (N_{\perp}n^{\mu} + N^a_{\|}x^{\mu}_{,a})dt + x^{\mu}_{,a}\,dx^a. \tag{3.4}$$

We may thus re-express the metric in terms of the function $N_{\perp}$, usually called lapse function, and

the components of the vector $\mathbf{N}_{\|}$, commonly referred to as shift vector. The physical meaning of the shift vector is roughly speaking to measure the displacement on the spatial hypersurfaces as one moves from one to the next, following the time-evolution. Upon insertion, the metric is thus given as

$$g = (-N_{\perp}^2 + q_{ab}N_{\|}^a N_{\|}^b)dt \otimes dt + q_{ab}N_{\|}^b(dx^a \otimes dt + dt \otimes dx^a) + q_{ab}dx^a \otimes dx^b. \tag{3.5}$$

Here q denotes the pullback $q = \phi^* g$ of the metric under the embedding of our spatial slices. It therefore constitutes an induced metric on Σ_t and is commonly referred to as the spatial metric. One may now proceed to determine the components of the inverse metric in similar fashion, we will therefore only state the result

$$g^{-1} = -\frac{1}{N_{\perp}^2}\partial_t \otimes \partial_t + \frac{N_{\|}^a}{N_{\perp}^2}(\partial_t \otimes \partial_a + \partial_a \otimes \partial_t) + (q^{ab} - \frac{N_{\|}^a N_{\|}^b}{N_{\perp}^2})\partial_a \otimes \partial_b. \tag{3.6}$$

3.1.2. The Hamiltonian

So far we have simply recast the initial metric in a more convenient form. As our next step we need to determine the Hamiltonian in this formulation, in order to then deduce the Schrödinger equation. We begin by considering the action of a scalar field in a general spacetime. The generalization to higher spin gauge theories is conceptually no different, however technically much more involved. For example, the quantization of the photon field in the Lorentz gauge forces us to work with an altered action, enforcing constraints on the states by hand. Calculations are also more cumbersome, as the longitudinal modes must be kept along with their corresponding functionals. The extension to spinor fields also does not add anything conceptually new. The Hamiltonian of the theory is of course of the Dirac type and thus results in a Grassman functional differential equation. As we are primarily interested in the qualitative features of such theories in the close vicinity to singular points of the metric, we do not expect spin to play a major role, at least within the bosonic sector. This does not exclude a qulitative distinction between bosonic and fermionic fields; however, we do not consider the latter here for now.

The action of a minimaly coupled scalar field is

$$S = -\frac{1}{2}\int d^4x\sqrt{-g}\,\left[g^{-1}(\phi,\phi) + (m^2 + \xi R)\phi^2\right]. \tag{3.7}$$

Here R denotes the Ricci scalar and g the determinant of the metric. Insertion of the expression for the inverse metric given above in terms of the lapse function and shift vector yields the following expression for the Lagrange density

$$\mathcal{L} = \frac{1}{2}\sqrt{q}N_{\perp}\left[-\frac{(\partial_t\phi)^2}{N_{\perp}} + 2\frac{N_{\|}^a}{N_{\perp}^2}(\partial_a\phi)(\partial_t\phi) + (q^{ab} + \frac{N_{\|}^a N_{\|}^b}{N_{\perp}^2})(\partial_a\phi)(\partial_b\phi) + (m^2 + \xi R)\phi^2\right]. \tag{3.8}$$

The canonical momentum field is still defined by the variation of the action with respect to $\dot{\phi}$

$$\pi := \frac{\delta \mathcal{L}}{\delta(\partial_t \phi)} = \frac{\sqrt{q}}{N_\perp}\left[\partial_t \phi - N^a_\parallel \partial_a \phi\right]. \tag{3.9}$$

The corresponding Hamiltonian is then again obtained by means of a Legendre transform

$$H = \int_{\Sigma_t} d^3x \left[\frac{N_\perp}{\sqrt{q}}\pi^2 + N^a_\parallel \partial_a \phi - \mathcal{L}\right]. \tag{3.10}$$

As the second term is not quadratic in the fields it represents a constraint. The remainder then results in the Hamiltonian density

$$\mathscr{H} = \frac{1}{2}\sqrt{q}\left[q^{-1}\pi^2 + q^{ab}\partial_a\phi\,\partial_b\phi + (m^2 + \xi R)\phi^2\right] \tag{3.11}$$

It is noteworthy that the kinetic and potential terms in (3.11) scale very differently with the metric factors. The kinetic term scales inversely to the mass term, or what would be the potential term had we chosen to include a potential. This is of great significance as it implies that a possible time-dependence of the background implies a certain hierarchy between the terms in (3.11). For generic backgrounds it is thus possible to have regimes where the kinetic factor dominates over the potential factor and vice versa. In the former case we expect the theory to trivialize, becoming effectively free, whilst in the latter the theory enters something akin to a strong coupling regime. Interestingly it will turn out that in the vicinity of some space-time singularities one enters such an era of asymptotic trivialization, i.e. kinetic dominance. This may seem counter-intuitive at first, however a physical interpretation seems straightforward. As interactions are local in the sense that they are associated with some natural range, an ever contracting space-time forces a coincidence limit in which they dominate. On the other hand should the geometry be such that the time-like separation of any two events diverges one expects interactions to become negligible. As we shall see later most space-times fall in one of these two categories. Equipped with a Hamiltonian density we may now write down a Schrödinger equation for the free field.

$$-i\partial_t \Psi_t[\phi,t] = \int_{\Sigma_t} d^3x \left[\frac{N_\perp}{\sqrt{q}}\pi^2 + N^a_\parallel \partial_a \phi - \mathcal{L}\right]\Psi[\phi,t] \tag{3.12}$$

3.2. Functional Space

Given the Schrödinger equation in a general space-time we can follow the same program as in the flat case of the previous section in order to construct a space of wave-functionals. We must replace the canonical momentum operator π with its functional representation through the kernel $-i(\delta/\delta\phi)\delta(\phi - \phi')$. If we adopt the spacetime coordinates to the foliation i.e. we

choose $x^0 = t$, we can set $N^a_{\|} = 0$ and we arrive at the expression

$$i\partial_t \Psi[\phi] = \frac{1}{2}\int_{\Sigma_t} d^3x \sqrt{-g}\left[-\frac{g_{00}}{g}\frac{\delta^2}{\delta\phi^2} + q^{ab}\partial_a\phi\partial_b\phi + (m^2+\xi R)\phi^2\right]\Psi[\phi]. \tag{3.13}$$

This is the Schrödinger equation as it pertains to quantum fields in a generic space-time, provided it admits an appropriate slicing.

3.2.1. The Ground State

We may now attempt to solve (3.13) in order to obtain a functional representation of any state in our theory. Naturally, a state of particular interest is the ground state, in the sense defined in the flat section. On the given hypersurface Σ_t the time-independent Schrödinger equation $H\Psi[\phi] = E\Psi[\phi]$ is well defined for the instantaneous eigenfunctionals of the Hamiltonian. With this consideration one arrives at the Ansatz for the ground state

$$\begin{aligned}\Psi^{(0)}[\phi](t) &= N^{(0)}(t)\mathcal{G}^{(0)}[\phi](t), \\ \mathcal{G}^{(0)}[\phi](t) &:= \exp\left[-\frac{1}{2}\int_{\Sigma_t} d\mu(x)d\mu(y)\phi(x)K(x,y,t)\phi(y)\right],\end{aligned} \tag{3.14}$$

through simple powercounting. In the above we have defined the covariant integration measure $d\mu(x) := \sqrt{q}d^3x$, thus the kernel $K(x,y;t)$ transforms as a scalar under coordinate transformations. We make this choice to make the covariance or non-covariance of expressions more transparent, however other authors may choose a different convention [8, 9]. While the general procedure is the same as in the case of Minkowski space, there are important differences that one needs to be aware of when interpreting the results.

The first immediate difference is in the nature of the "ground state". While in the Minkowski example the Hamiltonian and therefore its eigenvalues were time-independent, this will no longer be the case for general background geometries. In fact, in most interesting cases this will not be the case and the eigenenergies will explicitly depend on time. This means that the Gaussian wave-functional which we identify with, and refer to as the ground state does not in general correspond to the state of lowest energy, at least for all times. We will still refer to it as the ground state however, as it remains a basis on which to expand the state space. At a more technical level this may be seen from the fact that even in non-generic space-times (such as FLRW) with a preferred slicing, the Hamiltonian is time-dependent. While one can always work with the instantaneous ground state for a given fixed t, the expectation value of the renormalized stress energy tensor $\langle\psi|\, T_{\alpha\beta}\,|\psi\rangle$ associated to such a state will not necessarily be small, as the corresponding state fails to be a Hadamard state [1] as defined in [13].

[1] Private communication Prof. Stefan Hollands

Normalization

One of the main differences between the static Minkowski and the general case is the nature of the normalization. While in the static case it suffices to choose a (formally infinite) constant $\mathcal{N}$ to normalize the state functional, this is no longer the case in dynamical space-times. Here we must allow the normalization to be a function of time, while it still retains its character as a normalization constant in the sense that it does not functionally depend on the field. This can be seen by inserting the general Ansatz (3.14) into the Schrödinger equation (3.13). In order to simplify the notation we will adopt a generalized matrix notation, dropping the integral signs wherever this is unambiguously possible. Once more we split equation (3.13) into a field-dependent and a field-independent part. The latter will serve as defining relation for the Normalization. Since the mass and curvature dependent term will always be quadratic in the fields, we consider a free massless field here.

$$i\partial_t \mathcal{N}(t) e^{-\frac{1}{2}\phi K \phi} = \frac{\delta^2}{\delta \phi^2} \mathcal{N}(t) e^{-\frac{1}{2}\phi K \phi}, \tag{3.15}$$

giving

$$i\left[\dot{\mathcal{N}}(t) - \frac{1}{2}\phi \dot{K} \phi \mathcal{N}(t)\right] e^{-\frac{1}{2}\phi K \phi} = \mathcal{N}(t)\left[\mathrm{tr}K + (-\phi K)^2\right] e^{-\frac{1}{2}\phi K \phi}. \tag{3.16}$$

From the field-independent part we may therefore deduce that the normalization satisfies the following expression

$$i\partial_t \ln\left(\mathcal{N}^{(0)}(t)\right) = \frac{1}{2}\int_{\Sigma_t} d^3\mathbf{x}\sqrt{-g}K(\mathbf{x},\mathbf{x};t)\,, \tag{3.17}$$

where we have reinstated all integrals and measures. This may be easily integrated to give the full time-dependence of the normalization factor

$$\mathcal{N}^{(0)}(t) = \mathcal{N}^{(0)}(t_0)\exp\left[-\frac{i}{2}\int_{t_0}^{t} d\tau\sqrt{-g_{00}}\int_{\Sigma_\tau} d\mu(\mathbf{x})K(\mathbf{x},\mathbf{x};t)\right]. \tag{3.18}$$

The time-dependence of the normalization factor thus resides solely in the functional trace of the kernel. It is important to point out that, unlike in the usual case, it is not possible to simply define $\mathcal{N}$ as the inverse of the functional integral of $\|\Psi_t\|^2$, as is sometimes done in the literature, since this would mean that the resulting state is no longer a solution to the functional Schrödinger equation (3.13)! This is particularly important as it implies that the norm of a general state will no longer necessarily equal one at all times, in all geometries. While this is often met with skepticism, it is a simple consequence of the functional nature of the states involved. Furthermore, on a dynamical background it is to be expected that the norm may change as the underlying geometry dictates the dispersion of the oscillators making up the field. In the semi-classical approximation we are dealing in, the background is not resolved in terms of dynamical degrees of freedom, and it is therefore possible to “leak" probability into the background.

3.2.2. Relation to the Wave Equation

So far, all of the relations have been given in terms of the integration kernel $K(\mathbf{x},\mathbf{y};t)$. In general it must be determined from the Schrödinger equation by considering the field-dependent parts of (3.16), including the potential terms. In full generality for a free, massive scalar field this Ansatz leads to a Ricatti equation

$$\begin{aligned} i\partial_t\left(\sqrt{q_{\mathbf{x}}}\sqrt{q_{\mathbf{y}}}K(\mathbf{x},\mathbf{y};t)\right) = &\int d^3z\,\sqrt{-g_{\mathbf{z}}}\sqrt{q_{\mathbf{x}}q_{\mathbf{y}}}K(\mathbf{x},\mathbf{z};t)K(\mathbf{z},\mathbf{y};t) \\ &-\sqrt{q_{\mathbf{x}}q_{\mathbf{y}}}\sqrt{-g_{00}(\mathbf{x})}(-\Delta_x+m^2+\xi R)\delta^{(3)}(\mathbf{x},\mathbf{y})\,. \end{aligned} \tag{3.19}$$

As we can see (3.19) will be very complicated in a general space-time. It is therefore useful to simplify it as much as possible. Fortunately, a general equation of the Ricatti-type can be put into the so-called normal form, through which we associate the kernel with solutions of the wave equation.

Normal Form

Consider the following form for an ordinary Ricatti equation with regard to the unknown function $y(x)$

$$y' = y^2 + q(x)y + s(x). \tag{3.20}$$

This is precisely the form that we encountered above. As is well known, this equation is related to a solution $u(x)$ of the more standard Sturm-Liouville type problem

$$u'' = -q(x)u' + s(x)u = 0, \tag{3.21}$$

by virtue of the transformation

$$y(x) = -\frac{\partial}{\partial x}\ln u(x). \tag{3.22}$$

Furthermore, we see in (3.19) that the term linear in y is absent; thus the corresponding equation for u will have the form of an harmonic oscillator equation with a time-dependent frequency. In the following, we will show that this may be used to link the solutions of (3.19) to the solutions of the mode- or wave equation on the corresponding background space-time. In most cases this facilitates the solution tremendously.

Huygen's Principle

In order to establish the connection, we apply Huygen's principle to an arbitrary solution φ of the wave equation. Note that the term Huygen's principle is often used ambiguously and may refer to several different concepts pertaining to the propagation of waves, including within this thesis. To avoid confusion we will therefore always make explicit which formulation of Huygen's principle we are dealing with. Presently, we refer to the most common meaning,

whereby the wavefront at some time is made up out of the superimposed wave fronts at earlier times. We can therefore write

$$\varphi(t,\mathbf{x}) = i\int_{t_0}^{t} dt'\sqrt{-g_{00}}\int_{\Sigma_t} d^3x'\sqrt{q_{x'}}K(\mathbf{x},\mathbf{x}';t')\varphi(\mathbf{x}',t'). \tag{3.23}$$

Taking the time derivative of both sides we find

$$-i\frac{1}{\sqrt{g_{00}}}\frac{\partial}{\partial t}\varphi(t,\mathbf{x}) = \int_{\Sigma_t} d^3x'\sqrt{q_{x'}}K(\mathbf{x},\mathbf{x}';t)\varphi(\mathbf{x}',t). \tag{3.24}$$

After inserting this into the Ricatti equation for the kernel (3.19), as well as multiplying both sides by $\varphi(t,\mathbf{y})$ and integrating over y we find

$$\begin{aligned} i\int_{\Sigma_t} d^3y\,\varphi(t,\mathbf{y})\partial_t\left[\sqrt{q_x}\sqrt{q_y}K(\mathbf{x},\mathbf{y};t)\right] = \\ -i\int_{\Sigma_t} d^3z\sqrt{q_z}\sqrt{q_y}K(\mathbf{x},\mathbf{y};t)\partial_t\varphi(t,\mathbf{z}) + \sqrt{-g_x}(\triangle - m^2 - \xi R)\varphi(t,\mathbf{x}). \end{aligned} \tag{3.25}$$

After renaming the integration variable and using (3.24) once more we arrive at the standard covariant form of the mode equation

$$\partial_t[g^{00}\sqrt{-g}\partial_t\varphi] + \sqrt{-g}(\triangle - m^2 - \xi R)\varphi = 0. \tag{3.26}$$

We thus conclude that any kernel $K(\mathbf{x},\mathbf{y};t)$ fulfilling Huygens principle as stated in (3.24) will also be a solution of the kernel equation (3.19). Furthermore, the kernel is fully determined by the solutions to the wave-equation. This simplifies computations tremendously as it allows us to solve for the kernel directly using only the solutions to the wave equation. To see this we once again use (3.24) by considering its Fourier transformed version

$$\begin{aligned} -\frac{i}{\sqrt{-g_{00}}}\partial_t\varphi(t,x) &= \int d^3y\sqrt{q_y}\int\frac{d^3k}{(2\pi)^3}\int\frac{d^3p}{(2\pi)^3}e^{ik\cdot x}e^{i(p-k)\cdot y}\hat{K}(k,t)\hat{\varphi}(t,p) \\ &= \sqrt{q}\int\frac{d^3k}{(2\pi)^3}e^{ik\cdot x}\hat{K}(k,t)\hat{\varphi}(t,k). \end{aligned} \tag{3.27}$$

Taking the fourier transform of the LHS above we therefore get for the Kernel that

$$\boxed{\hat{K}(t,k) = -\frac{i}{\sqrt{-g}}\frac{\partial}{\partial t}\ln\hat{\varphi}(t,k).} \tag{3.28}$$

In fact, although it does provide some insight into the physical meaning of the kernel itself, one does not have to employ Huygens principle to arrive at this result. Viewed as transformation of variables (3.28) brings the kernel equation into linear normal form in the sense discussed above. The close resemblance of (3.28) and (3.22) is of course not accidental.

It is often more practical to work with the mode functions directly. This is both due to the fact that these have usually been studied in quite some detail already and that the physical interpretation is more straightforward. In particular, it is easier to provide the initial data in terms of mode solutions, especially as it is much closer to the more familiar Heisenberg Green function formalism. For example in inflation, one imposes the condition that the early time behavior must resemble free Minkowski evolution deep inside the horizon, to fix the initial data and select the appropriate Hankel functions specifying the Bunch Davies vacuum. Using (3.28) we can easily derive the real part of the kernel

$$2\,\mathrm{Re}\{\hat{K}\} = \frac{i}{\sqrt{-g}}\left(\frac{\hat{\varphi}\partial_t\hat{\varphi}^* - \hat{\varphi}^*\partial_t\hat{\varphi}}{|\hat{\varphi}|^2}\right), \tag{3.29}$$

which will become important when evaluating the norm of the wave functional later on. To close, we give the expressions derived in the flat space-time section again, this time for general backgrounds and in terms of the wave solutions. While they are very similar of course, care must be taken in order to account for the additional factors that stem from the non-trivial metric factors in all spatial integration measures. With the conventions laid out earlier, the absolute value of the normalization will be given by

$$|N(t)|^2 = |N(t_0)|^2 \exp\left(-\frac{1}{2}\mathrm{vol}(\Sigma)\int\frac{d^3\mathbf{k}}{(2\pi)^3}\ln\frac{|\hat{\varphi}(t,\mathbf{k})|^2}{|\hat{\varphi}(t_0,\mathbf{k})|^2}\right), \tag{3.30}$$

which can also be re-expressed in terms of the trace over the imaginary part of the kernel in position space. The field-dependent part will likewise be given by

$$\int\mathscr{D}\phi\,||G[\phi,t]||^2 = \int\mathscr{D}\phi\; e^{-\phi\mathrm{Re}K\phi} \propto \det\left[\frac{i}{2}\frac{\sqrt{q(t)}}{\sqrt{g}}\frac{\hat{\varphi}\partial_t\hat{\varphi}^* - \hat{\varphi}^*\partial_t\hat{\varphi}}{|\hat{\varphi}|^2}\right]^{-1/2}, \tag{3.31}$$

as only the real part of the kernel contributes here.

4. Completeness Concepts

In the following chapter we use the Schrödinger formalism developed so far to introduce the concept of quantum completeness as it pertains to space-time solutions. At its core it is a generalization of existing concepts that have long been in use for both the classical and the quantum theory of point particles to the theory of quantum fields. The question of completeness always arises in some form when using models to approximate physical systems. Even though there are numerous different concepts in use to answer this question, the underlying principle is always to see whether the inadequacies of the model give rise to physically unacceptable behavior within the framework of the theory built upon it. A simple example of this is the Coulomb-type potential,

$$V(r) \sim -\frac{1}{r} \tag{4.1}$$

that may be used to model a variety of physical situations, ranging from the gravitational field of some far away source to the electrical potential experienced by the electron in a hydrogen atom. The potential is clearly divergent at the origin and therefore any physical configuration that ends up there will obtain an infinite amount of energy, a state which is clearly not satisfactory from a physical standpoint. Naturally such singular behavior has no bearing on the actual physical reality but is rather a consequence of the superficial nature of our model. In the case of the hydrogen atom we have knowingly not taken into account the structure of the proton and resolving the singular nature of the potential would require us to do so. While it is general consensus that there can be no such thing as a "true" singularity in nature, we are almost always in a position where our incapability to capture the full physics necessitates the use of such singular models. To ask whether a system is complete or not is hence to ask whether it will become sensitive to the compromises we have made in setting it up, or if it is "safe" when left on its own. For example, in the case of the hydrogen atom the wave function of the electron does not give any probabilistic support to the problematic region in question, and therefore no problem will be encountered in the evolution despite the problematic nature of the potential. It is thus quantum mechanically complete. Classically however, there are initial conditions that allow us to probe the problematic point, and the potential is consequently incomplete classically. Completeness is therefore an important criterion to judge whether a given model will remain safe within the confines of its scope for all possible initial conditions or not.

In the following we will introduce the concepts of completeness as they have been established in the literature. Starting from the rather straightforward concepts related to a classical point

particle and quantum mechanics, we will develop an intuition for the relevant concepts. In the following we examine the various notions of completeness that exist in general relativity, where the notion becomes more complicated. Finally, we will see how to merge the two approaches and define the concept of semi-classical quantum completeness for a space-time manifold.

4.1. Completeness for Point Particles

Here we present the notion of completeness for the classical and quantum mechanical point particle on a Minkowski background.

4.1.1. Classical Completeness

The classical motion of a point particle is given entirely by the Lagrangian or Hamiltonian dynamics induced by its respective Hamiltonian. As we are only interested in the trivial flat geometry for now, the kinetic term of the Hamiltonian will always be of similar form and the entirety of the information about the properties of a system are contained within its potential V. For simplicity we will assume only motion on the half line, therefore the configuration space is given by $\mathbb{R}^+$ and the phase space is given by $(x(t), v(t)) \in \mathbb{R}^+ \times \mathbb{R}$. Furthermore we assume the potential $V(x)$ to be continuously Lipschitz differentiable on every compact subset of $\mathbb{R}^+$. The Hamiltonian will in this case take the form

$$H = \tfrac{1}{2}v^2(t) + V(x(t)). \tag{4.2}$$

In this very restricted setting, the only thing that stands in the way of completeness is the particle reaching zero or infinity in a finite amount of time. In this case, it can no longer remain within the confines of the phase space, and therefore the motion is "incomplete". Furthermore, if the particle cannot reach the edge of the configuration space, it is guaranteed that any local solution to the equation of motion is indeed a global one. Demanding that the motion be complete is therefore equivalent to the demand that the particle does not reach zero or infinity in finite time. This equivalent to the definition given in [14] which may be phrased as follows

Definition. *The classical motion generated by a potential V is called **complete** at 0 or ∞ if there exist no initial conditions for which the solution to the equations of motion $x(t)$ reaches 0 or ∞ respectively in a finite amount of time.*

In this simple setting it possible to unambiguously classify all possible potentials. In order to be complete at 0 the potential must be unbounded there, thus guaranteeing that no initial velocity is large enough to overcome the potential barrier. To prevent an escape to infinity we must simply ensure that the potential is not attractive enough in order to enable a finite time of travel.

4.1.2. Quantum Mechanical Completeness

The concept of quantum mechanical completeness differs from that of the classical point particle insofar as we do not have the actual trajectory available to us. Instead, the theory obtains a probabilistic interpretation, the probability density being given by the solutions to the Schrödinger equation

$$i\partial_t \Psi = H\Psi. \tag{4.3}$$

where, remaining on $\mathbb{R}^+$, the Hamiltonian H is given formally as the operator

$$H = -\frac{1}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x). \tag{4.4}$$

Assuming that the potential is a real valued, continuous function, H will always be a symmetric operator on $\mathbb{R}^+$. The time-evolution is then given, by Stone's theorem, through a unitary continuous one-parameter group, provided the Hamiltonian is self-adjoint. Previously, in the classical case, we used a definition of completeness which reflected our desire that the classical evolution does not reach the edge of phase space and unique with respect to given initial conditions. As the evolution of the state is now described in terms of a ray in Hilbert space, we must adapt our definition of completeness accordingly. In the spirit of the above, the minimal requirement we may ask for is the Hamiltonian H to be essentially self-adjoint. This means that the evolution is globally unique in the sense that every essentially self-adjoint operator will possess a unique self-adjoint extension, that may then be used to define the evolution group in the sense of Stone's theorem. The thus induced unitary evolution will also guarantee that the state remains normalized and therefore in the $L^2(\mathbb{R}^+)$ that is our Hilbert space. Again, as we have little choice for the kinetic part of the Hamiltonian, this condition will depend on the chosen potential $V(x)$.

Definition. *A potential $V(x)$ is called **quantum-mechanically complete** if the Hamiltonian $H = -d^2/dx^2 + V(x)$ is essentially self-adjoint on the smooth functions on $\mathbb{R}^+$.*

Unlike in the classical case, it is therefore not as straightforward to determine whether the evolution is complete or not. A useful condition given by [14] is the following

Theorem. *A Hamiltonian $H = -d^2/dx^2 + V(x)$ will be essentially self-adjoint if and only if for some $\lambda \in \mathbb{C}$ at least one solution to*

$$-\varphi'' + V(x)\varphi = \lambda\varphi$$

is not square integrable. In this case it is called to be in the limit point case.

Unfortunately, a direct comparison of different potentials reveals that the classical and the quantum mechanical definitions do not always agree. In fact one may find examples that satisfy any combination of the criteria. In particular, the coulomb type potential where $V(r) = -e^2/r$ mentioned at the outset, will be obviously classically incomplete as it is bounded above by

zero, while it is easy to show that the respective Hamiltonian will be essentially self-adjoint. The converse is also possible, owing to the fact that a quantum-mechanical particle will be capable of tunneling through potential regions that would turn back the classical particle, and therefore "escape" to infinity. An interesting example for this is once more given in [14] as

$$V(x) = \frac{1}{x^2} - x^4 + \sum_{k=1}^{\infty} \sigma_k(x) \tag{4.5}$$

where the functions $\sigma_k(x)$ are chosen such that for every integer $n \in \mathbb{N}$, $V(n) = n$. As the potential is unbounded at both zero and infinity, the classical motion is complete. The proof follows from the observation that $V_0 = 1/x^2 - x^4$ is not quantum-mechanically complete at zero. This can be directly confirmed, using the following theorem

Theorem. *Let $V \in C^2(\mathbb{R}^+)$ and assume that $V(x) \to -\infty$ as $x \to \infty$. Further, assume that*

$$\int_c^{\infty} \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\frac{d}{dx}\sqrt{-V}}{(-V)^{3/2}} \right) V^{-1/4} dx < \infty$$

for some c. Then V is in the limit point case if and only if $\int_c^{\infty} \frac{d}{dx}\sqrt{-V} = \infty$.

The fact that it is possible to choose $\sigma_k(x)$ that are narrow enough to ensure that the potential defined in (4.5) makes H non essentially self-adjoint then follows from the Kato-Rellich theorem for perturbations of operators. The theorem above does however show, that there is some relation between quantum mechanical and classical completeness insofar as it shows that a classically complete V will be quantum-mechanically complete, provided its derivatives remain small. Due to the sharpness of the peaks in (4.5) this is of course not the case here.

4.1.3. Completeness in General Relativity

So far we have only considered the dynamics on trivial i.e. flat backgrounds. Since our goal is to define a notion of completeness that may be applied to fields in general backgrounds, it is instructive to first consider the behavior of point particles thereon. There are several conceptual differences to the previously studied examples. Firstly, unlike before, the velocity terms will play a more important role. On the flat geometry in the classical case, the kinetic term cannot influence the completeness or un-completeness of a given system. In some sense, the only role it plays is to determine the energy budget of a given solution via the corresponding initial conditions. As a system is only complete when all admissible initial conditions are well behaved, it is sensible to speak only of the potential in these strictly kinematical considerations. In the setting of general relativity this is very different however, as the kinetic term itself may become dynamical, depending on the space-time model. Secondly, we must address the possibility of the background itself becoming ill-defined or singular. This opens up a new perspective on the question of completeness. In principle, there seem to be two distinct logical possibilities to console the appearance of singularities within the framework of Einsteins theory with the physical

reality we observe today. The first and perhaps most prevalent rests on the fact that, being a classical theory, general relativity cannot be fundamental. Thus the appearance of singularities may only signal the breakdown of a approximation to the 'true' underlying theory. One would then expect this fundamental theory of gravity to be void of such singularities. Unfortunately, owing to its perturbative non-renormalizabiliy, no quantum theory of gravity is available to date, and there seems little chance to give a definitive verdict on the question whether such a theory remedies the existence of singularities in the near future. This point of view is supported by semi-classical considerations. It is well known within the framework of quantum field theory in curved space-times that a dynamical space-time leads to the production of particles. This leads to a new source on the right hand side of the Einstein equation

$$G_{\mu\nu} = 8\pi T_{\mu\nu}, \tag{4.6}$$

which subsequently alters the metric. One assumes that these back-reactions will modify the metric in such a way that the resulting metric is no longer singular. In lack of a theory of quantum gravity it is of course not certain that this will happen, nor is it possible to describe such a transition form one background to another as of now. Furthermore there are many singular space-times that are static and therefore may not even be able to provide such a mechanism.

The second logical possibility lies in the realization that a singularity must not be observable and therefore must not bear any physical significance per se. In fact, one is easily tempted to simply equate the physical space-time with the semi Riemannian manifold that is used to model it, within the scope of general relativity. In its barest form the physical space-time is a set of events that satisfy certain causal relations between them. While the description in terms of manifolds has proven very fruitful, they themselves are not observable and thus physical. In this sense the physically relevant question is whether singularities necessarily lead to un-physical predictions. If, by some mechanism, singularities are shielded from physically observable consequences, their existence must not rule out the viability of space-time models. The situation is then comparable to an electron moving in a coulomb potential. Albeit the potential diverges in the limit $r \to 0$, there is no physical state that can realize this configuration as the probability to find the electron at the origin is strictly zero for all hydrogen wave functions. This perspective offers the advantage that it can be studied without the necessity of a quantum theory of gravity and the conclusions drawn should be independent of the completion that such a theory may eventually have to offer. As we shall see later, similar to the classical vs quantum completeness of a point particle, this interpretation opens up the possibility for the system under scrutiny to be complete, even when the underlying space-time is not.

The diffeomorphism invariance of general relativity makes it futile to single out individual points to anchor our notion of completeness, like we have done for the classical particle. Following the standard treatment, we define the mathematical model of space-time as a pair $(\mathcal{M}, g)$, where $\mathcal{M}$ is a connected, Hausdorff, C^∞ manifold (usually of dimension four) and g is a Lorentzian metric on $\mathcal{M}$. It is widely known that many exact solutions to (4.6) exhibit singularities, so one usually defines $\mathcal{M}$ upon the removal of such points. To be precise, one defines $(\mathcal{M}, g)$ by omitting all singular points such that the resulting manifold may not be extended smoothly any further. The trajectories a point particle will follow on this geometry are then given by the solutions to the geodesic equation

$$\dot{\xi}^\mu \nabla_\mu \dot{\xi}^\nu = 0, \tag{4.7}$$

where the over-dot denotes differentiation with respect to proper time and ∇_μ the covariant derivative with respect to the Levi-Cevita connection. As before, we require the trajectory to be well defined for all times, therefore the simplest definition of completeness in general relativity is that of geodesic completeness

Definition. *A spacetime $(\mathcal{M}, g)$ is **g-geodesically complete** if and only if every geodesic may be extended for arbitrary values of proper time.*

The definition above best replicates the spirit of the mechanical completeness of a system given earlier. One can further distinguish between *time-like*, *space-like* and *null* geodesic completeness depending on the nature of the inextendible geodesic. Null and time-like completeness are thereby a natural criterion, as the former directly pertains to the motion of mass-less particles, while the latter implies the possibility of observers appearing literally out of nowhere. It is unclear what the role of space-like geodesics may be, as there are no physical particles that move along space-like geodesics. In their work [15] Hawking and Ellis therefore suggest requiring only null and time-like completeness as a minimal criterion for the completeness of a space-time. There are examples of space-times that are complete in any one of the above senses, but incomplete in the other two as was shown by [16]. For example, the Reisner-Nordström black hole is time-like complete but null-incomplete. It should be mentioned that, even though this definition works perfectly well for freely falling observers it has been shown that there are space-times that, albeit geodesically complete, contain inextendible curves of bounded acceleration of finite length [17], [18]. This is problematic, as any reasonable definition of completeness must hold beyond freely falling particles.

A more general definition of completeness was first formally introduced by Schmidt [19]. For a more detailed discussion we refer to [15] as an excellent review. The basic idea of this definition is to consider the orthonormal frame-bundle $(O(\mathcal{M}), \pi, \mathcal{M})$ over the space-time manifold $\mathcal{M}$, and to construct a Euclidean metric on $O(\mathcal{M})$. This bears the advantage that one may define a distance function $\rho(x, y)$ as greatest lower bound for the length of all curves from x to

y. This is naturally not possible on the original Lorentzian manifold $\mathcal{M}$. One may proceed to define m-completeness as the property that any Cauchy sequence with respect to ρ converges to a point in $\mathcal{M}$:

$$u = \int_{\lambda(t)} \sqrt{\sum_i V^i V^i} dt. \tag{4.8}$$

Here, $\mathbf{V} = (\partial/\partial t)_{\lambda(t)}$ denotes the tangent vector to the C^1 curve under consideration. At the point p we may choose a orthonormal basis of the tangent vectorspace $T_p\mathcal{M}$ as $\{\mathbf{E}_a\}$, a running from one to four, and decompose the tangent vector according to this choice of basis $\mathbf{V} = V^i \mathbf{E}_i$. The integration is then to be understood as the sum of all points along the curve λ. The basis $\{\mathbf{E}_a\}$ is thus parallel transported along the curve to give meaning to the above expression. Obviously, the result depends on our initial choice of basis. However, all orthonormal frames are related through $GL(n)$ transformations, i.e. we have $\tilde{\mathbf{E}}_i = B_i^j \mathbf{E}_j$, where B is some invertible matrix. Therefore, there is some real constant C such that

$$C \sum_i V^i V^i \leq \sum_i \tilde{V}^i \tilde{V}^i \leq \frac{1}{C} \sum_i V^i V^i. \tag{4.9}$$

This implies that if a particular choice of basis will lead to a finite value of u all others will too. The definition reduces to that of the affine parameter in the case of geodesics, but is more general. We can therefore introduce the notion of bundle completeness [15]

Definition. *A space-time $(\mathcal{M}, g)$ is called **bundle-complete** if there is an endpoint for every continuously differentiable curve as measured by the generalized affine parameter.*

This notion extends the concept of geodesic completeness in the sense that it implies it; however, geodesic completeness does not imply bundle-completeness. Bundle-completeness may be defined on any space-time admitting a connection.

4.2. Semi-Classical Completeness

In the previous section we have outlined numerous definitions of completeness that are already in use for various settings. In the classical cases we have seen how these relate to a test particle remaining on a "well-behaved" trajectory, i.e. one that remains within the configuration space and does not suddenly begin or end. As the concept of a trajectory is ill-defined for a quantum mechanical particle, we have argued that the natural analog of this reasoning is to demand the Hamiltonian to be essentially self-adjoint, thereby guaranteeing that the state will be normalizable and represented by a ray in Hilbert space. As we have seen that classical and quantum-mechanical completeness are at times in tension, a natural question to ask is what happens in systems where we choose to quantize the particle on a classical background. We will discuss this first for the example of single particles before generalizing to field theory.

4.2.1. Quantum Mechanical Considerations on Curved Space-times

The question about the behavior of a relativistic quantum test particle on a classical, and potentially singular, background was first discussed by Horowitz and Marolf [20]. The approach therein is almost identical to the proceeding section. Considering a static space-time with a time-like killing vector field ξ^μ the wave equation may be rewritten in the form

$$\frac{\partial^2 \psi}{\partial t^2} = VD^i(VD_i\psi) - V^2 m^2 \psi, \tag{4.10}$$

where t denotes the Killing parameter, D_i is the spatial covariant derivative and $V = -\xi^\mu \xi_\mu$. When taking the right hand side of this equation as the defining relation for the operator

$$A := -VD^i(VD_i) + V^2 m^2, \tag{4.11}$$

we note that A is symmetric and positive on the smooth functions with compact support on the spatial hypersurfaces. Furthermore, due to the fact that it is real and therefore its deficiency indices will always be equal, it has self-adjoint extensions. As before, we will consider the system to be complete if A is essentially self-adjoint. In this case it is possible to "take the square root" of A and write the formal solution to the wave function as

$$\psi(t) = \exp\left[-it\sqrt{A}\right]\psi(0). \tag{4.12}$$

So far the treatment is no different from the flat cases considered before. Once again we may construct examples of space-times that are geodesically complete, yet are quantum mechanically incomplete and vice versa. One such example is given charged dilatonic black holes in four dimensions. They are characterized by extrema of the action

$$\mathcal{S} = \int \mathrm{d}^4x\sqrt{-g}[\, R - 2(\nabla\phi)^2 - e^{-2a\phi}F^2], \tag{4.13}$$

where ϕ is the dilaton, a the dilaton coupling and F the Maxwell field. As we have seen before, the operator A will be essentially self-adjoint if and only if one of the solutions to the respective eigenvalue equation is not normalizable near zero. In their work [20] show that the L^2-norm of these solutions can be expressed in terms of an integral involving only the dilatonic coupling

$$\|\varphi\|_2 = \int \mathrm{d}\rho\ \rho^{-4/(1+a^2)}. \tag{4.14}$$

It is immediate, that this integral will diverge whenever $a^2 \leq 3$. From this we may infer, that quanta approaching the time-like singularity will be repulsed and a quantum mechanical test particle may enjoy a complete evolution.

4.2.2. Field Theory

Unfortunately, the generalization of these concepts to non-static space-times is far from straightforward. In a general time-dependent background it is not possible to give any sensible quantum theory of a single particle. Instead we must turn to the theory of fields if we are to investigate the behavior of quantized degrees of freedom on these backgrounds. This requires a change both in the conceptual and technical framework. The second is simply due to the fact that much of the mathematical apparatus we have relied on to investigate the quantum mechanical setting is simply not well defined in the context of field theory. Especially the properties of unbounded operators in field space can be only hinted at by analogy, as a rigorous framework for the analysis of infinite dimensional manifolds of the field space is unavailable. However, some of the concepts that we have leaned on in the previous definitions must too be abandoned. In particular, the assumption of a strictly unitary time evolution, and therefore self-adjoint Hamiltonians must no longer be valid in curved, dynamical space-times. In principle, our task is to define an evolution operator evolving the initial field configuration in time

$$\Psi_t = \mathcal{E}(t,t_0)\Psi_{t_0}, \tag{4.15}$$

and to then investigate whether the ensuing evolution is complete in the sense that it is unique and steers clear of potentially singular points on the background metric. It was shown by Ashtekar and others [21–23], that the evolution operator transforming the field configuration from one spatial hyper-surface to the next will not be unitary in general. In the context of the Schrödinger quantization this is reflected in the fact that the norm of the wave functional $\|\Psi[\phi]\|_2$ is not constant with time. It seems unreasonable therefore, to further insist on a strictly self-adjoint Hamiltonian as a criterion for the completeness of field evolution. Instead, we will relax the condition to requiring that the evolution does not cause the norm to exceed the bound placed on in to ensure a probabilistic interpretation of the theory

$$\|\Psi[\phi]\|_2(t) \leq 1, \ \forall t. \tag{4.16}$$

While the norm may decrease and still admit for a viable probabilistic interpretation of the theory, an evolution which results in the increase of the norm will not. We will therefore define [1]

Definition. *A globally hyperbolic space-time $(\mathcal{M},g)$ is defined to be quantum complete (to the left) with respect to a free field theory, if the Schrödinger wave functional of the free test fields can be normalized at the initial time t_0, and if the normalization remains bounded from above by its initial value for all t.*

The loss of probability does not present a conceptual problem, but is rather an indication that the perturbative ground-state is not persistent. In this case probability is simply transferred to the background, as it is not resolved by dynamical degrees of freedom.

The Schwarzschild Space-time

The first application of the definition of a quantum complete space-time was to the interior Schwarzschild metric [1], which we briefly discuss in the following. As the Schwarzschild metric describes the gravitational field of a spherically symmetric body, and reduces to a $1/r$-potential for the remote observer it can be considered the most direct analog of the potentials studied earlier and therefore a natural testing ground. It will turn out that this space-time is in fact an example for a geodesically incomplete space-time that admits a quantum complete description of scalar fields near the geodesic border. Just like in the quantum mechanical case, it is an interesting question whether there are dynamical space-times that are quantum incomplete but geodesically complete, however no such example has been found yet to the best of our knowledge.

Naturally we are interested in the singularity at the center of the black hole and not the spurious singularities that may appear around the horizon, therefore we immediately specialize to the interior of the black hole given by the metric

$$ds^2 = -h(\tau)^{-1}dt^2 + h(\tau)dr^2 + \tfrac{1}{4}r^2 r_s^2 d\Omega_2, \tag{4.17}$$

where we have defined the Schwarzschild radius $r_s = 2M$, the dimensionless parameter $\tau := 2t/r_s$, the function $h(\tau) := (2-\tau)/\tau$ and the induced line element of a two sphere of radius $\tau r_s/2$. In this case the Ricatti equation determining the evolution of the functional kernel is a rather complicated one

$$i\partial_\tau \hat{K}(k,\tau) = \sqrt{-g}\tfrac{r_s}{2}\left(\sqrt{q}^{-1}\hat{K}^2(k,\tau) - q^{ab}k_a k_b + m^2\right), \tag{4.18}$$

where q^{ab} again refers to the induced metric on the spatial slices. Rather than attempting to evaluate the kernel in terms of the mode functions of the Schwarzschild interior, it is possible to solve this equation directly (at least asymptotically) by transforming it to the standard form, allowing for the determination of the imaginary and real parts of the kernel [1]

$$\mathrm{Im}\hat{K}(k,\tau) \to -\frac{1}{M^3\sin(\theta)}\frac{1}{\tau^3|\ln\tau|} \tag{4.19}$$

$$\mathrm{Re}\hat{K}(k,\tau) \to |\mathrm{Im}(C)|\frac{|\mathrm{Im}\hat{K}(k,\tau)|}{|\ln\tau|}. \tag{4.20}$$

Note that unlike in the Minkowski case, the kernel develops a non-trivial imaginary part, which is in fact the dominant contribution. With these results one can infer that the norm of the wave-functional approaches zero as we close in on the singular hypersurface.

$$\|\Psi\|_2(\tau) \to |\ln \tau|^{-\nu(\Sigma)}(\tau^{3/4}|\ln \tau|)^{N(\Lambda)} \to 0, \tag{4.21}$$

where $N(\Lambda)$ and $\nu(\Sigma)$ are the usual UV and IR regulators respectively. We can therefore conclude that the Schwarzschild space-time is quantum complete in the sense of the definition above. Moreover, the probabilistic support for field configurations at the geodesic border vanishes. This in turn implies that there is no quantum mechanical observable that is capable of probing the classically singular point. Therein lies the importance of the quantum completeness principle, as there is no measurement process that allows us to probe the geodesic incompleteness of the background, much like in the example of the hydrogen atom.

5. The Kasner Space-time

In this section we use the tools developed so far to analyze the behavior of quantum probes in the vicinity of the singularity of a Kasner universe. This space-time is of particular importance as it generalizes a wide variety of space-like singularities by virtue of the BKL conjecture, which claims that universally the approach to such singular points will end in a series of successively alternating Kasner epochs. Furthermore it is an interesting cosmological model, allowing for a smooth transition into a period of de Sitter-like expansion, providing a viable precursor to inflation. The phenomenological aspects of such a transition have been studied [24, 25] and provide a series of potentially measurable effects.

The main motivation for considering a Kasner universe comes from the so-called Belinskii-Khalatnikov-Lifschitz (BKL) model. In their 1970 seminal paper [26] Belinski, Khalatnikov and Lifschitz addressed the problem of a cosmological singularity from a very general perspective. Their main motivation was to study whether the initial singularity, famously displayed by many of the known solutions to the Einstein equations, was a general feature thereof or simply due to the many simplifying assumptions that had to be made to arrive at said solutions. In particular, they strove to determine the most general solution of the Einstein equations, generality being defined through the number of arbitrary functions of the coordinates contained within, to investigate whether such a solution contained a singularity. A sufficiently general solution should therefore be able to accommodate a large number of initial conditions, which are given by the matter distribution, the relative motion of matter etc. at a chosen moment in time. As an example, the Friedmann cosmological solutions would not be considered general from this standpoint, as the requirements of homogeneity and isotropy pose severe restrictions on the class of eligible initial data sets. In this way they hoped to shed some light on the question which features of singularities are universal and which only arise due to the highly idealized settings in which we choose to study them.

Inspired by the cosmologically relevant Friedmann solutions, they considered space-times with a singular point in time, i.e. a singular space-like hypersurface in the observable past. This does not include space-times where the singular region is bounded in space, such as for example the Schwarzschild geometry. As such, their work is of particular interest for the later application of our quantum framework to cosmological settings, maintaining the greatest possible generality. In short, their work suggests that the close vicinity of the singular point space-time universally mimics a Kasner-type behavior. The addition of matter does not seem to change

this trend but rather introduces a rapid rotation between different Kasner metrics. The only exception is given by stiff matter obeying the equation of state $\rho = \varepsilon$. Before we present their argument, concluding the classical discussion, we briefly introduce the Kasner and generalized Kasner solutions.

We then proceed to highlight the main phenomenological results pertaining to the Kasner space-time and how they are related to current cosmological observations. Kasner-like geometries lead to a large amplification of gravitational waves [25, 27], which ultimately leads to a destabilization of the geometry and can trigger a transition to more commonly used isotropic models. Signatures of such a transition leave an imprint on observational data today and are therefore in principle testable.

Finally we show how to quantize fields in a Kasner geometry and apply the apparatus developed in the previous sections to their Schrödinger form. We demonstrate that the Kasner singularity does not face inconsistencies as it is probed with quanta. This is due to the fact that the time evolution asymptotically becomes a contraction semi-group, hindering the migration of such quanta to the geodesic border. This behavior may be interpreted in terms of the BKL conjecture, as the velocity dominance displayed by the Einstein equations leads to a sufficient dilution of interactions as one approaches the singularity.

5.1. Kasner Solution

Kasner first introduced his solution to the Einstein field equations in 1921 [28]. The Kasner solution is a homogeneous an-isotropic vacuum solution of Bianchi-type I and basically represents one step back from the usual FLRW models in terms of symmetry. The line element of $(d+1)$-dimensional Kasner space is given by

$$ds_d^2 = -dt^2 + \sum_{i=1}^{d} t^{2p_i} (dx^i)^2. \tag{5.1}$$

The Kasner solution represents a vacuum solution of the Einstein equations and therefore the Ricci-tensor vanishes. The exponents p_i are subject to the so-called Kasner conditions, whereby they are required to lie in the intersection of the plane given by

$$p_1 + p_2 + \cdots + p_d = 1 \tag{5.2}$$

and the so-called Kasner sphere, parameterized by the condition

$$p_1^2 + p_2^2 + \cdots + p_d^2 = 1. \tag{5.3}$$

Due to the conditions above, the exponents p_i are not independent. When considering the four dimensional case, as we shall henceforth, there is only one independent exponent. Following [26], we define the parameter $u > 1$ to give a parameterization of the exponents p_i

$$\begin{aligned} p_1 &:= \frac{-u}{1+u+u^2}, \\ p_2 &:= \frac{1+u}{1+u+u^2}, \\ p_3 &:= \frac{u(1+u)}{1+u+u^2}, \end{aligned} \tag{5.4}$$

guaranteeing the ordering $p_1 < p_2 < p_3$. Interestingly we have that

$$p_1\left(\frac{1}{u}\right) = p_1(u),\ p_2\left(\frac{1}{u}\right) = p_3(u),\ p_3\left(\frac{1}{u}\right) = p_2(u).$$

There is no choice allowing for a complete degeneracy among the indices, thus the spacetime modeled by the Kasner line element will always be an-isotropic. Furthermore, for genuine Kasner spaces, one of the indices will always be negative, while the remaining two are positive. We also observe that there are only two cases in which two exponents are equal up to permutation of indices, namely $(p_1,p_2,p_3) = \{(1,0,0),(-\frac{1}{3},\frac{2}{3},\frac{2}{3})\}$. For later reference it is important to note that the Kasner conditions also imply that the determinant of the metric will always scale as t^2 since:

$$\det(-g) = \prod_{j=1}^{n} t^{2p_j} = t^{2\Sigma p_j} = t^2.$$

With one exception, the Kasner metric will always exhibit a space-like singularity at the time $t = 0$. This is evident from the components of the Riemann curvature tensor that take the form

$$R_{0i0i} = \frac{p_i(1-p_i)t^{2p_i}}{t^2}, \quad R_{ijij} = \frac{p_i p_j t^{2p_i} t^{2p_j}}{t^2}. \tag{5.5}$$

The components vanish for the choice of one exponent being equal to one, in which case the resulting spacetime will be simply a flat patch of Minkowski space. This is also apparent from the coordinate transformation

$$\tilde{t} = t\cosh(x_i),\ \tilde{x}_i = t\sinh(x_i), \quad \text{for} \quad p_i = 1.$$

For all other choices, the Kasner conditions force the Riemann tensor to diverge in the limit $t \to 0$, as do scalar invariants such as the Kretschmann scalar for example, which scales as

$$\mathscr{K} = \frac{f(u)}{t^4}, \tag{5.6}$$

where $f(u)$ is a regular positive function of the parameter u, with only one root $f(0) = 0$, corresponding to the choice $p_i = 1$. This implies that the singularity at $t = 0$ is indeed physical from a classical perspective, excluding the spurious $u = 0$ case. Furthermore, Kasner space is

geodesically incomplete in the sense discussed previously. This is straightforward to see from the observation that, in the limit of small angular displacements, the Kasner metric is equivalent to the Schwarzschild metric

$$ds^2 = -\left(1-\frac{2m}{r}\right)dt^2 + \left(1-\frac{2m}{r}\right)^{-1}dr^2 + r^2\left(d\theta^2+\sin(\theta)^2 d\varphi^2\right), \tag{5.7}$$

near the singularity. This is particularly interesting from the point of view of universality, as it shows that many of the conclusions we draw for Kasner space directly transfer to the Schwarzschild example. The isometry is seen by replacing θ with the new coordinate ρ, which we assume to be small. Equation (5.7) then reduces to

$$ds^2 = \left(\frac{2m}{r}\right)dt^2 - \left(\frac{2m}{r}\right)^{-1}dr^2 + r^2\left(d\rho^2+\rho^2 d\varphi^2\right) \tag{5.8}$$

if one aproaches the singularity. One is now in a position to make the following redefinition of coordinates,

$$t = \left(\frac{3}{4m}\right)^{1/3} z, \quad r = \left(\frac{9m}{2}\right)^{1/3}\tau^{2/3}, \quad \rho e^{i\varphi} = \left(\frac{2}{9m}\right)^{1/3}(x+iy), \tag{5.9}$$

reducing the line element to that of the Kasner space-time for the axis-symmetric choice of exponents $(p_1,p_2,p_3) = (-\frac{1}{3},\frac{2}{3},\frac{2}{3})$. The existence of in-extensible geodesics of finite proper length for the Kasner space-time then simply follows from the existence of such geodesics in the corresponding Schwarzschild limit.

5.2. The Belinskii-Khalatnikov-Lifshitz Model

We will now review the seminal work of BKL to elucidate the significance of the Kasner solution for a general description of space-like singularities.

5.2.1. Generalized Kasner Space

For the case of an-isotropic homogeneous space-times, a distinction is to be made between the exact Kasner solution discussed above and so-called generalized solutions or generalized Kasner space. In these cases the metric reduces to the one given in (5.1) only in the limit approaching the singular hypersurface. As such, it is much more general in the sense explained earlier. This class of solutions is of particular importance insofar as the exact Kasner solution has a vanishing Ricci tensor and thus is a vacuum solution, thereby severely restricting the possible initial data that may be considered. In order to provide a viable cosmological model, such an omission is of course not feasible. The consideration of generalized Kasner spaces allows for the inclusion of matter, while maintaining the Kasner-like nature near the singularity. We will see however that this does not significantly alter the evolution close to the singular point,

as is nicely summed up in a phrase coined by John Wheeler: "[near the singularity]... matter doesn't matter".

In following the treatment of [26], we will define generalized Kasner space to be any space with the spatial line element

$$dl^2 = (a(t)^2 l_\alpha l_\beta + b(t)^2 m_\alpha m_\beta + c(t)^2 n_\alpha n_\beta) dx^\alpha dx^\beta, \tag{5.10}$$

where

$$a(t) = t^{p_l},\ b(t) = t^{p_m},\ c(t) = t^{p_n} \text{ and } \mathbf{l}, \mathbf{m}, \mathbf{n} \in \mathbb{R}^3. \tag{5.11}$$

At this stage the p_i are labeled by the arbitrary spatial vectors $\mathbf{l}, \mathbf{m}, \mathbf{n}$ that do not necessarily coincide with the coordinate axis. Furthermore we do not require that they satisfy the Kasner conditions. Even though this may already seem very restrictive, when considering only the leading terms in an analytical expansion, a wide variety of models falls into this class, at least asymptotically. The question is now, how much can be said about the singularity without specifying any particular time dependence of the functions a, b and c. It is known that for any synchronous reference frame the Einstein equations in vacuum will take the form

$$R_0^0 = -\frac{1}{2}\frac{\partial}{\partial t}\kappa_\alpha^\alpha - \frac{1}{4}\kappa_\alpha^\beta \kappa_\beta^\alpha, \tag{5.12}$$

$$R_\alpha^\beta = \frac{1}{2\sqrt{-g}}\frac{\partial}{\partial t}\sqrt{-g}\kappa_\alpha^\beta - {}^{(3)}R_\alpha^\beta, \tag{5.13}$$

$$R_\alpha^0 = \frac{1}{2}(\kappa_{\alpha;\beta}^\beta - \kappa_{\beta;\beta}^\alpha), \tag{5.14}$$

where κ_α^β is the time derivative of the induced metric on the spatial hypersurface, and ${}^{(3)}R_\alpha^\beta$ is the corresponding pullback of the Ricci tensor. In this case one can therefore easily verify by insertion that the given components of the Ricci tensor can be written as

$$R_0^0 = \frac{\ddot{a}}{a} + \frac{\ddot{b}}{b} + \frac{\ddot{c}}{c}, \tag{5.15}$$

while the non-vanishing spatial components to leading order in $1/t$ are (provided that ${}^{(3)}R_\alpha^\beta$ does not contain higher order terms)

$$R_l^l = -\frac{\partial_t(\dot{a}bc)}{abc},\ R_m^m = -\frac{\partial_t(a\dot{b}c)}{abc},\ R_n^n = -\frac{\partial_t(ab\dot{c})}{abc}. \tag{5.16}$$

As we assumed that the functions a, b and c are analytical in t, all of the terms in equation (5.15) will be of the order $1/t^2$. From equations (5.15) and (5.16) it follows that the exponents p_l, p_m and p_n must indeed satisfy the Kasner conditions, when demanding the space-time remains vacuum. When ${}^{(3)}R_\alpha^\beta$ does contain higher orders, this is not quite as simple to see; however, the

result remains valid. We conclude from this that, without posing any severe restrictions on the functions a, b and c, the behavior near the singular point in vacuum will always converge to a Kasner solution.

Further [26] argue that the addition of matter does not change this general form in a significant way, as we can verify by considering the corresponding expressions for the evolution of matter

$$\frac{1}{\sqrt{-g}}\frac{\partial}{\partial x^i}\sqrt{-g}\sigma u^i = 0, \tag{5.17}$$

$$(p+\varepsilon)u^k\left(\frac{\partial u_i}{\partial x^k} - \frac{1}{2}u^l\frac{\partial g_{kl}}{\partial x^i}\right) = -\frac{\partial p}{\partial x^i} - u_i u^k\frac{\partial p}{\partial x^k}. \tag{5.18}$$

Here u_i denotes the four velocity, ε the energy density and σ the entropy density of matter. Insertion of the ultra-relativistic equation of state shows that none of the components of the energy momentum tensor scale to lower order in $1/t$ than the Ricci tensor. Therefore in the limit $t \to 0$ the presence of matter does not affect the space-time geometry to lowest order. Furthermore, the insertion of the relevant terms shows that the energy momentum tensor is in fact divergent as we approach the singular hypersurface, and thus the singularity is physical.

5.2.2. Metric Perturbations

More generally, [26] consider the effect of metric perturbations in the approach to the singular point of a generic homogeneous space-time. This restricts us to the consideration of Bianchi type VIII and IX spaces only. The authors argue that, subject to a perturbation characterized by a function λ of the coordinates the diagonal metric factors a^2, b^2 and c^2 take the form

$$a^2 = \frac{2|p_1|\Lambda}{\cosh(2|p_1|\lambda\tau)}, \tag{5.19}$$

$$b^2 = b_0^2\exp[2\Lambda(p_2 - |p_1|\tau)]\cosh(2|p_1|\lambda\tau), \tag{5.20}$$

$$c^2 = c_0^2\exp[2\Lambda(p_3 - |p_1|\tau)]\cosh(2|p_1|\lambda\tau), \tag{5.21}$$

where b_0, Λ and c_0 are constants of integration and we have transformed the time variable according to

$$\tau = \frac{1}{\lambda}\ln(t) + \text{const.} \tag{5.22}$$

In the limit of $\tau \to \infty$ these expressions are identical to the power laws discussed earlier. For $\tau \to -\infty$ we can once more cast these expressions into power laws by solving for the new exponents. Remember that we are approaching the singular point from the future time direction and that therefore the initial conditions lie at larger times. We can therefore re-express the line element in terms of the following, altered scale factors

$$a \sim t^{p_l'},\ b \sim t^{p_m'},\ c \sim t^{p_n'}, \tag{5.23}$$

where now

$$p_l' = \frac{|p_1|}{1-2|p_1|},\ p_m' = -\frac{2|p_1|-p_2}{1-2|p_1|},\ p_n' = \frac{p_3-2|p_1|}{1-2|p_1|}. \tag{5.24}$$

The effect of such perturbations is therefore that one so-called Kasner epoch is replaced by another, whereby the contracting dimension is shifted from the **l** to the **m** direction. Moreover, the process starts over, switching the contraction onto the next direction every time, as during the transition the **l**-scale factor $a(t)$ reaches a maximum, while the **m**-scale factor $b(t)$ reaches a minimum and subsequently increases again. This leads to an enhancement or damping of the respective perturbation terms causing the succession of Kasner epochs. The way in which the negative power bounces between the differing time directions can be modeled by the parameterization given above. If we define

$$p_l = p_1(u), \quad p_m = p_2(u), \quad p_n = p_3(u) \tag{5.25}$$

the new exponents will be given by

$$p_l' = p_2(u-1), \quad p_m' = p_1(u-1), \quad p_n' = p_3(u-1); \tag{5.26}$$

therefore the bigger of the two positive powers remains positive, while the other switches roles with the previously negative power. The consequences of these oscillations are best described by the original formulation of the authors: *Consequently, the evolution of our model towards a singular point consists of successive periods ... in which distances along the two axes oscillate and along the third axis decrease monotonically; the volume decreases according to a law which is near to* $\sim t$ [26]. Again, the general behavior is not changed by the presence of matter, as the corresponding contributions are sub-leading in the limit considered.

5.2.3. Effect of Scalar and Vector Fields

In a subsequent paper [29], the authors show that for the case of a massless scalar field with a "stiff" equation of state ($p = \rho$), the generally quite stochastic oscillations turn into an exactly Kasner-like behavior. We will examine later the effects of this presence on the quantum completeness of the system. Given the Lagrangian

$$\int d^4x\sqrt{-g}(-\partial_\mu\varphi\partial^\mu\varphi + R) \tag{5.27}$$

we have the field equations

$$\Box\varphi = 0, \tag{5.28}$$

$$R_{\mu\nu} = \partial_\mu\varphi\partial_\nu\varphi. \tag{5.29}$$

Under the assumption that the metric only depends on time, this system has a simple exact Kasner-like solution

$$ds^2 = -dt^2 + t^{2p_1}dx_1^2 + t^{2p_2}dx_2^2 + t^{2p_3}dx_3^2, \tag{5.30}$$

$$\varphi(t) = q\ln t, \tag{5.31}$$

Subject to the slightly altered conditions

$$p_1 + p_2 + p_3 = 1, \qquad p_1^2 + p_2^2 + p_3^2 = 1 - q^2, \tag{5.32}$$

at $q = 0$ this is of course simply the Kasner solution and the above analysis holds unaltered. In the cases for which $q \neq 0$ it is now possible to have all of the p_i positive as was not the case before (see discussion above). In particular [30] prove that the asymptotic solution to 7.11 and 5.29 will always be given by

$$ds^2 = -dt^2 + \left(t^{2p_1}l_i l_j + t^{2p_2}m_i m_j + t^{2p_3}n_i n_j\right)dx^i dx^j, \tag{5.33}$$

$$\varphi(t) = q\ln t + \varphi_0, \tag{5.34}$$

where the p_i's and q are subject to the same conditions as before but may now be functions of the spatial coordinates, as are the vectors l, m, n. As the Kasner condition fixing the determinant of the metric to be t^2 remains unaltered, the analysis of the above regularity does not change, since the rate at which the spatial volume contracts remains the same, independent on the particular choice of exponents. Furthermore, [30] show that the addition of vector fields does not change this general picture, but results in a generalized Kasner geometry near the singular point. We can therefore conclude, that the presence of scalar and vector fields does not interfere with the geometrical nature of the approach to the singular point. This is particularly important as we wish to probe the space-time with quantized test-fields later on. Such an investigation is naturally only warranted if it stands to reason that the presence of such fields does not dramatically alter the qualitative behavior. As we have seen, the work of BKL lends additional credibility to this assumption.

5.2.4. Velocity Dominance

An important consequence of the behavior described above is the fact that the gravitational equations exhibit so-called velocity dominance. This means that the dynamical equations reduce to a second order non-linear differential equation in time alone. This dominance of the time-like over the spatial gradients effectively means that spatial points decouple, as the equations are the same for every spatial point. We shall see later that this effect is crucial to the consistency of the quantum theory. Velocity dominance is an essential component of the BKL model. In fact, the implication goes in both directions, and it is possible to arrive at a Kasner-like solution by assuming velocity dominance. In [2] we have shown this direction and for

completeness we will elaborate on the argument here. The notation and geometric concepts are mainly taken from the books of Kobayashi and Nomizu [31] and [32]. As mentioned previously, the generalized Kasner space-time is characterized by the property that it is a purely time-dependent metric which can be written asymptotically as

$$g = -dt^2 + t^{2p_1}dx_1^2 + t^{2p_2}dx_2^2 + t^{2p_3}dx_3^2, \tag{5.35}$$

with the three Kasner exponents p_1, p_2, and p_3 fulfilling the two relations introduced earlier.

Kasner space-times are vacuum solutions of Einstein's equations; in particular the Ricci tensor is zero. Our goal is to prove that these type of solutions arise naturally when the manifold has a singular spatial hypersurface, close to which time gradients dominate over spatial gradients. Our approach will be to show that from these general assumptions the Kasner solution arises, with minimal assumptions. We start with the defining equation for a general metric, g, which is a vacuum solution of the Einstein equations;

$$\mathfrak{Ric} \equiv 0. \tag{5.36}$$

In order to understand this equation from a geometrical viewpoint, we have to understand the interpretation of the Ricci tensor. Loosely speaking, the Ricci tensor gives something like an average over the curvature of all planes involving specific vectors, given by the indices of its components. Furthermore, the Ricci tensor is a measure of the volume change along a geodesic of a curved space-time compared to the volume change along a flat space-time's geodesic. This can be expressed through

$$\frac{D^2}{d\tau^2}\delta V - \frac{D^2_{\text{flat}}}{d\tau^2}\delta V = -\delta V \mathfrak{Ric}(T,T). \tag{5.37}$$

Here δV is the volume change and $\frac{D^2}{d\tau^2}$ the Fermi-Walker derivation with respect to an affine parameter τ. It reduces to the standard covariant derivative in all inertial frames. The direction in which the volume moves is given by the vector T.

As we have seen, in differential geometry the criterion for a complete manifold is the existence of a complete connection. A connection is considered complete if geodesic curves $\gamma(\lambda)$, on the manifold, can always be parameterized by an affine parameter range $-\infty \leq \lambda \leq \infty$. This means the singular structure is encoded in the connection Γ, which is the Levi-Civita or Riemannian connection since we have Riemannian (or pseudo-Riemannian) manifolds. Hence we can perform a gradient analysis, on the level of the connection, neglecting spatial gradients when compared to time gradients.

The Riemannian connection $\Gamma = g^{-1}dg$ is given in a local normal coordinate neighborhood by

$$\Gamma^{\alpha}_{\mu\nu} = \frac{1}{2}g^{\alpha\beta}\left(\frac{\partial g_{\beta\mu}}{\partial x^{\mu}} + \frac{\partial g_{\nu\beta}}{\partial x^{\nu}} - \frac{\partial g_{\mu\nu}}{\partial x^{\alpha}}\right). \tag{5.38}$$

Note, for the following discussion we adopt the notation of [31] [32] in order to ensure consistency of the formulae. In particular, the Latin indices refer to the index set of the four dimensional manifold. One important step in the calculation of BKL is the choice of the coordinate frame. We choose similarly to work in normal coordinates (in physics often referred to as synchronous gauge). A normal coordinate system at a point x is a coordinate neighborhood where the $\frac{\partial}{\partial x^i}$ form an orthonormal frame. By parallel displacement along geodesics the normal coordinates can be attached to every point in a neighborhood U of x.

By the choice of a normal coordinate neighborhood we can re-express the metric in the form

$$g = -dt^2 + h_{ij}dx^i dx^j, \tag{5.39}$$

with the metric of the three dimensional hypersurface h. In this case it is intuitive to identify the vertical and horizontal subspace; we have split the space-time such that we have a purely spatial sub-manifold $\mathscr{S}$, described by h. The three-metric is, in the general case, a function of all coordinates, including time.

In order to proceed we make use of the Gauß-Codazzi-Mainardi equations, allowing us to rewrite the Riemann tensor of the four manifold $R(X,Y,Z)$ as

$$\begin{aligned} R(W,Z,X,Y) =& \mathscr{R}(W,Z,X,Y) + g(\alpha(X,Z),\alpha(Y,W)) \\ & - g(\alpha(Y,Z),\alpha(X,W)), \end{aligned} \tag{5.40}$$

where we have the Riemann tensor of the hypersurface $\mathscr{R}(X,Y,Z)$ lifted to the four dimensional space-time and the second fundamental form $\alpha(X,Y) = h(X,Y)\xi$, often referred to as the extrinsic curvature, which is the lifted metric of the sub-manifold $\mathscr{S}$. In local coordinates:

$$R_{ijkl} = \mathscr{R}_{ijkl} + K_{ik}K_{jl} - K_{il}K_{jk}, \tag{5.41}$$

with extrinsic curvature $K_{ij} = \frac{1}{2}\partial_t h_{ij}$. Concerning the spatial metric h the indices only run over the spatial components, i.e. the 0-component is excluded, unlike for expressions involving g. (We see in a normal coordinate neighborhood we could split the manifold into a spatial submanifold and the subspace normal to it.) For the Riemann tensor one may proceed in the same fashion and project onto the parts contributing to the vertical and horizontal subspace.

Since we are interested in the behavior close to a singular hypersurface, we assume, that spatial gradients are irrelevant when compared to time gradients. This corresponds in the ge-

ometrical picture to the restriction to the normal component of the Riemann tensor $R(X,Y)Z$

$$^{\perp}R(X,Y)Z = \left(\tilde{\nabla}_X \alpha\right)(Y,Z) - \left(\tilde{\nabla}_Y \alpha\right)(X,Z), \tag{5.42}$$

with $\tilde{\nabla}_X \alpha$ being the covariant derivative of α with respect to the connection in the tangent space $T(M)+T(M)^{\perp}$. The corresponding connections are ∇_X for $T(M)$ and D_X for $T(M)^{\perp}$. In general

$$\begin{aligned}\tilde{\nabla}_X \alpha(Y,Z) =& D_X\left(\sum_i h^i(Y,Z)\xi_i\right) \\ &- \sum_i \{h^i(\nabla_X Y,Z) + h^i(Y,\nabla_X Z)\}\xi_i.\end{aligned} \tag{5.43}$$

Remarkably, the normal component is given exclusively by the second fundamental form. This gives us almost all the prerequisites to evaluate equation (5.36). One could of course contract the Riemann tensor, but we propose a more elegant way, using the structure equation for a connection form ω and its curvature form Ω

$$d\omega(X,Y) = -\frac{1}{2}[\omega(X),\omega(Y)] + \Omega(X,Y). \tag{5.44}$$

On the bundle of orthonormal frames we can state the above equation as

$$\Psi^B_A = d\psi^B_A + \sum_k \psi^k_A \wedge \psi^B_k + \sum_r \psi^r_A \wedge \psi^B_r. \tag{5.45}$$

Here Ω corresponds to Ψ and ω to ψ. The indices denoted by capital letters range over the whole four manifold whereas k and r are restricted to the subspace normal to $\mathscr{S}$, which is in fact only the 0-component. We may use this structure equation in order to derive the equation of Gauß and Codazzi

$$\Psi^i_j = \Omega^i_j + \sum_r \psi^i_r \psi^r_i, \tag{5.46}$$

(where Ω denotes the curvature form of the orthonormal bundle of the spatial metric to the orthonormal bundle of the full four dimensional metric). Note for a tangent bundle of a Riemannian manifold the curvature form corresponds to the Ricci tensor when using the canonical form θ^i

$$\Omega^i_j = \frac{1}{2}\sum_{k,l} R^i_{kjl}\theta^k \wedge \theta^l. \tag{5.47}$$

From this analysis we see that in a normal coordinate neighborhood we get two contributions to the four-dimensional Ricci tensor, one coming from the lift of the three dimensional curvature form and the second from the squared connection form. Expressing these quantities by the

second fundamental form we get for the components of the Ricci tensor the three relations:

$$(\mathfrak{Ric})^0_0 = -\frac{\partial}{\partial t}K^k_k - K^l_k K^k_l, \tag{5.48}$$

$$(\mathfrak{Ric})^0_i = \frac{\partial}{\partial x^k}K^k_i - \frac{\partial}{\partial x^i}K^k_k, \tag{5.49}$$

$$(\mathfrak{Ric})^j_i = -^{(3)}(\mathfrak{Ric})^j_i - \frac{1}{\sqrt{\det(h)}}\frac{\partial}{\partial t}\left(\sqrt{\det(h)}K^j_i\right). \tag{5.50}$$

All three equations have to satisfy (5.36). (Looking at the 00-component we can identify two different contributions, the first part comes from the lifted curvature form on the spatial sub-manifold and the second from the squared connection forms.)

To proceed, we will perform the gradient expansion explicitly and show similarity to the previously derived relations. In normal coordinates (i.e. $g_{00} = -1$, $g_{0i} = 0$ and $g_{ij} = h_{ij}$) after exploiting that $\partial_x h \ll \partial_t h$, we have only two types of non-vanishing Christoffel symbols

$$\Gamma^t_{ij} = \frac{1}{2}\frac{\partial h_{ij}}{\partial t}, \tag{5.51}$$

$$\Gamma^j_{it} = \frac{1}{2}g^{jk}\frac{\partial h_{ik}}{\partial t}. \tag{5.52}$$

These Christoffel symbols allow us to calculate the Ricci tensor with the general formula

$$\begin{aligned}(\mathfrak{Ric})_{ij} =& \frac{\partial \Gamma^l_{ij}}{\partial x^l} - \frac{\partial \Gamma^l_{il}}{\partial x^j} \\ &+ \Gamma^m_{ij}\Gamma^l_{lm} - \Gamma^m_{il}\Gamma^l_{jm}.\end{aligned} \tag{5.53}$$

From this we derive the following three equations for the different types of components of the Ricci tensor

$$(\mathfrak{Ric})_{00} = -\frac{1}{2}\frac{\partial}{\partial t}\left(h^{ik}\frac{\partial h_{ki}}{\partial t}\right) - \frac{1}{4}h^{lk}\frac{\partial h_{ki}}{\partial t}h^{im}\frac{\partial h_{ml}}{\partial t}, \tag{5.54}$$

$$(\mathfrak{Ric})_{0i} = \frac{1}{2}\frac{\partial}{\partial x^l}\left(h^{lk}\frac{\partial h_{ki}}{\partial t}\right) - \frac{1}{2}\frac{\partial}{\partial x^i}\left(h^{jk}\frac{\partial h_{kj}}{\partial t}\right), \tag{5.55}$$

$$(\mathfrak{Ric})_{ij} = \frac{1}{2}\frac{\partial^2 h_{ij}}{\partial t^2} - \frac{1}{4}\frac{\partial h_{ki}}{\partial t}h^{km}\frac{\partial h_{mj}}{\partial t}. \tag{5.56}$$

The 00 and the 0i-component are easily compared to the form derived above by the structure equation; the third will be a bit more involved. (Nevertheless, what is immediately visible is that the 00- and the 0i- components are similar to the pure choice of the normal coordinates; everything arising from these components will not depend on the gradient analysis.)

We will now make the Ansatz of a diagonal metric, simplifying calculations. It is easy to see that the 0i-components then trivially obey (5.36) and the 00-component reduces drastically to

$$(\mathfrak{Ric})_{00} = -\frac{1}{2}\left[\frac{\partial}{\partial t}\left(h^{ii}\frac{\partial h_{ii}}{\partial t}\right) + \frac{1}{2}\left(h^{ii}\frac{\partial h_{ii}}{\partial t}\right)^2\right] = 0. \tag{5.57}$$

Since $(\mathfrak{Ric})_{0i}$ is trivially zero we can find a solution to (5.57) by taking the following ansatz for h:

$$h = t^{k_1}dx_1^2 + t^{k_2}dx_2^2 + t^{k_3}dx_3^2, \tag{5.58}$$

(This is justified since no spatial derivatives occur) and we obtain a system of coupled differential equations for the three metric components, only containing time derivatives. Using this Ansatz we get for the part coming from the lifted Ricci tensor

$$\Omega \to \frac{k_1 + k_2 + k_3}{2t^2} \tag{5.59}$$

and similarly from the squared connection form

$$\omega \wedge \omega \to -\frac{k_1^2 + k_2^2 + k_3^2}{4t^2}. \tag{5.60}$$

When we now consider (5.57) and additionally propose the identification $k_i = 2p_i$, then we see immediately that we obtain the defining conditions for Kasner space-times. From the lifted curvature form Ω, as well as the requirement that the Ricci tensor vanishes, we obtain the Kasner plane condition

$$\Omega : p_1 + p_2 + p_3 = 1 \tag{5.61}$$

and from the squared connection forms ω we get the Kasner sphere

$$\omega^2 : p_1^2 + p_2^2 + p_3^2 = 1. \tag{5.62}$$

Only if these conditions are both met does this metric describe the behavior close to a space-like singularity properly.

5.3. Anisotropic Pre-Inflation

As we have shown, Kasner space-time has a number of very interesting classical properties that seem to possess some degree of universality near spatial singularities. As our work is primarily interested in the behavior of quantum probes in the vicinity of such points, it seems a prime candidate for further inspection. The question of the consistency of Kasner space-time with respect to such probes is even more pressing as it has been considered by a wide variety of authors as a model for a pre-inflationary era, for example [24, 25, 33, 34].

Inflation extends the cosmic history prior to the decelerated Friedmann cosmology observed today, with an accelerated expansion stage, which is known to be past-directed time-like and null geodesic incomplete, and which initially borders on a space-like singularity. A pure de Sitter phase, representing an extremely good approximation to all inflationary models at early times and therefore close to the initial singularity, is subjected to a divergent time-evolution towards said singularity. The coincidence limit renders this space-time quantum incomplete in the sense discussed earlier. Without imposing an initial boundary condition at the Big Bang, finite amplitude tensor fluctuations at finite times will be amplified to trans-Planckian values when evolved backwards [35]. The failure of the no boundary proposal imposes a general obstruction to de Sitter cosmology close to the geodesic border and serves as a plea for a pre-inflationary phase. As we will see, Kasner space-times are not stable under quantum fluctuations and can therefore provide only a transient description of any cosmology. However, this instability is precisely what provides a mechanism for a smooth transition to inflation. More specifically, inflation can emerge from spatially anisotropic but homogeneous cosmologies as described by Kasner-type space-times. These cosmologies develop forward instabilities towards approximate isotropic spaces in inflating space-time regions. We have seen that Kasner space-times develop backward instabilities triggering Bianchi type-II like transitions between different anisotropic cosmologies, leading to successions of Kasner geometries [26]. Furthermore, Kasner space-times are past-directed time-like and null geodesic incomplete as well. However, we shall see that the anisotropy gives rise to a contractile evolution semi-group that prohibits quanta from reaching the geodesic border. It is therefore quantum complete in the sense introduced earlier. This further improves the standing of Kasner-like geometries as pre-inflationary candidate cosmologies from a consistency standpoint.

In the following we will first demonstrate how Kasner space-times are unstable and how this allows for a transition to an isotropic expansion phase. We then include some comments on how these may have an observable impact on cosmological observations. To close, we demonstrate that Kasner space-time is quantum complete.

5.3.1. Stability of Kasner Space-times

One of the features that makes the Kasner universe an attractive candidate for a pre-inflationary phase is the fact that it is unstable in its forward evolution due to the amplification of gravitational waves, at least at early times. This was first demonstrated for specific, Kasner-like geometries [25, 34]. Therein the authors discovered a trend toward an isotropization of the space-time that ultimately triggered the transition towards the isotropic inflationary epoch. Later, the general case was examined by Kofman et al. and found to be compatible with these observations [27].

The Weyl Tensor

The main obstacle to a Kasner universe as cosmological model is the fact that its manifest an-isotropy is in blatant contradiction to the extremely high degree of isotropy that we observe today. If the universe was at some stage close to a Kasner-like evolution, we must therefore ask whether and how this an-isotropy was lost in order to be compatible with the perfectly isotropic Friedmann models that succeeded it. As the destabilization of the Kasner geometry stems mostly from the amplification of gravitational waves, the Weyl tensor features prominently in this discussion. Furthermore, as it describes the directional distortion due to the background geometry rather than the change of volume, it can be thought of as a more or less direct measure of an-isotropy. The Weyl tensor $C_{\alpha\beta\gamma\delta}$ is given by the traceless part of the Riemann curvature tensor $R_{\alpha\beta\gamma\delta}$. As the Kasner solution is a vacuum solution of the Einstein equations the Ricci tensor and Riemann scalar, comprising the trace part of the curvature tensor, vanish identically. Therefore, in a pure Kasner universe the Weyl tensor is equal to the Riemann tensor. The non-trivial components are

$$C_{titi} = \frac{p_i(1-p_i)t^{2p_i}}{t^2}, \qquad C_{ijij} = \frac{p_i p_j t^{2p_i} t^{2p_j}}{t^2}. \tag{5.63}$$

Given the restrictions placed on the p_i by the Kasner conditions (5.2), (5.3) we immediately see that the Weyl tensor diverges as we approach the singular point $t \to 0$. The geometry is completely characterized by the Weyl tensor, also at the perturbation level.

Perturbations

In order to see how the perturbations of the background will eventually destabilize the entire system we must first adopt a notation that allows us to trace their evolution. Following [27] we therefore define a new parameter $\varpi \in [0, 3\pi/2]$ such that

$$p_i = \frac{2}{3}\sin(\varpi_i) + \frac{1}{3}, \qquad \varpi_i := \varpi - \frac{2\pi i}{3} \tag{5.64}$$

will always satisfy the Kasner conditions. The spatial part of the metric can then be written as

$$\gamma_{ij}(t) = \left(\frac{t}{t_0}\right)^{2/3} \mathrm{diag}\left[\left(\frac{t}{t_0}\right)^{2q_i}\right] \tag{5.65}$$

with the shorthand

$$q_i = p_i - \frac{1}{3}. \tag{5.66}$$

This implies that the q_i are given by

$$q_i = \frac{2}{3}\sin(\varpi_i), \tag{5.67}$$

and suggests the further introduction of

$$Q_i := \frac{3}{2} q_i, \tag{5.68}$$

such that $Q_i \in [-1,1]$. With these definitions the metric can be expressed in terms of conformal time η

$$ds^2 = S(\eta)[-d\eta^2 + \gamma_{ij}(\eta) dx^i dx^j]. \tag{5.69}$$

The function $S(\eta)$ is given by

$$S(\eta) = \sqrt{\frac{\eta}{\eta_0}} \quad \text{with} \quad \eta_0 = \frac{3}{2} t_0. \tag{5.70}$$

Thus we see that $t = \frac{2}{3} S(\eta)\eta$ and the spatial metric is given as

$$\gamma_{ij}(\eta) = \text{diag}\left[\left(\frac{\eta}{\eta_0}\right)^{3q_i}\right]. \tag{5.71}$$

In terms of these coordinates it makes sense to define the comoving Hubble parameter $\mathcal{H}$ as the logarithmic derivative of $S(\eta)$ with respect to conformal time. Furthermore the shear tensor is introduced as

$$\sigma_{ij} := \frac{d}{d\eta} \gamma_{ij}(\eta). \tag{5.72}$$

In cosmic time the shear tensor is therefore just given by $\sigma_{ij}(t) = \sigma_{ij}/S$. Finally, the square of the Weyl tensor

$$\begin{aligned} C^2 &= 6\mathcal{C}^2 (1+2Q_i)^2 (1-Q_i) \\ &= -81 \mathcal{C}^2 p_1 p_2 p_3, \end{aligned} \tag{5.73}$$

where we defined $\mathcal{C}^2 = \frac{1}{S^4 \eta^4}$. Moving forward, one introduces perturbations to the metric above yielding a perturbed metric of the form

$$ds^2 = S^2(\eta)[-(1+2A)d\eta^2 + 2B_i dx^i d\eta + (\gamma_{ij} + h_{ij}) dx^i dx^j]. \tag{5.74}$$

The perturbations A, B and h may be then further split in to scalar, vector and tensor components in the usual manner. When following this program one finds that the initially six degrees of freedom permitted by the overall symmetry group are further reduced through four constraint equations. Thus, we end up with two physical degrees of freedom, which are identified, just as in the Friedman case, with the two independent polarizations of the gravitational wave. We will denote these as $\lambda \in \{+, \times\}$ in the traditional manner. Unlike in the usual cosmological setting however, these two tensor modes do not decouple, making actual computations immensely more

complicated. However, the evolution equations will be of the schematic form

$$E_\lambda = T^{(1)}_{\lambda\lambda'}(\eta)a(\eta_0) + T^{(2)}_{\lambda\lambda'}(\eta)b(\eta_0), \tag{5.75}$$

where the $T^{(i)}$ are transfer functions depending on time and three-momentum, and a and b reflect the initial conditions. As a measure for the impact of the waves on the background [27] suggest the ratio between the square of the full Weyl tensor and the square of its value on the background $\bar{C}^2$

$$\Xi := \frac{C^2}{\bar{C}^2}. \tag{5.76}$$

Specifically, we are interested in how the amplitude of the gravitational waves will evolve with time. The initial conditions are chosen such that the two polarizations are uncorrelated initially

$$\langle a_\lambda(\mathbf{k}) b^*_{\lambda'}(\mathbf{k}')\rangle = 0 \tag{5.77}$$

and satisfy the same initial power spectrum

$$\langle a_\lambda(\mathbf{k}) a^*_{\lambda'}(\mathbf{k}')\rangle = \langle b_\lambda(\mathbf{k}) b^*_{\lambda'}(\mathbf{k}')\rangle = \delta(\mathbf{k}-\mathbf{k}')\delta_{\lambda\lambda'}P_{\text{initial}}(k_i). \tag{5.78}$$

From here [27] derive the early and late time behavior of the perturbation to second order $\Xi^{(2)}(\mathbf{k},\eta)$, as the first order vanishes identically. For the general case, in which the modes are aligned with a principle axis, this expansion of the Weyl tensor for late times yields

$$\Xi^{(2)}(\mathbf{k},\eta) \sim \frac{4k^2\eta^2}{3}\frac{\left(\frac{\partial T_\lambda}{\partial \ln \eta}\right)^2 + k^2\eta^2 T_\lambda^2}{(1+2Q_1)^2(1-Q_1)} \to \frac{8k^3\eta^3}{3\pi(1+Q_1)^2}. \tag{5.79}$$

We see that the general perturbation $\Xi^{(2)}(\mathbf{k},\eta)$ converges to $\Xi^{(2)}(k_1,\eta)$, which is divergent at late times. In general there will always be two types of modes T_λ, one growing and one decaying. The growing mode gives the dominant contribution to $\Xi^{(2)}$ at late times of course, while its contribution at early times remains bounded. The decaying mode will be the dominating contribution at early times, while it only leads to a redefinition of the phase at late times.

We see that at late times the perturbation part will always dominate the background Weyl tensor $\bar{C}$, and therefore it cannot be maintained that the Kasner geometry persists. As stated earlier, for the vacuum case the entire geometrical information is contained within the Weyl tensor. Therefore, when the perturbation to the Weyl tensor becomes large compared to its background value, it is no longer reasonable to assume that the Kasner metric is a good description of the geometry. In particular, this does not depend on the choice of initial conditions $a(\eta_0)$ and $b(\eta_0)$. At early times, the conclusion is not as clear cut, for an appropriate choice of initial conditions, such that the decaying mode is not present, allows for a safe limit $\eta \to 0$, while their presence will lead to a breakdown similar to the late-time behavior. However, this is not guaranteed, as it is for the late time situation, and there are initial conditions that allow a stable

evolution right up to the singular point. Notwithstanding this geometrical stability, this statement cannot be made as easily for the case in which matter is present, in the full quantum case. The volume element will of course scale as t^2 by virtue of the Kasner conditions; therefore, it is to be expected that the matter density diverges close to the singular hypersurface. In this case, semi-classically we do expect back-reactions on the metric via the coupling to the expectation value of the energy momentum tensor.

5.3.2. Quantum Complete Pre-Inflation

The prelude to inflation considered in this work is given by an an-isotropic Bianchi type-I cosmology with a sequence of Kasner space-times characterizing the neighborhood of its geodesic boundary, as suggested by the work of BKL. The main observational constraint on such a pre-inflationary phase is posed on its duration. It is well known that, in order to explain the homogeneity and isotropy observed today, the duration of inflation must have been no less than around $N = 62$ e-folds. To be consistent with current observation the pre-inflationary epoch can therefore not last for too long in order for it not to infringe on the necessary amount of inflation. At the same time, models in which the number of $e-$folds exceeds $N = 62$ significantly lead to a total smoothing of possible in-homogeneity or an-isotropy from earlier times. While this is of course possible, it is much less attractive, as it would render the search for such remnants of the earlier universe in the form of primordial gravitational waves much more difficult [36]. A Kasner-like pre-inflationary phase is consistent with observational bounds on the e-folds because of the fast developing forward instability [27] that we have discussed in detail above. This, along with the work of BKL, makes it one of the most promising candidates for our investigation. Most of the arguments and proofs of the remaining part of this chapter can be found in more concise form in our publication [2].

The Model

Any space-time $(\mathcal{M}, g)$ considered in this prelude is a multiple warped product manifold of the form $\mathcal{M} = \mathcal{I} \times_{w_1} \mathbb{R} \times_{w_2} \mathbb{R} \times_{w_3} \mathbb{R}$ furnished with a tensor field

$$g = -\pi^* (\mathrm{d}t \otimes \mathrm{d}t) + \sum_{a=1}^{3} (w_a \circ \tau)^2 \, \sigma_a^* (q_a) \ , \tag{5.80}$$

with positive warping functions $w_a \in C^\infty(\mathcal{I})$ $(a \in \{1,2,3\})$. By τ and σ_a we denote the projections onto the base (time interval) $\mathcal{I}$ and the fibers (in our case one-dimensional subspaces), respectively, and π^* and σ_a^* are the corresponding pullbacks. The pairs $(\mathbb{R}, q_a)$ denote the flat Riemannian Fiber manifolds with respect to the base manifold $(\mathcal{I}, -\mathrm{d}t \otimes \mathrm{d}t)$. Kasner space-times are multiple warped products of this type with warping functions $w_a = \mathrm{id}_{\mathcal{I}}^{p_a}$, where $p_a \in \mathbb{R}$

denote the Kasner exponents introduced earlier. As we have seen, the Kasner exponents are required to lie in the intersection of the Kasner plane $p_1 + p_2 + p_3 = 1$ and the Kasner sphere $p_1^2 + p_2^2 + p_3^2 = 1$. Kasner space-times can be characterized as Ricci-flat Einstein manifolds which are globally hyperbolic, future-directed time-like and null geodesic complete, but past-directed time-like and null geodesic incomplete. Since they are vacuum solutions, Kasner geometries can only be an approximate description close to the geodesic border of an an-isotropic space-time such as the more general Bianchi type-I models relevant for this work. Bianchi type-I geometries are multiple warped product manifolds $\mathcal{M}_B$ of the type (5.80).

Both, inflationary Friedmann and Kasner universes belong to the Bianchi I class of space-times, the only difference lies in the an-isotropy of Kasner which has to be diluted by the scalar field dynamics of the inflaton. String theoretical models propose an inflationary potential of the form [37]

$$V = V_{\mathrm{dS}} \left(1 - \exp\{(-\phi/\phi_0)\}\right)^2 . \tag{5.81}$$

V_{dS} and ϕ_0 are constants, fixed by the prescribed initial conditions. For a classical scalar field $\phi : \mathcal{M}_B \to \mathbb{R}$ in a Bianchi type-I space-time this amounts to a Hamiltonian density

$$\mathcal{H} = \mathcal{T}(\pi; g) + \mathcal{V}(\phi; g). \tag{5.82}$$

The constants can be fixed such that the correct amplitude for the metric fluctuations are obtained, i.e. $\phi_0 = M_{\mathrm{Pl}} \cdot 10^{-3}$ and $V_{\mathrm{ds}} = \left(10^{13}\mathrm{GeV}\right)^4$, the slow roll part is away from the minimum and the potential is almost flat there $V \approx V_{\mathrm{ds}}$. Around the minimum, the potential is approximately quadratic in the field. More concretely, we start with small velocity condition $\dot{\phi}^2 \ll V_{\mathrm{ds}}$ with minimal potential energy V_0. In the presence of a cosmological constant the expression for the scale factors $a_i(t)$ is known to be [34]

$$a_i(t) = a_i^{\mathrm{in}} \left(\sinh(3H_{\mathrm{ds}}t)\right)^{\frac{1}{3}} \left(\tanh\left(\tfrac{3}{2}H_{\mathrm{ds}}t\right)\right)^{p_i - \frac{1}{3}} . \tag{5.83}$$

Clearly, $1/H_{\mathrm{dS}}$ is the characteristic time scale for isotropization driven by V_{dS}: Consider the Weyl tensor as a tensor of type $(0,4)$ given by $C = R - \frac{1}{2}(\mathrm{Ric} - \frac{1}{4}Sg) * g - \frac{1}{24}Sg * g$, where R denotes the type-$(0,4)$ Riemann tensor, Ric is the Ricci tensor and S the curvature scalar. For any symmetric tensors T_1, T_2 of type $(0,2)$, $T_1 * T_2$ denotes the Kulkarni-Nomizu product. Throughout the evolution up to the end of inflation $\mathrm{Ric} \approx \frac{1}{4}Sg$, so $C \approx R - \frac{1}{24}Sg * g$. The Ricci decomposition is therefore $|R|^2 \approx |C|^2 + |\frac{1}{24}Sg * g|^2$. At early times $t \ll 1/H_{\mathrm{dS}}$ this decomposition into irreducible components with respect to the orthogonal group is dominated by the an-isotropic contribution, $|R|^2 \approx |C|^2 = |p_1 p_2 p_3|(2/t)^4$. The asymptotic behavior of the conformal tensor renders any de Sitter-like source initially irrelevant, which is why the Kasner solution is a good description of the geometry in the vicinity of the initial cosmic singularity. In contrast, at late times $t \gg 1/H_{\mathrm{dS}}$ the Ricci decomposition is dominated by the approximate de Sitter source $|R|^2 \approx |\frac{1}{24}Sg * g|^2$ because $|C|^2 \approx \exp\{(-6tH_{\mathrm{dS}})\}$. At this later stage, the approx-

imate de Sitter source damps away the an-isotropic contributions to the curvature and therefore approximate isotropy is reached.

In the slow-roll regime $\mathcal{T} \ll V_{\mathrm{dS}}$ at early times $t \ll 1/H_{\mathrm{dS}}$ the an-isotropic expansion history is given by a Kasner solution with warping functions $w_a(t)/w_a(t_{\mathrm{in}}) \approx (t/t_{\mathrm{in}})^{p_a}$ for $a \in \{1,2,3\}$. At these early times the approximate de Sitter source $H_{\mathrm{dS}}^2 = (8\pi/3)G_{\mathrm{N}}(V_{\mathrm{dS}} + \mathcal{O}(\mathcal{K}/V_{\mathrm{dS}}))$ is effectively decoupled from space-time and Kasner geometries can emerge. In the following we restrict ourselves to axis-symmetric Kasner models (only two distinct scale factors) and especially to the case $(p_1,p_2,p_3) = (\frac{2}{3},\frac{2}{3},-\frac{1}{3})$[1]. The reason for this choice is primarily technical as will become obvious shortly.

Solutions to the Mode Equation

We have already seen that the functional Kernel determining the ground state in the Schrödinger representation can be constructed from the mode functions that are the solution to the wave equation. Consequently we briefly review the main properties of the wave equation on a Kasner background. In the simple massless case, we are therefore concerned with solutions to

$$\Box\varphi = 0. \tag{5.84}$$

The D'Alambert operator for the pure Kasner space-time is given by:

$$\Box = \partial_t^2 + \frac{1}{t}\partial_t - \sum_{j=1}^{3} \frac{1}{|t|^{2p_j}}\partial_j^2. \tag{5.85}$$

As it is usually easier and more intuitive to work in momentum space, we introduce the Fourier transform as follows:

$$\hat{f}(k,t) = \int_{\mathbb{R}^n} f(x,t)e^{i2\pi\langle x,k\rangle}d^n x,$$

such that the solution to (5.84) is given by :

$$\varphi(t,x) = \int_{\mathbb{R}^3} \hat{\varphi}(k,t)e^{-i2\pi\langle x,k\rangle}d^3k,$$

where $\hat{\varphi}$ is the solution to the Cauchy problem given by:

$$\ddot{\hat{\varphi}}(t) + \frac{\dot{\hat{\varphi}}(t)}{t} + 4\pi^2 \sum_{j=1}^{3} \frac{k_j^2}{|t|^{2p_j}}\hat{\varphi}(t) = 0. \tag{5.86}$$

Note that the brackets denote the standard Euclidean inner product as we have explained in the Appendix. For the general case exact analytical expressions of the solution to (5.86) are not

[1] There is another possibility of choice for the exponents $(p_1,p_2,p_3) = (1,0,0)$. This model admits only an artificial symmetry and is isometric to an accelerated frame in Minkowski space.

known. However, it is possible to give solutions to several special or asymptotic cases [38].

Closed analytical expressions are available only in the axis-symmetric case, i.e. with two of the Kasner exponents coinciding. The first possibility for this is when two of the exponents vanish, and we are left with one non-trivial exponent p which will equal one. The wave equation

$$\ddot{\hat{\varphi}}(t)+\frac{\dot{\hat{\varphi}}(t)}{t}+4\pi^2\left(\frac{k_1^2}{t^2}+k_2^2+k_3^2\right)\hat{\varphi}(t)=0 \tag{5.87}$$

is then solved in terms of Bessel functions of first and second type:

$$\hat{\varphi}(\mathbf{k},t)=c_1 J_{2\pi i k_1}\left(2\pi t\sqrt{k_2^2+k_3^2}\right)+c_2 Y_{2\pi i k_1}\left(2\pi t\sqrt{k_2^2+k_3^2}\right). \tag{5.88}$$

As in this case the singularity is only fictitious, we will not expand on this case and only note that asymptotically the expressions coincide with those of the flat space derived in an earlier chapter, as the mode solutions simplify to plane waves.

The more interesting case is that where all of the Kasner exponents are unequal to zero. The only axis-symmetric choice of the Kasner exponents compatible with the Kasner conditions is given by $(p_1,p_2,p_3)=(-\frac{1}{3},\frac{2}{3},\frac{2}{3})$. In this case the wave equation becomes

$$\ddot{\hat{\varphi}}(t)+\frac{\dot{\hat{\varphi}}(t)}{t}+4\pi^2\left(k_1^2t^{2/3}+(k_2^2+k_3^2)t^{-4/3}\right)\hat{\varphi}(t)=0. \tag{5.89}$$

Depending on the distribution of the initial momentum $\mathbf{k}$, the exact solutions take a more or less compact form. Below we give an overview of the known solutions in terms of the unknown, and possibly complex integration constants c_1 and c_2, that can be found in [38].

$$\hat{\varphi}(\mathbf{k},t)=\hat{\varphi}'(\mathbf{k},t_0)\ln\left(\frac{t}{t_0}\right)t_0+\hat{\varphi}(\mathbf{k},t_0), \qquad \text{for } \mathbf{k}=0, \tag{5.90}$$

$$\hat{\varphi}(\mathbf{k},t)=c_1 J_0\big(\frac{3}{2}\pi k_1 t^{4/3}\big)+c_2 Y_0\big(\frac{3}{2}\pi k_1 t^{4/3}\big) \qquad \text{for } k_1\neq 0,\ k_2^2+k_3^2=0, \tag{5.91}$$

$$\hat{\varphi}(\mathbf{k},t)=c_1 J_0\big(6\pi\sqrt{k_2^2+k_3^2}t^{1/3}\big)+c_2 Y_0\big(6\pi\sqrt{k_2^2+k_3^2}t^{1/3}\big) \text{ for } k_1=0,\ k_2^2+k_3^2\neq 0, \tag{5.92}$$

and finally,

$$\hat{\varphi}(\mathbf{k},t)=e^{\frac{3}{2}\pi i|k_1|t^{4/3}}\mathrm{HeunB}(0,0,0,\delta_k,L_k t^{2/3})\left[\int_{t_0}^{t}dx\frac{c_1 e^{-3\pi i|k_1|x^{4/3}}}{x\mathrm{HeunB}(0,0,0,\delta_k,L_k t^{2/3})^2}dx+c_2\right] \tag{5.93}$$

when $k_1\neq 0,\quad k_2^2+k_3^2\neq 0$ and where HeunB denotes the Biconfluent Heun function.

Additionally we have defined the functions

$$\delta_k := -18\pi^2 \frac{k_2^2 + k_3^2}{L_k}, \tag{5.94}$$

and

$$L_k := (1+i)\sqrt{3/2\pi|k_1|}. \tag{5.95}$$

While the form of the solutions may seem daunting, they all possess a very simple form in the early time regime, as we argue in [2].

Theorem. *For a non-flat Kasner universe the solution to the wave equation approaches that of the axis-symmetric case for which* $\mathbf{k} = 0$ *in the sense that*

$$\hat{\varphi}(\mathbf{k},t) - c_1 \ln\left(\frac{t}{t_0}\right) t_0 - c_2$$

approaches zero as $t \to 0$*, for an appropriate choice of integration constants.*

As we are only interested in the vicinity of the singularity, this will simplify the discussion substantially. Since the d'Alembert operator is

$$\Box = \partial_t^2 + t^{-1}\partial_t - t^{-2p_a}\partial_a^2$$

with the spatial index running in $a \in \{1,2,3\}$. The Ansatz

$$\varphi(t,x) = T(t)R(x)$$

gives an ordinary second-order differential equation for T with singular coefficients:

$$(\partial_t^2 + t^{-1}\partial_t - \kappa' t^{-2\alpha}\,\mathrm{id})T \approx 0.$$

Here α is the largest Kasner exponent, κ' is determined from the solution of R and $\approx$ denotes equality up to irrelevant contributions, i.e. contributions which are less singular than those given. We introduce a pivotal time scale t_* and $\varepsilon\tau := t/t_*$, where $\varepsilon > 0$ is a smallness parameter. Then

$$(\partial_\tau^2 - \tau^{-1}\partial_\tau)T \approx \kappa\varepsilon^{2(1-\alpha)}\tau^{-2\alpha}T.$$

Since $p_a \in [-1/3, 1[$ the largest Kasner exponent is smaller than one. In the limit $\varepsilon \to 0$ the asymptotic solution is $T \approx c_1 + c_2\ln(\varepsilon\tau)$ with $c_1, c_2 \in \mathbb{C}$. These results are also in agreement with the different proof to be found in [38].

This completes the proof of the above claim, as close the geodesic border the exact solutions which are known agree with our asymptotic solution $\varphi(t,x) = C_1(x) + C_2(x)\ln(t/t_*)$, where $C_i\,(i \in \{1,2\})$ are smooth complex valued functions on Σ_t. Note therefore that this asymptotic

form is, unlike the exact solutions, not restricted to the axis-symmetric case. For simplicity we will choose $t_* = t_{\rm in}$ for the pivotal time scale such that $\varphi(t_{\rm in},x) = C_1(x)$, $\dot{\varphi}(t_{\rm in},x) = \frac{1}{t_{\rm in}} C_2(x)$ and $\varphi(t,x) = \varphi(t_{\rm in},x) - t_{\rm in}\dot{\varphi}(t_{\rm in},x) \mid \ln(t/t_{\rm in}) \mid$ for $t \in]0,t_{\rm in}]$.

Evolution semi-Group

We now consider a family of formal evolution operators $\{\mathcal{E}_g(t,t_0) : 0 \leq |t-t_0| < \infty\}$ on the generalized functional $L^2(\mathcal{C}(\Sigma_t),\mathcal{D}\phi)$ in order to study the dynamical behavior of the inflaton field as we approach the singular point. Such a family is a strongly continuous semi-group if $\mathcal{E}_g(t_0,t_0) = {\rm id}_{L^2}$, $\mathcal{E}_g(s,t)\mathcal{E}_g(t,t_0) = \mathcal{E}_g(s,t_0)$ for all $s,t,t_0 \in]0,\infty[$ with $s,t \leq t_0$ (which reflects our convention that the flow of time runs from t_0 towards 0), and if for each $\Psi_t \in L^2(\mathcal{C}(\Sigma_t),\mathcal{D}\phi)$ the map $\mathcal{I} \subset \mathbb{R} \to L^2(\mathcal{C}(\Sigma_t),\mathcal{D}\phi)$, defined by $t \mapsto \mathcal{E}_g(t,t_0)\Psi$ is continuous. Such evolution semi-groups arise naturally in the Schrödinger-picture quantum theory of fields in curved space-times, as we have seen above. A probabilistic interpretation is only possible for a special class of evolution semi-groups: a contractile evolution semi-group satisfies the additional requirement $\|\mathcal{E}_g(t,t_0)\| \leq 1$ for all $t \leq t_0$ in the time interval $\mathcal{I}$. Here the operator norm is defined as usual, $\|\mathcal{E}_g(t,t_0)\| := \inf\{C \geq 0 : \|\mathcal{E}_g(t,t_0)\Psi\|_2 \leq C\|\Psi\|_2 \text{ for all } \Psi_t \in L^2(\mathcal{C}(\Sigma_t),\mathcal{D}\phi)\}$.

As in the case of unitary evolution groups we obtain the generator of $\mathcal{E}_g(t,t_0)$ by differentiation with respect to t. Set $h_g(t) := ({\rm id}_{L^2} - \mathcal{E}_g(t,t_0))/|t-t_0|$ and consider only $\Psi_t \in L^2(\mathcal{C}(\Sigma_t),\mathcal{D}\phi)$ for which $h_g(t)\Psi_t$ exists in the limit $|t-t_0| \to 0$. We denote this limit by $h_g(t_0)\Psi_{t_0}$ and call $h_g(t_0)$ the infinitesimal generator of $\mathcal{E}_g(t,t_0)$. Of course, $h_g = H[\Phi,\Pi;g]$, where H denotes the Hamiltonian composed of configuration field operators Φ and conjugated momentum field operators Π in $L^2(\mathcal{C}(\Sigma_t),\mathcal{D}\phi)$. For simplicity we focus on a simple local quantum theory with a Hamiltonian density $\mathcal{H} = \mathcal{T}(\Pi;g) + \mathcal{V}(\Phi;g)$. On the hypersurface Σ_t the functional Laplacian is $\mathcal{T} := \sqrt{g_{tt}}\,\Pi\circ\Pi/2$, where $\mathcal{V}$ denotes the effective potential with $\sqrt{g_{tt}}\,g^{-1}_{\Sigma_t}({\rm d}\Phi,{\rm d}\Phi)$ included. The infinitesimal generator $H[\Phi,\Pi;g]$ and the evolution operator $\mathcal{E}_g(t,t_0)$ are related as follows:

$$\mathcal{E}_g(t,t_0) = T_{\leftarrow}\exp\left\{\left\{-{\rm i}\int_{t_0}^{t} {\rm d}t' H[\Phi,\Pi;g](t')\right\}\right\} \tag{5.96}$$

$$H[\Phi,\Pi;g](t') = \int_{\Sigma_{t'}} {\rm d}\mu\ \mathcal{H}(\Phi,\Pi;g_{\Sigma_{t'}})\,. \tag{5.97}$$

Here ${\rm d}\mu$ is the covariant measure on Σ and $T_{\leftarrow}$ denotes the time-ordering starting at $t_0 > t$.

We now turn to the crucial condition for the generator of an evolution semi-group. Consider a dual element $S \in [L^2(\mathcal{C}(\Sigma_t),\mathcal{D}\phi)]^*$ which satisfies $\|S\| = \|\Psi\|_2$ and $S(\Psi_t) = \|\Psi_t\|_2^2$. We can think of S as a normalized tangent functional to Ψ_t. The Hahn-Banach theorem guarantees that each wave functional $\Psi_t \in L^2(\mathcal{C}(\Sigma_t),\mathcal{D}\phi)$ has a normalized tangent functional. The generator h_g of $\mathcal{E}(t,t_0)$ is called accretive if for each $\Psi_t \in L^2(\mathcal{C}(\Sigma_t),\mathcal{D}\phi)$ we have ${\rm Im}(S(h_g\Psi_t)) \leq 0$. The relation between contractile and accretive is almost straight forward: h_g is the generator of a contractile evolution semi-group if and only if h_g is accretive.

The Ground State Functional

With the asymptotic solution to the wave equation known, we may now proceed to compute the ground state functional along the lines illustrated earlier. In the following we consider smooth functions on Σ_t and linear functionals on the algebra of these smooth functions, but our notation will not distinguish between them. The bi-linear functional $\mathcal{K}_t$ can be described by on-shell configuration fields in $\mathcal{S} = \{\varphi : \mathcal{I} \times \Sigma_{t\in\mathcal{I}} \to \mathbb{C} : (\Box - m^2)\varphi = 0\}$ as we have shown. Huygens' principle, in the form discussed in the earlier chapters, relates the kernel functional with on-shell configuration fields as follows

$$J\,[-\mathrm{i}\partial_t \varphi] = [J]\mathcal{K}_t[\varphi] \tag{5.98}$$

for any smooth detector source J. For smooth fields (5.98) implies $-\mathrm{i}\partial_t\varphi = K_t \star \varphi$, with $K_t \star \varphi$ denoting the covariant convolution of the bi-local kernel function and the configuration field on Σ_t. Using $\mathcal{F}^{-1}\widehat{K}_t \star \mathcal{F}^{-1}\widehat{\varphi} = \mathcal{F}^{-1}\widehat{K}_t\widehat{\varphi}$, where the Fourier transforms are with respect to the convolution variable, and $\partial_t\mathcal{F}^{-1}\widehat{\varphi} = \mathcal{F}^{-1}\partial_t\widehat{\varphi}$, Huygens's principle (5.98) can be written as

$$\frac{-\mathrm{i}}{\sqrt{\det(q)}}\,\partial_t \ln\frac{\widehat{\varphi}(t,k)}{\widehat{\varphi}(\tau,k)} = \widehat{K}(t,k)\;, \tag{5.99}$$

where τ is an arbitrary reference time in $\mathcal{I} =]0, t_{\mathrm{in}}]$. As a result the kernel function is given by

$$K_t(x,y) \approx -\frac{\mathrm{i}}{t^2 \ln\left(t/t_{\mathrm{in}}\right)}\left[\delta\left(x-y\right) - \frac{R(x,y)}{\ln\left(t/t_{\mathrm{in}}\right)}\right]. \tag{5.100}$$

Here $R := \mathcal{F}^{-1}\widehat{C_1}/\widehat{C_2}$. To leading order in $\ln^{-1}(t/t_{\mathrm{in}})$ $(t \in]0, t_{\mathrm{in}}[)$ the kernel function is given by a purely imaginary contact term. This contribution alone is a particular solution to Huygens's principle (5.98). It is universal in the following sense: let us introduce a functional generalization of the Dirac measure $\delta : \mathcal{C}_0^\infty(\Sigma_t) \times \mathcal{C}_0^\infty(\Sigma_t) \to \mathbb{C}$, defined by $[f_1]\delta[f_2] := f_1[f_2]$. Note that our notation does not distinguish between elements of $\mathcal{C}_0^\infty(\Sigma_t)$ and linear functionals on $\mathcal{C}_0^\infty(\Sigma_t)$. A particular kernel functional solving (5.98) is given by

$$[f_1]\mathcal{K}_t[f_2] = -\mathrm{i}[f_1]\delta[f_2\,\partial_t \ln\left(f_2/f_{2\mathrm{in}}\right)]$$

and can be extended to a bi-linear functional associated with propagating waves. On its own it accounts only for the wave front at the location of the detector described by the current density J, but does not contain information about spatial correlations between wave fronts on Σ_t, which is partially contained in the bi-linear functional $\mathcal{R}$ associated with R. This contribution, however, is already sub-leading in the vicinity of the geodesic border. Hence events at different spatial locations on Σ_t are approximately uncorrelated close to the geodesic border. In other words, towards the geodesic singularity the space-time probes consisting of quantum fields are reduced to decoupled point-like degrees of freedom.

Close to the classical equilibrium configuration of the inflaton potential (5.81) we make the same Ansatz for the Schrödinger wave functional as before:

$$\Psi_t[\phi] = \Psi_t^{(0)}[\phi] \times \exp\{(\mathscr{D}_t[\phi])\} \,. \tag{5.101}$$

Here $\Psi_t^{(0)}$ denotes the ground state functional

$$\begin{aligned}
&\Psi_t^{(0)}[\phi] = \mathcal{N}_t^{(0)} \mathcal{G}_t^{(0)}[\phi] \,, \\
&\mathcal{N}_t^{(0)} = \mathcal{N}_{t_{\rm in}}^{(0)} \exp\left\{ \left\{ +\tfrac{\mathrm{i}}{2} \int_{t_{\rm in}}^{t} \mathrm{d}\tau \int_{\Sigma_\tau} \mathrm{d}\mu \, \tfrac{1}{2}\Pi^2[\phi] \mathcal{K}_\tau[\phi] \right\} \right\} , \\
&\mathcal{G}_t^{(0)}[\phi] = \exp\left\{ \left\{ -\tfrac{1}{2}[\phi] \mathcal{K}_t[\phi] \right\} \right\} ,
\end{aligned} \tag{5.102}$$

and $\mathscr{D}_t[\phi]$ generates non-Gaussian deformations of the ground state due to inflaton self-interactions caused by the potential (5.81). Note that $\mathscr{D}_t[\phi] = \sum_{n\geq 2} \mathscr{D}_t^{[n]}[\phi]$ is a sum of nonlinear functionals starting at quadratic order.

Next, we consider the wave functional of the ground state in the vicinity of the geodesic border, which we shall denote by Σ_0. Using the expansion of the bi-local kernel in terms of the mode solutions we can express the normalization to leading and sub-leading order

$$\frac{\mathcal{N}_t^{(0)}}{\mathcal{N}_{t_{\rm in}}^{(0)}} \approx \exp\left\{ -\tfrac{1}{2} \mathrm{vol}_{\rm ps} \int_{t_{\rm in}}^{t} \frac{\mathrm{d}\tau}{\tau \ln(\tau/t_{\rm in})} \right\} \exp\left\{ \tfrac{1}{2} R(0) \mathrm{vol}\,(\Sigma_t) \int_{t_{\rm in}}^{t} \frac{\mathrm{d}\tau}{\tau \ln^2(\tau/t_{\rm in})} \right\} , \tag{5.103}$$

where $\mathrm{vol}_{\rm ps} = \mathrm{vol}(\Sigma_t)\,\mathrm{vol}(T^*\Sigma_t)$ denotes the time-independent coordinate phase space volume, and $R(0)$ is the regularized value of the complex-valued bi-local function R in the coincidence limit. As anticipated, the kernel function requires regularization in the spatial coincidence limit on any hypersurface $\Sigma_t\,(t \in]0, t_{\rm in}])$ (just as it would in Minkowski space). In particular, since $\mathrm{vol}_{\rm ps}$ is time-independent, this requirement is logically independent from the existence of a geodesic border and subsequently not owed to the geometry under scrutiny. Therefore, it is sufficient to introduce crude cut-off regulators for the purposes of this argument, as they will not alter the results qualitatively. We find

$$\left[\ln\left(\mathcal{N}_\tau^{(0)} \right) \right]_{t_{\rm in}}^{t} \approx -\frac{\mathrm{vol}_{\rm ps}}{2} \left[\ln\left(\ln\left(\tau/t_{\rm in} \right) \right) \right]_{t_{\rm in}}^{t} - \frac{\mathrm{vol}(\Sigma_t)}{2} R(0) \left[\ln^{-1}\left(\tau/t_{\rm in} \right) \right]_{t_{\rm in}}^{t} \,.$$

In the limit in which we approach Σ_0, the ground state normalization $\mathcal{N}_t^{(0)} \propto \exp\{(\Gamma_t)\}$ is exponentially suppressed with a damping factor $\Gamma_t \approx (-\mathrm{vol}_{\rm ps}/2)\ln(|\ln(t/t_{\rm in})|)$ up to an irrelevant phase in leading order. The real part of the damping factor monotonically approaches minus infinity when t goes to zero.

In order to study $\mathcal{G}^{(0)}$ we decompose the bi-local kernel function into its real and imaginary parts $R = \mathrm{Re}(R) + \mathrm{i}\,\mathrm{Im}(R)$ and its associated bi-linear functional $\mathcal{R} = \mathcal{R}_{\mathrm{re}} + \mathrm{i}\mathcal{R}_{\mathrm{im}}$ accordingly. Then

$$\begin{aligned}\mathcal{G}_t^{(0)} &\approx \exp\left\{\frac{\mathrm{i}}{2}\frac{1}{t^2\ln(t/t_{\mathrm{in}})}[\phi]\left(\delta - \frac{\mathcal{R}_{\mathrm{re}}}{\ln(t/t_{\mathrm{in}})}\right)[\phi]\right\} \\ &\times \exp\left\{\frac{1}{2}\frac{1}{t^2\ln^2(t/t_{\mathrm{in}})}[\phi]\mathcal{R}_{\mathrm{im}}[\phi]\right\}\end{aligned} \tag{5.104}$$

towards the geodesic border Σ_0. Note that for any bi-linear functional $\mathcal{A} \in \{\delta, \mathcal{R}_{\mathrm{re}}, \mathcal{R}_{\mathrm{im}}\}$ appearing in (5.104) the combination $t^{-2}\mathcal{A}$ is time independent. Therefore $\mathcal{G}^{(0)}[\phi] \to 1$ in the limit $t/t_{\mathrm{in}} \to 0$ for any field configuration. As a result $\Psi_t^{(0)}[\phi] \to 0$ towards Σ_0, which implies

$$\lim_{t\to 0}\left\|\Psi_t^{(0)}\right\|_2 = 0\,. \tag{5.105}$$

The ground state wave functional does not yield probabilistic support to any field configuration at the geodesic border.

Non-Gaussianities

The vanishing support of the ground state at the geodesic border extends to the entire stack of excited states that can be constructed therefrom. To see this, we may once more consider the ladder operators constructed in an earlier chapter. Applying the creation operators to the ground state functional we may infer that they can be interpreted geometrically as directional derivatives in field space,

$$a^\dagger[f_\lambda] \propto -2\int_{\Sigma_t} d^3x f_\lambda(x)\frac{\delta}{\delta\phi(x)}. \tag{5.106}$$

Following the usual path of expressing the first excited state as

$$\Psi_{1\lambda}[f,\Phi] := a^\dagger[f_\lambda]\Psi_0[\Phi]. \tag{5.107}$$

we see that in any amplitude, the consideration of excited states amounts to an insertion of on-shell fields convoluted with the mode functions f_λ. In particular we see proportionality to the ground-state amplitude:

$$||\Psi_{1\lambda}||^2 = 2\langle f_\lambda, f_\lambda\rangle_K ||\Psi_0||^2, \tag{5.108}$$

where

$$\langle f_{\lambda'}, f_\lambda\rangle_K := \int_{\Sigma_t} d\mu(x)d\mu(y) f^*_{\lambda'}(x)\mathrm{Re}\{K\}(x,y;t)f_\lambda(y). \tag{5.109}$$

Note that the on shell information of the fields only enters at the level of the excited states. This is the main difference between the ground state and the excited states; in the former the scalar field configurations need not satisfy any on-shell conditions. Only the spatial support of the fields is relevant, while the excited states become sensitive to on shell information mediated by the kernel overlap. The exact result of the integral (5.109) will now depend on how the mo-

mentum is distributed among the spatial directions and may be extremely difficult to calculate, especially since an exact solution for the $f_\lambda(x)$ is needed, whilst usually not available. Nonetheless it is easy to see from the asymptotics of both the kernel and the $f_\lambda(x)$, that it will in our case become time independent in the $t \to 0$ limit. Asymptotically, the on-shell fields are given by $\ln(t)$ and the real part of K by $1/(t^2 \ln^2(t))$; which cancels the time-dependence of f_λ and $\det(q)$ from the integration.

In general a state that is populated with n particle excitations can be written as:

$$\Psi_{n\lambda} = a^\dagger[f_{\lambda_n}] \cdots a^\dagger[f_{\lambda_1}]\Psi_0. \tag{5.110}$$

Using the commutation relations derived in Chapter 2 we see that:

$$||\Psi_{n\lambda}||^2 = \sum_{j=1}^{n} \Big[\langle f_{\lambda_n}, f_{\lambda_j} \rangle_K \Psi_0^* a[f_{\lambda_1}] \cdots a[f_{\lambda_{n-1}}] \tag{5.111}$$
$$\cdots a^\dagger[f_{\lambda_{j+1}}] a^\dagger[f_{\lambda_{j-1}}] \cdots a^\dagger[f_{\lambda_1}]\Psi_0 \Big].$$

However in the sum above only the term for which $n = j$ contributes, as all other terms have a mismatch of creation and annihilation operators, resulting in the destruction of a particle with on shell data that was not previously created. We hence straightforwardly conclude that

$$||\Psi_{n\lambda}||^2 = \prod_{j=1}^{n} \langle f_{\lambda_j}, f_{\lambda_j} \rangle_K ||\Psi_0||^2. \tag{5.112}$$

We therefore see that the ground state bequeaths its quantum completeness to the entirety of Fock space elements constructed from it, as the asymptotic behavior derived previously cannot alter the time-dependence in the limit $t \to 0$. In particular, since we are still close to the singular hypersurface, we can neglect the momentum dependence of the integrals in (5.109) and consider the scaling with time alone. Due to a cancellation of the time dependencies of the kernel, the mode functions and the integration measure, the integral becomes asymptotically time independent and we write,

$$\langle f_{\lambda'}, f_\lambda \rangle_K \sim const., \tag{5.113}$$

Thus, creating excited modes does not alter the scaling of $|\Psi|^2$ for early times and the regularity properties shown remain intact. The main result is that probability amplitudes of excitations decrease in the same way as the ground state. Furthermore transition amplitudes from one to another excitation vanish also in the limit of small times.

The last question that remains to be answered is whether the self-interactions of the inflaton field due to its potential (5.81) can have an effect. In general it is of course impossible to

find exact solutions to interacting theories and we have to employ perturbation theory to study the effect of switching on interactions in our system. As we are working in the Schrödinger framework we will therefore consider standard Rayleigh-Schrödinger perturbation theory of the states constructed for the free case above. The crucial question is whether or not the interaction term can induce significant fluctuations in occupation numbers or not. In both time-dependent and time-independent perturbation theory, this information is encoded in the transition matrix element $\langle M|H_{\text{int}}|N\rangle$, where $|N\rangle$ and $|M\rangle$ denote N and M particle states, respectively. In our case, said matrix element takes the following path integral form:

$$\begin{aligned}\langle\Psi_M^{(0)}|e^{-J\phi}|\Psi_N^{(0)}\rangle = \int \mathcal{D}[\phi]\Psi_0^{*(0)}[\phi]a[f_{\lambda_1}]\cdots a[f_{\lambda_M}] \\ \times e^{-J\phi}a^\dagger[f_{\lambda_N}]\cdots a^\dagger[f_{\lambda_1}]\Psi_0^{(0)}[\phi].\end{aligned} \tag{5.114}$$

If we remind ourselves of the interpretation of the creation operators as directional derivatives in field space (5.106), we recognize that the most general term in (5.114) will be of the form:

$$\begin{aligned}\left(\prod_i \int d^3x f_{\lambda_i}(x)\right)\left(\prod_j \int d^3x f^*_{\lambda_j}(x)\right) \\ \times \int \mathcal{D}[\phi](-J)^a \tilde{K}^b \phi^c e^{-\phi K\phi - J\phi}.\end{aligned} \tag{5.115}$$

In our particular case J will be proportional to a delta distribution and therefore $(-J)^a$ will evaluate to a constant times determinant factors upon full contraction[2]. Since $\tilde{K}$ does not depend on ϕ, we may pull it out of the path integral and rewrite the remainder as a functional differentiation of a shifted Gaussian integral with respect to J. The resulting expression is, up to the two finite products over f, given by:

$$(\sqrt{\det q})^a \tilde{K}^b \frac{\delta^c}{\delta J^c} \exp\left(\frac{1}{2}J\Delta J\right)||\Psi_0^{(0)}[\phi]||^2, \tag{5.116}$$

Δ being the inverse of K i.e. $\int K(x,z)\Delta(z,y) = \delta(x,y)$. The regularity and, more importantly, the vanishing of these terms in the limit of $t \to 0$ is now a simple consequence of the fact that all factors independently go to 0 in this limit. The functional differentiation will only improve this behavior by multiplication of additional factors of $\sqrt{\det q}\int d\mu(x')\Delta(x',x)J(x')$. Since the matrix element $\langle\Psi_M^{(0)}|e^{-J\phi}|\Psi_N^{(0)}\rangle$ measures the ability of the interaction term to excite a N particle state to an M particle state, the vanishing of these matrix elements implies that the theory trivializes in the vicinity of the singular hypersurface. This counter intuitive result may be made sense of by considering the peculiar nature of the underlying geometry. While the volume element monotonically approaches zero, the an-isotropy of the contraction forces at least one direction to expand very rapidly. Therefore, two events however close they may be

[2]Terms such as $J\phi$ are understood to be the functional generalization of matrix multiplication and we have surpressed the corresponding integrals for notational convenience

initially (barring complete coincidence) will be forced infinitely apart during the approach of the geodesic border. As the interaction terms are local, the potential part of the Hamiltonian becomes sub-leading in the approach of the singular point, rendering the theory effectively free. This can be viewed as a direct consequence of the BKL-conjecture, stating that velocity terms will always dominate close to the singularity. This explains the relative importance of the kinetic terms over the interaction terms, which contain only spatial gradients.

Conclusion

While Kasner space times border at a geodesic singularity, they do not leak information across the geodesic border. There is no physical characterization of Σ_0 in terms of measurement processes and observables. By direct Kernel methods we have shown that $\{\mathcal{E}_g(t,t_{\text{in}}) : t \in]0,t_{\text{in}}]\}$ is a contraction semi-group describing the ground state evolution in asymptotic Kasner space times. Since $\mathcal{E}_g(t,t_{\text{in}})$ has an explicit kernel, we can qualify asymptotic Kasner geometries as quantum complete preludes to inflation (via intermediary Bianchi type-I cosmologies) by direct kernel methods. The succession from asymptotic Kasner geometries via Bianchi type-I to inflationary space-times is, therefore, a quantum complete sequence of physical space-times, which is consistent with the results in [39]. The analysis extends to interacting and excited fields, by virtue of the velocity dominance as postulated by BKL. The singular potential in an-isotropic cosmologies has no effect on the consistency of scattering processes. In turn, extending inflation by an an-isotropic prelude with asymptotic Kasner geometry results in a quantum complete inflationary paradigm.

6. Dual-Null Formalism

6.1. Introduction

One of the main shortcomings of the Schrödinger formalism in the context of general relativity is its reliance on the explicit performance of a 3+1 split of the underlying space-time. From a standpoint of general covariance it hardly seems natural to single out the temporal evolution of spatial slicings in such a way. It is therefore interesting in its own right to consider more general types of evolution. Furthermore, there are many examples of physically interesting systems to which the usual approach of separating into equal-time hypersurfaces seems ill suited. This may be due to the fact that the surfaces of interest are in fact not space-like, such as for example the light-like Cauchy horizon of the Reisner Nordström metric, or simply due to the fact that the space-time under consideration does not admit such a slicing in the first place. Probably the most prominent example of the latter is the pp-wave class of space-times which are not globally hyperbolic. Nonetheless gravitational wave metrics have been of great interest, as they likely provide exactly soluble backgrounds for string theory [40, 41].

The main obstacle to any attempt at extending the well-established Lagrangian and Hamiltonian formulation of temporal evolution is of course the definition of a well-posed initial value problem. Global hyperbolicity guarantees the existence of a Cauchy surface and therefore appropriate initial conditions for a unique time-evolution. However, as pointed out by [42], the causal structure of general relativity depends to a much larger extent on null-surfaces, and it seems natural to ask whether it is possible to define null-evolution in close analogy to the usual temporal one. It turns out that it is in fact possible to define the so-called dual-null formulation describing the evolution of initial data on two intersecting null-surfaces in terms of the generalized momenta on the respective surfaces and the configuration on the intersection. The formalism was first introduced for the gravitational field [43] [44] and extended to the Klein-Gordon field in [42].

In the following we will closely follow these references to give a brief introduction to the general formalism. We will then demonstrate how the formalism can be adapted in the example of pp-wave space-times, making use of the null-structure of their singularity to define a Schrödinger-type evolution for a scalar field thereon.

6.2. Temporal Dynamics

Before expounding the dual-null formalism we present a quick recapitulation of the well-known Lagrangian and Hamiltonian approaches to facilitate comparison. In our conventions we will closely follow the redoubtable [45]. Classically, the Lagrangian is built around the configuration variable q and its velocities $\dot{q}$. More technically, we consider a vector bundle Q over the configuration bundle C. The classical position fields then live in the module of smooth sections over Q which we will denote by SQ. Naturally, the velocities then inhabit the corresponding tangent bundle TSQ. Evolution is temporal in the sense that we consider a time interval $t \in [0,T]$, where t is our evolution parameter and we extend all of our fields to $C \times [0,T]$ by $\dot{q} = dq/dt$.

The Lagrangian density $\mathscr{L}$, which in our high-riding formalism is now a map from the tangent bundle TSQ to the module of smooth sections of the bundle of scalar densities, then governs the evolution of our system, by way of the principle of least action. From this we immediately obtain the famed Euler-Lagrange equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\delta\mathscr{L}}{\delta\dot{q}}\right) = \frac{\delta\mathscr{L}}{\delta q}. \tag{6.1}$$

Assuming the Lagrangian density is independent of a certain generalized velocity $\tilde{q}$, the left-hand side of the corresponding Euler-Lagrangian is zero, and thus $\delta\mathscr{L}/\delta\tilde{q}$ is automatically a constant of motion.

The Hamiltonian formulation is based accordingly on the conjugated momenta on the corresponding cotangent bundle $(q,p) \in T^*SQ$. The Hamilton density can thus be defined with the help of the Laplace transform $\Lambda : TSQ \to T^*SQ$

$$\Lambda(q,\dot{q}) = \left(q, \frac{\delta\mathscr{L}}{\delta\dot{q}}\right). \tag{6.2}$$

This gives the familiar form of the Hamilton density

$$\mathscr{H}(q,p) = ((0,p) - \mathscr{L})\Lambda^{-1}(q,p), \tag{6.3}$$

which is usually denoted less stringently

$$\mathscr{H} = p\dot{q} - \mathscr{L}. \tag{6.4}$$

The dynamics are then of course given in terms of the equally well-known Hamilton equations

$$\frac{\mathrm{d}}{\mathrm{d}t}q = \frac{\delta\mathscr{H}}{\delta p}, \qquad \frac{\mathrm{d}}{\mathrm{d}t}p = -\frac{\delta\mathscr{H}}{\delta q}. \tag{6.5}$$

Again there may be gauge degrees of freedom, which now will result in a reduced set of Hamil-

ton equations accompanied by constraints of the form $\delta\mathscr{H}/\delta\tilde{q} = 0$. In general a constraint is not necessarily conserved and thus the time derivative of the constraint equation is an independent constraint. Interestingly this is not the case for the Einstein field [44].

6.3. Dual-Null Dynamics

When considering the context of general relativity the formulation of dynamics in terms of temporal evolution does not seem entirely natural. After all, the very essence of relativity lies in the equal treatment of spatial and time-like directions. Furthermore, a Cauchy surface is not necessary for the definition of a well-defined initial value problem. As pointed out by Hawking and Ellis in [15], the minimal requirement is the existence of an achronal set $\mathscr{A}$ and some global flow respecting this property. In essence, achronality requires some set of which no two constituent points can be connected by a time-like curve. In this light null dynamics seems to be a natural attempt to venture beyond temporal dynamics. While essentially the formulation of null dynamics is very similar to the ordinary evolution, the increase in generality comes at a price, of course. We will see that now that our initial configuration is prescribed on the intersection of two null surfaces, every configuration variable has not one but two velocities associated to it. This will lead to two dynamical momentum fields for every configuration variable and thus inexorably require additional integrability conditions.

6.3.1. Lagrangian Null Dynamics

Again, the starting point is a configuration vector bundle Q over some compact and orientable manifold, which is now of co-dimension two in space-time. The configuration fields are again the smooth sections of Q, denoted SQ. As space for the velocities we must now consider the direct sum of two tangent bundles, i.e. $(q, q^+, q^-) \in TSQ \oplus TSQ$, where the upper index now labels the velocity along the null surfaces of our choosing. In anticipation of future applications we shall denote them S^+ and S^-, respectively. There are now two independent evolution directions and thus two evolution parameters $\xi \in \mathscr{U} = [0,U]$ and $\eta \in \mathscr{V} = [0,V]$. Once more the fields on C are extended to $C \times \mathscr{U} \times \mathscr{V}$ via

$$q^+ = \frac{\partial q}{\partial \xi}, \qquad q^- = \frac{\partial q}{\partial \eta}. \tag{6.6}$$

The dual Lagrangian $\mathscr{L}$ can again be varied to obtain the dynamical equations by means of the principle of least action.

$$
\begin{aligned}
0 &= \delta \int_{\mathscr{U}\mathscr{V}S} \mathrm{d}\xi \mathrm{d}\eta \, \mathscr{L} \\
&= \int_{\mathscr{U}\mathscr{V}S} \mathrm{d}\xi \mathrm{d}\eta \left(\frac{\delta \mathscr{L}}{\delta q} \delta q + \frac{\delta \mathscr{L}}{\delta q^+} \delta q^+ + \frac{\delta \mathscr{L}}{\delta q^-} \delta q^- \right) \\
&= \int_{\mathscr{U}\mathscr{V}S} \mathrm{d}\xi \mathrm{d}\eta \left(\frac{\delta \mathscr{L}}{\delta q} - \frac{\mathrm{d}}{\mathrm{d}\xi} \left(\frac{\delta \mathscr{L}}{\delta q^+} \right) - \frac{\mathrm{d}}{\mathrm{d}\eta} \left(\frac{\delta \mathscr{L}}{\delta q^-} \right) \right) \delta q \\
&+ \int_{\mathscr{V}S} \left[\frac{\delta \mathscr{L}}{\delta q^+} (\delta q^+) \right]_0^U \mathrm{d}\eta + \int_{\mathscr{U}S} \left[\frac{\delta \mathscr{L}}{\delta q^-} (\delta q^-) \right]_0^V \mathrm{d}\xi .
\end{aligned} \tag{6.7}
$$

As usual in the case of vanishing variations at the boundaries, we obtain the equations of motions equivalent to (6.1)

$$
\frac{\mathrm{d}}{\mathrm{d}\xi} \left(\frac{\delta \mathscr{L}}{\delta q^+} \right) + \frac{\mathrm{d}}{\mathrm{d}\eta} \left(\frac{\delta \mathscr{L}}{\delta q^-} \right) = \frac{\delta \mathscr{L}}{\delta q} . \tag{6.8}
$$

6.3.2. Hamiltonian Null Dynamics

Similarly the momentum fields are now $(q, p^+, p^-) \in T^*SQ \oplus T^*SQ$ and the Hamiltonian density is once more derived from the Laplace transformation

$$
\mathscr{H}(q, p^+, p^-) = ((0, p^+, p^-) - \mathscr{L}) \Lambda^{-1}(q, p^+, p^-), \tag{6.9}
$$

or in more familiar terms

$$
\mathscr{H} = p^+(q^+) + p^-(q^-) - \mathscr{L} . \tag{6.10}
$$

The Hamiltonian equations are

$$
\frac{\mathrm{d}}{\mathrm{d}\xi} q = \frac{\delta \mathscr{H}}{\delta p^+}, \qquad \frac{\mathrm{d}}{\mathrm{d}\eta} q = -\frac{\delta \mathscr{H}}{\delta p^-}, \qquad \frac{\partial p^+}{\partial \xi} + \frac{\partial p^-}{\partial \eta} = -\frac{\delta \mathscr{H}}{\delta q} . \tag{6.11}
$$

The treatment of constraints is more subtle; however, with the latter application in mind it is out of our purview, and we refer the reader to [42] for details. Note that the notation here is counter-intuitive since the momentum variable p^+ is part of the dual tangent space T^*SQ and thus not parallel to q^+ and vice versa for p^-. In fact, it lies in the plane, S^- or S^+, respectively and is thus orthogonal. See figure 7.2 for comparison.

Integrability Conditions

In order to remain consistent, it is necessary to impose integrability conditions. This is most transparently done in the Hamiltonian formulation. By the construction of the evolution space above, the derivatives with respect to the two evolution parameters ξ and η commute. It thus follows immediately from the Hamilton equations that

$$
\frac{\partial}{\partial \xi} \frac{\delta \mathscr{H}}{\delta p^-} = \frac{\partial}{\partial \eta} \frac{\delta \mathscr{H}}{\delta p^+} . \tag{6.12}
$$

If we make use of the Hamiltonian equations once more, this may be expanded into a rather lengthy expression

$$\left(\frac{\delta\mathscr{H}}{\delta p^+}\left(\frac{\delta}{\delta q}\right)+\frac{\partial p^+}{\partial\xi}\left(\frac{\delta}{\delta p^+}\right)+\frac{\partial p^-}{\partial\xi}\left(\frac{\delta}{\delta p^-}\right)\right)\frac{\delta\mathscr{H}}{\delta q^-}$$
$$=\left(\frac{\delta\mathscr{H}}{\delta p^-}\left(\frac{\delta}{\delta q}\right)+\frac{\partial p^+}{\partial\eta}\left(\frac{\delta}{\delta p^+}\right)+\frac{\partial p^-}{\partial\eta}\left(\frac{\delta}{\delta p^-}\right)\right)\frac{\delta\mathscr{H}}{\delta q^-}. \tag{6.13}$$

This additional condition on the Hamiltonian equations relates the four derivatives along the respective evolution parameter to the momentum fields p^+ and p^-. We see that this integrability condition contains the derivatives $\frac{\partial p^-}{\partial\xi}$ and $\frac{\partial p^+}{\partial\eta}$, which are not present in the Hamiltonian equations. For the formulation of an evolution problem, these present a major obstacle as it seems unreasonable to prescribe them as initial information and there are now too many equations to determine them uniquely. Fortunately for us, it is possible to steer clear of this issue. Considering the three types of bilinears

$$A=\left(\frac{\delta}{\delta p^+}\otimes\frac{\delta}{\delta p^+}\right)\mathscr{H},\quad B=\left(\frac{\delta}{\delta p^+}\otimes\frac{\delta}{\delta p^-}\right)\mathscr{H},\quad C=\left(\frac{\delta}{\delta p^-}\otimes\frac{\delta}{\delta p^-}\right)\mathscr{H}, \tag{6.14}$$

we see that restriction to the case

$$A=C=0 \tag{6.15}$$

cures the problem of over determination. The above is known as the dual-null condition and is less restrictive than it might appear at first sight. In most problems we are concerned with Hamiltonians where the kinetic part depends quadratically on the velocities and the potential is independent of them. In these cases it can be shown that the dual-null condition is satisfied for space-time examples where the initial surfaces S^+ and S^- are null in space-time [42]. While this is hardly a panacea for the general settings one may like to consider, this is precisely the situation that we will encounter later in our discussion of the plane-wave space-times.

Hamiltonian Constraints

The occurrence of constraints in the dual-null formulation differs slightly from temporal dynamics, insofar as the Hamiltonian equations corresponding to primary constraints do not reduce to constraint equations. This is due to the fact that there are now two associated momenta which do not necessarily both vanish. The procedure is analogous to the temporal case however, by defining a reduced Hamiltonian on the constraint submanifold using the invertible part of Λ. The non-invertible velocities then furnish Lagrange multipliers of the constrained momenta giving rise to the reduced Hamiltonian equations.

6.3.3. Application to Field Theory

We close this introductory discussion by applying the formalism to the simple case of a scalar field in Minkowski space. Again, we closely follow [42], wherein one can also find a neatly presented discussion of the Maxwell field, which does not concern us now however. We thus consider flat space-time $(\mathbb{M}, g)$

$$ds^2 = -dt^2 + d\mathbf{x}^2. \tag{6.16}$$

The dual-null basis $(u, v; e)$ naturally coincides with the choice of light-cone coordinates $u := t + z$ and $v := t - z$. In this case the metric takes the simple form

$$ds^2 = -dudv + \delta_{ij} dx^i dx^j, \tag{6.17}$$

or more explicitly

$$g = \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

We can then identify the evolution parameters with the u and v directions, i.e. $u = \frac{\partial}{\partial \xi}$ and $v = \frac{\partial}{\partial \eta}$. In this chart the gradient operator on $\mathbb{M}$ decomposes into

$$\nabla = (\frac{\partial}{\partial \xi}, \frac{\partial}{\partial \eta}, \nabla_{\Omega_2}), \tag{6.18}$$

where ∇_{Ω_2} is just the gradient on the 2-sphere. The simplest possible case is that of a free scalar field; its action given by

$$S = -\frac{1}{2} \int \mathrm{d}^4 x \sqrt{-g} \, [\nabla_\mu \phi \nabla^\mu \phi + m^2 \phi^2]. \tag{6.19}$$

From (6.17) it is straightforward to see that the Lagrangian density in the dual-null formulation reduces to

$$\mathscr{L} = \phi^+ \phi^- - \frac{1}{2} \nabla_{\Omega_2} \phi \nabla_{\Omega_2} \phi - \frac{1}{2} m^2 \phi^2. \tag{6.20}$$

We can now use the previously derived results to read off the equations of motion, which simply give the Klein-Gordon equation in dual-null form

$$2 \frac{\partial^2 \phi}{\partial \xi \partial \eta} = \Delta_{\Omega_2} \phi - m^2 \phi^2. \tag{6.21}$$

The derivation of the Hamiltonian density is equally straightforward. The conjugated momentum fields are given by

$$\pi^+ = \frac{\delta \mathscr{L}}{\delta \phi^+} = \phi^-, \qquad \pi^- = \frac{\delta \mathscr{L}}{\delta \phi^-} = \phi^+ \tag{6.22}$$

This gives the Hamiltonian density as

$$\mathscr{H} = \pi^+\phi^+ + \pi^-\phi^- - \mathscr{L} = \pi^+\pi^- + \nabla_{\Omega_2}\phi\nabla_{\Omega_2}\phi + \frac{1}{2}m^2\phi^2, \tag{6.23}$$

from which we obtain the equivalent Hamiltonian equations

$$\frac{\partial\phi}{\partial\xi} = \frac{\delta\mathscr{H}}{\delta\pi^+} = \pi^-, \quad \frac{\partial\phi}{\partial\eta} = \frac{\delta\mathscr{H}}{\delta\pi^-} = \pi^+, \quad \frac{\partial\pi^+}{\partial\xi} + \frac{\partial\pi^-}{\partial\eta} = -\frac{\delta\mathscr{H}}{\delta\phi} = \Delta_{\Omega_2}\phi - m^2\phi. \tag{6.24}$$

The integrability condition again only reduces to Schwartz's theorem applied to the field ϕ and therefore may be inverted to give

$$\frac{\partial\pi^+}{\partial\xi} = \frac{\partial\pi^-}{\partial\eta}, \tag{6.25}$$

reducing the equations of motion to the simple form

$$\frac{\partial\phi}{\partial\xi} = \pi^-, \quad \frac{\partial\phi}{\partial\eta} = \pi^+, \quad \frac{\partial\pi^+}{\partial\xi} = \frac{\partial\pi^-}{\partial\eta} = \frac{1}{2}(\Delta_{\Omega_2}\phi - m^2\phi). \tag{6.26}$$

We see that the initial data for the π and ϕ is prescribed on the two null surfaces and their intersection respectively. Moreover the above defines a well-posed evolution problem for the field ϕ. In particular, this formulation may be quantized as we shall see later in more detail when discussing the plane-wave space-time.

7. Plane Wave Space-Times

The plane wave solutions to the Einstein field equations were first discussed in 1923 in a paper by Brinkmann on space-times that are conformally equivalent to Minkowski space. Subsequently, they were studied by Rosen, Bondi and others with the most comprehensive and perhaps best known review on the topic due to Ehlers and Kundt in 1962 [46]. In 1965 it was discovered by Sir Roger Penrose [47] that these space-times have the extraordinary property of focusing all incoming geodesics into a single point, thereby excluding the existence of a Cauchy surface and therefore the possibility of a global embedding into any hyperbolic pseudo-Euclidean space. This is of course extremely inconvenient for the formulation of local dynamics on this background and will be the main point of interest for us later on. Setting the absence of a Cauchy surface aside, pp-wave space-times have many very convenient features, lending themselves to quantum mechanical investigation. For example, it was also shown in 1965 by Günther [48] that the d'Alambertian for the metric of the gravitational plane wave satisfies Huygens's principle. It can in fact be shown that it is the only vacuum space-time other than Minkowski space of which this is true [49]. This remarkable property is an integral reason for the fact that plane wave space-times do not cause the production of particles in the semi-classical framework of quantum field theories on curved space-times, as shown by Gibbons [50]. More recently there has also been a resurgence in interest from various fields within the string theory community due to the fact that plane waves represent exactly soluble string theory backgrounds. For example, it was shown that the action for the type IIB superstring on a plane wave space Ramond Ramond background is quadratic in the superstring fields and may thus be explicitly quantized [41]. Plane waves have also given new insight on the famed AdS/CFT-correspondence [51] wherein pp-waves describe the first correction to the flat space spectrum of strings on $AdS_5 \times S^5$ at large t'Hooft coupling for some states. Consequently, research on plane wave space-times is very much relevant to this day and a better understanding of the puzzling nature of the physical ramifications of the focussing singularity would be extremely beneficial. In this section we will therefore give a brief oversight of the general characteristics of the plane wave solution and how they are relevant to our purposes. We will also discuss the qualitative differences to the situation in the Kasner and Schwarzschild cases as presented earlier.

7.1. Classical Properties of the Plane Wave Singularity

We begin the discussion by presenting the classical behavior of the plane wave background. This will fix the notation and highlight the essential difficulties to be addressed later.

7.1.1. Types of Plane Waves

Rosen Coordinates

The most accessible path towards deriving the plane wave metric is by considering the familiar perturbation of Minkowski space by a small fluctuation $g = \eta + h$. Inserted into the Einstein equations, this Ansatz results in a wave equation for the perturbation h, which is discussed in virtually every textbook on General Relativity. The solutions are transversely polarized gravitational waves, with the two possible polarizations commonly denoted as h_+ and $h_\times$. It is customary to choose the direction of propagation along the z-axis, resulting in the simple line element

$$ds^2 = -dt^2 + (\delta_{ij} + h_{ij}(z+t))dy^i dy^j. \tag{7.1}$$

In light-cone coordinates we replace $U = (z+t)$ and $V = \frac{1}{2}(z-t)$, transforming the line element to the form

$$ds^2 = 2dUdV - \gamma_{ij}(U)dy^i dy^j, \tag{7.2}$$

where we have defined $\gamma_{ij}(U) := \delta_{ij} + h_{ij}(U)$. Interestingly (7.2) remains a solution of the Einstein equations independent of any weak field limit or the "size" of the perturbation h. We can therefore choose an arbitrary matrix-valued function $\gamma(U)$ while remaining in the space of exact solutions. This coordinate system is known as the *Rosen* coordinates. The Rosen coordinates have the main advantage that they display most of the symmetries of the space-time in a more or less obvious way. For example the Killing vector fields $\frac{\partial}{\partial y_i}$ and $\frac{\partial}{\partial V}$ may be readily read off and it is also easily verified that the vectors

$$y^i \frac{\partial}{\partial V} + \frac{\partial}{\partial y_i} \int_0^U ds\, \gamma^{ij}(s) \tag{7.3}$$

are Killing too. The main downside to Rosen coordinates is that they do not cover the entirety of space-time in a single patch (as we shall see later) and that they contain spurious coordinate-singularities, whenever the function $\gamma(u)$is ill-defined.

Brinkmann Coordinates

So as not to contend with said singularities one often chooses the so-called Brinkmann coordinates. If we consider the most general line element admitting a covariantly constant null vector field (in our case this is $\partial/\partial V$) we end up with a metric of the form [40]

$$ds^2 = 2dudv + K(u,x^c)du^2 + 2A_a(u,x^c)dx^a du + g_{ab}(u,x^c)dx^a dx^b, \tag{7.4}$$

where the latin indices a,b,c refer to the two remaining spatial directions. The sub-class of metrics for which that is quadratic in its spatial part i.e. $g_{ab} = \delta_{ab}$ are called the plane-fronted waves with parallel rays. This is in reference to the fact that the wave fronts at $u = \text{const.}$ are planar, and the existence of a null vector parallel to the wave front. It is much more commonly abbreviated as the class of pp-waves.

Plane waves are an even more specific case of pp-waves for which $A_a = 0$ and $K(u,x^c)$ is quadratic in the spatial directions. The resulting metric in terms of the so-called Brinkmann coordinate system is

$$ds^2 = 2dudv + H_{ab}(u)x^a x^b du^2 + \delta_{ab}dx^a dx^b. \tag{7.5}$$

The function $H(u,\mathbf{x}) := H_{ab}(u)x^a x^b$ specifies the amplitude of the wave and is therefore often called the profile function. In these coordinates the Christoffel symbols are particularly simple,

$$\Gamma^v_{uu} = \partial_u H, \quad \Gamma^a_{uu} = -\partial_a H, \quad \Gamma^v_{au} = \partial_a H \tag{7.6}$$

resulting in only one non-vanishing component of the Riemann and Ricci tensors respectively

$$R_{uabu} = \partial_a \partial_b H, \qquad R_{uu} = \nabla^2 H, \tag{7.7}$$

where ∇ refers to the gradient on the two-sphere spanned by the x^a. As we can see, the only non-vanishing component of the Ricci-tensor corresponds to the energy density. This is apparent from the only non-trivial component of the Einstein equations

$$T_{00} = -\frac{1}{8\pi G}\operatorname{tr} H. \tag{7.8}$$

The demand that energy density be positive, also known as the weak-energy condition, therefore immediately requires the trace of H_{ab} to be negative

$$H^a_a \leq 0. \tag{7.9}$$

This may obviously be accomplished by choosing H to be traceless. This case, referred to as a gravitational plane wave, has the Weyl and Riemann tensors coinciding. The other commonly studied case is that in which $H_{ab} = f(u)\delta_{ab}$ and is referred to as a null electromagnetic plane wave and its Weyl tensor vanishes.

The relation to Rosen coordinates may not be immediately clear. In order to transform (7.5) to (7.2) and vice versa we introduce a vielbein E as follows

$$x^a = E^a_i y^i. \tag{7.10}$$

Being a vielbein E satisfies

$$g_{ij} = E^i_a E^j_b \delta_{ab}, \tag{7.11}$$

where E^i_a denotes the inverse vielbein and we enforce the condition

$$\dot{E}^i_a E_{ib} - \dot{E}^i_b E_{ia} = 0, \tag{7.12}$$

stemming from the Wronski determinant, requiring independence of solutions. Here and subsequently an overdot will denote a derivative with respect to u. In this manner one obtains the following for the transition between Rosen and Brinkmann coordinates

$$\begin{aligned} U &= u, \\ V &= v + \frac{1}{2}\dot{E}_{ai} E^i_b x^a x^b \\ y^i &= E^i_a x^a. \end{aligned} \tag{7.13}$$

The profile function is finally given by

$$H_{ab} = \ddot{E}_{ai} E^i_b. \tag{7.14}$$

Multiplying both sides by the inverse vielbein we obtain a harmonic oscillator-type equation

$$\ddot{E}_{ai} = H_{ab} E_{bi}. \tag{7.15}$$

As pointed out in [40] this oscillator equation has $2d$ linearly independent solutions. The condition that the Wronskian between them must vanish and (7.12) then reduces this number to the d solutions that label the Rosen coordinates. They can thus be constructed from the Brinkman coordinates by solving the oscillator equation and constructing the vielbein from a maximally commuting set of solutions. From this g_{ij} follows algebraically via (7.11).

7.1.2. Focusing of Geodesics

While many of the singularities that are encountered when choosing Rosen coordinates can be shown to be spurious coordinate singularities, plane wave space-times do generally exhibit singular behavior nonetheless. A first hint at this is to consider the geodesic deviation equation

$$\frac{D^2}{D\tau^2}\delta x^\mu = -R^\mu_{\nu\lambda\rho}\dot{x}^\nu \dot{x}^\lambda \delta x^\rho, \tag{7.16}$$

for the separation vector between two geodesics x^μ. Specifically, when choosing the affine parameter such that we compare two neighboring geodesics at equal u, this gives

$$\frac{\mathrm{d}^2}{\mathrm{d}u^2}\delta x^a = H_{ab}\delta x^b. \tag{7.17}$$

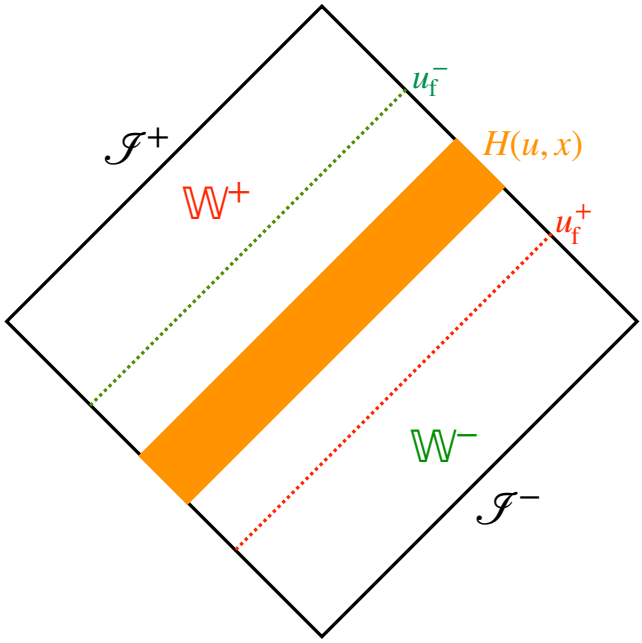


Figure 7.1.: The Penrose diagram of the pp-wave space-time shows the full Brinkmann chart $(\mathbb{W}^4, g)$, with embedding $\iota : \mathscr{U} \times \mathscr{V} \times \mathcal{S} \to \mathcal{M}$, ranging from $\mathscr{I}^-$ to $\mathscr{I}^+$. The outgoing wave is depicted by the orange bar $H(u,x)$ which divides the manifold in two parts. Additionally, we see the two Einstein-Rosen patches $\mathbb{W}^- = (-\infty, u_{\mathrm{f}}^-) \times \mathscr{V} \times \mathcal{S}$ and $\mathbb{W}^- = (\infty, u_{\mathrm{f}}^+) \times \mathscr{V} \times \mathcal{S}$, which end at the null-singularities at the focussing points $u_{\mathrm{f}}^{\pm}$ displayed by the dashed lines.

We see that, if the profile function is chosen accordingly, we do get physical divergences of tidal forces. In particular, for gravitational plane waves, the vanishing of the trace of H imposed by the weak energy condition will guarantee the existence of a negative eigenvalue. Effectively this leads to an attractive force between geodesics and thus has a focusing effect.

To see that plane waves invariably suffer from such a focusing singularity, we will shortly recapitulate the argument given by Penrose in [47]. We start by considering a metric of the Brinkmann form (7.5) as it is free of spurious singularities and covers the entire manifold. Furthermore we restrict to the special case of a so-called Sandwich wave, by restricting the support of $H(u)$ to some finite interval

$$H_{ab}(u) \neq 0 \text{ for } u_1 < u < u_2; \text{ and } H_{ab}(u) = 0 \text{ else.} \tag{7.18}$$

Thus, asymptotically space-time is flat and the effects of the plane wave are only felt in a intermediate region of compact support. The situation is illustrated by the Penrose diagram depicted in figure 7.1. The choice of a sandwich wave simplifies the argument substantially; however, as Penrose points out, this does not come at a cost of generality; general plane waves may be treated in similar fashion albeit the expressions involved become more complicated. Let

Q be any point in the incoming flat region of the sandwich wave, i.e. with coordinates

$$x_a = 0, \qquad v = v_0, \qquad u = u_0 < u_1. \tag{7.19}$$

Define the *complete null cone* K_3 of Q as the set of all points lying on the null geodesics that pass through Q. In the vicinity of Q the complete null cone just takes the familiar form of the Minkowski light-cone, given by

$$0 = (u-u_0)(v-v_0) - \delta_{ab}x^a x^b. \tag{7.20}$$

We define the function

$$f_{ab}(u) := (u-u_0)^{-1}\delta_{ab}, \tag{7.21}$$

such that near Q we can re-write the expression for the complete null cone as

$$v = f(u)_{ab}x^a x^b + v_0. \tag{7.22}$$

If the function f is chosen in such a manner that the hypersurface defined by (7.22) remains null, (that is, with a null normal vector) then even in the curved region of space-time (7.22) serves as a defining equation for K_3. This poses the following restriction on f:

$$\partial_u f_{ab} + f_{ac}f_{cb} + H_{ab} = 0. \tag{7.23}$$

Taking the trace of the above expression and making use of both the weak energy condition and Schwartz' inequality we see that

$$\partial_u f_{aa} + \frac{1}{2}f_{aa}f_{bb} = -\frac{1}{2}(f_{ac}f_{ac}\delta_{bc}\delta_{bc} - f_{ac}\delta_{ac}f_{ac}\delta_{ac}) - H_{aa} \leq 0. \tag{7.24}$$

Therefore,

$$\frac{\partial^2}{\partial u^2}\exp\left(\frac{1}{2}\int f_{aa}(u)du\right) \leq 0. \tag{7.25}$$

It is now a simple matter to show that f will become singular somewhere. We see from (7.21) that in the limiting case of $u_0 \to -\infty$ the function f tends to zero. Thus for sufficiently early u, the complete null cone is simply given by the plane of constant $v = v_0$, as seen from (7.22). Therefore,

$$\frac{\partial}{\partial u}\exp\left(\frac{1}{2}\int f_{aa}(u)du\right) = 0 \tag{7.26}$$

for early u. However, as the second derivative satisfies the inequality (7.25) we can conclude that $\exp\left(\frac{1}{2}\int f_{aa}(u)du\right)$ will become zero for some value of u. This in turn is only possible if one of the components of f_{ab} becomes infinite for some value $u_f > u_1$ of u. We now assume that this point is reached after the wave has subsided $(u_1 > u_f)$. Then, taking a large negative value for u_0 will only slightly change (7.22) for values of u close to u_1 and therefore we still

have $u_f > u_1$. While no explicit proof of this is given in [47], it is straightforward to see as all the involved expressions are continuous functions of the coordinates away from u_1. It follows that the complete null cone of the point Q encounters a physical singularity once the wave has passed. Again we see that the nature of the singularity is to focus the incoming light-cone at u_f. In the flat region $u > u_2$ the condition (7.23) reduces to

$$(f^{-1})_{ab} = \delta_{ab}, \tag{7.27}$$

which has a very simple solution

$$(f^{-1})_{ab} = u\delta_{ab} - q_{ab} \tag{7.28}$$

for some constant and symmetric matrix q_{ab}. Thus f_{ab} will diverge whenever u is an eigenvalue of q_{ab}. As q is symmetric, we can diagonalize it. For the electromagnetic plane wave the eigenvalues are degenerate and we have $q_{ab} = u_f \delta_{ab}$. This means that the entirety of the light-cone emanating from Q will reconverge at a point R with the coordinates $(u_f, v_0, 0, 0)$. This is referred to as anastygmatic focusing.

The case of a gravitational plane wave is more subtle as the eigenvalues of q_{ab} are now no longer equal. Here, unlike before, there is a single geodesic through Q that does not pass through R, namely the one running parallel to the direction of propagation i.e. $u = \text{const} = u_0, x_a = 0$. When the light-cone enters the flat space-time region $u > u_2$, we can solve the geodesic equation using (7.28) and obtain

$$x_a = (u\delta_{ab} - q_{ab})m_b \tag{7.29}$$

where m_b is constant for every geodesic. In this case we may choose coordinates such as to diagonalize q with two distinct eigenvalues λ_1 and λ_2. In this case $x_1 = 0$ when $u = \lambda_1$, such that all geodesics pass through some point of the space-like line given by $x_1 = 0$, $v = v_0$, $u = \lambda_1$.

Conclusions on the Nature of the Singularity

Both cases imply that there are null geodesics passing through the initial point Q arbitrarily close to the parallel geodesic Q_1 that pass through a fixed point R not on Q_1. We therefore see that the focusing of geodesics is unavoidable even in the general case. For specific examples, as we shall shortly see, one does not have to go to these lengths in order to diagnose geodesic incompleteness. In most instances, one can directly observe that the metric becomes degenerate at the focal point. Nonetheless, the general proof of geodesic incompleteness is important as it shows, that the singularity is not some by-product of an overly idealized choice of wave form. From the classical perspective it is unavoidable even for more realistic plane-wave profiles.

We have to point out here that this singularity is somewhat different from the Schwarzschild and Kasner cases, as it is possible to extend the geodesics beyond the focal point in a smooth

way. Of course, uniqueness is lost and therefore one cannot call the space-time geodesically complete in this sense. The most obvious discrepancy is the fact that, unlike in the aforementioned cases, all curvature invariants of plane-fronted waves vanish. This is immediately apparent from the fact that the only possibly non-vanishing component of the Ricci-tensor is R_{uu} and it is simply impossible to find any contraction of indices not amounting to zero. A more stringent proof can also be given, arguing that for any point x in the pp-wave space-time there exists a homothety[1] with fixed point x excluding the possibility of any non-vanishing invariant [52]. Furthermore, there is no horizon that could possibly shield the focal point from outside observation, as the light-cone maintains its orientation throughout the approach. This is in stark contrast to the Schwarzschild case where the light-cone begins to tilt and even flip at the Schwarzschild radius. As we remember, this tilting leads to the Kasner-like expansion in at least one direction. As this behavior seems to be absent here, it will be interesting to study in detail the influence this has on the behavior of the wave functional near the focal point.

7.2. Quantum Propagation on pp-Wave Space-times

Before we study the Schrödinger quantization of fields in this setting we give a short overview of the main results pertaining to the propagation of quantum fields on pp-waves. This will serve to build some intuition on the general behavior of quantum systems in this background, as well as laying the technical groundwork for later developments. Although the literature on this subject is vast, we will only cover results that are directly connected to application we have in mind, meaning that this overview is far from complete.

7.2.1. Particle Creation on pp-Waves

One of the most prominent results of the semi-classical approach inherent to quantum field theories in curved space-times is that of particle creation. In the standard quantization of fields we begin by choosing an orthonormal set of solutions to the classical equations of motion ϕ_k and then expand the field operator in terms of these excitations

$$\hat{\Phi} = \int_k \phi_k \hat{a} + \phi_k^* \hat{a}^\dagger, \tag{7.30}$$

whereby we pair the creation operator $\hat{a}^\dagger$ with the positive frequency modes and the annihilation operator $\hat{a}$ with the negative frequency modes. Aside from the usual normalization condition on the Wronskian we are completely free in our choice of mode functions, granting us the freedom to change to a different set of $\{\phi_k\}$ related to the former by a Bogoliubov transformation. The physical meaning of the creation and annihilation operators acting on the Fock-space is therefore only given in conjunction with a choice of mode functions and thereby gives rise to the famed ambiguity in the choice of physical vacuum. In flat space we are doubly lucky. Firstly,

[1] Homothety hereby refers to a scaling transformation of the associated affine space

the symmetries of Minkowski space single out a unique choice of mode functions such that the resulting vacuum is invariant under said symmetries. Secondly, in flat space all representations are unitarily equivalent and therefore particle number is a globally well-defined concept. In curved space-times we are not so fortunate. Not only is there not enough symmetry to uniquely fix a vacuum state, but all representations are now unitarily in-equivalent, meaning that our potentially arbitrary choice will have physical consequences. It is consequently paramount for any discussion of quantum phenomena on a dynamical space-time to include an outlook on this issue.

Plane-fronted waves, in particular sandwich waves, are unique in this regard. As we shall see, they enjoy an evolution that is free of particle creation; in some sense this makes them the closest analogue to Minkowski space among all dynamical space-times. This should not come as a surprise for several reasons. As mentioned previously they are the only dynamical space-time on which the scalar wave operator satisfies the Huygens principle [49]. In loose terms this means that the solutions to the wave equation do not "have long tails", meaning that a disturbance to the background by suddenly turning on a source has a sharp beginning and end. Systems not enjoying this property lead to a "less compact" response. A related but not equivalent way of viewing the Huygens principle is to say that solutions of the wave equation do not back-scatter off the background itself. Intuitively it is clear how this property would affect particle production, which after all is very closely linked, in the sense defined above, to the behavior of the mode functions. Technically it remains to show that there is no mixing of positive and negative frequency modes. Sandwich waves are particularly useful in this context, as they are essentially equal to Minkowski space, apart from a compact patch, and therefore allow an unambiguous particle definition in both the remote past and future. In some sense one may even regard them to simply be two "glued together" Minkowski patches, and the absence of particle production hardly surprises.

The Scalar Wave Equation

In order to see the absence of particle production explicitly we require an expression for the solutions to the scalar wave equation

$$\frac{1}{\sqrt{-g}}\partial_\mu \sqrt{-g}\, g^{\mu\nu}\, \partial_\nu \phi = 0. \tag{7.31}$$

Expressed in Rosen coordinates this becomes

$$(2\partial_u\partial_V + \partial_u\sqrt{\gamma}\,\partial_V - \gamma^{ij}\partial_i\partial_j)\phi = 0. \tag{7.32}$$

Fortunately, an exact solution is known [49], taking the form

$$\phi(\mathbf{y}) = \Omega(u)e^{i\phi_k}, \qquad \Omega(u) := \left|\gamma^{-1}\right|^{1/4} = \frac{1}{\sqrt{|E(u)|}}. \tag{7.33}$$

The phase is given by

$$\phi_k = k\cdot y + k_0 V + \frac{F^{ij}k_i k_j}{2k_0}. \tag{7.34}$$

In Brinkmann coordinates the equation takes the form

$$(2\partial_u\partial_v + H(u,\mathbf{x})\partial_v^2 - \partial_a\partial^a)\phi = 0 \tag{7.35}$$

and is obviously solved by the same function. As the amplitude is only dependent on u, thus being the same in both coordinate systems, the only change is in the phase which now includes the shear term that comes from the transformation of the V-component (7.13).

$$\phi_k = \frac{k_0}{2}\Xi_{ab}x^a x^b + k_i E^i_a x^a + k_0 v + \frac{F^{ij}k_i k_j}{2k_0}, \tag{7.36}$$

where

$$\Xi_{ab} = \dot{E}_{ai}E^i \tag{7.37}$$

is often referred to as the shear or deformation tensor. In the case of sandwich waves this gives rise to a natural restriction on the vielbein such that the asymptotic behavior reduces to that on Minkowski space in the remote past and future

$$\lim_{u\to\pm\infty} E^a_i(u) = \delta^a_i. \tag{7.38}$$

This also identifies the positive frequency solutions as those for which $0 \leq k_0$.

Bogoliubov Coefficients

The absence of particle production was first shown by Gibbons [50], and we give his elegant argument for calculation of Bogoliubov coefficients here. In general one may try to solve the (massive) scalar wave equation with an Ansatz of the form

$$\phi = Ae^{iS}, \tag{7.39}$$

yielding

$$\Box^2 A/A = (\nabla S)^2 - m^2. \tag{7.40}$$

In this case the WKB approximation reduces to requiring S to satisfy the Hamilton-Jacobi equation, implying that the left hand side vanishes. As the eikonal approximation is exact in this case, we see that A^{-2} is the determinant orthogonal to the geodesics whose normals are ∇S. As we have already seen that the V dependence of the mode solutions is given simply by e^{ik_0V}, we can

see that the scalar product between two solutions

$$(\phi,\psi) = (2i)^{-1/2}\int dV dx^1 dx^2 \left(\bar{\phi}\frac{\partial\psi}{\partial v} - \psi\frac{\partial\bar{\phi}}{\partial v}\right) \tag{7.41}$$

will always be equal to 0 for differing values k_0, no matter what the u dependence looks like. It follows that all Bogoliubov coefficients connecting two different sets of bases for the mode solutions must vanish (unless the transformation is the trivial one). The result of this simple but powerful argument is that there can be no particle creation, irrespective of the amplitude of the wave, which is a function of u only.

7.2.2. Scattering on and with pp-Waves

Due to the closed and simple form of the mode solutions it is possible to calculate the inner product between positive frequency in and out states, encoding the amplitude for in to out scattering on a pp-wave [53, 54], and therefore get an explicit expression for the S-matrix elements. For two solutions associated with the momenta $\{k_0,k\}$ and $\{l_0,l\}$ the inner product at $u=0$ becomes

$$(\phi_{\text{in}},\phi_{\text{out}}) = 2k_0\delta(k_0-l_0)\Omega(0)\int d^2x \exp i\left[\frac{l_0}{2}\Xi_{ab}(0)x^a x^b + (k_a + l_i E_a^{-i}(0)x^a) + \frac{F^{ij}(0)l_i l_j}{2l_0}\right].$$

The resulting Gaussian integral can be performed and gives

$$(\phi_{\text{in}},\phi_{\text{out}}) = 2k_0\delta(k_0-l_0)\left(\frac{2\pi}{il_0}\right)e^{-i(s_l+r_{k,l})}|b|^{-1/2}, \tag{7.42}$$

where the two phases are given by

$$s_l := \frac{F^{ij}(0)l_i l_j}{2l_0} \tag{7.43}$$

and

$$r_{k,l} := -\frac{1}{2l_0}(k_a - l_i c_a^i)c^{an}(b^{-1})_n^d(k_d - l_j c_d^j), \tag{7.44}$$

and we have parameterized in terms of the two by two matrices b and c as

$$E_{ia} = u b_{ia} + c_{ia}. \tag{7.45}$$

The above results again demonstrate that the S-Matrix remains unitary without particle creation. They can also be generalized to higher spins without substantial changes to the qualitative outcome [54].

These properties also allow interesting conclusions to be drawn on gravitational scattering in flat space. It is well known that, even at tree level, the scattering of gravitons violates the

unitarity bound at Planckian energies. The search for a UV-completion of General Relativity has of course been the holy grail of high energy physics for many decades, and has given rise to many theories that attempt to provide a framework in which these scattering amplitudes are unitary. Some, such as String theory, have even had success in this endeavor; however, it remains unclear how and if they are realized in nature. Instead one may also call into question the assumption of asymptotic in- and out-states that is necessary to derive these amplitudes. If we assume that some of the involved gravitons carry Planckian energy, it seems questionable to assume back-reactions to be negligible, since the gravitational coupling only increases with energy. One of the first to propose a method of taking back-reaction into account was 't Hooft. His suggestion was to replace the incoming transplackian particles by gravitational shock waves as the ones introduced above [55]. The basic idea is to exploit the fact that a plane wave can be thought of as the exact solution of the back-reaction on the geometry, while its relatively forthcoming properties may enable us to actually solve the scattering problem. In the Regge limit such a reduction of a non-perturbative generalization of the graviton to a perturbative calculation on a plane wave was performed by [56], coming to the conclusion that the relevant amplitudes are in fact unitarized.

The main problem with all of these approaches is of course the behavior near the focusing singularity. While, unlike for example the Schwarzschild space-time, the geometry itself does not induce a massive response to the singularity (such as the divergence of curvature scalars), the focusing effect will nonetheless lead to major divergences for external fields. Obviously, if some form of matter is present, its density will diverge as it is focused. Therefore particles that partake in the scattering will cause back-reaction on the plane wave itself as their energy momentum density grows approaching the focal points. This effect may be estimated by considering the energy-momentum tensor of a scalar field in a plane wave geometry. From the form of (7.33) we see that the dominant contribution to the energy-momentum tensor will be given by

$$T_{uu} \sim \partial_u \phi \partial_u \phi \sim \left(\partial_u \left|\gamma_{ij}\right|^{-1/4}\right)^2. \tag{7.46}$$

As we have seen, the focussing effect will cause the metric γ to become degenerate at the focal points and therefore the energy-momentum tensor will diverge. In this case, we can no longer safely assume that the geometry of the problem is given by (7.5). In fact, as the right hand side of the Einstein equations grows unbounded, we do not even expect the deviations from the exact solution to be perturbative in any well-defined sense.

As it has such a severe impact, it is an intriguing question whether a quantum field can actually occupy this classically ill-defined configuration. We have seen for the Schwarzschild and Kasner examples that it may be the case that the evolution near the focal points actually prevents this configuration from being reached as probabilistic support vanishes. Should this be the case, one could hope that a perturbative treatment of back-reactions can be successful, even

in the proximity of the focal points. Should it turn out that this is not the case one is forced to come to the conclusion that in the presence of matter fields, the geometry is incomplete and unstable against quantum fluctuations. To establish this we will consider a Schrödinger description of quantum fields in the vicinity of the singular points in the next section.

7.3. Schrödinger Quantization on Plane Waves

In this section we will describe how the null reduction approach may be used to give a well-defined Schrödinger quantization on plane-wave metrics. While the construction is general to any space-time that admits a double-null foliation, it is greatly simplified by the sandwich plane-wave geometry. This is owed to the fact that in both asymptotic regions we can make the comparison to ordinary Minkowski space in light-cone coordinates and that the wavefront gives us a preferred null surface on which to base the foliation. We will then look at a specific choice of sandwich wave to answer how the definitions and notions regarding quantum completeness apply to this setting. We conclude by giving a back of the envelope prediction of how the inclusion of back-reaction might alter the results derived.

7.3.1. The Schrödinger Equation

The first objective is to write down the Schrödinger equation in its null reduced form. In order to do so we must determine the form of the Hamiltonian along the lines of the previous chapter. We therefore consider the tangent space TCQ to CQ such that we can define the velocity fields $(q, q^+, q^-) \in TCQ \oplus TCQ$. From here it is clear that the evolution space is given by $\mathscr{V} \times \mathscr{U}$ and q^+ is the velocity field tangent to the outgoing v-direction and q^- is tangent to the ingoing u-direction. The Hamilton density is constructed by the Legendre transformation [42] of the Lagrange density $\mathcal{L}$

$$\mathcal{H}(q, p^+, p^-) = ((0, p^+, p^-) - \mathcal{L})\Lambda^{-1}(q, p^+, p^-). \tag{7.47}$$

Here the conjugate fields are $p^\pm \in T^*CQ$ and

$$\begin{aligned} &\Lambda : TCQ \oplus TCQ \to T^*CQ \oplus T^*CQ \\ &\Lambda : (q, q^+, q^-) \mapsto (q, \tfrac{\delta \mathcal{L}}{\delta q^+}, \tfrac{\delta \mathcal{L}}{\delta q^-}), \end{aligned} \tag{7.48}$$

denotes the invertible Laplace transformation.

The identification of the conjugate momenta $p^{\pm}$ with the functional derivative of $\mathcal{L}$ with respect to the velocity fields $q^{\pm}$ follows from the Hamilton equations given previously

$$p^{+} = \frac{\partial q}{\partial u} = \frac{\delta \mathcal{H}}{\delta q^{+}}, \quad p^{-} = \frac{\partial q}{\partial v} = \frac{\delta \mathcal{H}}{\delta q^{-}}, \quad \frac{\partial q^{+}}{\partial u} + \frac{\partial q^{-}}{\partial v} = -\frac{\delta \mathcal{H}}{\delta q}. \tag{7.49}$$

As stated before, there is an additional integrability condition which takes the form

$$\frac{\partial}{\partial u}\frac{\delta \mathcal{H}}{\delta q^{-}} = \frac{\partial}{\partial v}\frac{\delta \mathcal{H}}{\delta q^{+}}. \tag{7.50}$$

Fortunately, it was demonstrated by Hayward that these will always be satisfied for the case of a double null foliation [57] and we therefore need not worry about them here. This is especially easy to see in the context of the plane wave background chosen, as the integrability conditions simply reduces to Schwartz's theorem for the exchange of partial derivatives.

Hence, we proceed to consider a free massless scalar field theory on a pp-wave background, minimally coupled to the geometry. The action in its standard form is given by

$$S = -\tfrac{1}{2}\int \mathrm{d}^4x\sqrt{-g}\left[g(\nabla\phi,\nabla\phi) + \zeta\mathcal{R}\phi^2\right] \tag{7.51}$$

with the covariant derivative ∇, Ricci scalar $\mathcal{R}$, and coupling constant ζ. Rewriting this action in terms of the Brinkmann coordinates and using the embedding ι given by the dual-null foliation, yields

$$S = -\frac{1}{2}\int_{\mathbb{W}^4} \mathrm{d}^4x\sqrt{-g}\left(-\phi^{+}\phi^{-} + H(u,x)\phi^{+}\phi^{+} + \frac{1}{2}\delta(\nabla\phi,\nabla\phi) + \zeta\mathcal{R}\phi^2\right). \tag{7.52}$$

Here, δ denotes the induced Euclidean flat metric on $\mathcal{S}$ and the ∇ are understood to be the spatial derivatives. Considering ι, the boundary and initial data for the velocity fields with respect to the u- and v-direction are given by $\phi^{+} \restriction \Sigma_{-} = \{0\}\times\mathscr{V}\times\mathcal{S}$, and $\phi^{-} \restriction \Sigma_{+} = \mathscr{U}\times\{0\}\times\mathcal{S}$, while the spatial data is given by $\phi \restriction \{0\}\times\{0\}\times\mathcal{S}$. An illustration of the dual-null foliation can be found in FIG. 7.2 where the velocity fields and the hypersurfaces are shown explicitly. From here, it is obvious why the evolution in this foliation is an initial value problem on $\mathcal{S}$ combined with a boundary condition at $\mathscr{I}^{+}$ or $\mathscr{I}^{-}$.

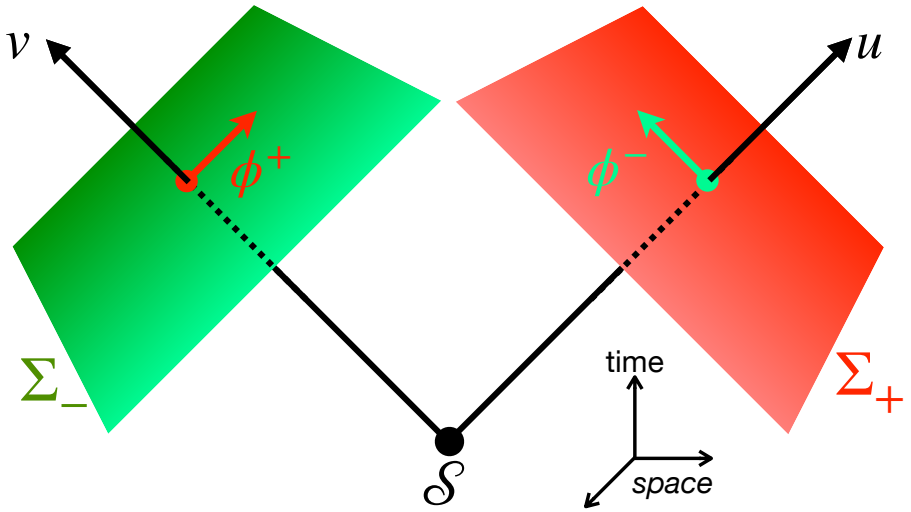


Figure 7.2.: Sketch of the dual-null foliation (spatial dimensions partially suppressed): attached to the two dimensional space-like surface $\mathcal{S}$ on which the spatial fields live, are the ingoing and outgoing null-vectors along $v \in \mathscr{V}$ and $u \in \mathscr{U}$ respectively. Perpendicular to the null-directions are the three-surfaces Σ_- and Σ_+ to which the velocity fields are restricted $\phi^\pm \restriction \Sigma_\mp$. Points in the two-dimensional spatial sub-manifold are represented by intersections of the three dimensional sub-manifolds Σ_+ and Σ_- at certain values of the light-cone coordinates.

Applying (7.47) to (7.52), we find the Hamilton density in Brinkmann coordinates to be

$$\mathcal{H} = \frac{\sqrt{-g}}{2}\left(2\pi^+\pi^- + H(u,x)\pi^-\pi^- + \delta\left(\nabla\phi,\nabla\phi\right)\right). \tag{7.53}$$

This is the general form for a Hamilton density in Brinkmann coordinates; however, for an outgoing wave, the only non-zero component of the Ricci tensor is $R_{uu} = -\mathrm{tr}(H)$, which is zero for gravitational waves as we have seen before. Hence, we have safely set $\mathcal{R} \equiv 0$ in the above equation. Furthermore, to replace the mixing terms in the Legendre transformation we used the Hamiltonian equations

$$\pi^- = \frac{\delta\mathcal{H}}{\delta\phi^-} = \phi^+, \tag{7.54}$$

$$\pi^+ = \frac{\delta\mathcal{H}}{\delta\phi^+} = \phi^- - H(u,x)\phi^+. \tag{7.55}$$

We see that the outgoing momentum is not affected by the wave since it propagates parallelly while the ingoing momentum that crosses the wave experiences a distortion which will lead to the inevitable focusing. Hence, the first term on the right hand side of (7.47) becomes $\pi^-\phi^- = \phi^+\phi^-$ and $\pi^+\phi^+ = \phi^-\phi^+ - H(u,x)\phi^+\phi^+$ such that we can complete the Legendre transformation using (7.54) and (7.55) to get (7.53). Although the Hamilton density in Einstein-Rosen coordinates misses the term proportional to $H(u,x)$ and therefore speciously looks simpler, the spatial metric will be given by γ and has a non-trivial U-dependence.

Once the Hamiltonian is known, we can proceed to writing down the Schrödinger equation

for the quantum test field. Due to the construction of the foliation, the null-reduced Hamiltonian retains its property of generating the Hamiltonian flow in phase space, thus determining the dynamics just as in the prior cases. The interpretation of the resulting wave functional is therefore analogous to before. Just as in the prior studies of Gibbons [50], the role of and auxiliary time variable will be played by the light-cone coordinate u, which is acceptable as long as we are only considering ingoing modes. While this technically limits the consideration to a specific choice of initial conditions, it is sufficient to study the cases that we are most interested in, namely quantum test particles interacting with the plane wave as they approach the focusing singularity.

In the usual cases with time-direction t the differential operator describing the Schrödinger equation $P\psi = 0$ with Hamilton operator $\hat{H}(t)$ is given by

$$P = i\partial_t - \hat{H}(t). \tag{7.56}$$

Recalling the definition of the light-cone coordinates chosen along the $z-$direction; $u = t - z$ and $v = t + z$ from the earlier sections, this can be recast as follows such that $2\partial_t \to \partial_u + \partial_v$. In these coordinates the Schrödinger operator becomes

$$\hat{P} = i(\partial_u + \partial_v) - 2\hat{H}(u,v). \tag{7.57}$$

As stated, in full generality the evolution problem is more involved than in the standard case due to the superposition of evolution directions. In the functional Schrödinger representation, the differential operator will be constructed using (7.53) and proceeds along the lines of the previous cases but has to be adapted to the null foliation.

Importantly, it is necessary to provide a quantization scheme that clearly identifies the canonical momentum associated to the configuration variable, which we have chosen to be given by the ingoing fields. To do so we will work with the form of the canonical commutation relations which is commonly employed when using light-cone coordinates [58]. The following commutation relations can be shown to hold on every individual three-surface $\Sigma_\pm$ and the two dimensional $\mathcal{S}$:

$$\left[\pi^\pm, \phi^\pm\right]_{\Sigma_\mp} = -i\delta^{(2)}(x,x')\delta(\xi_\pm, \xi'_\pm), \tag{7.58}$$

$$\left[\phi^+, \phi^-\right]_{\mathcal{S}} = -i\delta^{(2)}(x,x'), \tag{7.59}$$

where $\xi_+ = v$ and $\xi_- = u$.

With this prescription in place, we may fix the canonical momentum conjugate to our field variables to be $\pi^\pm$. The corresponding momentum operator in the Schrödinger representation

is given accordingly by the respective functional derivative

$$\pi^{\pm} \to -i\frac{\delta}{\delta\phi^{\pm}}. \tag{7.60}$$

Inserting this into the expression for the Hamiltonian (7.53) gives us the adequate functional Schrödinger operator on which to base the analysis.

$$\mathcal{H} = \frac{\sqrt{-g}}{2}\left(-2\frac{\delta}{\delta\phi^{+}}\frac{\delta}{\delta\phi^{-}} - H(u,x)\frac{\delta}{\delta\phi^{+}}\frac{\delta}{\delta\phi^{-}} + \delta\left(\nabla\phi,\nabla\phi\right)\right). \tag{7.61}$$

Thus, in general the Ansatz for the free ground state functional becomes more complicated, as we still retain the full dependence on both evolution directions. In particular there is no a priori reason to exclude the possibility of the evolution kernel mixing ingoing and outgoing modes; thus it is convenient to introduce a matrix notation as follows:

$$\Psi[f](u,v) = N(u,v)\exp\left(-\frac{1}{2}[f]\mathcal{K}(u,v)[f]\right), \tag{7.62}$$

with $\mathcal{C}(\Sigma_+)\times\mathcal{C}(\Sigma_-) \ni f(x) = (\phi^+(x),\phi^-(x))^T$ being the field vector and the kernel matrix $\mathcal{K}_{AB}(u,v)$ where $A,B \in \{+,-\}$. The individual entries of $\mathcal{K}$ appearing in (7.62) are bi-local functionals $\mathcal{K} : \mathcal{C}(\Sigma_\pm)\times\mathcal{C}(\Sigma_\pm) \to \mathbb{C}$, $(f_1,f_2) \mapsto [f_1]\mathcal{K}[f_2]$ of the form

$$[f]\mathcal{K}[f] = \iint_{\Sigma_{A,B'}} \mathrm{dvol}_{A,B'} f^A(x) K_{AB}(x,x') f^B(x'). \tag{7.63}$$

It should be noted that the f^A are only defined on the corresponding Σ_A while the x-dependence in K_{AB} has to be interpreted with respect to the entire coordinate patch $\mathbb{W}^4$. The primed index B' denotes that the three surface or volume integration respectively, is associated to the primed coordinate. From here we see that $\mathcal{K}_{AB}$ develops a dependence on both the u and v coordinate. The field independent part of (7.62) once more plays the role of a normalization. Just as in the flat case, this is given by the trace of the functional kernel K_{AB}

$$\frac{N(u,v)}{N(u_0,v_0)} = \exp\left(-\frac{i}{2}\int_{u_0}^{u}\int_{v_0}^{v}\int_{\mathcal{S}} \mathrm{d}^4x\sqrt{-g}\sum_{A,B} K_{AB}(x,x)\right). \tag{7.64}$$

Just as in the standard case, it will in general not be possible to solve the expressions given exactly. In particular, the possible mixing of the ingoing and outgoing velocity fields complicates matters further. In this work however, we are in the fortunate position that the chosen plane wave background exhibits a large degree of symmetry that is almost uniquely suited to our approach and therefore simplifies the equations dramatically. The first simplification is due to the fact that there is no dynamical mixing between outgoing and ingoing velocity fields, as has been shown by a number of investigations into the quantum evolution on plane wave space-

times [50, 53, 54, 56]. This leads to an effective decoupling of the two evolution directions, allowing for the separation of the ingoing fields ϕ^- traveling along the u-direction and the outgoing fields. The two sets of initial data are evolved independent of each other. Intuitively this is clear, as we would not expect the ϕ^+ fields that travel parallel to the wavefront to be affected by it. Σ_- can therefore be seen as an achronal set in the sense of Hawking and Ellis [15]. This allows for a so-called null-reduction, in which we set the outgoing fields $\phi^+(v) \equiv 0$ per default, then (7.53) as well as (7.62) will only depend on u as an auxiliary time variable and the Schrödinger operator will reduce to [59]

$$P = i\partial_u - 2H(u). \tag{7.65}$$

Subsequently, the kernel matrix $K_{AB}(x,x)(u)$ has only a single non-trivial component which is given by $K_{--}(u)$. An equation for $K_{--}(u)$, which we will refer to simply as $K(u)$ from now on, may once again be derived from inserting the Ansatz into the functional Schrödinger equation. The general Ricatti-type form of the evolution equation will be retained, and the same transformation can be used to bring it to standard form

$$K_k(u) = \frac{-i}{\sqrt{-g}}\partial_u \ln\left(\frac{\varphi^-(u;k)}{\varphi^-(u_0;k)}\right). \tag{7.66}$$

Once more the $\varphi^-(u;k)$ denote solutions to the scalar wave equation, whose initial conditions are compatible with the null reduction performed earlier. This restriction on the functional space is the only essential deviation from what we have seen and discussed so far. As we have seen, the exact solutions of the wave equation are known on the given geometry and we may therefore give an explicit expression for the kernel. Using $\varphi_k^-(u,x) = \Omega(u)e^{i\phi_k}$ where $\Omega = |\det(\gamma)|^{-1/4}$ and the phase is once more given by

$$\phi_k = \frac{k_0}{2}\Xi_{ab}x^a x^b + k_i E^i_a x^a + k_0 v + \frac{F^{ij}k_i k_j}{2k_0}, \tag{7.67}$$

we can insert these results into (7.66) to obtain

$$K_k(u) = \frac{1}{\sqrt{-g}}\left[\frac{k_0}{2}\dot{\Xi}_{ab}x^a x^b + k_i\dot{E}^i_a x^a + \frac{\gamma^{ij}k_i k_j}{2k_0} - i\frac{\dot{\Omega}}{\Omega}\right]. \tag{7.68}$$

Again, the kernel will in general be complex, with the real part resulting in the main contribution to the functional part of Ψ, while the imaginary part enters the normalization.

7.3.2. Shock Waves in Brinkmann Coordinates

To investigate the behavior of the probing field, as we approach the focal point, we will now specify to a particular type of plane wave. The following sections are based on [3]. Shock waves are characterized by the delta function support of the actual wave $H \sim \delta(u-u_0)$ and are the simplest to study. Due to the compact nature of the wave in the u-direction it represents the closest analogue to the flat Minkowski example, insofar as it is essentially given by two differing Minkowski patches “glued" together with different boundary conditions. Specifically, we choose the profile function

$$H_{ab}(u) = \lambda^{(a)}\delta(u)\delta_{ab}, \tag{7.69}$$

describing a shock wave-front residing at $u = 0$. The real number $\lambda^{(a)}$ represents the physical amplitude of the wave in the x^a-direction. The vielbein corresponding to this choice is given by the oscillator equation (7.15) together with the condition, that the Minkowski values must be reproduced at the boundaries $\mathscr{I}^{\pm}$. The oscillator equation can easily be integrated giving as a result

$$E^{\pm}_{ia} = \delta_{ia}\left(1 \mp \lambda^{(a)} u\Theta(\mp u)\right), \tag{7.70}$$

$\Theta(u)$ being the Heaviside theta-distribution. Insertion of (7.70) into the expressions for the Rosen coordinates shows that the metric becomes degenerate at the value $u^{\pm}_{\mathrm{f}} = \mp 1/\lambda^{(a)}$. We therefore see explicitly that the focal length of the wave is given by the inverse of its amplitude. It is straightforward to compute the spatial metric from here, resulting in a diagonal matrix

$$(\gamma)_{ij} = \begin{pmatrix} (1+\lambda^{(1)}u\Theta(u))(1+\lambda^{(1)}u\Theta(u) & 0 \\ 0 & (1+\lambda^{(2)}u\Theta(u))(1+\lambda^{(2)}u\Theta(u). \end{pmatrix} \tag{7.71}$$

It is trivial to read off the determinant, which is given by

$$\gamma = (1+\lambda^{(1)}u\Theta(u))^2(1+\lambda^{(2)}u\Theta(u))^2. \tag{7.72}$$

Furthermore, we require the shear tensor

$$\Xi_{ab} = \delta_{ab}\frac{-\lambda^{(a)}\Theta(u)(1+\lambda^{(b)}u\Theta(u))}{(1+\lambda^{(a)}u\Theta(u))^2}, \tag{7.73}$$

where the expression above is exact. While there is an additional term when directly plugging the given form of the vielbein into the required expressions, this term is directly proportional to a factor of $u\delta(u)$ and therefore vanishes everywhere. As the shear tensor measures the distortion of neighboring geodesics, it is an effective measure of the focussing after the wave front. Such a focal point will always be present if $\lambda^{(a)}$ is smaller than zero. Due to the condition imposed on gravitational waves that $H(u,v)$ must be traceless, such an eigenvalue is guaranteed to exist. As we can see, γ^{ij} diverges for $u \to u_{\mathrm{f}}$ as well as Ξ_{ab}, Ω, and E^i_a while (7.70) and γ_{ij} approach

zero. The u-derivative of the shear tensor is then given by

$$\dot{\Xi}_{ab} = \delta_{ab}\left[\frac{(\lambda^{(a)}(\lambda^{(b)}u+2)-\lambda^{(b)})\lambda^{(a)}\Theta(u)}{(1+\lambda^{(a)}u\Theta(u))^3}+h(u)\right]. \tag{7.74}$$

Becoming singular at the focal point, (7.74) will also develop a divergence at $u=0$ because the second term $h(u)$ is just proportional to the shock wave $H_{ab}(u)\propto\delta(u)$ for all $u\in\mathbb{R}$. However, this divergence is only fictitious and roots in the particular choice of $H(u,x)$ which will be cured by a smooth and therefore more realistic profile function. In this case the contribution will remain finite. Since we are not interested in the plane-wave itself, we will ignore this term due to the vanishing support at $u\neq 0$.

We are now in a position to calculate the ground state wave functional from the various metric dependent factors we have derived above. In order to gain an intuition for the general structure, we will specialize to a specific metric. To make things as simple as possible, we choose the linearly polarized plane-wave [56] with $\lambda^{(1)}=1$ and $\lambda^{(2)}=-1$, or equivalently, $H_{ab}(u)=\sigma^z_{ab}\delta(u)$, where $\sigma^z_{ab}=\mathrm{diag}(1,-1)$. The focal points will therefore be located at $u_\mathrm{f}=1$; the problematic value being the negative eigenvalue in this situation. The vielbein, being a linear function in u, degenerates in this case once the focal point is reached, signaling the focusing singularity. This choice further simplifies (7.74) since we are only interested in the immediate vicinity of the focusing singularity, $u\approx 1$ where $\Theta(u_\mathrm{f}\pm\Delta u)=1$ for $0<\Delta u<1$, such that the second term in (7.74) remains zero. The most singular term in the derivative of the shear tensor, which will eventually enter our expression for the kernel through (7.68), is then given by

$$\dot{\Xi}_{22}\to 1/(1-u)^2, \tag{7.75}$$

which diverges at the focal point. Closer inspection reveals that all of the other contributions to the real part of (7.68) scale similarly.

With this, we can evaluate the asymptotic behavior of the field independent part or normalization of $\Psi[\phi^-](u)$. In the normalization $|N|^2(u)$ only the imaginary part of the kernel K plays a role, as the real part amounts merely to a phase. The imaginary part of (7.68) is given entirely through the logarithmic derivative of Ω. Inserting the expressions for the vielbein into the solution of the wave equation we see that

$$\Omega = |(1+\lambda^{(1)}u\Theta(u))(1+\lambda^{(2)}u\Theta(u))|^{-1/2} \tag{7.76}$$

and therefore

$$\frac{\dot{\Omega}}{\Omega} = \frac{-(\lambda^{(1)}+\lambda^{(2)}+2\lambda^{(1)}\lambda^{(2)}u)\Theta(u)}{2((1+\lambda^{(1)}u\Theta(u))(1+\lambda^{(2)}u\Theta(u)))}. \tag{7.77}$$

The expression can be simplified by setting $\lambda^{(1)} = 1$, $\lambda^{(2)} = -1$ to match our previous choice. Furthermore, as we are only interested in the approach of the focal point we concentrate on the region where $u > 0$, eliminating many of the Θ-functions to yield an exceptionally simple result

$$\dot{\Omega}/\Omega = u/(1-u^2). \tag{7.78}$$

As we see, the normalization seems divergent in the limit $u \to 1$, even after performing the u-integration in (7.64), which yields $\ln\left(1-u^2\right)$ in the exponent. This is however due to the general feature of the kernel itself diverging in its coincidence limit. When writing out the full contribution to the norm of the wave functional, we find for $0 < u_0 < 1$

$$\frac{|N(u)|^2}{|N(u_0)|^2} = |1-u^2|^{\mathrm{vol}(\Sigma_-)} \tag{7.79}$$

where the volume factor $\mathrm{vol}(\Sigma_-)$ comes from the integration over the hypersurface Σ_- in (7.64) and is simply an infrared regulator. For all values $u < 0$ the normalization is simply equal to one, as we would expect, due to the fact that space-time here is equal to a flat Minkowski patch.

The field-dependent part may be treated in similar fashion. Contrary to the normalization, only the real part of K gives a contribution in this case. As the covariant volume element, given by the determinant of the spatial metric, is constant in Brinkmann coordinates, the pertaining expressions become very simple. Altogether, we find that

$$\left\|\exp\left(-[\phi^-]\mathcal{K}[\phi^-]\right)\right\|_2^2 = \sqrt{\left|\frac{C}{\mathrm{Det}(-g\mathrm{Re}(K))}\right|} \propto |1-u|^{\frac{\Lambda}{2}}, \tag{7.80}$$

The last expression on the right hand side is the leading term in the vicinity of the focal points. All remaining terms are sub-dominant. The constant C has been used to absorb various integration constants such as to de-clutter the notation. The cut-off Λ was introduced as a means to regulate the infinite dimensionality of the field space. Of course, the determinant is truthfully given by an infinite product of eigenvalues; however, in the present case the u-dependency may be factored as it is the same for all modes. We see that the field dependent part rapidly approaches zero as we near the focal point, suggesting the functional remains normalizable.

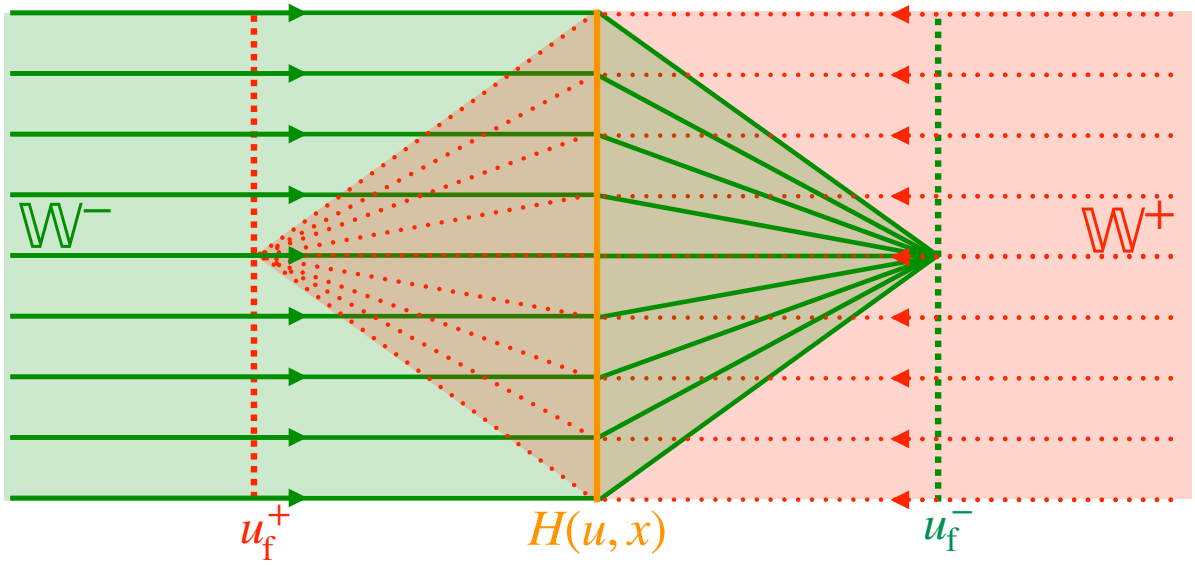


Figure 7.3.: The Focusing of the different Einstein-Rosen patches $\mathbb{W}^-$ and $\mathbb{W}^+$ is shown in terms of the green and red lines. Einstein-Rosen coordinates do not extend beyond the null singularities such that $\mathbb{W}^-$ is given by the green shaded and $\mathbb{W}^+$ by the red shaded area. The diamond-shaped overlap in the middle belongs to both patches. Brinkmann patches $\mathbb{W}^4$ have non-degenerate focal planes and the volume form remains constant throughout. This is in contrast to Einstein-Rosen coordinates where $\mathrm{vol}(\Sigma_{\mathrm{f}^-}) \to 0$ at the null-singularities. The orange line in the center shows the location of the shock wavefront.

7.3.3. Einstein Rosen Coordinates

The computation in Einstein Rosen coordinates is more complex, as the metric does not possess a u-independent determinant. Furthermore, the momentum dependence of the eigenvalues is such that a more rigorous regularization than a simple cut-off is needed. The Einstein Rosen coordinates are more similar to the Kasner and Schwarzschild cases studied earlier, in the sense that the space-time actually terminates at the singular point. Unlike the Brinkmann coordinates, for which the focal points are not special in any way, the Einstein Rosen patch terminates there. This is most clearly reflected by the determinant of the metric degenerating at the focal points, thus making the volume form degenerate as well. The intuitive picture is therefore a contracting space-time that reaches a vanishing total volume at the focusing singularity. Einstein Rosen coordinates can be thought of as two separate patches, one ingoing and one outgoing, that overlap to from the Brinkmann patch. This is illustrated in Figure 7.3.

We can use the diffeomorphism connecting the two coordinate systems, as it was given in (7.13) along with the vielbein, which is patch independent, to derive the form of the functional kernel in the Einstein Rosen case. To do so, we must again consider the solutions to the wave equation as a function of ingoing momentum

$$\hat{\phi}(\mathbf{k},U) = \int d\mathbf{y}^2 e^{-i\mathbf{p}\cdot\mathbf{y}} \Omega(U) e^{i\phi_k(\mathbf{y},U)} \tag{7.81}$$

The term proportional to the shear tensor is precisely canceled by the shift in the v-coordinate

$$K(U) = \frac{1}{\sqrt{-\gamma}}\left[\frac{\gamma^{ij}k_i k_j}{2k_0} - i\frac{\dot{\Omega}}{\Omega}\right]. \tag{7.82}$$

In this form, it is easy to see that it reduces to the expression derived in Minkowski space in the limit of large U, since the imaginary part will vanish as Ω becomes a constant. Close to the focal plane however, both the real and imaginary parts are non-trivial. The calculation of the normalization is by now a straightforward issue. Making use of the simpler expressions for the mode solutions ϕ_k we may once more employ (7.64). The result is extremely similar to the one previously derived,

$$\frac{|N(U)|^2}{|N(U_0)|^2} = |1-U^2|^{\mathrm{vol}(\Sigma_-)}; \tag{7.83}$$

however, we must bear in mind that due to the explicit time dependence of the volume element, the expression is completely different in nature. Due to the fact that the covariant volume tends to zero, we see that the normalization remains constant as we approach the focal point

$$\lim_{U\to 1}|1-U^2|^{\mathrm{vol}(\Sigma_-)} = 1 \quad \text{with} \quad \lim_{U\to 1}\mathrm{vol}(\Sigma_-) = 0. \tag{7.84}$$

As stated earlier the analysis of the field dependent part of the functional requires more care. It is of course given by the same formal functional determinant as in (7.80), however due to the time-dependence of γ the behavior is different. Due to the simplicity of the metric it is not hard to find the explicit form of the determinant as

$$\mathrm{Det}(-\gamma\mathrm{Re}(K)) = \prod_{k_1,k_2}\left(\frac{1+U}{1-U}k_1^2 + \frac{1-U}{1+U}k_2^2\right). \tag{7.85}$$

This result is very similar to the Minkowski result, as it can once more be seen as a product of two dimensional harmonic oscillators, subject to the dispersion relation dictated by the time-dependent metric. Owing to the simplicity and symmetry of the metric, the result can be regularized in terms of zeta functions.

ζ-Regularization

Fortunately determinants very similar to (7.85) have been studied extensively in a wide variety of contexts. One such example is the calculation of the generating functional in fermionic Thrirring models where, structurally, a very similar determinant arises [60]. To begin with, we must choose a toroidal compactification for the two spatial directions in order to discretize the momenta k_1 and k_2 and make sense of the infinite product. As the spatial slice under consideration here is isotropic, we choose to consider the field in a square of length L with periodic boundary conditions to achieve this. The individual modes then become discrete and we can define the eigenvalues

$$\lambda_k^{(1)}(U) := \frac{1+U}{1-U}\left(\frac{2\pi k_1}{L}\right)^2, \quad \lambda_k^{(2)}(U) := \frac{1-U}{1+U}\left(\frac{2\pi k_2}{L}\right)^2. \tag{7.86}$$

With these definitions the Determinant (7.85) can be factored as

$$\prod_k \lambda_k := \prod_k \lambda_k^{(1)}\lambda_k^{(2)} = \prod_{n\in\mathbb{Z}^2}\left(\frac{2\pi}{L}\right)^2 \rho^{\mu\nu}\left(\tfrac{1}{2}\mathbb{1}_\mu + c_\mu + n_\mu\right)\left(\tfrac{1}{2}\mathbb{1}_\nu + c_\nu + n_\nu\right), \tag{7.87}$$

where the n_μ are now the reference coordinates on the torus and the matrix ρ is given by

$$\rho = \begin{pmatrix} \frac{1+U}{1-U} & 0 \\ 0 & \frac{1-U}{1+U} \end{pmatrix}, \tag{7.88}$$

which is the same general form as given in [60]. In particular we show that functions of the form (7.87) can be identified with certain Epstein ζ-functions. We can proceed with the regularization along similar lines in terms of the analytical continuation of ζ-functions. To this end we will define a generalized ζ-function from the eigenvalues above

$$\zeta(s) := \sum_k (\lambda_k)^{-s}. \tag{7.89}$$

It follows from the properties of the ζ-function that the desired determinant will then be given by the derivative of this ζ-function evaluated at $s = 0$. To derive the corresponding expression, we make use of the Mellin transform

$$\zeta(s) = \frac{1}{\Gamma(s)}\sum_n \int \mathrm{d}t\, t^{s-1} e^{-t\lambda_k} \tag{7.90}$$

and the generalized Poisson resummation formula

$$\sum_{\mathbb{Z}} \exp\left[-\pi h^{\mu\nu}(n_\mu - a_\mu)(n_\nu - a_\nu)\right] = \sum_{\mathbb{Z}} \sqrt{h}\exp\left[-\pi h_{\mu\nu} n^\mu n^\nu - 2\pi i n^\mu a_\mu\right]. \tag{7.91}$$

Inserting (7.91) into (7.90), we can explicitly perform the t-integration to derive the following identity

$$\zeta(s) = \frac{\Gamma(s-1)}{\Gamma(s)}\pi^{2s-1}\sqrt{\rho}\sum_n(\rho_{\mu\nu}n^\mu n^\nu)^{\frac{s-1}{2}} \times \exp\left[-2\pi n^\mu\left(c_\mu + \tfrac{1}{2}\mathbb{1}_\mu\right)\right]. \tag{7.92}$$

Taking the derivative, we find the following simpler looking result

$$\zeta'(0) = \pi^{-1}\sqrt{\rho}\sum_n(\rho_{\mu\nu}n^\mu n^\nu)^{-\frac{1}{2}}. \tag{7.93}$$

We may therefore make use of the known properties of the Epstein ζ-functions [61]. In general, they are defined rather unwieldy as

$$\begin{aligned}\zeta_E(s,c,\mathbf{r}) := \sum_{\mathbf{m}\in\mathbb{Z}^2}(c + r_1m_1^2 + r_2m_2^2)^{-s} &= \sqrt{\frac{\pi}{r_1\cdot r_2}}\frac{\Gamma(s-\frac{1}{2})}{\gamma(s)}c^{\frac{1}{2}-s} \\ &+ \frac{2\pi^s c^{\frac{1-2s}{4}}}{\Gamma(s)\sqrt{r_1\cdot r_2}}\sum_{\mathbf{n}\in\mathbb{Z}^2}\left(\frac{n_1^2}{r_1}+\frac{n_2^2}{r_2}\right)^{\frac{1}{2}(s-\frac{1}{2})} \times K_{\frac{1}{2}-s}\left(2\pi\sqrt{c}\sqrt{\frac{n_1^2}{r_1}+\frac{n_2^2}{r_2}}\right).\end{aligned} \tag{7.94}$$

For the present case we may expand the previously defined result in terms of these Epstein ζ-functions

$$\zeta(s) = \tfrac{1}{4}\zeta_E\left(s,c,(\tfrac{\pi^2}{L_1^2},\tfrac{\pi^2}{L_2^2})^T\right) - \frac{1}{4}\zeta_E(s,c,\tfrac{\pi^2}{L_1^2}) - \frac{1}{4}\zeta_E(s,c,\tfrac{\pi^2}{L_2^2}), \tag{7.95}$$

where we have absorbed the metric factors in the functions $L_1 := \rho_{11}(U)L$ and $L_2 := \rho_{22}(U)L$. The expressions may now be treated individually to obtain a finite result. As the constant shift c can be sent smoothly to zero in our case, the second and third terms can be expressed in terms of ordinary Riemann ζ-functions

$$\zeta_E(s) \to \left(\frac{\pi^2}{L^2}\right)\zeta_R(2s). \tag{7.96}$$

In this case evaluating the first derivative at $s = 0$ is analogous to the Minkowski case and gives

$$-\zeta_E(s,c,\tfrac{\pi^2}{L_1^2}) - \zeta_E(s,c,\tfrac{\pi^2}{L_1^2}) \to \ln(L_1L_2) + 2\ln(2). \tag{7.97}$$

Remembering the definitions of the L_i as well as the matrix ρ, the expression above is independent of U and therefore only contributes a finite constant to the value of the functional determinant at the focal point. The divergent k-dependence has disappeared and we obtain a finite value without UV-divergences. The infra-red divergence linked to the infinite size of space remains of course, and is regulated by the cut off length L. The mixed term in (7.95) can be shown to vanish in the limit we are interested in and does not contribute to the overall determinant.

In conclusion we can therefore say that once the UV-divergences are removed the functional determinant, coming from the path integral over $\|\Psi\|^2$ in (7.80) takes a U-independent value at the focal point. We can therefore arrange for the constant C to normalize the entire expression to one. Similar approaches to the one presented here can be found in both [62] and more recently in [63]. A different, heuristic argument that may be extended to this case is given by Hawking [64], where the integral of the k-modes is estimated in terms of the infra-red regulator and shown to approach a finite value. All in all this result is not surprising, as we may think of the Einstein Rosen patches to be essentially Minkowski space away from the wavefront. Therefore we expect the wave functional to behave similarly and thus tend towards a normalizable constant.

Conclusion

We conclude that the wave functional remains normalized throughout its evolution on the plane wave background. More importantly, as we approach the focal point u_f the normalization becomes identical to one and thus $\|\Psi\|_2^2(U) \to 1$, meaning that, unlike in the previous examples, the singular point can be probed with quantum fields. Moreover, the probabilistic support at the focal point is equal to one and it is therefore not possible to evade the classical singularity, unlike in the examples studied in [1, 2]. The space-time must be classified as complete in the sense described above. In our opinion, the main distinction from the previous examples is the isotropic contraction in the spatial directions. This forces a true coincidence limit upon the possible quantum probing devices, and therefore causes a degeneracy at the focal points. Furthermore, the evolution is essentially Minkowski-like, resulting in a probability of exactly equal to unity at geodesic border. We must keep in mind that throughout this investigation we have maintained the semi-classical approximation, ignoring back-reactions on the metric itself. It has long been suggested, that an inclusion of these might ameliorate the problems caused by the focal properties, and we will investigate this possibility in the next section. We see that we obtain a different value for the normalization in the Einstein Rosen and Brinkmann coordinates and must comment how these results may be reconciled. This effect is related to the phenomenon of gravitational memory. Owing to the fact that Brinkmann coordinates non-trivially extend the Einstein-Rosen metric, a direct comparison is not altogether straightforward. This is mainly due to the difference in the functional spaces that define the domain on which the path integration in (7.80) is understood. The space of solutions to the wave equation on Brinkmann space $P_B\phi = 0$ is a unification of the solution spaces associated to both individual Einstein-Rosen patches. Therefore the path integral measure includes the sum over solutions that lack an interaction with the plane wave in the past as illustrated by Figure 7.3. One may verify explicitly, that the solution space to $P_B\phi = 0$ consists of solutions that exhibit gravitational memory effect since they have passed through the wave and solutions that behave simply as plane waves. Considering the explicit form of the mode solutions for $u > 0$, (7.67) describes two different

kind of modes in Brinkmann space-time, one kind corresponding to the (green) $\mathbb{W}^-$ patch that show a gravitational memory because of the non-trivial vierbeins $E^-_{ia} = \delta_{ia}(1+\lambda^{(a)}U)$, while the other modes belong to the (red) $\mathbb{W}^+$ patch that have $E^+_{ia} \equiv \delta_{ia}$, that is to say, they have an empty gravitational memory in the future development.

The inclusion or omission of these modes in the path integral will have a direct impact on the probabilistic measure induced. In order to make a fair comparison between the two cases we therefore consider a finite region in the patch where both coordinates overlap, i. e. on the right hand side of the diamond depicted in Figure 7.3. To have a direct comparison with the Einstein-Rosen result, which correctly captures the experience of an "infalling" measuring device, approaching and transiting the wave, we need to project out modes with empty gravitational measurement. The remaining modes with a non-empty gravitational memory will be confined within a region on the right side of the diamond that, to a Brinkmann observer, will continuously shrink until it ends at a caustic, thereby rendering the evolution the same as for the local Einstein-Rosen observer.

7.4. Inclusion of Backreactions

So far, we have only considered the case wherein the background geometry remains fixed, allowing only for the quantum fields to become dynamical. This approach is only logical if we are to study the properties of a given space-time and is on the same footing as for example the famous Hawking Penrose singularity theorems. However, as we have seen, the focal properties of the space-time will inevitably lead to very high energy densities at or near the focal points. This is true already for the classical case as the dominant contribution to the stress energy tensor will scale as [56]

$$T_{uu} \sim \frac{1}{(1-u)^3}, \tag{7.98}$$

which clearly diverges as $u \to 1$. As our prior investigation has shown, this divergence remains present at the quantum level, as the expectation value of the stress energy tensor inherits this problem. With the right hand side of the Einstein equations inevitably exceeding any chosen scale at some point, it is hence unreasonable to assume that the space-time persists in its unaltered form all the way up to the singular point. One may speculate that, as a safeguard against the potential theoretical breakdown at the focal points, nature would react in such a way that the singularity is mollified. In most cases the consistent evolution of the back-reacted Einstein equations is not tractable and the present one offers no exception. In this section we will therefore develop a self-consistent approximation scheme to estimate the qualitative changes one would encounter when allowing for back-reactions.

To do so, we note that the leading term in the stress energy tensor may by expressed in terms of the tetrad E

$$T_{uu} = (\partial_u \varphi^-)^2 \approx \left(\partial_u \sqrt{|E|}^{-1}\right)^2 \sim \frac{\dot{\mathcal{E}}^2}{\mathcal{E}^3}, \tag{7.99}$$

where we defined $\mathcal{E} := |\det(E)|$. As we have seen in the introduction to the plane wave spacetime, there is only one non-trivial component of the Ricci tensor, namely the uu-component. Again it is possible to express this in terms of the tetrad alone

$$R_{uu} = \frac{\ddot{\mathcal{E}}}{\mathcal{E}}. \tag{7.100}$$

As in this case the Einstein tensor coincides with the Ricci tensor, we can self-consistently determine a solution to the uu-component of the Einstein equations by using (7.99) as a source term for the Einstein equation given by (7.100). In this manner, we can derive a corrected tetrad E that will in turn yield a new Einstein Rosen metric via this tetrad. This will give us some insight into the way in which the leading u-behavior is modified by the inclusion of matter. We must point out that in doing so, we only take into account the leading behavior in terms of u which is equivalent to the assumption that we do not leave the space of possible plane wave solutions. We comment on the validity of this assumption at a later time. First, equating (7.99) and (7.100) we obtain

$$\mathcal{E} = \frac{1}{\ln(1-u)}, \tag{7.101}$$

where we have neglected all terms that are sub-leading as $u \to 1$. Next we construct a new Einstein Rosen metric. Comparing to (7.71) we see that the entries are given directly by the tetrad. Originally, one of the entries will approach a constant, while the other one degenerates as we approach the focal point. In order to focus only on the divergent terms as well as keeping things as simple as possible, we will therefore set the entry tending towards a constant equal to one. While this is technically not a full solution, the proper generalization being given by metrics of the Stoyanov type, it will certainly be a very good approximation close to the focal plane. The remaining metric element is then given by (7.101) and yields the approximate metric

$$\gamma = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{\ln^2(1-u)} \end{pmatrix}. \tag{7.102}$$

With this we may proceed to repeat the analysis along the lines followed previously. The shear tensor becomes very simple in this case and is computed iteratively using the new γ. The only non-trivial component is

$$\dot{\Xi}_{22} = \frac{1-\ln(1-u)}{(1-u)^2 \ln^2(1-u)}. \tag{7.103}$$

This too is divergent, however due to the logarithmic factors in the denominator, the divergence is less severe as u approaches 1. Approximating $K(u) \sim \dot{\Xi}_{22}$ shows that $\mathrm{Det}(-g\mathrm{Re}(K))^{-1/2}$ decreases less rapidly than previously but will become zero eventually as well. The same holds

for the imaginary part of the kernel

$$\frac{\dot{\Omega}}{\Omega} = -\frac{1}{2(1-u)\ln(1-u)}. \tag{7.104}$$

The qualitative behavior is thus unchanged; however, the strength of the contraction near the focal point lessened in severity.

We can see that the inclusion of back-reactions softens divergent behavior in u; however, it does not eliminate it altogether. In some ways this is related to the restriction made earlier, maintaining the class of plane wave space-times as only possible solutions. Naturally, this preserves the focal properties, which are a inherent property of all plane wave solutions as we have seen. The only possibility of evading this focal property altogether is by permitting a mixing of ϕ^- and ϕ^+ modes by allowing for a disturbance of the wave in the v-direction. In doing so we would then pass to a more general class of space-times and many of the properties used above would have to be re-investigated. In particular, while it would lead to a de-focusing, the mixing of modes would inevitably lead to particle production, which was absent previously. Thereby, the separated treatment of the various kernel entries would no longer be justified. While the possibility of including a v-dependence in the profile function $H(u,v)$ has been studied [65], the program followed here would require significant extensions to arrive at a conclusive result in these situations. Nonetheless we think that our results strongly suggest that the overall trend points towards the direction of back-reactions regulating the singular nature of the space-time, and in a more realistic setting may even compensate it altogether.

8. Numerical Calculation of Determinants in Curved Space-time

So far our calculations have been based largely around the computation of functional kernels for the Schrödinger wave-functional and the evaluation of their determinants in order to extract the time-evolution in some asymptotic region at least. Owing to the overall computational complexity of the equations involved, an analytical treatment is only available whenever the asymptotic behavior simplifies tremendously. We have seen that the velocity dominance often times comes to our rescue in these situations, making an analytical treatment tractable. However it is of course of interest how these calculations may be extended to regions not immediately bordering on the singular hypersurface. In these cases only a numerical approach to the computation of the functional determinants involved seems viable. While they have not been applied directly to the functional Schrödinger approach as of yet, numerical methods for the evaluation of determinants very similar to those appearing therein have already been developed within the context of false vacuum decay. In the following section we will therefore give an oversight of false vacuum decay in general and the methods pertaining to the evaluation of functional determinants in particular. We will discuss how these may be adjusted to be applied in curved space-times and finally use them to compute the full and renormalized functional determinant pertaining to the decay amplitude of a scalar field in a de Sitter background. de Sitter space is particularly important in expansionary phases of the universe, such as inflation or the current epoch, therefore studying the dependence of the decay rate of false vacuum on the rate of expansion or cosmological constant can lead to a better understanding of these phases. We close with some remarks on how these methods may be used in the setting of Schrödinger quantization in general backgrounds.

8.1. Vacuum decay in flat space-time

Most computations of scattering amplitudes of physical processes generally employ the path integral formulation of quantum field theory expanded around a space-time independent background [66,67], or more precisely around homogeneous expectation values. The corresponding partition function is then (for a more detailed review on the path integral formulation see for example [68])

$$\langle \Omega_{\rm out}|\mathcal{E}(t_f,t_i)|\Omega_{\rm in}\rangle = Z[0] \equiv \int_{\Omega_{\rm in}}^{\Omega_{\rm out}} \mathscr{D}[\phi] \mathrm{e}^{\frac{i}{\hbar}S[\phi]}, \tag{8.1}$$

which corresponds to the transition between the two vacua $\Omega_{\rm in}$ and $\Omega_{\rm out}$. This enters the computation in the form of boundary conditions for the right hand side, where it is understood that the functional integration covers all field configurations that satisfy $\phi(t_i,\mathbf{x}) = \Omega_{\rm in}(\mathbf{x})$ and $\phi(t_f,\mathbf{x}) = \Omega_{\rm out}(\mathbf{x})$. In order to be able to compute S-matrix elements and more general expectation values, one adds an external source to the action,

$$S[\phi,J] = \int \mathrm{d}^4x\, \mathcal{L} + J(x)\phi(x) \tag{8.2}$$

where $\mathcal{L}$ stands for the Lagrangian density of the model. Then one defines the generating functional for connected n-point functions by

$$W[J] \equiv \ln Z[J] \tag{8.3}$$

such that the computation of expectation values for operators coupled to external sources is achieved by taking functional derivatives with respect to the external source at $J = 0$, for example:

$$\langle \phi(x)\phi(y)\rangle_{\rm connected} = \frac{\delta W}{\delta J(x)\delta J(y)}\bigg|_{J=0} = \langle \phi(x)\phi(y)\rangle - \frac{1}{Z[0]}\langle\phi(x)\rangle\frac{1}{Z[0]}\langle\phi(y)\rangle; \tag{8.4}$$

however, we will not be interested in n-point functions of fields but only in the vacuum to vacuum transition between non trivial field configurations, which are related to tunneling phenomena via the nucleation of true vacuum bubbles [69,70].

Let us therefore consider a field theory of a single real scalar field $\phi(x)$, subject to a potential $V(\phi(x))$ which is analytic and displays more than one local minimum as in Fig. 8.1. The Lagrangian density corresponding to this theory is

$$\mathcal{L} = \frac{1}{2}(\partial_x\phi(x))^2 - V(\phi(x)), \tag{8.5}$$

where $V(\phi(x))$ is such that there exist at least two solutions to $\frac{\partial}{\partial\phi}V(\phi(x)) = 0$, say for field values $\phi_\pm$. This feature of the potential implies the existence of an additional saddle point in the path integral, meaning an overlap of the two minima. As we will see, there exist field configura-

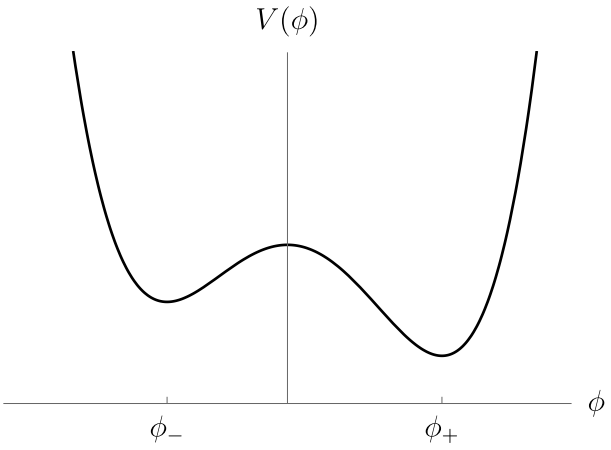


Figure 8.1.: Example of a scalar potential displaying two non-degenerate minima. The higher local minimum is referred to as the false vacuum, while the right hand side global minimum represents the true vacuum.

tions that interpolate between these two field values for which the action is finite. Generically, one of these field values will be associated with a higher potential. In order to make things simple we shall choose $\phi_+ > \phi_-$ and $V(\phi_+) \leq V(\phi_-)$, and add a constant to the potential in order to have $V(\phi_-) = 0$. Under this setup, a static field configuration $\phi(t,\mathbf{x}) = \phi_-$ will a have a zero action, while a field configuration located around the other minimum, $\phi(t,\mathbf{x}) = \phi_-$, will have a negative action. As both minima are saddle points of the theory, one could expand the action around a scalar field "sitting" in either one of the minima (i.e. having an expectation value equaling one or the other). These two settings are what is usually referred to as false/true vacuum, where false corresponds to the minimum associated with a higher potential.

We are interested in tunneling phenomena between these two configurations. To describe them, the corresponding expansion is not made around homogeneous expectation values, but around a field configuration that spends an infinitely long time close to each of the minima. This solitonic configuration, known as bounce, can be shown [70], [71] to correspond to imaginary energy values, and therefore the transition amplitude is interpreted as a decay rate from false to true vacuum. This can again easily bee seen from the time-evolution operator

$$e^{-iE_0 t}\left|0\right\rangle = e^{-i\mathrm{Re}E_0 t} e^{\mathrm{Im}E_0 t}\left|0\right\rangle, \tag{8.6}$$

meaning that the decay rate is given by

$$\Gamma = 2\,\mathrm{Im}\,E_0. \tag{8.7}$$

To compute the transition from one vacuum state to the other we will need to employ a Wick

rotation and compute the limit where time is taken to infinity:

$$\langle\phi_+|e^{iHT}|\phi_+\rangle = \int_{\phi_+}^{\phi^+} \mathscr{D}[\phi]\exp\left(\frac{i}{\hbar}\int_{-T}^{T} dt\, d^3\mathbf{x}\,\mathcal{L}\right) \tag{8.8}$$

here T is a real parameter that can be analytically continued to the complex plane. Let us then employ the substitution $T \to i\mathcal{T}$, with $\tau \in \mathbb{R}$ to get to the following expression

$$\langle\phi_+|e^{-H\mathcal{T}}|\phi_+\rangle = \int_{\phi_+}^{\phi^+} \mathscr{D}[\phi]\exp\left(\frac{i}{\hbar}\int_{-i\mathcal{T}}^{i\mathcal{T}} dt\, d^3\mathbf{x}\,\mathcal{L}\right) \tag{8.9}$$

the next step is to perform the analytic continuation of the time variable within the integration, $t \to i\tau$ which leads to:

$$\langle\phi_+|e^{-H\mathcal{T}}|\phi_+\rangle = \int_{\phi_+}^{\phi^+} \mathscr{D}[\phi]\exp\left(-\frac{1}{\hbar}\int_{-\mathcal{T}}^{\mathcal{T}} d\tau\, d^3\mathbf{x}\,\Delta^4\phi(x) + V(\phi(x))\right) \tag{8.10}$$

The formal expression on the left hand side can be written in terms of energies of the eigenstates of the theory by the complete insertion of a set of such states:

$$\langle\phi_+|e^{-H\mathcal{T}}|\phi_+\rangle = \sum_n \langle\phi_+|n\rangle e^{-E_n\mathcal{T}}\langle n|\phi_+\rangle \underset{\mathcal{T}\to\infty}{\sim} e^{-E_0\mathcal{T}}\langle\phi_+|0\rangle\langle 0|\phi_+\rangle, \tag{8.11}$$

where in the last step we have made use of the fact that only the state with the lowest energy survives. Putting everything together, using (8.7) we can therefore express the decay rate as

$$\Gamma = \frac{2}{\mathcal{T}}\,\mathrm{Im}\left(\ln Z_E[0]\right) \tag{8.12}$$

To include higher order corrections coming from one-loop contributions and background gradients we can employ the effective action construction [66], combined with a semi-classical expansion in $\hbar$.

8.2. Vacuum decay in de Sitter Space-time

In order to study the aforementioned effects on curved backgrounds we will discuss false vacuum decay on a de Sitter geometry. Being a dynamical background some amendments need to be added to the previous methods. We will start by considering a global coordinate patch to parameterize the Euclidean version of de Sitter space. This is achieved by

$$ds^2 = d\tau^2 + \frac{1}{H^2}\sin^2(H\tau)d\mathbf{x}^2, \tag{8.13}$$

where $\tau \in [0, \pi/H]$ and H is the Hubble constant.

8.2.1. The Model

As a first approach, we neglect the evolution of the scale factor according to the Friedmann equations and assume the scalar field ϕ has an energy scale such that its evolution will not have an impact on the de Sitter background. As a benchmark we will use $H = 1$ in all numerical calculations. We consider a standard curved space-time Lagrangian for a scalar field subject to a potential V, which exhibits two different local minima and allows therefore for tunneling between them, namely

$$S = \int \mathrm{d}^4x\sqrt{-g}\left[\frac{1}{2}g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - V(\phi)\right], \tag{8.14}$$

where ϕ is a real scalar field and $g_{\mu\nu}$ is the metric. As we assume it is a fixed background, this is once again a semi-classical approximation. The potential is chosen such as to feature at least two different local minima and to be polynomial in the field

$$V(\phi) = V_0 - \frac{m^2}{2}\phi^2 - \frac{b}{3!}\phi^3 + \frac{\lambda}{4!}\phi^4. \tag{8.15}$$

Again we perform a Wick rotation of the entire action by means of the substitution $t \to i\tau$,

$$S[\phi] \to -i\int \mathrm{d}\tau\mathrm{d}^3\mathbf{x}\sqrt{g_E}\left[\frac{1}{2}g_E^{ij}\partial_i\phi\partial_j\phi + V(\phi)\right] \equiv -S_E[\phi], \tag{8.16}$$

denoting by g_E the positive-definite Euclidean metric. This has the effect of creating a saddle point in the path integral while at the same time changing the sign of the potential. To understand the gradients of ϕ, $\partial_\mu\phi$, we expand the action around our background

$$\phi \to \phi_b + \phi^{(1)}, \tag{8.17}$$

where ϕ_b is the solution to the tree-level equation of motion, with appropriate boundary conditions, which will be discussed later in Sec.8.2.2

The expansion is

$$S_E = \int \mathrm{d}^4x\sqrt{g_E}\left[\frac{1}{2}g_E^{ij}\left(\partial_i\phi_b + \partial_i\phi^{(1)}\right)\left(\partial_j\phi_b + \partial_j\phi^{(1)}\right) + V\left(\phi_b + \phi^{(1)}\right)\right] \tag{8.18}$$

$$= \int \mathrm{d}^4x\sqrt{g_E}\left[\frac{1}{2}g_E^{ij}\partial_i\phi_b\partial_j\phi_b + V(\phi_b) + g_E^{ij}\partial_i\phi_b\partial_j\phi^{(1)} + \left.\frac{\partial V}{\partial\phi}\right|_{\phi=\phi_b}\phi^{(1)} + \frac{1}{2}g_E^{ij}\partial_i\phi^{(1)}\partial_j\phi^{(1)} + \frac{1}{2}\left.\frac{\partial^2 V}{\partial\phi^2}\right|_{\phi=\phi_b}\phi^{(1)}\phi^{(1)}\right]. \tag{8.19}$$

with Latin indices representing Euclidean coordinates, i.e. $i, j = 1,2,3,4$ and τ understood as x^4. Here the linear terms in ϕ vanish by construction as they are proportional to the equation of

motion. The derivatives of the potential are explicitly

$$\frac{\partial V(\phi)}{\partial \phi} = -m^2\phi - \frac{b}{2}\phi^2 + \frac{\lambda}{6}\phi^3 \tag{8.20}$$

$$\frac{\partial V^2(\phi)}{\partial \phi^2} = -m^2 - b\phi + \frac{\lambda}{2}\phi^2. \tag{8.21}$$

We split the action $S_E = B + S_E^{(1)}\left[\phi^{(1)}\right]$, where $S_E^{(1)}[\phi]$ contains bi-linear terms for ϕ with operators evaluated over the ϕ_b background and higher dimensional terms do not contribute at the one-loop level,

$$B = \int \mathrm{d}^4x \sqrt{g_E}\left[\frac{1}{2}g_E^{ij}\,\partial_i\phi_b\partial_j\phi_b + V(\phi_b)\right] \tag{8.22}$$

$$S_E^{(1)}[\phi^{(1)}] = \int \mathrm{d}^4x \sqrt{g_E}\left[\frac{1}{2}g_E^{ij}\,\partial_i\phi^{(1)}\partial_j\phi^{(1)} + \frac{1}{2}\left.\frac{\partial^2 V}{\partial\phi^2}\right|_{\phi=\phi_b}\phi^{(1)}\phi^{(1)} + \mathcal{O}\left((\phi^{(1)})^3\right)\right] \tag{8.23}$$

Truncating S_E to second order, we obtain a Gaussian path integral

$$Z[0] = \int \mathscr{D}\phi \exp\left(-\frac{1}{\hbar}B - \frac{1}{\hbar}S_E^{(1)}\right) = \exp\left(-\frac{1}{\hbar}B\right)\int \mathscr{D}\phi \exp\left(-\frac{1}{\hbar}S_E^{(1)}\right) \tag{8.24}$$

We can compute the path integral containing the fluctuations as follows:

$$S_E^{(1)}\left[\phi^{(1)}\right] = \int \mathrm{d}^4x\left[-\frac{1}{2}\phi^{(1)}\partial_i\left(\sqrt{g_E}\,g_E^{ij}\,\partial_j\phi^{(1)}\right) + \sqrt{g_E}\,\frac{V''(\phi)}{2}\phi^{(1)^2} + \mathcal{O}\left(\phi^{(1)^3}\right)\right] \tag{8.25}$$

$$= \int \mathrm{d}^4x\left[-\frac{1}{2}\phi^{(1)}\left[\partial_i\sqrt{g_E}\,g^{ij}\partial_j - \sqrt{g_E}\,\frac{\partial^2 V(\phi)}{\partial\phi^2}\right]\phi^{(1)} + \mathcal{O}\left(\phi^{(1)^3}\right)\right] \tag{8.26}$$

$$= \int \mathrm{d}^4x\left[\frac{1}{2}\phi^{(1)}\left[-\partial_i\sqrt{g_E}\,g_E^{ij}\,\partial_j + \sqrt{g_E}\,\frac{\partial^2 V(\phi)}{\partial\phi^2}\right]\phi^{(1)} + \mathcal{O}\left(\phi^{(1)^3}\right)\right] \tag{8.27}$$

where an integration by parts was performed to obtain the first line. We then define the operator of fluctuations as

$$G_b^{-1}(x,y) = \left(-\partial_i\sqrt{g_E}\,g_E^{ij}\partial_j + \sqrt{g_E}\left.\frac{\partial^2 V}{\partial\phi^2}\right|_{\phi=\phi_b}\right)\delta(x-y). \tag{8.28}$$

In order to regularize the functional determinant, we consider the ratio with the determinant of the corresponding false vacuum solution

$$G_-^{-1}(x,y) = \delta(x-y)\left(-\partial_i\sqrt{g_E}\,g_E^{ij}\,\partial_j + \sqrt{g_E}\left.\frac{\partial^2 V}{\partial\phi^2}\right|_{\phi=\phi_-}\right). \tag{8.29}$$

This will enable us to extract a finite result for the Gaussian path integral and we obtain schematically

$$Z[0] \propto \left| \frac{\det'\left(G_b^{-1}(x,y)\right)}{\det\left(G_-^{-1}(x,y)\right)} \right|^{-\frac{1}{2}} \mathrm{e}^{-B}, \tag{8.30}$$

where the prime indicates that the determinant does not include negative and zero modes. The proportionality factor will be discussed later when we examine the non-positive modes.

In a more general setting, where gravitational effects are included, the fluctuations of the metric can lead to non-trivial constraints on the fluctuation operator. Expressions for such cases have been found [72, 73], from which we can specialize to our de Sitter case. The parametrization we are using follows Dunne's previous work [74, 75] where the following formula for the fluctuation integral is derived including fluctuations around the scale factor

$$a(\tau) = \frac{1}{H}\sin(H\tau) \tag{8.31}$$

in Euclidean de Sitter space:

$$S_E^{(1)}\left[\phi^{(1)}\right] = \pi^2 \int \mathrm{d}^3x d\tau \phi^{(1)} \left[-\frac{d}{d\tau}\frac{a^3(\tau)}{Q(\tau)}\frac{d}{d\tau} + a^3(\tau)U(\tau) \right] \phi^{(1)}, \tag{8.32}$$

where the dot denotes derivative with respect to τ and where we have defined

$$Q(\tau) = 1 + \frac{\kappa a^2 \dot{\phi}}{2(\Delta_3 - 3K)}, \tag{8.33}$$

and

$$U(\tau) = \frac{V''(\phi)}{Q} - \frac{\Delta_3}{Qa^2} + \kappa\left[\frac{2\dot{\phi}^2}{Q} - \frac{5a\dot{a}\dot{\phi}V'(\phi) - a^2V''(\phi)^2 - 6\dot{a}^2\dot{\phi}^2}{Q^2(\Delta_3 + 3k)}\right]. \tag{8.34}$$

8.2.2. Computing the classical background

In order to compute the decay rate of the false vacuum, we must first find the saddle-point field configuration known as the bounce, ϕ_b. Motivated by the proofs of minimization in the flat space cases [70], we look for an $O(4)$ symmetric solution to the equation of motion, which greatly simplifies to

$$\ddot{\phi} + 3H\cot(H\tau)\dot{\phi} = V'(\phi), \tag{8.35}$$

where the dot denotes differentiation with respect to τ and $'$ denotes derivatives with respect to ϕ.

The bounce has the boundary conditions $\phi_b(0) = \phi_+$ and $\phi_b(\pi/H) = \phi_-$, corresponding to starting at the true vacuum and then rolling up to the false vacuum at infinite time. Notice that in the de Sitter case without a thin wall approximation, there is a friction term in the EOM

Eq. (8.35), which changes sign. This is the reason a bounce solution with the above boundary conditions exists, in contrast to the flat space case, where the bounce solution does not actually reach the true vacuum when a thick wall is considered. An example of the profile of the bounce configuration for our study is shown in Fig. 8.2.

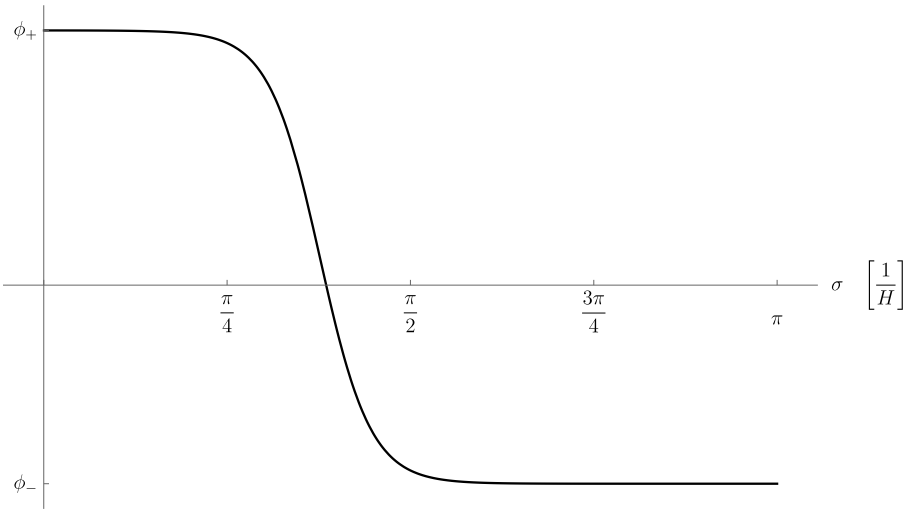


Figure 8.2.: Profile of the bounce solution that interpolating between the true and false vacuum of the potential V.

8.3. Functional Determinant of the Fluctuation Operator

We will now discuss how to evaluate the functional determinant (8.30) numerically. The fluctuation operator for the general case when variations of the metric are considered (8.32) has been determined previously by [72, 75]. Here however we will specialize to the case where the de Sitter background remains fixed, making the fluctuation operator more straightforward. A short computation gives it as

$$G_b^{-1}(x,x') = \delta(x-x')H^{-3}\sin^3(H\tau)\left(-\partial_\tau^2 - 3H\cot(H\tau)\partial_\tau - H^2\csc^2(H\tau)\Delta_3 + V''(\phi_b)\right). \tag{8.36}$$

Zero modes

As the determinant of any operator may be thought of as a product over all its eigenvalues, our first task is to find those which are equal to zero. The removal of these eigenvalues is usually achieved by a replacement with collective coordinates, thereby avoiding the determinant to equal zero trivially. A typical zero-mode is related to translations of the bounce $\partial_\mu\phi_b$. If ϕ_b satisfies the equations of motion

$$\frac{1}{\sqrt{g_E}}\partial_i\left(\sqrt{g_E}\,g_E^{ij}\,\partial_j\phi_b\right) = V'(\phi_b), \tag{8.37}$$

we can take an extra derivative to arrive at the following

$$\begin{aligned}
0 &= \partial_k \left\{ \frac{1}{\sqrt{g_E}} \partial_i \left(\sqrt{g_E}\, g_E^{ij}\, \partial_j \phi_b \right) - V'(\phi_b) \right\} \\
&= \left(-\frac{1}{2} g_E^{-3/2}\, \partial_k g_E \right) \partial_i \left(\sqrt{g_E}\, g_E^{ij}\, \partial_j \phi_b \right) + \frac{1}{\sqrt{g_E}} \partial_i \left[\partial_k \left(\sqrt{g_E}\, g_E^{ij} \right) \partial_j \phi_b \right] \\
&\quad + \frac{1}{\sqrt{g_E}} \partial_i \left[\sqrt{g_E}\, g_E^{ij}\, \partial_j \partial_k \phi_b \right] - V''(\phi_b)\, \partial_k \phi_b \\
&= -\left(\frac{1}{2} g_E^{-3/2}\, \partial_k g_E \right) \partial_i \left(\sqrt{g_E}\, g_E^{ij} \right) \partial_j \phi_b - \left(\frac{1}{2 g_E}\, \partial_k g_E \right) g_E^{ij} \partial_i \partial_j \phi_b \\
&\quad + \frac{1}{\sqrt{g_E}} \partial_i \left[\partial_k \left(\sqrt{g_E}\, g_E^{ij} \right) \partial_j \phi_b \right] + \frac{1}{\sqrt{g_E}} \partial_i \left(\sqrt{g_E}\, g_E^{ij}\, \partial_j \partial_k \phi_b \right) - V''(\phi_b)\, \partial_k \phi_b .
\end{aligned} \tag{8.38}$$

However, if $k \neq \tau$, we get zero-modes in each of the three spatial directions, $\partial_k \phi_b$, because the metric is independent of such coordinates and the first three terms in the last line cancel, leaving the fluctuation operator of q. (8.28) acting on $\partial_k \phi_b$. In this case it is known we have then the following three normalized zero mode eigenfunctions [71]

$$\phi_{0,k} = \frac{1}{\sqrt{B}} \partial_k \phi_b . \tag{8.39}$$

This is the expected result, as our model exhibits translational invariance in all of the spatial directions. Unlike in the flat case, time translation invariance is lost due to the dynamical background and therefore the fourth zero mode is absent. Let us come back to the path integral over the fluctuations, Eq. (8.24), to see how by using the idea of collective coordinates, one can avoid the possible infinity coming from the integration over zero-modes [76]. Consider a basis of functions $\{\phi_n\}$ for the vector space of fluctuations around ϕ_b, assuming we can label the eigenvalues by n and were degeneracies might exist. The field ϕ therefore decomposes into

$$\phi(x) = \phi_b(x) + \sum_{n,k} c_{n,k} \phi_{n,k}(x), \tag{8.40}$$

where k labels any possible degenerate eigenvalues. After factoring out the exponential containing the bounce, the path integral measure takes the form:

$$\mathscr{D}\phi = \prod_{n,k} \frac{1}{\sqrt{2\pi\hbar}} \mathrm{d}c_n \tag{8.41}$$

so that we integrate over all possible coefficients of the expansion eigenfunctions. From Eq. (8.40), we can see that the effect of performing a translation in any direction other than τ by an infinitesimal amount Δx_k leads to the infinitesimal change in the path:

$$\delta\phi_k = \phi(x + \Delta x_k) - \phi(x) = \partial_k \phi_b \Delta x_k . \tag{8.42}$$

We also know however that $\phi_{0,k} \propto \partial_k \phi_b$ so a shift in the coefficient $c_{0,k}$ implies

$$\delta\phi_k = \phi_{0,k} \mathrm{d}c_{0,k}. \tag{8.43}$$

Putting together the last two equations we can deduce the following exchange of integration variables

$$\mathrm{d}c_{0,k} = \frac{\partial_k \phi_b}{\phi_{0,k}} \mathrm{d}x_k = \sqrt{B}\, dx_k. \tag{8.44}$$

Returning to the ratio of functional determinants we therefore have

$$\left| \frac{\det\left(G_b^{-1}(x,y)\right)}{\det\left(G_-^{-1}(x,y)\right)} \right|^{-1/2} = 2\pi^2 \left(\frac{B}{2\pi\hbar}\right)^{3/2} \left| \frac{\det'\left(G_b^{-1}(x,y)\right)}{\det\left(G_-^{-1}(x,y)\right)} \right| \tag{8.45}$$

after extracting the three directions different from τ and including the solid angle of the 3-sphere covered in the integration. With this procedure we may therefore remove the zero modes from the integration by replacing them by the corresponding factor given above.

8.3.1. Gel'fand Yaglom Results

As we have outlined in the appendix, it is not necessary to actually compute all individual eigenvalues in order to extract the determinant. Instead the famous theorem by Gel'fand Yaglom [77] gives a rather simple way to compute the entire determinant from a single initial value problem. In order to apply such a procedure here, we must first bring the fluctuation operator to a more manageable form. The spectrum of the fluctuation operator is determined by the so-called Jacobi equation

$$\frac{1}{a^3}\frac{\mathrm{d}}{\mathrm{d}\tau}\left(\frac{a^3}{Q}\frac{\mathrm{d}\Phi}{\mathrm{d}\tau}\right) + U[a,\phi]\Phi = \lambda\Phi, \tag{8.46}$$

where Φ is a fluctuation, λ the corresponding eigenvalue, and U and Q were defined in (8.34) and (8.33) respectively. Due to the fact that we are considering the background to be strictly de Sitter, we have $Q = 1$ and $U = V''(\phi) - \frac{\Delta_3}{a^2}$ here.

The Gel'fand-Yaglom approach can be used to calculate the determinant ratio in terms of the asymptotics of the solutions to the Jacobi equation (8.46). Making use of the spherical symmetry of the problem, we can further label all modes by their corresponding angular momentum ℓ. For every individual ℓ we obtain

$$\frac{\det G_{b,\ell}^{-1}(\tau,\tau')}{\det G_{-,\ell}^{-1}(\tau,\tau')} = \frac{\Phi^{(\ell)}(\tau_{\max})}{\Phi_{\mathrm{fv}}^{(\ell)}(\tau_{\max})}, \tag{8.47}$$

where $\Phi^{(\ell)}$ are eigenfunctions for the eigenvalue 0 for their corresponding fluctuation operator. The calculation is greatly facilitated by the fact that the false vacuum solution solution is known analytically,

$$\Phi^{(\ell)}_{\mathrm{fv}}(\tau) = \frac{N}{\sin(H\tau)} P^{\alpha}_{\ell+1}\left(\cos(H\tau)\right) \qquad \text{with} \qquad \alpha = -\frac{1}{2} + i\sqrt{\frac{V''(\phi_{\mathrm{fv}})}{H^2} - \frac{9}{4}}, \tag{8.48}$$

where $P^{\alpha}_{\ell+1}$ are the Legendre functions of the first kind. With the definition of the auxiliary function

$$T^{(\ell)}(\tau) := \frac{\Phi^{(\ell)}(\tau)}{\Phi^{(\ell)}_{\mathrm{fv}}(\tau)}, \tag{8.49}$$

it is thus necessary to solve the differential equation

$$-\ddot{T} - \left[2\frac{\dot{\Phi}^{(\ell)}_{\mathrm{fv}}}{\Phi^{(\ell)}_{\mathrm{fv}}}\right]\dot{T} + \left[U - V''(\phi_{\mathrm{fv}}) + \frac{\Delta_3}{a^2}\right] T = 0, \tag{8.50}$$

subject to the initial conditions $T(0) = 1, \dot{T}(0) = 0$, to finally obtain

$$\frac{\det G^{-1}_{b,\ell}(\tau,\tau')}{\det G^{-1}_{-,\ell}(\tau,\tau')} = T^{(\ell)}(\tau_{\max}). \tag{8.51}$$

Equation (8.50) can now be solved numerically for every value of l. The un-renormalized functional determinant will then be given by the sum over all ℓ

$$\det\Lambda^{(l)} = \frac{1}{2}\sum_{\ell=0}^{\infty}(\ell+1)^2 \ln T^{(\ell)}(\tau_{\max}). \tag{8.52}$$

The accuracy of the solution for $T_\ell(\tau_{\max})$ depends of course on the size of fluctuations by which $T_\ell(\tau)$ fluctuates around this value towards the edge of the domain. As most of the time-dependent factors in the equation (8.50) are only rapidly changing in the middle of the domain this is rarely a problem here, as can be seen in figure 8.3, showing the solution for $T_\ell(\tau)$ for an exemplary value of ℓ.

A plot of the partial determinants is shown in figure 8.4 and is in excellent agreement with [75]. From the pre-factor we immediately see that the sum will not converge unless all contributions up to $\mathcal{O}(\ell^{-3})$ are canceled for large ℓ (remember that only odd powers of ℓ are present in the expansion). We will label the corresponding terms by α and β respectively

$$\ln\frac{\det\Lambda^{(\ell)}}{\det\Lambda^{(\ell)}_{\mathrm{fv}}} = \frac{\alpha}{\ell+1} + \frac{\beta}{(\ell+1)^3} + \mathcal{O}\big((\ell+1)^{-5}\big). \tag{8.53}$$

In the flat case a treatment for these contributions is known in terms of a WKB analysis [74] and we will consider this treatment in the next section.

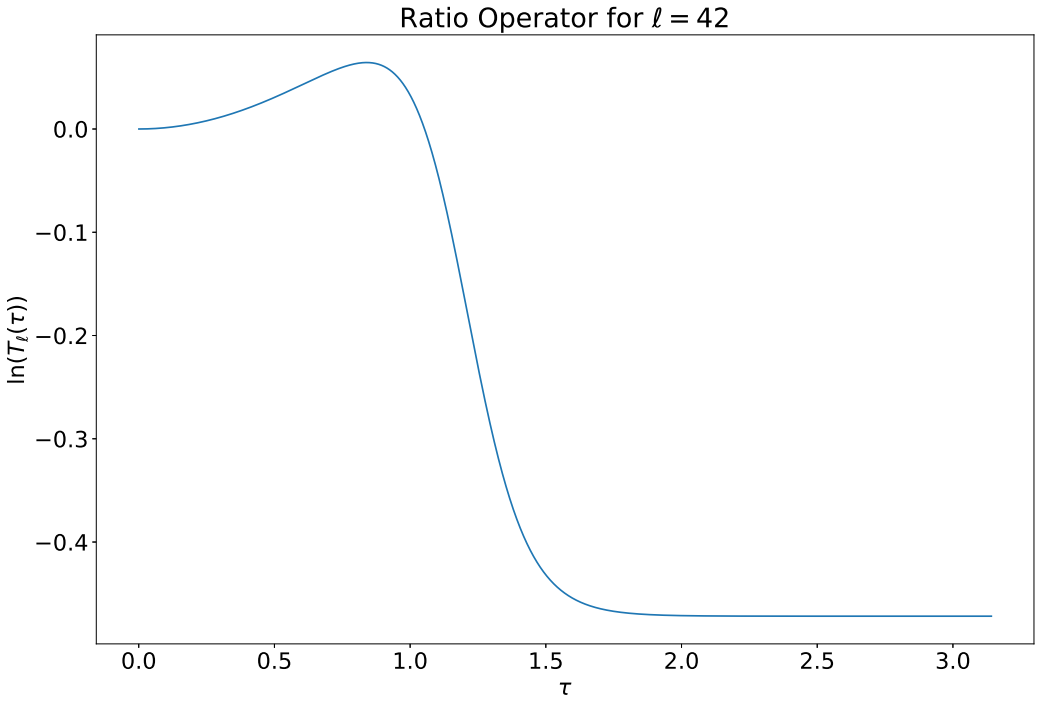


Figure 8.3.: The ratio operator T as a function of time. As we can see, T rapidly approaches a constant for late times. Therefore, obtaining the value of $T_\ell(\tau_{\max})$ is fairly in-sensitive to the choice of $\tau_{\max}$

Negative Modes

Additionally to the zero modes, related to the translational symmetry of the problem, we know that there must be at least one mode of negative eigenvalue present in order to give the appropriate imaginary contribution to the energy in the tunneling process. It was shown by Coleman that for the present case there is only a single negative mode, which lies in the $\ell = 0$ sector [78]. In order to extract it we again consider the fluctuation equation setting $\ell = 0$

$$\ddot{\Phi} + 3\frac{\dot{a}}{a}\dot{\Phi} - V''(\phi)\Phi = \lambda\Phi. \tag{8.54}$$

Since we have compactified the temporal direction, we expect the spectrum of the fluctuation operator to be discrete, and since there is only one negative mode, it will belong to the fluctuation with the lowest eigenvalue. Numerically the lowest eigenvalue can be determined to be $\lambda = -3.52959$. The corresponding eigenfunction can be determined straightforwardly and is shown in figure 8.5.

8.3.2. Renormalization

As we have seen, the sum over all ℓ contributions will diverge and therefore give an infinite answer for the determinant. This behavior is already known from Minkowski space and is

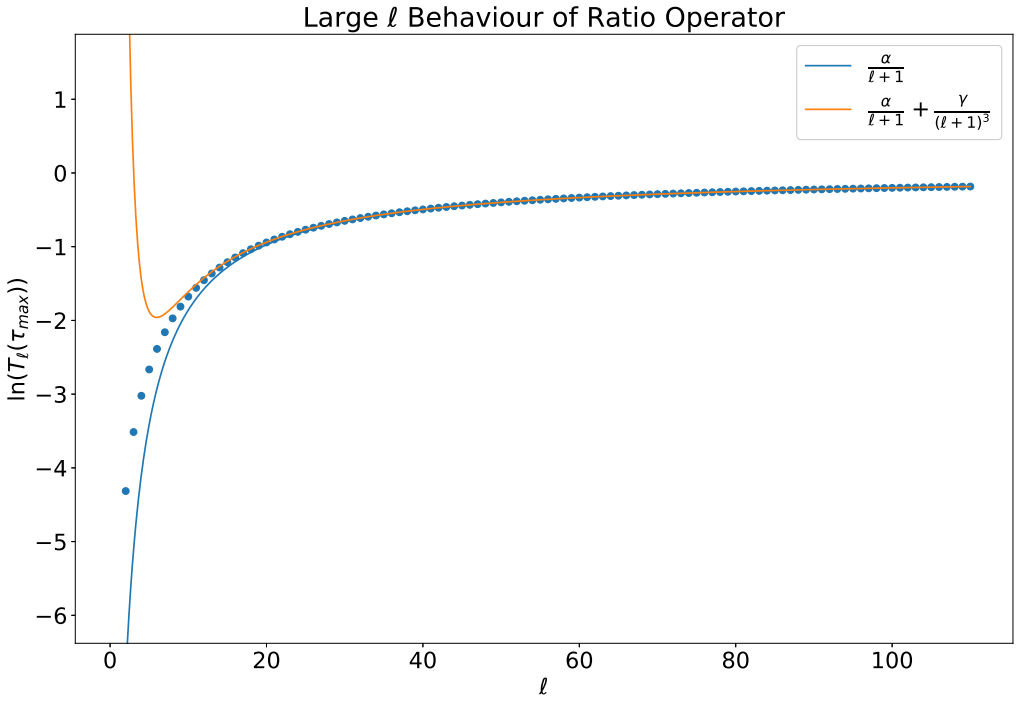


Figure 8.4.: The individual dots show the partial determinants $T^{(\ell)}$. The enveloping functions indicate divergent the large-ℓ behavior that has to be subtracted. Here we have used $\alpha = -20.459$ and $\gamma = 330.353$

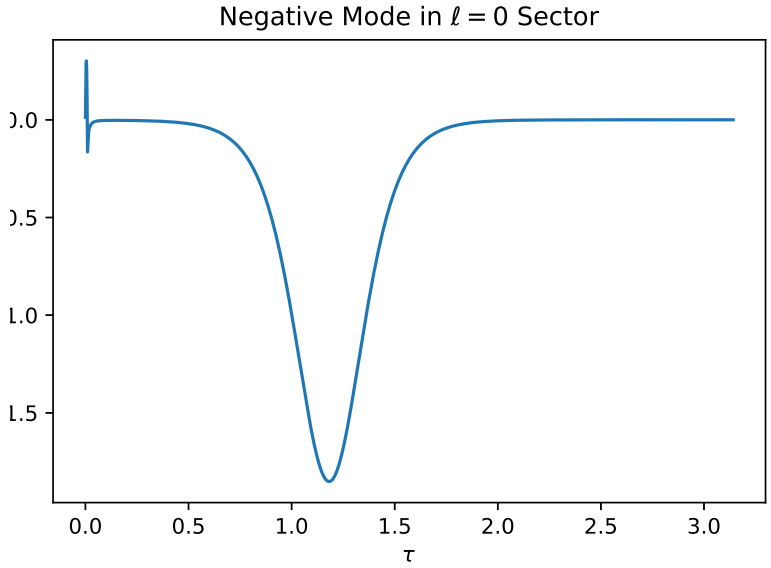


Figure 8.5.: The Eigenfunction belonging to the negative eigenvalue $\lambda = -3.52959$

treated by the extraction and subsequent subtraction of the divergent modes at large ℓ. This is the main reason we restrict ourselves to a fixed background. If we were to allow for fluctuations in the geometry, an according subtraction procedure would have to be carried out to remove the divergences stemming therefrom, which is obviously not possible, owing to the non-renormalizability of gravity. We follow the techniques described by Dunne et. al. [74] to renormalize the model by means of the WKB approximation. We expect the large ℓ behavior to be given to great accuracy by the WKB solution, and thus subtract the analytical expressions obtained in this way form the numerical results already discussed.

We begin by considering the large-ℓ limit of the Jacobi equation

$$\ddot{\Phi} + 3\frac{\dot{a}}{a}\dot{\Phi} - \left[V''(\phi) + \frac{\ell(\ell+2)}{a^2}\right]\Phi = 0 \tag{8.55}$$

First we need to bring this into a form such that the WKB approximation can be used. In order to do so we must first absorb the linear term in the derivatives to obtain a Schrödinger-type equation. Consider therefore an equation of the type

$$\ddot{\varphi} + \omega^2(\tau)\varphi = 0. \tag{8.56}$$

and define

$$\varphi := c(\tau)\Phi. \tag{8.57}$$

As we want to solve for ω, we insert this into the expression above to obtain

$$c\ddot{\Phi} + 2\dot{\Phi}\dot{c} + \ddot{c}\Phi + \omega^2 c\Phi = 0. \tag{8.58}$$

A simple comparison of coefficients is now enough to see that we must identify

$$2\frac{\dot{c}}{c} = 3\frac{\dot{a}}{a} \tag{8.59}$$

and

$$\frac{\ddot{c}}{c} + \omega^2 = -U. \tag{8.60}$$

This straightforwardly yields the frequency

$$\omega^2 = -\left(\frac{3}{4}\frac{\dot{a}^2}{a^2} + \frac{3}{2}\frac{\ddot{a}}{a} + U(a,\phi,\ell)\right). \tag{8.61}$$

The Jacobi equation for the false vacuum solution is identical with the exception of a different fluctuation potential

$$U_{\mathrm{fv}} := V''(\phi_{\mathrm{fv}}) + \frac{\ell(\ell+2)}{a^2} \tag{8.62}$$

thus,

$$\omega_{\mathrm{fv}}^2 = -\left(\frac{3}{4}\frac{\dot{a}^2}{a^2} + \frac{3}{2}\frac{\ddot{a}}{a} + U_{\mathrm{fv}}(a, \phi_{\mathrm{fv}}, \ell)\right). \tag{8.63}$$

In order to see the validity of the WKB Ansatz we check the remainder of the Jacobi equation. For the fluctuation alone the Ansatz to solve equation (8.55) is given by

$$\Phi = \frac{1}{\sqrt{\omega}} \mathrm{e}^{\pm i \int_0^{\tau_{\max}} d\tau\, \omega}, \tag{8.64}$$

where ω takes the form stated earlier. The validity of the WKB approximation is subject to the condition that

$$\left|\frac{\dot{\omega}}{\omega^2}\right| \ll 1. \tag{8.65}$$

As expected this condition is satisfied for all large values of ℓ. We expect the accuracy of the Ansatz to increase with growing ℓ as well as a larger mass for the scalar field as compared to the Hubble rate. In fact, for the infinite mass limit we expect to recover the Minkowski result. This is not surprising as in this case the de Broigle wavelength of the quantum particles becomes essentially negligible compared to the curvature scale, given by H and therefore see the background as essentially flat. Inserting the Ansatz back into (8.55) we obtain the following for the first order approximation. As can be seen the Ansatz solves the equation very well even for

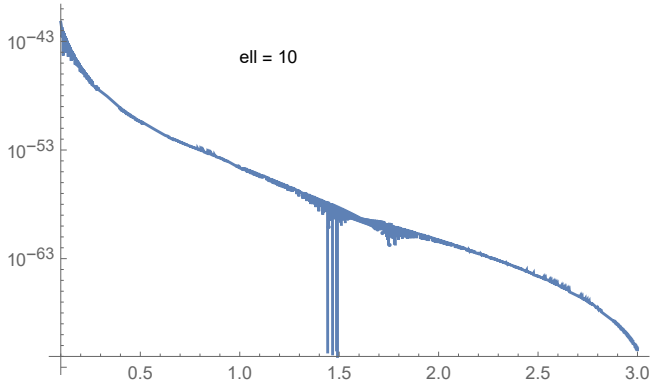


Figure 8.6.: The remainder of the Jacobi operator applied to the fluctuation Ansatz to first order in WKB for $\ell = 10$.

moderate values of ℓ. The same can be verified for the second order Ansatz; however there is no appreciable change in the plots for high values of ℓ as the corrections are extremely small. Not shown here explicitly is the fact that the approximation increases in accuracy as the mass is increased. This was verified separately.

Using now the definition of T above we can write the WKB approximation as

$$T^{(\ell)}(\tau_{\max}) = \sqrt{\frac{\omega_{\mathrm{fv}}}{\omega}} \mathrm{e}^{\pm i \int_0^{\tau_{\max}} d\tau (\omega - \omega_{\mathrm{fv}})}. \tag{8.66}$$

From this first order solution we may now extract the leading $1/\ell$ term of the total summation.

The obtained result is exact agreement with the one found by Dunne [75].

$$\alpha = \frac{1}{2}\int \mathrm{d}\tau\, a(\tau)\,\left\{V''(\phi_b) - V''(\phi_{\mathrm{fv}})\right\}. \tag{8.67}$$

To obtain the next order we must iterate the WKB procedure, refining the Ansatz using the new frequency

$$\omega_{(2)} = -\left(\frac{1}{4}\frac{\ddot{\omega}_{(1)}}{\omega_{(1)}^2} - \frac{3}{8}\frac{\dot{\omega}_{(1)}}{\omega_{(1)}^3}\right). \tag{8.68}$$

The corresponding solution will then be accurate up to contributions $\mathcal{O}(\ell^{-3})$ and therefore capture the entire divergent behavior in need of regularization. The corresponding coefficient is given by

$$\gamma = -\frac{1}{8}\int \mathrm{d}\tau\, a\left\{(V''(\phi_b) - V''(\phi_{\mathrm{fv}}))(-2 - 2\dot{a}^2 + a^2(V''(\phi_b) + V''(\phi_{\mathrm{fv}}))\right\}. \tag{8.69}$$

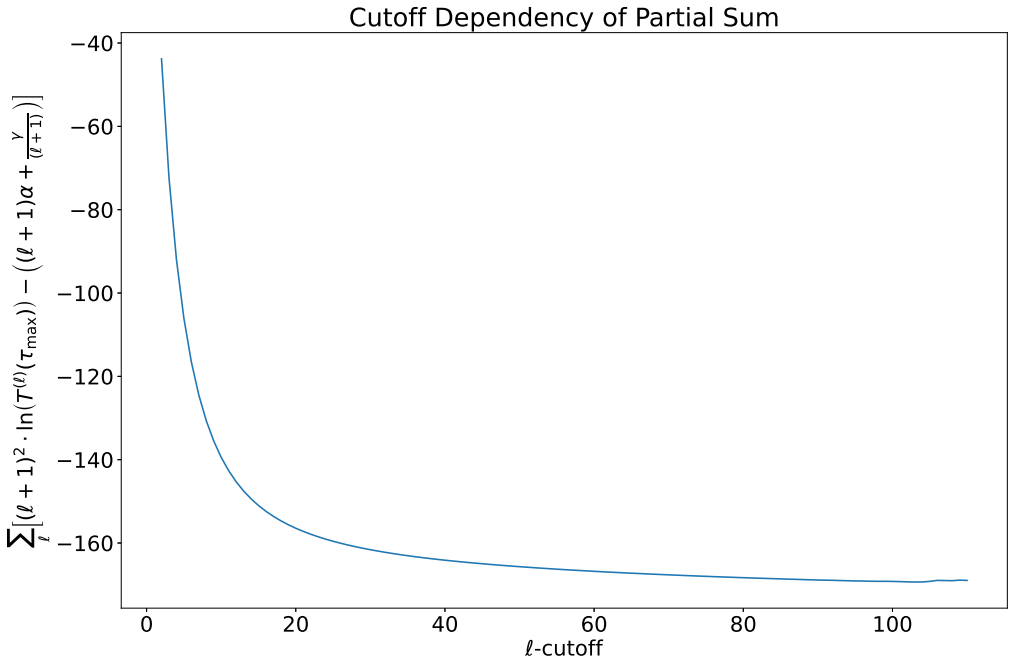


Figure 8.7.: The renormalized determinant as a function of the ℓ cut-off. We see the rapid convergence for higher values of ℓ

This is very similar in appearance to the factor that was postulated by Dunne, however it differs by factors that would be absent in the flat space analog he uses as a basis for his estimate and is therefore numerically different. Subtracting the corresponding terms should render the sum in Eq. (8.52) finite. A plot of the resulting series can be found in Fig. 8.7 and shows that we do in fact obtain a good convergence of the total sum as $\ell \to \infty$. However due to the very delicate and highly oscillatory nature of the associated Legendre functions as a false vacuum solution, it is numerically very difficult to reach the point of exact cancellation, as they become

numerically very unstable for values of $\ell > 80$. More care needs to be taken therefore in order to improve upon the accuracy of the actual determinant, which we can momentarily only give up to an uncertainty of around three percent. A separate verification of these results using Green function techniques, together with the inclusion of gradient effects and tadpole contributions can be found in [79].

Summary

In the past section we have seen how it is practically possible to compute the functional determinant of an operator in the case of a specific example. While many of the techniques applied can be taken directly into the Schrödinger formalism, some work remains to be done on the path of a reliable numerical framework to be applied to the previous chapters. Firstly, in order to make progress, we heavily relied on the Wick rotation and analytic continuations to obtain convergent expressions. While this has been studied extensively within the context of false vacuum decay, very little has been done for the Schrödinger formulation of QFT. While it should in principle be straightforward by analogy there is still some thought required on the physical interpretation of the Euclidean action within this framework. While this problem may be easy to circumvent, the more pressing issue is that of boundary conditions. As the spectrum of any operator necessarily depends on the boundary conditions imposed, little can be done in situations where they are not known. In the case of false vacuum decay they are naturally given by the process under consideration, however in the general setting of the previous examples they are not. In the Kasner and plane wave cases it was possible to extract the analytic properties of the time evolution operator, and therefore of the functional kernel for a large class of initial conditions. In order to apply the techniques demonstrated here to these or similar cases, boundary conditions must be prescribed explicitly, which will seldom be possible close to singular surfaces. Notwithstanding the integration of numerical methods into the Schrödinger formalism can be very fruitful whenever one wishes to look at specific scenarios in which conditions can be found and these issues are under control.

A. The Fourier Transform in Curved Space

As we expect the kernel to depend only on the difference $\mathbf{x}-\mathbf{y}$, we may begin by exploiting translation invariance by way of the Fourier transform, as the resulting equation in momentum space is much less unwieldy. Unfortunately, the definition of a Fourier transform on a general manifold is a subtle issue. Following our path of formal manipulation we push aside these subtleties and begin with the covariant definition of the delta distribution $\delta(x,y)$:

$$\int_{\Sigma_t} d^3y\sqrt{q_y}\delta(x,y)f(y) := f(x). \tag{A.1}$$

Furthermore, we must define a measure in k-space, where the question arises how said measure must transform under coordinate transformations such as to make the entire construction covariant. Using the Darboux theorem, we know the canonical volume form is given by

$$dx^1 \wedge dx^2 \wedge dx^3 \wedge dk_1 \wedge dk_2 \wedge dk_3,$$

determining the index position of the index of k. Subsequently we arrive at the conclusion, that the following notation for our plane waves has the Eucledian scalar product in the exponent, and the subsequent expression is a standard consequence of distributional analysis, irrespective of geometry.

$$\int \frac{d^3k}{(2\pi)^3} e^{ik\cdot(x-y)} := \int \frac{d^3k}{(2\pi)^3} e^{ik_a(x^a-y^a)} = \delta(x^a-y^a). \tag{A.2}$$

From this, we infer

$$\int d^3x e^{i(k_a-p_a)x^a} = (2\pi)^3\delta(k-p). \tag{A.3}$$

Therefore, the Fourier transformation defined as

$$f(x) = \int \frac{d^3k}{(2\pi)^3} e^{ik\cdot x}\hat{f}(k), \quad \hat{f}(k) = \int dx e^{-ik\cdot x} f(x), \tag{A.4}$$

is valid in curved space and in particular consistent with the above. Even though it may seem strange, it may be brought to covariant form using the defining relation (A.1). With this construction at hand we may now write down the unambiguous form of the Fourier transform of (3.19).

For convenience and later use we choose to restrict (3.19) to the class of Bianchi I space-

times and therefore factors of $\sqrt{g_{00}}$ may be set to one. Applying the definitions used above consistently gives the following expressions:

$$\begin{aligned}
&\int_{\Sigma_t} d^3z\sqrt{q_z}\sqrt{q_x}\sqrt{q_y}K(x,z;t)K(z,y;t), \qquad (A.5)\\
&= q^{3/2}\int_{\Sigma_t} d^3z \int \frac{d^3k}{(2\pi)^3}\int \frac{d^3p}{(2\pi)^3} e^{ik\cdot(x-z)}e^{ip\cdot(z-y)}\hat{K}(k,t)\hat{K}(p,t),\\
&= q^{3/2}\int \frac{d^3k}{(2\pi)^3}\int \frac{d^3p}{(2\pi)^3}\int_{\Sigma_t} d^3 e^{i(p-k)\cdot z}e^{ik\cdot x}e^{-ip\cdot y}\hat{K}(k,t)\hat{K}(p,t),\\
&= q^{3/2}\int \frac{d^3k}{(2\pi)^3} e^{ik\cdot(x-y)}\hat{K}^2(k,t),
\end{aligned}$$

where we have made use of (A.3) in the last line. We infer from (A.1) that $\delta(x,y) = \delta(x-y)\sqrt{q}$ and use the representation (A.2) to write the last term on the right hand side as

$$\sqrt{q_x}\sqrt{q_y}\big(\triangle - m^2 - \xi R\big)\delta^{(3)}(x,y) = \sqrt{q}\int \frac{d^3k}{(2\pi)^3}\big[k^2 - m^2 - \xi R\big]. \qquad (A.6)$$

Since the measure now does not depend on time, we can exchange the differentiation and integration on the left hand side of (3.19) and put the pieces together to obtain, for the Fourier transformed kernel,

$$\boxed{i\partial_t\big(q\hat{K}(\mathbf{k},t)\big) = q^{3/2}\hat{K}^2(\mathbf{k},t) + \sqrt{q}\Omega^2(\mathbf{k},t),} \qquad (A.7)$$

where we have defined $\Omega^2(k,t) := q^{ab}k_a k_b - m^2 - \xi R$.

B. Unitarity and S-matrix

When defining a unitary time evolution it is a necessary consequence that the norm of a given state remains constant. Therefore it is equal in the Heisenberg and Schrödinger pictures

$$\langle \Psi | \Psi \rangle_S = \langle \Psi | \Psi \rangle_H. \tag{B.1}$$

In the Schrödinger picture the time-evolution of the state is given by

$$|\psi_t\rangle = e^{-iHt} |\psi_0\rangle, \tag{B.2}$$

and the S-matrix is therefore usually defined as

$$S = \mathbb{1} + iT = e^{-iHt}. \tag{B.3}$$

Whenever H is Hermitian, it follows immediately that the S-matrix will be unitary. The amplitude of a scattering experiment with initial state $|i\rangle$ and final state $|f\rangle$ is then usually denoted by

$$\langle f | T | i \rangle = (2\pi)^4 \delta^{(4)}(p_i - p_f) \mathcal{M}(i \to f). \tag{B.4}$$

It follows directly from the unitarity of the S-matrix that

$$i(T^\dagger - T) = T^\dagger T \tag{B.5}$$

Taking to above expression and wedging it between the final and initial state, then yields the well known optical theorem, upon one insertion of unity on the right hand side,

$$\mathcal{M}(i \to f) - \mathcal{M}^*(f \to i) = i \sum_X \int d\Pi_X (2\pi)^4 \delta^{(4)}(p_i - p_X) \mathcal{M}^*(i \to X) \mathcal{M}^*(f \to X), \tag{B.6}$$

relating various tree level processes to the one loop level. If we were now to suppose, that the initial and final states are the same $|i\rangle = |f\rangle := |A\rangle$, the optical theorem states

$$2 \operatorname{Im} \mathcal{M}(A \to A) = \sum_X \int d\Pi_X (2\pi)^4 \delta^{(4)} |\mathcal{M}(A \to X)|^2, \tag{B.7}$$

where we have suppressed the momentum conservation for simpler reading. As we can see the right hand side will always be larger than zero, as we are integrating only over strictly positive values. Now if we were to assume that the Hamiltonian is not Hermitian, as can be the case in

effective field theories, or when the absence of a time-like killing vector field does not allow for unitary evolution, we can split it into it's Hermitian and non-Hermitian parts as follows

$$H = H_{\mathrm{H}} + H_{\mathrm{NH}}. \tag{B.8}$$

In order to keep things as simple as possible, we will assume a very straightforward non-Hermitian part

$$H_{\mathrm{NH}} = i\alpha\mathbb{1}, \;\; \alpha \in \mathbb{R}. \tag{B.9}$$

The S-matrix will then be equal to

$$S = e^{-iH_{\mathrm{H}}t} e^{\alpha t} \tag{B.10}$$

Naturally, for the case that $\alpha \neq 0$ it will no longer be unitary. Moreover, for $\alpha > 0$ the evolution will cause the norm of the state to increase, while for $\alpha < 0$ it will decrease with time as $SS^{\dagger} = e^{2\alpha t}$. We also know, that

$$i(T^{\dagger} - T) = T^{\dagger}T + \mathbb{1} - S^{\dagger}S. \tag{B.11}$$

Therefore, we can conclude that whenever

$$\mathrm{Im}\,\mathcal{M}(A \to A) < 0 \tag{B.12}$$

unitarity must necessarily be broken. In other words, the vacuum persistence amplitude develops an imaginary contribution, whenever the full theory fails to follow a unitary time-evolution. One should stress however, that this does not necessarily mean a breakdown of predictability. Cases such as the ones studied in the previous thesis are also known from other areas, effective field theories in particular. Here it is known for the theory of unstable particle decay. Owing to the fact that the heavy particles considered therein are unstable, the time-evolution of the entire system is non-unitary. However, it is still possible to conduct sensible scattering experiments with unitary amplitudes. One such approach is to perform perturbation theory with respect to the ratio of the decay width Γ and the mass of the particle M. It is then possible to define a perturbative series in Γ/M, that is unitary order by order (that is up to contributions suppressed by a higher order of Γ/M) [80].

C. Gel'fand Yaglom Technique

The Gel'fand Yaglom theorem provides us with an easy way to compute the determinant of a given functional operator. We will give a brief explanation of the technique here. This exposition is largely based on notes from the lecture given by Graham Shore at the Saalburg Summer School, the rigorous details and proofs can be found in [81, 82].

Assume that we are interested in the spectrum of some differential operator $\mathcal{D}$ given on some domain $D(\mathcal{D})$ and assume for simplicity that the eigenvalues λ_n are discrete. Let F be some function whose zeros are given by the eigenvalues of $\mathcal{D}$, therefore $F(\lambda_n) = 0$, $\forall n \in \mathbb{N}$. From this property it follows that the logarithmic derivative of F will have simple poles at all λ_n, each with residue one. We can therefore again make use of the ζ-function to write

$$\zeta(s) = \frac{1}{2\pi i}\int_\gamma \mathrm{d}\lambda\ \lambda^{-s}\frac{\mathrm{d}\ln F(\lambda)}{\mathrm{d}\lambda} \tag{C.1}$$

The contour γ encloses the eigenvalues in the λ plane and a branch cut was chosen along the negative real line as usual. If the contour is deformed in such a way, that it encloses the branch cut along the negative real λ-axis the integral may be split into two parts, each of which picks up an additional phase factor of $e^{\pm i\pi s}$. An illustration of this is shown in figure C.1. In this case, the we can rewrite it as

$$\zeta(s) = -\frac{\sin(\pi s)}{\pi}\int_{-\infty}^{0} \mathrm{d}\lambda\ \lambda^{-s}\frac{\mathrm{d}\ln F(\lambda)}{\mathrm{d}\lambda}. \tag{C.2}$$

Taking a derivative with respect to s, we see that the value of the ζ-function is given solely by the values of F at the boundary

$$\zeta'(0) = \ln F(-\infty) - \ln F(0). \tag{C.3}$$

As we have seen, the ζ-function may be easily used to define the determinant of a given operator through the expression,

$$\det\mathcal{D} = \exp\left(\zeta'_{\mathcal{D}}(0)\right). \tag{C.4}$$

The only task at hand is therefore to find the function F. This is usually achieved by considering the same operator with different boundary conditions. Consider therefore eigenfunctions of $\mathcal{D}$, given by ϕ_n where the label indicates that the corresponding eigenvalue is λ_n, satisfying Dirichlet boundary conditions. Assume the ϖ_λ are also eigenfunctions of $\mathcal{D}$ with the following

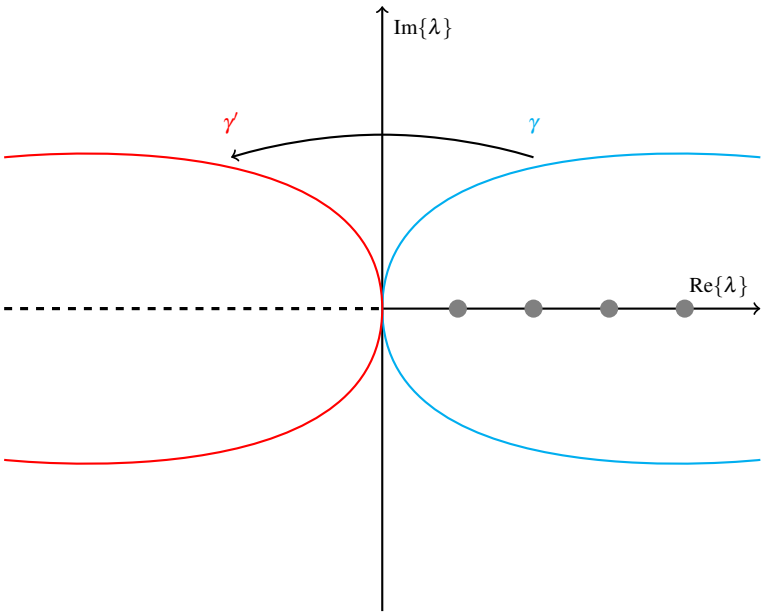


Figure C.1.: The rotation of the integration contour

boundary conditions

$$\mathcal{D}\varpi_\lambda = \lambda\varpi_\lambda, \;\; \varpi_\lambda(0) = 0, \; \varpi'_\lambda(0) = 1. \tag{C.5}$$

We have restricted the domain of the eigenfunctions to the interval $[0,1]$ for simplicity but the argument allows for arbitrary intervals. If λ is to be an eigenvalue of the initial problem we must therefore have $\varpi_\lambda(1) = 0$. We can therefore define the function

$$F(\lambda) := \varpi_\lambda(1). \tag{C.6}$$

This implies that

$$\zeta'(0) = \ln \frac{\varpi_{\lambda=0}(1)}{\varpi^{\text{free}}_{\lambda=0}(1)}. \tag{C.7}$$

This simplifies the calculation of the entire determinant to solving the appropriate equation for the eigenfunction ϖ_λ and then taking its value at the boundary.

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