A Class of Almost Equilibrium States in Robertson-Walker Spacetimes

Dissertation
zur Erlangung des Doktorgrades
des Department Physik
der Universität Hamburg

vorgelegt von
Muharrem Küskü
aus Kalkandere

Hamburg
2008

Gutachter der Dissertation	Prof. Dr. K. Fredenhagen
	Prof. Dr. W. Buchmüller
Gutachter der Disputation:	Prof. Dr. K. Fredenhagen
	Prof. Dr. V. Schomerus
Datum der Disputation:	29.07.2008
Vorsitzender des Prüfungsausschusses:	Prof. Dr. J. Bartels
Vorsitzender des Promotionsausschusses:	Prof. Dr. J. Bartels
Dekan der Fakultät für Mathematik, Informatik und Naturwissenschaften:	Prof. Dr. A. Frühwald

Abstract

In quantum field theory in curved spacetimes the construction of the algebra of observables of linear fields is today well understood. However, it remains a non-trivial task to construct physically meaningful states on the algebra. For instance, we are in the unsatisfactory situation that there exist no examples of states suited to describe local thermal equilibrium in a non-stationary spacetime. In this thesis, we construct a class of states for the Klein-Gordon field in Robertson-Walker spacetimes, which seem to provide the first example of thermal states in a spacetime without time translation symmetry. More precisely, in the setting of real, linear, scalar fields in Robertson-Walker spacetimes we define on the set of homogeneous, isotropic, quasi-free states a free energy functional that is based on the averaged energy density measured by an isotropic observer along his worldline. This functional is well defined and lower bounded by a suitable quantum energy inequality. Subsequently, we minimize this functional and obtain states that we interpret as 'almost equilibrium states'. It turns out that the states of low energy, which were recently introduced in [Olb07b], are the ground states of the almost equilibrium states. Finally, we prove that the almost equilibrium states satisfy the Hadamard condition, which qualifies them as physically meaningful states.

Zusammenfassung

In der Quantenfeldtheorie in gekrümmter Raumzeit ist die Konstruktion der Algebra der Observablen linearer Felder heutzutage gut verstanden. Es ist jedoch eine nicht-triviale Aufgabe physikalische Zustände auf der Algebra zu konstruieren. Zum Beispiel sind wir in der unzufriedenstellenden Situation, dass keine Zustände bekannt sind, die es erlauben ein lokales thermales Gleichgewicht in einer nicht-stationären Raumzeit zu beschreiben. In dieser Arbeit konstruieren wir ein Klasse von Zuständen für das Klein-Gordon Feld in Robertson-Walker Raumzeiten, die das erste Beispiel thermaler Zustände in einer Raumzeit ohne Translationssymmetrie bezüglich der Zeit darstellen dürften. Genauer gesagt definieren wir für das reelle, lineare, skalare Feld in Robertson-Walker Raumzeiten ein Funktional für die freie Energie auf der Menge der homogenen, isotropen, quasifreien Zustände, welches auf der gemittelten Energiedichte basiert, die ein isotroper Beobachter auf seiner Weltlinie misst. Dieses Funktional ist wohldefiniert und von unten beschränkt, dank einer geeigneten Quanten-Energie-Ungleichung. In der Folge minimieren wir dieses Funktional und erhalten so Zustände, welche wir als Fast-Gleichgewichts-Zustände ("almost equilibrium states") interpretieren. Es stellt sich heraus, dass die Zustände niedriger Energie ("states of low energy"), welche kürzlich in [Olb07b] definiert wurden, die natürlichen Grundzustände der Fast-Gleichgewichts-Zustände sind. Schließlich beweisen wir, dass die Fast-Gleichgewichts-Zustände die Hadamard-Bedingung erfüllen, was sie als physikalisch sinnvolle Zustände auszeichnet.

Dedicated to the memory of Bernd Kuckert.

Contents

1 Introduction

There are plenty of reasons to investigate quantum fields in curved spacetimes. Accepting for the time being that we don't know how to formulate a quantum theory of gravity, we may still have the desire to investigate the physics in the intermediate regime, where the quantum nature of fields is already apparent and spacetime is curved, but the quantum nature of gravitation plays no crucial role. That such a theory can produce interesting results is undoubted since the discovery of the Hawking effect, which establishes a remarkable connection between two seemingly distinct branches of physics, namely, gravitational (black hole) physics and thermodynamics. The latter field is also of major importance in modern cosmology, where the cosmic microwave background (CMB), its isotropy on large scales, and its anisotropy at small scales remains a startling puzzle. It is also remarkable that cosmological observations, e.g., the ones leading to the postulation of dark matter and dark energy, nowadays become a major trigger for particle physics research. For example, the Large Hadron Collider (LHC) at CERN, scheduled to start operating this year, is hoped to provide clues on the constituents of dark matter. Surely, the interplay between cosmology and particle physics will increase in the years to come.

The formulation of quantum field theory in curved spacetime is hampered by the fact that the traditional formulation relies heavily on Poincaré symmetry, which is lacking in a general curved spacetime. Consequently, notions like 'particles' and 'vacuum', which depend on Poincaré symmetry, are not well defined in this setting. Furthermore, quantum field theory becomes ambiguous because of the appearance of unitarily inequivalent Hilbert space representations of the algebra of observables. An expanding, homogeneous, isotropic universe is described by a Robertson-Walker metric, which is non-stationary and comes in three types, of which two have curved spacelike sections. Owing to the present symmetry, the curvature of the spacelike sections does not pose a serious problem for the formulation of quantum field theory. On has analogues of the Fourier transform, and the quantum field can be written, as usual, as an integral over modes, albeit the coefficients in the mode decomposition, which in stationary spacetimes are interpreted as creation and annihilation operators, loose their meaning. However, non-stationarity, i.e., the absence of time translation symmetry, brings about, among others, the problems mentioned above. In particular, the lack of a timelike Killing field results in a failure of energy conservation and, consequently, the lack of a Hamiltonian, which generates time-evolution in the non-stationary case.

A thorough analysis of these problems is viable within the algebraic approach to quantum field theory, which can be rigorously formulated for quantum fields on curved

backgrounds. In this approach, one first constructs the algebra of observables for the quantum system, satisfying, for instance, the canonical commutation relations. In a second step, one constructs states with desired properties as linear functionals on the algebra. This course of action disentangles, effectively, problems tied to the algebra of observables from problems arising at the level of representations and states. While the first step is, at least for free fields, to a large degree understood, the second one is, put mildly, less explored. One has to admit, that the number of known examples for physically meaningful states in curved spacetimes is small. For example, to date, there are no explicitly known thermal states with respect to global time evolution in a non-stationary spacetime.

A different problem – which is already present in flat spacetime –, namely, the lower unboundedness of point-like energy densities in quantum field theory has led to the so-called quantum inequalities. These uncertainty-type inequalities give lower bounds on the averaged energy densities measurable in (a class of) quantum states, where the averaging procedure involves a sampling function with suitable properties. Quantum inequalities were established in flat spacetimes as well as in arbitrary globally hyperbolic spacetimes. They are important in general relativity since they reestablish the macroscopic energy conditions, e.g., the weak energy condition, utilized for proving singularity theorems. Furthermore, it has been argued that they may serve as stability conditions for quantum systems on a mesoscopic scale between the Hadamard condition (microscopic scale) and passivity (macroscopic scale) [FV03].

The initial motivation for the project presented in this thesis can be stated as follows. Since there are, by quantum inequalities, locally meaningful energy-quantities even in curved spacetimes, how do the ground states and (thermal) equilibrium states of these 'energies' look like? Regarding ground states, the analysis carried out by Olbermann in [Olb07b] in the setting of real, linear, scalar fields in Robertson-Walker spacetimes resulted in the definition of states of low energy. These are pure, homogeneous, isotropic, quasi-free states that minimize the averaged energy density measured by an observer along a timelike curve. Moreover, it could be proven, by comparison with adiabatic vacuum states, that the two-point distributions of the states of low energy satisfy the Hadamard condition, which is a condition on the short distance behaviour of the two-point distribution to be satisfied by physically reasonable states. Encouraged by this result, we construct, in the same setting, a class of (thermal) almost equilibrium states with respect to the timelike averaged energy density.

The basic idea of our construction is the following. For a finite quantum statistical system in contact with a much larger reservoir at a constant positive temperature $\frac{1}{\beta}$, the free energy $\mathcal{F} = \mathcal{E} - \frac{1}{\beta}\mathcal{S}$, where $\mathcal{E}$ is the inner energy and $\mathcal{S}$ denotes the entropy, is the maximum amount of work that the system can perform. It turns out that the equilibrium state of such system is characterized uniquely by the property that it minimizes the free energy. Following this general principle, we define on the set of homogeneous, isotropic, quasi-free states of the Klein-Gordon field in Robertson-Walker spacetimes a free energy

functional, where a timelike averaged energy density takes the role of $\mathcal{E}$. We show that, owing to the symmetry of the spacetimes, this energy quantity has the form of an integral over the modes of the quantum field. In view of this, we associate to each mode an entropy functional and require the mode to evolve according to the KMS condition, i.e., as a system in thermal equilibrium at inverse temperature β. By a certain quantum inequality proved in [Few00], our free energy functional is bounded below within the class of Hadamard states. Indeed, we succeed in calculating the two-point distribution of the unique state that minimizes our free energy functional for a given sampling function. We call the resulting state an almost equilibrium state a inverse temperature β associated to the sampling function used for averaging the energy density. We finally prove that the almost equilibrium states satisfy the Hadamard condition. The last step is crucial since, as noted above, the quantum inequality on which we base our definition is valid only within the class of Hadamard states. At the same time, the Hadamard property proves the almost equilibrium states to be physically meaningful states.

Outline The outline of this thesis is as follows. In section 2 we give an account of the basics of quantum field theory in curved spacetimes. We consider both the quantization scheme via construction of a Hilbert space as well as the algebraic method. We introduce the notion of quasi-free states and Hadamard states. The main sources for this chapter are [Wal94] and [KW91] but the reader, who is not well acquainted with algebraic quantum field theory will also benefit from [Haa96] and [Emc72]. In section 3, we specialize to Robertson-Walker spacetimes and recall relevant facts about homogeneous, isotropic, quasi-free states of the Klein-Gordon field in this setting. In particular, we introduce the two-point distribution of such states. Most of the the material presented here can be found in the seminal paper [LR90]. We add to the known facts a characterization of the two-point distribution in terms of the mode solutions of the Klein-Gordon equation. Chapter 4 is devoted to quantum inequalities. A brief survey of the topic is followed by a quotation of the quantum inequality on which our construction is based [Few00]. Then, we calculate the specific expression for the averaged stress-energy tensor, since this will be part of the free energy that we will minimize. Section 5 is the main part of this thesis, in which we explain and accomplish the construction of the almost equilibrium states. As a necessary step for our construction, but maybe also interesting in its own right, we calculate the generator of KMS states on the Weyl algebra of a system with one degree of freedom. Then, we define the almost equilibrium states and prove that they are indeed Hadamard states. In section 6, a summary of the construction is given and supplemented by a few ideas on possible future projects.

2 Quantum field theory in curved spacetime

The overall setting of this thesis is quantum field theory in curved spacetime. This is a generalization of ordinary quantum field theory in the sense that the fields propagate on a curved Lorentzian manifold rather than flat Minkowski space. It may be seen as a semiclassical approach to 'quantum gravity' since the fields are quantized but the background spacetime is taken to be classical and fixed. Any backreaction of the field on the spacetime is, in principle, encoded in the semiclassical Einstein equations

$$G_{\mu\nu} + \Lambda \mathfrak{g}_{\mu\nu} = 8\pi \langle \boldsymbol{T}_{\mu\nu} \rangle \ , \tag{2.1}$$

though, to date, few is known about backreaction effects, due to some serious difficulties in calculating $\langle \boldsymbol{T}_{\mu\nu} \rangle$. See the discussion in [Wal94] on this point.

The absence of symmetries is a big obstacle for the traditional formulation of quantum field theory on a general spacetime. However, the algebraic quantum field theory, as defined in [HK64], has a well defined generalization to curved spacetimes [Dim80]. The fundamental object in the algebraic formulation is a net of local algebras on a spacetime. Such a net associates to each open region $\mathcal{O}$ in spacetime an algebra $\mathfrak{A}(\mathcal{O})$ of observables that are measurable in the region. The latest enhancement of the algebraic approach is the so-called locally covariant quantum field theory [BFV03]. In this approach a locally covariant quantum field theory is defined as a covariant functor between the category of globally hyperbolic Lorentzian spacetimes with admissible (isometric, orientation and time-orientation preserving, causally convex) embeddings as morphisms and the category of unital C*-algebras with certain homomorphisms as morphisms.

In the first section of this chapter, we introduce the necessary facts about globally hyperbolic spacetimes and the Cauchy problem thereon. Then, we present the quantization scheme in curved spacetime, where we follow the presentation found in the monograph [Wal94] and the review [KW91]. At last, we introduce the notions of quasi-free states and Hadamard states. Our presentation of the general theory is strongly biased by our needs in the later chapters.

2.1 Classical preliminaries

2.1.1 Spacetime structure

We adopt the common viewpoint that spacetime is modelled by a smooth (in the sense that it is C^∞, Hausdorff, paracompact, and connected) four-dimensional manifold $\mathcal{M}$ with Lorentzian metric $\mathfrak{g}_{\mu\nu}$. We also assume that the spacetime under consideration is orientable and time-orientable. Actually, we will restrict ourselves to the class of Robertson-Walker spacetimes, which fulfill these hypotheses. Following the loosely established tradition of field theorists, we choose the signature of the metric $\mathfrak{g}_{\mu\nu}$ to be $(+,-,-,-)$. According to this convention, a vector v^μ is called timelike if its norm $\mathfrak{g}_{\mu\nu}v^\mu v^\nu$ is positive, spacelike if the norm is negative, and null if it is zero. A curve $\gamma(t) : \mathbb{R} \to \mathcal{M}$ with tangent vectors $\dot{\gamma}^\mu(t)$ that are timelike everywhere is called a timelike curve. It is called a causal curve if the tangent vectors are timelike or null everywhere. For $\mathcal{K} \subset \mathcal{M}$ the causal future $J^+(\mathcal{K})$ and the causal past $J^-(\mathcal{K})$ are the sets of all points that can be reached from $\mathcal{K}$ by a future/past directed causal curve. A point $x \in \mathcal{M}$ is said to be the future endpoint of a causal curve if for every neighborhood $\mathcal{O}$ of x there is a t_0 such that $\gamma(t) \in \mathcal{O}$ for every $t \geq t_0$. A causal curve is said to be future inextendible if it has no future endpoint. Analogously, we can define past inextendible curves. A causal curve is called inextendible if it is future and past inextendible [HE73]. Less precisely, one can say that an inextendible curve can end only at infinity or at some initial or final singularity. The future(+)/past(-) domain of dependence $D^\pm(\Sigma)$ of Σ is the set of all $x \in \mathcal{M}$ such that every past/future inextendible causal curve through x intersects Σ [Wal84].

A Cauchy surface for a Lorentzian manifold $\mathcal{M}$ is a spacelike hypersurface which is intersected exactly once by every inextendible causal curve in $\mathcal{M}$ [Ful89]. Equivalently, the domain of dependence $D(\Sigma) = D^+(\Sigma) \cup D^-(\Sigma)$ of a Cauchy surface is the entire spacetime. A spacetime $(\mathcal{M}, \mathfrak{g}_{\mu\nu})$ is said to be stationary if there exists a one-parameter group of isometries $\Xi_t : \mathcal{M} \to \mathcal{M}$, $\Xi_t^* \mathfrak{g}_{\mu\nu} = \mathfrak{g}_{\mu\nu}$, $t \in \mathbb{R}$ whose orbits are timelike curves. Equivalently, there exists a global timelike Killing vector field ξ^μ satisfying Killing's equation $\nabla_\mu \xi_\nu + \nabla_\nu \xi_\mu = 0$, namely, the generator of Ξ_t. The spacetime is said to be static if it is stationary and if, in addition, there exists a spacelike hypersurface Σ that is orthogonal to the orbits of the isometry. In a local coordinate system $x^i, i = 1, 2, 3$, the metric of a static spacetime may be written as $ds^2 = N(\mathbf{x})^2 dt^2 - \mathfrak{h}_{ij}(\mathbf{x}) dx^i dx^j$, where $\mathfrak{h}_{ij}$ is the induced metric on the Cauchy surfaces, and $N \in C^\infty(\Sigma)$ is the lapse function. In this case, the timelike Killing vector field satisfies $\xi_{[\mu} \nabla_\nu \xi_{\rho]} = 0$. For completeness, we note that a spacetime is called ultrastatic if it possesses a timelike Killing vector field ξ^μ that is orthogonal to the spacelike hypersurfaces and obeys $\mathfrak{g}_{\mu\nu}\xi^\mu\xi^\nu = 1$. In this case, the lapse function is $N = 1$.

In order to guarantee the well posedness of the classical time evolution of a field, one usually assumes globally hyperbolicity of the underlying spacetime. There are different equivalent definitions of global hyperbolicity. For example, a spacetime $(\mathcal{M}, \mathfrak{g}_{\mu\nu})$ is called

globally hyperbolic if there are no closed causal curves in $\mathcal{M}$ and the collection of all causal curves joining two arbitrary points $x_1, x_2 \in \mathcal{M}$ is compact (in a suitable topology). Due to a theorem by Geroch [Ger70] an n-dimensional globally hyperbolic spacetime $(\mathcal{M}, \mathfrak{g}_{\mu\nu})$ can be foliated with a family of Cauchy surfaces that are diffeomorphic to an $(n-1)$-dimensional manifold Σ. This means that a globally hyperbolic spacetime has the topology $\mathcal{M} = \mathbb{R} \times \Sigma$. Global hyperbolicity is a condition on the geometry of spacetime that ensures the existence and uniqueness of global solutions to hyperbolic differential equations. In a broader sense, global hyperbolicity of Lorentzian spacetimes serves as an analog for the notion of completeness of Riemannian manifolds [BGP07]. Since quantum dynamics is usually modelled around classical dynamics, global hyperbolicity of the underlying spacetime is a reasonable assumption in a semiclassical approach like quantum field theory in curved spacetime. We refer the interested reader to [HE73, Wal84, BGP07] for further elaborations on this topic.

2.1.2 The Cauchy problem

A thorough and general treatment of the Cauchy problem on globally hyperbolic spacetimes can be found in the monograph [BGP07]. The results there are valid for arbitrary (complex) vector bundles on general globally hyperbolic manifolds. However, in order to keep in touch with the physical literature and to avoid unnecessary complexity, we will use the traditional formulation found in [Dim80, Wal94], keeping in mind the more general results.

In this thesis, we are concerned with the special case of a real, linear, scalar field ϕ on a globally hyperbolic spacetime $(\mathcal{M}, \mathfrak{g}_{\mu\nu})$ satisfying the Klein-Gordon equation,

$$(\Box_{\mathfrak{g}} + \mathrm{m}^2)\phi = 0 \ , \tag{2.2}$$

where $\Box_{\mathfrak{g}} = \mathfrak{g}^{\mu\nu}\nabla_\mu\nabla_\nu$ is the wave operator associated to $\mathfrak{g}_{\mu\nu}$ and $\mathrm{m} \geq 0$ is the mass parameter. By the global hyperbolicity of $\mathcal{M}$, the Klein-Gordon equation (2.2) has a well-posed initial value formulation. This means that there exist unique continuous linear operators

$$E^{\pm} : \mathscr{D}(\mathcal{M}) \to \mathscr{E}(\mathcal{M}) \ , \tag{2.3}$$

called the advanced fundamental solution, E^+, and retarded fundamental solution, E^-, with the following properties:

$$(\Box_{\mathfrak{g}} + \mathrm{m}^2)E^{\pm}f = f = E^{\pm}(\Box_{\mathfrak{g}} + \mathrm{m}^2)f \ , \tag{2.4}$$

$$\mathrm{supp}(E^+ f) \subset J^+(\mathrm{supp}\, f) \ , \tag{2.5}$$

$$\mathrm{supp}(E^- f) \subset J^-(\mathrm{supp}\, f) \tag{2.6}$$

for $f \in \mathscr{D}(\mathcal{M})$. We use the notation $\mathscr{D}(\mathcal{M}) := \mathrm{C}_0^\infty(\mathcal{M})$ and $\mathscr{E}(\mathcal{M}) := \mathrm{C}^\infty(\mathcal{M})$, denoting the set of (complex-valued) smooth functions (with compact support in the case of $\mathscr{D}$) on the manifold $\mathcal{M}$. The first of these properties says that E^+ and E^- are solutions to

the inhomogeneous Klein-Gordon equation. The other properties are sensible support properties. Combining the advanced and retarded fundamental solutions, one constructs the fundamental solution

$$E := E^+ - E^- : \mathscr{D}(\mathcal{M}) \to \mathscr{E}(\mathcal{M}) \tag{2.7}$$

of the Cauchy problem, which has the properties

$$(\Box_{\mathfrak{g}} + \mathrm{m}^2)Ef = 0 = E(\Box_{\mathfrak{g}} + \mathrm{m}^2)f \ , \tag{2.8}$$

$$\mathrm{supp}(Ef) \subset \big(J^+(\mathrm{supp}\, f) \cup J^-(\mathrm{supp}\, f)\big) \tag{2.9}$$

for $f \in \mathscr{D}(\mathcal{M})$.

There are different schemes available for the quantization of a classical fields, some of which start from complex solutions and some of which use real-valued functions. In this chapter we will be concerned with the latter spaces. Denote by $\mathscr{S} \subset \mathscr{E}(\mathcal{M}, \mathbb{R})$ the space of classical, real-valued, smooth solutions to the Klein-Gordon equation that have compact support on Cauchy surfaces, and denote by $\mathscr{T} := \mathscr{D}(\mathcal{M}, \mathbb{R})$ the test function space of real-valued, smooth functions of the fundamental solution. with compact support. Then the following lemma states some important properties

Lemma 2.1 ([Wal94]) *The map $E : \mathscr{T} \to \mathscr{S}$ satisfies the following three properties*

(i) E is onto, i.e., every $\phi \in \mathscr{S}$ can be expressed as $\phi = Ef$ for some $f \in \mathscr{T}$.

(ii) $Ef = 0$ if and only if $f = (\Box_{\mathfrak{g}} + \mathrm{m}^2)g$ for some $g \in \mathscr{T}$.

(iii) For all $\phi \in \mathscr{S}$ and all $f \in \mathscr{T}$, we have

$$\phi(f) := \int d^4x \ \phi(x)f(x) = \sigma(Ef, \phi) \ . \tag{2.10}$$

The fundamental solution plays an important role in the quantization procedures to be described later. For example, it determines the values of the commutators of the quantum fields. Even more important for us, it can be used to calculate the four-smeared two-point distribution from the three-smeared two-point distribution of the quantum fields, as we will see in section 3.3.1.

The fundamental solution E maps test functions on a globally hyperbolic spacetime to solutions that arise from initial data on some Cauchy surface. More precisely, this correspondence can be formulated as follows [Dim80]. Define for a given Cauchy surface Σ the restriction operator ρ_0 and the forward normal derivative ρ_1 by

$$\rho_0 : \mathscr{E}(\mathcal{M}, \mathbb{R}) \to \mathscr{E}(\Sigma, \mathbb{R}) \qquad \rho_1 : \mathscr{E}(\mathcal{M}, \mathbb{R}) \to \mathscr{E}(\Sigma, \mathbb{R}) \tag{2.11}$$

$$\phi \mapsto \phi|_\Sigma \ , \qquad \phi \mapsto (n^\mu \nabla_\mu \phi)|_\Sigma \ , \tag{2.12}$$

where n^μ denotes the unit forward normal to Σ and $n^\mu\nabla_\mu$ is the Lie derivative in this direction. Now, the following holds. Let Σ be any Cauchy surface and let $u, p \in \mathscr{D}(\Sigma, \mathbb{R})$ be any pair of smooth functions with compact support on the Cauchy surface Σ. Then, there exists a unique solution $\phi \in \mathscr{S}$ defined on all of $\mathcal{M}$ to the Klein Gordon equation (2.2) that is related to its initial values on Σ by $\rho_0(\phi) = u$ and $\rho_1(\phi) = p$. Furthermore,

$$\operatorname{supp}\phi \subset \left(\bigcup\nolimits_{\pm} J^{\pm}(\operatorname{supp} u)\right) \cup \left(\bigcup\nolimits_{\pm} J^{\pm}(\operatorname{supp} p)\right) \ , \tag{2.13}$$

i.e., for any closed subset of Σ the solution ϕ restricted to the corresponding domain of dependence depends only on the initial data in that subset.

2.1.3 Phase spaces

The quantum theory of linear systems is usually modelled after the classical theory as it becomes apparent in the 'Poisson bracket goes to commutator' rule. A sophisticated version of this rule is used for linear fields in curved spacetimes. Now, we introduce the classical part of this correspondence, namely, the classical phase space.

A classical phase space is a symplectic vector space, i.e., a pair $(\mathscr{V}, \sigma)$, where $\mathscr{V}$ is a vector space and σ is a bilinear form $\sigma : \mathscr{V} \times \mathscr{V} \to \mathbb{R}$ that is symplectic, $\sigma(f, g) = -\sigma(g, f)$, and non-degenerate, which means if $\sigma(f, g) = 0$ for all $f \in \mathscr{V}$ then $g = 0$. The space of solutions $\mathscr{S}$ to the Klein-Gordon admits a natural symplectic form defined by

$$\sigma_{\mathscr{S}}(\phi_1, \phi_2) := \int_\Sigma d^3x \sqrt{|\mathfrak{h}|}\ n^\mu(\phi_1\nabla_\mu\phi_2 - \phi_2\nabla_\mu\phi_1) \ . \tag{2.14}$$

The integral is evaluated on a Cauchy surface Σ, but σ is independent of the particular choice of Σ. This is due to the conservation, $\nabla_\mu j^\mu = 0$, of the current $j^\mu := \phi\nabla^\mu\phi' - \phi'\nabla^\mu\phi$ as can be shown by the application of Stokes' theorem to a timelike cylindrical spacetime volume bounded by portions of Cauchy surfaces. The space $(\mathscr{S}, \sigma_{\mathscr{S}})$ may be called the covariant phase space of the theory.

Alternatively, one can regard the canonical phase space. This is the space

$$\mathscr{M} := \{(u, p), u, p \in \mathscr{D}(\Sigma_t, \mathbb{R})\} \tag{2.15}$$

of initial values on Σ_t of the Klein-Gordon equation equipped with the symplectic form

$$\sigma_{\mathscr{M}}(F_1, F_2) := -\int_{\Sigma_t} d^3x\ (u_1p_2 - u_2p_1) \tag{2.16}$$

for $F_i := (u_i, p_i) \in \mathscr{M}$, $i = 1, 2$, where $p_i := \sqrt{|\mathfrak{h}|}(n^\mu\nabla_\mu u_i)$ is the canonical conjugate to the configuration variable u_i.

The relation between the distinct phase spaces can be summarized as follows: By the unique correspondence between the solutions to the field equation and the initial values

on a given Cauchy surface Σ_t, the spaces $\mathscr{S}$ and $\mathscr{M}$ are isomorphic, i.e., there exists an isomorphism $\mathcal{I}_t : \mathscr{M} \to \mathscr{S}$. This isomorphism induces a symplectic map $\sigma_{\mathscr{M}} = \mathcal{I}_t^* \sigma_{\mathscr{S}}$, where $\mathcal{I}_t^*$ denotes the pulled back isomorphism. Consequently, both phases spaces are equally well suited for quantization [TV99].

2.2 Quantization

Let us introduce some basic notions regarding algebras [BW92]. Let $\mathfrak{A}$ be an algebra over $\mathbb{C}$ with a map $^* : \mathfrak{A} \to \mathfrak{A}$ such that for all $A, B \in \mathfrak{A}$ and $\alpha, \beta \in \mathbb{C}$ we have $(\alpha A + \beta B)^* = \overline{\alpha} A^* + \overline{\beta} B^*$, $(AB)^* = B^* A^*$, and $(A^*)^* = A$. Then, * is called an involution and $\mathfrak{A}$ is called an involutive algebra or a *-algebra (star-algebra). If $\mathfrak{A}$ contains a unit element $\mathbb{1}$ such that $\mathbb{1}A = A\mathbb{1}$ for all $A \in \mathfrak{A}$ then it is called a unital *-algebra. If the *-algebra $\mathfrak{A}$ is also a Banach space where the norm satisfies $\|AB\| \leq \|A\|\|B\|$ for all $A, B \in \mathfrak{A}$ then $\mathfrak{A}$ is a Banach *-algebra. If, in addition, $\|A\|^2 = \|A^* A\|$ then $\mathfrak{A}$ is a C*-algebra. A *-subalgebra $\mathfrak{I}$ of $\mathfrak{A}$ is a *-ideal if $AB, BA \in \mathfrak{I}$ for all $A \in \mathfrak{A}$ and $B \in \mathfrak{I}$. A C*-algebra $\mathfrak{A}$ is called simple if it contains no non-trivial, i.e., different from 0 and $\mathfrak{A}$, closed *-ideals.

The observables of the quantized theory are represented by the self-adjoint elements of a suitable algebra, e.g., a (unital) *-algebra or, if a stronger structure is desired, a C*-algebra. So, owing to the different necessities, there exist several formulations of the algebra of observables, which are substantially equivalent, albeit technically inequivalent. In this section, we introduce the formulation in terms of a Weyl algebra, which is a C*-algebra. For a thorough treatment of the quantization scheme in curved spacetimes see [Wal94, KW91]. All relevant facts regarding Weyl algebras and their representations can be found in [BR97].

Based on each of the symplectic spaces defined in section 2.1.3, we can define an abstract C*-algebra that obeys the canonical commutation relations (CCR) via the Weyl construction. Consider a real symplectic vector space $(\mathscr{V}, \sigma)$.

Definition 2.2 A Weyl algebra $\mathfrak{W}(\mathscr{V}, \sigma)$ is a simple C*-algebra with unit generated by objects $W(f)$ that are labeled by functions $f \in \mathscr{V}$ and that satisfy the relations

(i) $W(0) = \mathbb{1}$,

(ii) $W(f)^* = W(-f)$,

(iii) $W(f_1)W(f_2) = \mathrm{e}^{-\frac{\mathrm{i}}{2}\sigma(f_1, f_2)} W(f_1 + f_2)$

for all $f, f_1, f_2 \in \mathscr{V}$.

Condition (iii) is the Weyl form of the canonical commutation relations (CCR); Thus, a Weyl algebra is often called a CCR algebra. The elements of $\mathfrak{W}$ represent the basic

observables of the quantum theory. They are bounded operators, which avoids possible domain problems, and they correspond, formally, to exponentiated field operators $W(f) = \mathrm{e}^{-\mathrm{i}\Phi(f)}$. This interpretation is mathematically well defined in regular representations (see section 2.2.2). Note that, since $\mathscr{V}$ is not given a topology, the elements $W(f)$ need not be continuous. Provided that $\sigma(f,g)$ is non-degenerate, the Weyl algebra is unique in the sense that given two Weyl algebras $\mathfrak{W}_1$ and $\mathfrak{W}_2$ there exists a unique *-isomorphism $\alpha : \mathfrak{W}_1 \to \mathfrak{W}_2$ such that for any $W_1 \in \mathfrak{W}_1$ and $W_2 \in \mathfrak{W}_2$, we have $\alpha \cdot W_1 = W_2$.

States

A state ω on the algebra of observables $\mathfrak{A}$ is a positive, $\omega(A^*A) \geq 0$, normalized, $\omega(\mathbb{1}) = 1$, linear functional $\omega : \mathfrak{A} \to \mathbb{C}$ for all $A \in \mathfrak{A}$. The set of all states is a convex set, i.e., a mixture $\omega := \lambda_1\omega_1 + \cdots + \lambda_n\omega_n$ of states $\omega_1, \ldots, \omega_n$ with $\lambda_i \geq 0$, $\sum \lambda_i = 1$ is again a state. A pure state is extremal in this set in the sense that it cannot be expressed as the sum of two other states with positive coefficients λ_i.

The general definition of states on an algebra is, on the one hand, clear and concise, but on the other hand, far to general for concrete applications. The space of states satisfying these conditions is enormous and requires further criteria that single out subspaces of states that are appropriate for a given physical situation. On a Weyl algebra one typically restricts attention to the class of regular states, which allows to introduce the quantum fields $\Phi(f)$ as self-adjoint generators of the Weyl elements $W(f)$. A further condition is to require the states to be quasi-free, i.e., to be completely specified by their two-point distribution, which makes the set of states tractable without removing most of the physically interesting states. Further conditions that we will use are homogeneity and isotropy, and the Hadamard condition. All these requirements will be introduced in due place.

The algebraic approach makes contact with the traditional Hilbert space formulation of quantum theory via the GNS theorem, which says that every state ω on a C*-algebra $\mathfrak{A}$ gives rise to a representation of $\mathfrak{A}$ on some Hilbert space.

Theorem 2.3 (GNS construction) *Let ω be a state on a C*-algebra $\mathfrak{A}$ with unit-element. Then, there exists a complex Hilbert space $\mathscr{H}_\omega$, a unit-preserving representation π_ω in terms of linear operators on $\mathscr{H}$, and a vector $\Omega_\omega \in \mathscr{H}_\omega$ such that*

$$\omega(A) = \langle \Omega_\omega, \pi_\omega(A)\Omega_\omega \rangle_{\mathscr{H}_\omega} \tag{2.17}$$

for all $A \in \mathfrak{A}$. The vector Ω_ω is cyclic, i.e., $\pi_\omega(\mathfrak{A})\Omega_\omega$ is dense in $\mathscr{H}_\omega$. The representation π_ω is unique up to unitary equivalence.

The triple $(\mathscr{H}_\omega, \pi_\omega, \Omega_\omega)$ is called the GNS triple and the representation is called the GNS representation.

The folium of a state ω is the set of all states that can be represented as density matrices ρ in the GNS representation of ω. So the folium consist of all states of the form

$$\omega(A) = \operatorname{Tr} \rho\pi(A) \ . \tag{2.18}$$

with a positive, trace class, i.e., $\operatorname{Tr} \rho < \infty$, operator ρ. An important theorem due to Fell [Fel60] states that the folium of a faithful representation of a C*-algebra is weakly dense in the set of all states. Since every physical experiment consists of a finite number of measurements and, furthermore, these measurements have limited accuracy, it is impossible to determine more than a weak neighborhood of a state. Thus, by Fell's theorem, it is impossible to find out in which folium the state lies. Note that, since all Weyl algebras are simple [Sim72], all their representations are faithful. For a discussion of further implications of Fell's theorem see [Haa96, Wal94].

The GNS representations of different states need not be unitarily equivalent. In fact, the Stone-von Neumann uniqueness theorem fails for systems with infinitely many degrees of freedom and it is known that infinitely many inequivalent, irreducible Hilbert space representations of the Weyl algebra exist (see, e.g., [Wal94]). Consequently, the folium of a single state does not encompass all possible algebraic states. This is in contrast to the finite case, where all irreducible regular representations, in particular, the Schrödinger and the Heisenberg representation, are unitarily equivalent.

A representation π on $\mathscr{H}_\pi$ of the Weyl algebra $\mathfrak{W}$ is called regular if the unitary groups $\lambda \mapsto \pi(W(\lambda f))$, $\lambda \in \mathbb{R}$ are strongly continuous for all f. If π is regular, one can, by Stone's theorem, introduce self-adjoint infinitesimal generators $\Phi_\pi(f)$ of the Weyl elements, which act on $\mathscr{H}_\pi$. These operators may then be used to define annihilation and creation operators (see theorem 2.5). A state ω on the Weyl algebra $\mathfrak{W}$ is said to be regular if its GNS representation is regular.

An automorphism α on a *-algebra $\mathfrak{A}$ is a one-to-one linear mapping of the algebra onto itself that is compatible with the algebraic structure, i.e., it satisfies $\alpha(A \cdot B) = \alpha(A) \cdot \alpha(B)$ and $\alpha(A^*) = \alpha(A)^*$ for all $A, B \in \mathfrak{A}$. A classical symplectic transformation on $(\mathscr{V}, \sigma)$ is a map that leaves the symplectic form invariant, i.e., a symplectic transformation is given by an operator $\mathcal{T} : \mathscr{V} \to \mathscr{V}$ such that $\sigma(\mathcal{T} f_1, \mathcal{T} f_2) = \sigma(f_1, f_2)$ for all $f_1, f_2 \in \mathscr{V}$. A symplectic transformation on a classical symplectic vector space corresponds directly to an automorphism on the associated Weyl algebra. For example, the time translation on stationary spacetime is implemented on the classical phase $(\mathscr{S}, \sigma_{\mathscr{S}})$ by a one-parameter group of symplectic transformations $\mathcal{T}_t : \mathscr{S} \to \mathscr{S}$, which gives rise to a one-parameter group of automorphisms

$$\alpha_t : \mathfrak{W} \to \mathfrak{W} \ , \quad \alpha_t(W(\phi)) := W(\mathcal{T}_t \phi)) \tag{2.19}$$

for all $\phi \in \mathscr{S}$. We note that a pair $(\mathfrak{A}, \alpha_t)$ of a C*-algebra $\mathfrak{A}$ and a strongly continuous automorphism group $\{\alpha_t\}_{t \in \mathbb{R}}$ acting on $\mathfrak{A}$ is called a C*-dynamical system. This kind of system provides the basis for the definition of KMS states (see section 5.1) and passive states (section 4.1.1).

Given a Hilbert space representation π of $\mathfrak{A}$ on some Hilbert space $\mathscr{H}$, we say that the symplectic transformation $\mathcal{T}$ is unitarily implementable if there exists a unitary transformation $U : \mathscr{H} \to \mathscr{H}$ such that

$$U\pi(A)U^{-1} = \pi(\alpha \cdot A) \tag{2.20}$$

for all $A \in \mathfrak{A}$. While there is no problem with the unitary implementation of time-translations in stationary spacetimes, the situation changes significantly for non-stationary spacetimes. The two-parameter family of symplectic transformations $\mathcal{T}_{t_2,t_1}$, describing time-evolution in that case, gives rise to a family of automorphisms α_{t_2,t_1} on the algebra. However, these automorphisms are no longer implementable as unitary operators on a Fock space, as it has been shown in [TV99] for the Klein-Gordon field on the torus $\mathbb{T}^2$ with non-flat Cauchy surfaces. One may actually conjecture that only transformations defined by the isometry group of a spacetime can be represented as unitary transformations on a Hilbert space.

2.2.1 Hilbert space quantization

In this section, we review the quantization of a linear, scalar field in a formalism that is close to the traditional Hilbert space quantization and directly applicable to curved spacetimes. The formalism starts with a real, symplectic vector space - in our case, the vector space $(\mathscr{S}, \sigma_{\mathscr{S}})$ of solutions to the Klein-Gordon equation. Then, on $(\mathscr{S}, \sigma_{\mathscr{S}})$ an inner product μ with suitable properties is chosen, which gives rise to a map $\boldsymbol{K}$ from $\mathscr{S}$ to a (complex) Hilbert space $\mathscr{H}$. The quantum field theory is then constructed on the symmetric Fock-space $\mathscr{F}_s(\mathscr{H})$ associated to the one-particle space $\mathscr{H}$. We do not give all details of the construction, just the general procedure. The authoritative references caring for all contingencies are [KW91, Wal94].

First, we need to construct an inner product structure on the real, symplectic vector space$(\mathscr{S}, \sigma_{\mathscr{S}})$. So, choose any positive, symmetric, bilinear map $\mu : \mathscr{S} \times \mathscr{S} \to \mathbb{R}$ such that

$$\frac{1}{4}\sigma_{\mathscr{S}}(\phi_1, \phi_2)^2 \leq \mu(\phi_1, \phi_1)\mu(\phi_2, \phi_2) \tag{2.21}$$

for all $\phi_1, \phi_2 \in \mathscr{S}$. Since $\sigma_{\mathscr{S}}$ is non-degenerate, the map μ defines a real inner product on the vector space $\mathscr{S}$.

One can show that there always exists a μ satisfying (2.21), but in a general curved spacetime there is no way to select a preferred one. While in the case of theories with finitely many degrees of freedom different choices of μ lead to unitarily equivalent theories, in the non-finite case the theories turn out to be, in general, unitarily inequivalent. In a stationary spacetime an operator $\boldsymbol{K}$ associated to μ can be defined that projects solutions in $\mathscr{S}$ onto the subspace of 'positive frequency solutions'. These solutions have positive frequency in a generalized sense, namely, with respect to the timelike Killing vector field ξ^μ present in a stationary spacetime [AM75, Kay78, Wal94].

For non-stationary spacetimes there is no unique subspace of positive frequency solutions on which $\boldsymbol{K}$ could project. Nevertheless, one can proceed with a non-unique decomposition of $\mathscr{S}$ by the following results due to Kay and Wald.

Theorem 2.4 ([KW91]) *Let $\mathscr{S}$ be a real vector space on which are defined both a bilinear symplectic form $\sigma_{\mathscr{S}}$ and a bilinear positive symmetric form μ satisfying* (2.21)*. Then, one can always find a complex Hilbert space $\mathscr{H}$ together with a real-linear map $\boldsymbol{K} : \mathscr{S} \to \mathscr{H}$ such that*

(i) the complexified range of $\boldsymbol{K}$, i.e., $\boldsymbol{K}\mathscr{S} + \mathrm{i}\boldsymbol{K}\mathscr{S}$, is dense in $\mathscr{H}$,

(ii) $\mu(\phi_1, \phi_2) = \Re \langle \boldsymbol{K}\phi_1, \boldsymbol{K}\phi_2 \rangle_{\mathscr{H}}$ for all $\phi_1, \phi_2 \in \mathscr{S}$,

(iii) $\sigma_{\mathscr{S}}(\phi_1, \phi_2) = 2\Im \langle \boldsymbol{K}\phi_1, \boldsymbol{K}\phi_2 \rangle_{\mathscr{H}}$ for all $\phi_1, \phi_2 \in \mathscr{S}$.

Moreover, the pair $(\boldsymbol{K}, \mathscr{H})$ is uniquely determined up to equivalence, where we say $(\boldsymbol{K}', \mathscr{H}')$ is equivalent to $(\boldsymbol{K}, \mathscr{H})$ if there exists an isomorphism $V : \mathscr{H} \to \mathscr{H}'$ such that $V\boldsymbol{K} = \boldsymbol{K}'$.

So, to every triple $(\mathscr{S}, \sigma_{\mathscr{S}}, \mu)$ there corresponds a pair $(\mathscr{H}, \boldsymbol{K})$. The pair $(\mathscr{H}, \boldsymbol{K})$ is called a one-particle Hilbert space structure. The equations given in theorem 2.4 are often stated in the form

$$\langle \boldsymbol{K}\phi_1, \boldsymbol{K}\phi_2 \rangle_{\mathscr{H}} = \mu(\phi_1, \phi_2) + \frac{\mathrm{i}}{2}\sigma_{\mathscr{S}}(\phi_1, \phi_2) \ . \tag{2.22}$$

A corresponding operator $\overline{\boldsymbol{K}} : \mathscr{S} \to \overline{\mathscr{H}}$ can be defined which projects into the subspace of 'negative frequency solutions', where $\overline{\mathscr{H}}$ is the complex conjugate Hilbert space to $\mathscr{H}$. To remind the reader, the complex conjugate space $\overline{\mathscr{H}}$ differs from $\mathscr{H}$ by the scalar multiplication: $c \odot f = \overline{c} \cdot f$, $f \in \mathscr{H}$, $c \in \mathbb{C}$, where the bar denotes complex conjugation. One may as well say that an antilinear isometry Γ satisfying $\Gamma^2 = 1$ makes the transition between the spaces $\mathscr{H}$ and $\overline{\mathscr{H}}$. It follows immediately that $\boldsymbol{K} + \overline{\boldsymbol{K}} = \mathbb{1}$.

Once having defined a one-particle structure $\boldsymbol{K}$, the remaining quantization procedure is straightforward. Define by

$$\mathscr{F}_s(\mathscr{H}) := \mathbb{C} \oplus \mathscr{H} \oplus (\mathscr{H} \otimes_s \mathscr{H}) \oplus \dots \tag{2.23}$$

the symmetric Fock space over the one particle Hilbert space $\mathscr{H}$. To each solution in $\mathscr{S}$ a corresponding operator $\sigma_{\mathscr{S}}(\Phi, \cdot)$ on the Fock space $\mathscr{F}_s(\mathscr{H})$ is defined by

$$\sigma_{\mathscr{S}}(\Phi, \phi) := \mathrm{i}a(\boldsymbol{K}\phi) - \mathrm{i}a^*(\boldsymbol{K}\phi) \ , \tag{2.24}$$

where the standard creation and annihilation operators a^*, a on $\mathscr{F}_s(\mathscr{H})$ satisfy

$$[a(\psi), a^*(\psi')] = \langle \psi, \psi' \rangle_{\mathscr{H}} \ , \tag{2.25}$$

$$a(\psi)\Omega = 0 \tag{2.26}$$

for all $\psi, \psi' \in \mathscr{H}$ and the vacuum state $\Omega := \mathbb{1} \oplus \mathbb{0} \oplus \mathbb{0} \oplus \ldots$. This concludes the construction of the quantum field theory.

The quantization scheme presented here, leads directly to a Fock space representation of the algebra. However, as already noted, these representations need not be unitarily equivalent. If $\mu_1 \neq \mu_2$ the resulting representations $\{\mathscr{F}_s(\mathscr{H}_1), \sigma_{\mathscr{S},1}(\Phi, \phi)\}$ and $\{\mathscr{F}_s(\mathscr{H}_2), \sigma_{\mathscr{S},2}(\Phi, \phi)\}$ may be unitarily inequivalent. It follows immediately that different notions of 'particles' arise by different choices of μ. In a spacetime without time translation symmetry no preferred choice for μ exists. On stationary spacetimes, owing to the existence of a timelike Killing field, a satisfactory definition of a preferred μ, and thus a meaningful notion of 'particles' can be given [AM75, Kay78].

The viewpoint taken in algebraic quantum field theory is that unitary equivalence on the level of representations is not fundamental to the quantum theory. Rather, the algebraic relations between the collection of operators $\{\sigma_{\mathscr{S}}(\Phi, \phi)\}$ on $\mathscr{F}_s(\mathscr{H})$ are important. Hence, one postulates that a net of local algebras satisfying these relations completely determines the quantum theory and the fields play a role similar to coordinates in differential geometry: useful tools for daily work, but dispensable for the essential assertions.

Before we come to the algebraic formulation, let us note that there is an alternative procedure for the selection of a representation. Rather than specifying the bilinear form μ, one may define a complex structure J, i.e., a bounded linear map satisfying $J^2 = -\mathbb{1}$, on $\mathscr{S}$ for which $-\sigma(\phi, J\phi)$ is a positive definite inner product. This procedure is, e.g., used in the geometric quantization programme [Woo92]. Its application and importance for quantum field theory in curved spacetimes is illustrated best in a series of papers by Ashtekar and Magnon-Ashtekar [AM75, AMA80a, AMA80b]. Both schemes, the choice of an inner product μ and the choice of a complex structure J are roughly equivalent. See, once more, [Wal94] for details.

2.2.2 The algebra of observables

The Weyl algebra

We have seen how a Fock space representation $\{\mathscr{F}_s(\mathscr{H}), \sigma_{\mathscr{S}}(\Phi, \phi)\}$ of the algebra of observables can be obtained via the choice of a bilinear form $\mu(\phi, \phi)$. Now, a Weyl algebra (see definition 2.2) can be defined through the unitary operators

$$W(\phi) := \mathrm{e}^{-\mathrm{i}\sigma_{\mathscr{S}}(\Phi,\phi)} \ . \tag{2.27}$$

These operators satisfy the Weyl relations

$$W(\phi)^* = W(-\phi) \ , \tag{2.28}$$

$$W(\phi_1)W(\phi_2) = \mathrm{e}^{-\frac{\mathrm{i}}{2}\sigma_{\mathscr{S}}(\phi_1,\phi_2)}W(\phi_1 + \phi_2) \ . \tag{2.29}$$

The C*-completion, which is known to exist, of the space generated by all $W(\phi)$ via formal finite sums $\sum_i \lambda_i W(\phi_i)$ comprises a Weyl algebra, which can be seen as the minimal algebra of observables of a quantum field theory in curved spacetime. This makes

sense, since the Weyl algebras arising from different choices of μ are always isomorphic even if the corresponding Fock space representations are unitarily inequivalent [Sla72].

A second Weyl algebra, which is isomorphic to the former via lemma 2.1, can be constructed as follows. Define using the third property of lemma 2.1 for each $f \in \mathscr{T}$ a smeared operator on $\mathscr{F}_s(\mathscr{H})$ by

$$\Phi(f) := \mathrm{i}a(\boldsymbol{K}(Ef)) - \mathrm{i}a^*(\boldsymbol{K}(Ef)) \ , \tag{2.30}$$

and to consider the Fock space $\{\mathscr{F}_s(\mathscr{H}), \Phi(f)\}$. The operators

$$W(f) := \mathrm{e}^{-\mathrm{i}\Phi(f)} \ , \tag{2.31}$$

where we set $W(f') := W(f)$ if $Ef = Ef'$ again define a Weyl algebra,

$$W(f)^* = W(-f) \ , \tag{2.32}$$

$$W(f_1)W(f_2) = \mathrm{e}^{-\frac{\mathrm{i}}{2}E(f,g)}W(f_1 + f_2) \ , \tag{2.33}$$

where

$$E(f_1, f_2) := \int d^4x f_1 E f_2 = \sigma_{\mathscr{S}}(Ef_1, Ef_2) \ . \tag{2.34}$$

The field algebra An abstract definition of a *-algebra $\mathfrak{A}$ of field operators for a real, linear, scalar field can be obtained as follows. Take the unit $\mathbb{1}$ and the formal smeared field operators $\Phi(f)$, where $f \in \mathscr{D}(\mathcal{M})$ and demand that

(i) $\Phi(f)$ is linear,

(ii) $\Phi(f)$ is hermitian: $\Phi(f) = \Phi(f)^*$,

(iii) $\Phi(f)$ satisfies the field equation: $\Phi([\Box_{\mathfrak{g}} + \mathrm{m}^2]f) = 0$,

(iv) $\Phi(f)$ satisfies the commutation relations. $[\Phi(f_1), \Phi(f_2)] = \mathrm{i}E(f_1, f_2)\mathbb{1}$.

To be precise, one takes the free algebra over the field of complex numbers generated by the symbols $\Phi(f), \Phi(f)^*$, and $\mathbb{1}$ and divides by the *-ideals generated by the properties stated above.

The formal correspondence between the field algebra and the Weyl algebra becomes mathematically well defined in regular GNS representations. For those representations, as already noted, the map $\lambda \mapsto \pi(W(\lambda f) = \pi(\mathrm{e}^{-\mathrm{i}\Phi(\lambda f)})$, $\lambda \in \mathbb{R}$ defines a strongly continuous unitary group for every f. Thus, by Stone's theorem, the operators $\Phi(f)$ are self-adjoint generators of these groups. These generators satisfy the requirements for a *-algebra of fields by lemma 2.1. The collection of all such operators may, equally well as their Weyl counterparts, be interpreted as the collection of fundamental observables of the theory. The same is valid for the collection of $\sigma_{\mathscr{S}}(\Phi, \phi)$ in a regular representation.

2.2.3 Quasi-free states

There is a distinct class of regular algebraic states, namely, the quasi-free states, also known as Gaussian states, which have GNS Hilbert spaces that look like the familiar Fock spaces built on a one-particle Hilbert space (see theorem 2.5 below). The class of quasi-free states contains the usual vacuum states in stationary spacetimes as well as other vacua obtained by mode decomposition of the field operators. In quantum statistical mechanics, quasi-free states represent the general form of equilibrium states for free bosonic systems [BR97, HR97]. Besides this, quasi-free states are well suited for calculations as they are exclusively determined by their two-point distribution.

A quasi-free state can be defined as an abstract linear functional of a special kind on the algebra of observables, or in a regular GNS representation by the requirement that it is completely fixed by the two-point distribution. Let us investigate the first possibility. To define a state on a Weyl algebra $\mathfrak{W}$, it suffices to specify its expectation values on the Weyl operators $W \in \mathfrak{W}$. As before, let μ be a real scalar product on $\mathscr{S}$ and consider the Weyl algebra $\mathfrak{W}(\mathscr{S}, \sigma_{\mathscr{S}})$. Define a functional $\omega_\mu : \mathfrak{W} \to \mathbb{C}$ by

$$\omega_\mu(W(\phi)) = \mathrm{e}^{-\frac{1}{2}\mu(\phi,\phi)} \tag{2.35}$$

for all $\phi \in \mathscr{S}$. Its action is extended to the whole algebra by linearity and continuity. Now, if μ satisfies (2.21) then ω_μ is positive on the whole algebra and thus a state. Any quasi-free state ω_μ can be realized in a representation as the vacuum state in a Fock space by the following theorem.

Theorem 2.5 ([KW91]) *Let $(\boldsymbol{K}, \mathscr{H})$ be the one-particle Hilbert space structure obtained from ω_μ by Theorem 2.4. The GNS-triple $(\mathscr{H}_{\omega_\mu}, \pi_{\omega_\mu}, \Omega_{\omega_\mu})$ of the state ω_μ is equivalent to a triple $(\mathscr{F}(\mathscr{H}), \pi^{\mathscr{F}}, \Omega^{\mathscr{F}})$ with the following properties.*

(i) The GNS space $\mathscr{F}(\mathscr{H}) := \mathscr{F}_s(\mathscr{H})$ is the symmetric Fock space built on $\mathscr{H}$.

(ii) The representation $\pi^{\mathscr{F}}$ is specified by $\pi^{\mathscr{F}}(W(\phi)) = \mathrm{e}^{-\overline{[a(\boldsymbol{K}\phi) - a^*(\boldsymbol{K}\phi)]}}$, where the bar denotes the closure.

(iii) The state $\Omega^{\mathscr{F}} := \mathbb{1} \oplus \mathbb{0} \oplus \mathbb{0} \oplus \dots$ is the (cyclic) Fock vacuum in $\mathscr{F}_s(\mathscr{H})$.

The purity of ω_μ is equivalent to the irreducibility of the representation $\pi^{\mathscr{F}}$. Moreover this is equivalent to the property that $\boldsymbol{K}\mathscr{S}$ alone, rather than $\boldsymbol{K}\mathscr{S} + \mathrm{i}\boldsymbol{K}\mathscr{S}$, is dense in $\mathscr{H}$ [KW91].

The two-point distribution of a quantum field in the state ω on the Weyl algebra $\mathfrak{W}(\mathscr{S}, \sigma_{\mathscr{S}})$ is defined by

$$\langle \sigma_{\mathscr{S}}(\Phi, \phi_1) \sigma_{\mathscr{S}}(\Phi, \phi_2) \rangle_\omega := -\frac{\partial^2}{\partial s \partial t} \left(\omega(W(s\phi_1 + t\phi_2)) \mathrm{e}^{-\mathrm{i}st\sigma(\phi_1,\phi_2)/2} \right) \Big|_{s=t=0} \tag{2.36}$$

provided that the right hand side exists. For quasi-free states, as defined by (2.35) the two-point distribution always exists and is given by

$$\omega^{(2)}(\phi_1, \phi_2) = \mu(\phi_1, \phi_2) + \frac{\mathrm{i}}{2}\sigma_{\mathscr{S}}(\phi_1, \phi_2) \ . \tag{2.37}$$

If one works with the field algebra of operators $\Phi(f)$, a quasi-free state ω can be defined, by the requirement that all odd n-point distributions vanish and the even ones are determined by the two-point distribution via the the recursion formula

$$\omega^{(2j)}(\Phi(f_1), \ldots, \Phi(f_{2j})) := \sum_{\sigma} \prod_{i=1}^{j} \omega^{(2)}(f_{\sigma(i)}, f_{\sigma(i+j)}) \tag{2.38}$$

for $j \in \mathbb{N}$, where the sum is taken over all permutations σ of $\{1, 2, \ldots, 2j\}$ with $\sigma(1) < \sigma(2) < \cdots < \sigma(j)$ and $\sigma(i) < \sigma(i+j), i = 1, \ldots, j$.

According to theorem 2.5, the two-point distribution $S(f_1, f_2)$ of a quasi-free state can be calculated in the GNS representation by

$$\begin{aligned} S(f_1, f_2) &:= \left\langle \Omega^{\mathscr{F}}, \Phi(f_1)\Phi(f_2)\Omega^{\mathscr{F}} \right\rangle && (2.39)\\ &= \langle \boldsymbol{K}Ef_1, \boldsymbol{K}Ef_2 \rangle_{\mathscr{H}} && (2.40)\\ &= \mu(Ef_1, Ef_2) + \frac{\mathrm{i}}{2}\sigma(Ef_1, Ef_2) && (2.41) \end{aligned}$$

Thus $S(f, f) = \mu(Ef, Ef) = \langle \boldsymbol{K}Ef, \boldsymbol{K}Ef \rangle_{\mathscr{H}}$ for $f \in \mathscr{D}(\mathcal{M})$ and we see that we can define the generator (2.35) of a quasi-free state either by the use of μ, S, or $\langle\ ,\ \rangle_{\mathscr{H}}$.

Saturating the inequality (2.21) turns out to be equivalent to the irreducibility of the GNS representation arising from ω_μ. Thus, (remember the comments after theorem 2.5) such a μ results in pure quasi-free states. However, already in stationary spacetimes, thermal equilibrium states at finite temperature are represented by quasi-free states which fail to satisfy the saturated version of (2.21), and in a spacetime with a non-compact Cauchy surface, states in the folium of a thermal equilibrium state do not, in general, lie in the folium of any pure quasi-free state [Wal94]. Thus, in order to incorporate thermal states, we cannot restrict ourselves to the case of pure states. Note that the common notion of a 'vacuum state' or, more generally, ground state corresponds to a pure, quasi-free state in the algebraic approach. We note that all pure, quasi-free state are Fock states and thus related through a Bogoliubov transformation [MV68].

2.2.4 Hadamard states

Even in the restricted class of quasi-free states there exist many states that cannot be considered physical; this should not be misunderstood as the statement that all physical states are quasi-free. A further condition that is believed to reasonably narrow down the class of states is the Hadamard condition. It has several formulations and was used

already for a long time (see, e.g., [DB60]) before Kay and Wald [KW91] put it on a sound mathematical foundation. The Hadamard condition essentially restricts the singularity structure of the two-point distribution at coinciding points such that it comes close the Minkowski vacuum state. On a heuristic level, one could say that in a Hadamard state the high frequency modes of the field are 'close' to their ground state.

The principle motivation for the Hadamard condition comes from the point-splitting renormalization scheme. The absence of a preferred vacuum state makes the normal ordering procedure of standard quantum field theory nonviable in a general curved spacetime. The point-splitting prescription is a replacement for normal ordering in the sense that it defines sensibly differences of stress-energy expectation values even in curved spacetime.

The basic idea is as follows. The calculation of the stress-energy tensor involves the calculation of objects like $\langle\phi(x)^2\rangle$. These objects are, in general, ill defined as they involve the calculation of products of two distributions at a point. Such products are only well defined in special cases, where the wavefront sets (see below) of the involved distributions 'fit' to each other [Hör03]. The point-split object $\langle\phi(x)\phi(x')\rangle$, however, makes sense as a bi-distribution on $\mathcal{M}$. Now, one demands that for physically reasonable states the singularity structure of $\langle\phi(x)\phi(x')\rangle$ as x' approaches x should be the same as for $\langle\Omega, \phi(x)\phi(x')\Omega\rangle$. This provided, the difference $\langle\phi(x)\phi(x')\rangle - \langle\Omega, \phi(x)\phi(x')\Omega\rangle$ is a smooth function, which allows taking the coincidence limit $x' \to x$.

States satisfying the Hadamard condition yield a renormalized stress-energy tensor $\boldsymbol{T}_{\mu\nu}$ that satisfies Wald's axioms [Wal94], which are believed to be reasonable physical assumptions on $\boldsymbol{T}_{\mu\nu}$. In brief, the assumptions are as follows. For states $\omega, \omega_1, \omega_2$:

(i) $\langle\boldsymbol{T}_{\mu\nu}\rangle_{\omega_1} - \langle\boldsymbol{T}_{\mu\nu}\rangle_{\omega_2}$ should be well defined by the point splitting procedure.

(ii) $\boldsymbol{T}_{\mu\nu}$ should be locally covariant.

(iii) $\langle\boldsymbol{T}_{\mu\nu}\rangle_{\omega}$ should be conserved, $\nabla^\mu \langle\boldsymbol{T}_{\mu\nu}\rangle_{\omega} = 0$, for all states ω.

(iv) In Minkowski spacetime, $\langle\Omega, \boldsymbol{T}_{\mu\nu}\Omega\rangle_{\omega} = 0$.

These assumptions fix the expectation value $\langle\boldsymbol{T}_{\mu\nu}\rangle_{\omega}$ uniquely up to a conserved local curvature term that is independent of ω. Actually, it is possible to locally construct a bi-distribution $\boldsymbol{H}(x, x')$ such that if

$$\boldsymbol{F}_\omega(x, x') := \langle\phi(x)\phi(x')\rangle_{\omega} - \boldsymbol{H}(x, x') \tag{2.42}$$

is a smooth function for a state ω then $\langle\boldsymbol{T}_{\mu\nu}\rangle_{\omega}$ is well defined. We refer the reader to [Wal94] for subtleties of the construction.

It has not only been proved that there exist many Hadamard states for the linear, scalar field in a globally hyperbolic spacetime; One also knows that the canonical ground state and the thermal equilibrium states in stationary, globally hyperbolic spacetimes are quasi-free Hadamard states [SV00]. Regarding interacting fields, the construction

of renormalized perturbative quantum field theory in a generic spacetime is possible for Hadamard states [BF00, HW01]. On the other hand, only few Hadamard states on curved spacetimes have been explicitly constructed. Among these are the ground states on ultrastatic spacetimes [FNW81, Jun96] and KMS states on ultrastatic spacetimes with compact Cauchy surfaces; Furthermore, we mention the adiabatic vacuum states of infinite order [Jun96, Jun02]. None of these examples deals with thermal states on a non-stationary spacetime.

The formulation by Kay

and Wald Let $t(x)$ be a any global time function that increases towards the future and let $t(x,x') := t(x) - t(x')$. Furthermore, let $\sigma(x,x')$ be the squared geodesic distance, i.e.,

$$\sigma(x,x') = \pm \left(\int_\gamma \left| \mathfrak{g}_{\mu\nu}(y(\tau)) \frac{dy^\mu(\tau)}{d\tau} \frac{dy^\nu(\tau)}{d\tau} \right|^{\frac{1}{2}} \mathrm{d}\tau \right)^2 , \tag{2.43}$$

where γ is the unique geodesic connecting x and x' with parametrization $y(\cdot)$ and the sign is plus for spacelike $y(\cdot)$ and minus for timelike $y(\cdot)$. The geodesic distance is well defined and smooth in the set $\mathcal{O}$ in $\mathcal{M} \times \mathcal{M}$, which is taken to be a neighborhood of the set of causally related points (x,y) such that $J^+(x) \cap J^-(y)$ and $J^+(y) \cap J^-(x)$ are contained within a convex normal neighborhood. A convex normal neighborhood of a point x is a neighborhood $\mathcal{U}$ of x such that there exists a unique geodesic connecting each pair of points in $\mathcal{U}$ and staying entirely within $\mathcal{U}$. A manifold can always be covered by such neighborhoods [HE73].

For each $n \in \mathbb{N}$ and $\epsilon \in \mathbb{R}, \epsilon > 0$ define a complex-valued function in $\mathcal{O}$ by

$$G_\epsilon^{t,n}(x,x') = \frac{1}{(2\pi)^2} \left(\frac{u(x,x')}{\sigma_\epsilon^t(x,x')} + v^{(n)}(x,x') \ln \sigma_\epsilon^T(x,x') \right) , \tag{2.44}$$

where

$$\sigma_\epsilon^t(x,x') = \sigma(x,x') + 2\mathrm{i}\epsilon t(x,x') + \epsilon^2 . \tag{2.45}$$

The smooth function $u(x,x')$ is the square root of the van Vleck-Morette determinant, and $v^{(n)}(x,x') \in \mathscr{E}(\mathcal{O})$ is a real function defined by the power series

$$v^{(n)}(x,x') := \sum_{m=0}^{n} v_m(x,x') \sigma(x,x')^m , \tag{2.46}$$

where the $v_m(x,x')$ are determined by the Hadamard recursion relations. The branch cut for the logarithm is taken to lie along the negative real axis. The field equations and commutation relations require that u and v are uniquely determined by the local geometry, i.e., by the metric $\mathfrak{g}_{\mu\nu}$ and its derivatives. Of course, $G_\epsilon^{t,n}(x,x')$ is singular for coinciding points x and x', but it is also singular for points connected by a null geodesic.

Let Σ be a Cauchy surface and let $\mathcal{N}$ be a causal normal neighborhood of Σ [KW91]. Denote by $\mathcal{O}'$ an open neighborhood in $\mathcal{N}\times\mathcal{N}$ of the set of causally related points such that the closure of $\mathcal{O}'$ in $\mathcal{N}\times\mathcal{N}$ is contained in $\mathcal{O}$. Now, define a function $\chi(x,x')\in\mathscr{E}(\mathcal{N}\times\mathcal{N})$ with the property

$$\chi(x,x')=\begin{cases}0\ , & \text{for } (x,x')\notin\mathcal{O}\\ 1\ , & \text{for } (x,x')\in\mathcal{O}'\ .\end{cases} \tag{2.47}$$

A state ω is said to be a Hadamard state if its two-point distribution satisfies the following requirement: for each $n\in\mathbb{N}$ there exists a C^n-function $w^n(x,x')$ on $\mathcal{N}\times\mathcal{N}$ such that for all $f_1,f_2\in\mathscr{D}(\mathcal{N})$ we have

$$S(f_1,f_2)=\lim_{\epsilon\to 0}\int\limits_{\mathcal{N}\times\mathcal{N}} d\mu(x)\ d\mu(x')f_1(x)f_2(x')\ \Lambda_\epsilon^{t,n}(x,x')\ , \tag{2.48}$$

where

$$\Lambda_\epsilon^{t,n}(x,x')=\chi(x,x')G_\epsilon^{t,n}(x,x')+w^n(x,x') \tag{2.49}$$

and the measures are the induced measures $d\mu(x):=d^4x\sqrt{|\mathfrak{g}|}$. The functions $w^n(x,x')$ depend on the individual state in the folium. Note that the function $\chi(x,x')$ introduces a localization of the singular object $G_\epsilon^{t,n}(x,x')$ in spacetime, which has the consequence that the Hadamard condition only cares for the ultraviolet modes of a field.

The microlocal formulation

For linear quantum fields the microlocal spectrum condition, which we will state below, is equivalent to the Hadamard condition. This has been shown by Radzikowski [Rad92, Rad96]. The microlocal spectrum condition has been investigated and extended to curved spacetimes and Wick powers of scalar fields in [BFK96]. In this sense, it is more general than the original Hadamard condition as it also can be generalized to non-linear fields. Microlocal analysis shifts the study of singularities of distributions from the base space to the cotangent bundle. The 'micro-localization' property makes this formulation well suited for curved spacetimes.

We define the notion of wavefront sets by first introducing the set of regular directed points. Let $u\in\mathscr{D}'(\mathbb{R}^n)$ be a distribution. A point (x,ξ) in the cotangent bundle of $\mathbb{R}^n$ is called a regular directed point of u if there exists a smooth function $\phi\in\mathscr{D}(X)$, $X\subset\mathbb{R}^n$ which does not vanish at x and such that for any $m\in\mathbb{N}$ there exists a constant B_m satisfying

$$|\widetilde{\phi u}(\xi')|\leq B_m(1+|\xi'|)^{-m} \tag{2.50}$$

for all ξ' in a conical neighborhood $U\subset\mathbb{R}^n\backslash\{0\}$ of ξ. A neighborhood U is called conical if $\xi\in U\ \Rightarrow\ t\xi\in U, t\in\mathbb{R}^+$. Now the wavefront set $\mathrm{WF}(u)$ of a distribution $u\in\mathscr{D}'(X)$ is the complement in $X\times\mathbb{R}^n\backslash\{0\}$ of the space of all regular directed points of u.

Theorem 2.6 (Microlocal spectrum condition) *A quasi-free state ω of the Klein-Gordon field on globally hyperbolic spacetime $\mathcal{M}$ is a (global) Hadamard state if and only if its two-point distribution has the wave-front set*

$$\mathrm{WF}(\omega^{(2)}(x_1, x_2)) = C^+ \ , \tag{2.51}$$

where

$$C^+ = \left\{ [(x_1, \xi_1), (x_2, \xi_2)] \in (T^*(\mathcal{M})\backslash 0) \times (T^*(\mathcal{M})\backslash 0); (x_1, \xi_1) \sim (x_2, -\xi_2); \xi_1^0 \geq 0 \right\} \ . \tag{2.52}$$

The notation $(x_1, \xi_1) \sim (x_2, \xi_2)$ means that x_1 and x_2 can be connected by a null geodesic such that ξ_1^μ is tangential to γ at x_1 and ξ_2^μ is the parallel transport of ξ_1^μ along γ at x_2.

So, singularities in the two-point distribution $\omega^{(2)}(x, x')$ only occur if x and x' are lightlike connected and the singularities have positive frequencies.

Wavefront sets have the property that for two distributions u, v it holds that

$$\mathrm{WF}(u + v) \subseteq \mathrm{WF}(u) \cup \mathrm{WF}(v) \ . \tag{2.53}$$

Thus, $\mathrm{WF}(u) \subseteq \mathrm{WF}(u - v) \cup \mathrm{WF}(v)$ and $\mathrm{WF}(u) = \mathrm{WF}(v)$ if $\mathrm{WF}(u - v) = \emptyset$, i.e., the distributions u and v have the same wavefront set, and hence the same singularity structure if the difference of u and v is a smooth function.

3 Scalar fields in Robertson-Walker spacetimes

Robertson-Walker spacetimes are a particularly important class of spacetimes to investigate. They are homogeneous and isotropic solutions of the Einstein equations. These assumptions on the geometry of spacetime determine the solutions up to three discrete types of spatial geometry – flat, closed, and open geometry – and an arbitrary positive function $a(t)$, which determines the expansion of the spacelike sections. Although these spacetimes do not possess a time evolution symmetry, they possess a preferred class of observers, namely, the ones who are orthogonal to the homogeneous surfaces. These are also called isotropic (or comoving) observers. Owing to the present symmetries, the field can be written, in the usual way, as an integral (or sum, for the closed geometry) over modes. The spatial dependence of the modes is known explicitly, but the time dependent part does not acquire the usual form $e^{\pm i\omega t}$. Rather, it satisfies a certain differential equation with time-dependent coefficients. A determination of solutions to this equation is possible by a method motivated by a WKB type approximation. This led Parker to define the adiabatic vacuum states [Par69]. The adiabatic vacuum states are defined such that the particle creation is minimized in an expanding universe. Later, the adiabatic vacuum states were redefined by Lüders and Roberts [LR90] in a more rigorous setting of quantum field theory in curved spacetime.

In this chapter we introduce, first, the quantum theory of the scalar field in the formulation used in [LR90]. We also give a brief account of adiabatic vacuum states. Then, we quote the important theorem on the general form of the two-point distribution of a homogeneous, isotropic, quasi-free state for the scalar field in Robertson-Walker spacetime. Finally, we calculate, as a preparation for the construction the almost equilibrium states, a 'four-smeared' version of the two-point distribution.

3.1 The algebra and the states

We have seen in chapter 2 how the Weyl algebra or the field algebra for a quantum field is constructed in a general, curved spacetime. There is an alternative way to obtain the algebra of observables, which goes back to Araki, namely, by constructing a self-dual algebra [Ara68, AS72, AY82]. The self-dual algebra is a different route to the construction of the CCR algebra, distinguished by the fact that one chooses a different set of generators that act on a complex vector space $\mathscr{K}$. This approach is used in [LR90],

where the Weyl algebra associated to a self-dual algebra is is taken as the algebra of observables.

The self-dual algebra

A self-dual algebra is based on a phase space triple $(\mathscr{K}, \Gamma, \boldsymbol{\gamma})$, where $\mathscr{K}$ is a complex linear space, Γ is an antilinear involution of $\mathscr{K}$, and $\boldsymbol{\gamma}$ is a Hermitian form on $\mathscr{K}$ satisfying

$$\boldsymbol{\gamma}(\Gamma f, \Gamma g) = -\boldsymbol{\gamma}(f, g)^* \ . \tag{3.1}$$

The space $\mathscr{K}$ serves as the test function space for creation and annihilation operators. The indefinite inner product $\boldsymbol{\gamma}(f, g)$ gives rise to the canonical commutation relations and the involution Γ combines complex conjugation with the interchange of test functions for creation and annihilation operators [AY82].

For the Klein-Gordon field on a globally hyperbolic spacetime $(\mathcal{M}, \mathfrak{g}_{\mu\nu})$ one defines

$$\mathscr{K} := \mathscr{D}(\mathcal{M})/[(\Box_{\mathfrak{g}} + \mathrm{m}^2)\mathscr{D}(\mathcal{M})] \ , \tag{3.2}$$

$$\boldsymbol{\gamma}(f, g) := \mathrm{i}G(\bar{f}, g) \ , \tag{3.3}$$

where $G(f, g) := \int d^4x \ fEg$, $f, g \in \mathscr{K}$, and Γ is defined by the requirement

$$\Gamma f = \bar{f} \ . \tag{3.4}$$

Note that $\mathscr{D}(\mathcal{M}) := \mathrm{C}_0^\infty(\mathcal{M})$ is a space of complex functions, as opposed to the space of real functions used in the construction in chapter 2, and the fundamental solution E is defined in equation (2.7). Equation (3.2) ensures that the corresponding field satisfies the Klein-Gordon equation. The involution Γ satisfies (3.1) by the properties of the Green's function $G(f, g)$.

On the phase space $(\mathscr{K}, \Gamma, \boldsymbol{\gamma})$ one constructs the self-dual CCR algebra $\mathfrak{A}(\mathscr{K}, \Gamma, \boldsymbol{\gamma})$ as follows. First, consider the complex, free, *-algebra over $\mathscr{K}$ generated by the symbols $\phi(f)$, their conjugates $\phi(f)^*$, and the identity $\mathbb{1}$, where $f \in \mathscr{K}$. Then, take the quotient of it by the two-sided *-ideal that is generated by the relations

$$\phi(f) \text{ is complex linear in } f \ , \tag{3.5}$$

$$\phi(f)^*\phi(g) - \phi(g)\phi(f)^* = \boldsymbol{\gamma}(f, g)\mathbb{1} \ , \tag{3.6}$$

$$\phi(\Gamma f)^* = \phi(f) \ . \tag{3.7}$$

for $f, g \in \mathscr{K}$. In order to circumvent problems with unbounded operators, one passes, as usual, from $\mathfrak{A}(\mathscr{K}, \Gamma, \boldsymbol{\gamma})$ to an associated Weyl algebra. The Weyl algebra $\mathfrak{W}(\mathscr{K}_{\Re}, \mathrm{i}\boldsymbol{\gamma})$ is based on the real linear space $\mathscr{K}_{\Re} := \{f \in \mathscr{K} : \Gamma f = f\}$ equipped with the real symplectic form $\mathrm{i}\boldsymbol{\gamma}(f, g)$:

$$W(f)W(g) = \mathrm{e}^{-\frac{1}{2}\boldsymbol{\gamma}(f,g)}W(f + g) \ . \tag{3.8}$$

Note that this is formally equal to (2.32) if $\mathscr{K}_{\Re}$ coincides with $\mathscr{T}$. A net of C*-algebras is obtained by taking $\mathfrak{A}(\mathcal{O})$ to be the C*-subalgebra generated by the Weyl elements $W(f)$, $f \in \mathscr{D}(\mathcal{M})$ with $\operatorname{supp} f \subset \mathcal{O}$.

Quasi-free states

A quasi-free state for a real, linear, scalar field is specified by its two-point distribution

$$S(f,g) = \omega_S(\phi(f)^*\phi(g)) \tag{3.9}$$

for $f, g \in \mathscr{K}$. This two-point distribution may be seen as a complex scalar product on the space $\mathscr{K}$. It specifies the corresponding quasi-free state in terms of Weyl operators by

$$\omega_S(W(f)) := e^{-\frac{1}{2}S(f,f)} \ . \tag{3.10}$$

The two-point distribution of a quasi-free state is a polarization on the phase space $(\mathscr{K}, \Gamma, \boldsymbol{\gamma})$. This means that $S(\cdot,\cdot)$ is a positive Hermitian form on $\mathscr{K}$ such that

$$S(f,g) - S(\Gamma g, \Gamma f) = \boldsymbol{\gamma}(f,g) \ . \tag{3.11}$$

Given $S(\cdot,\cdot)$ one defines a scalar product $(\cdot,\cdot)_S$ on $\mathscr{K}$ by

$$(f,g)_S = S(f,g) + S(\Gamma g, \Gamma f) \tag{3.12}$$

so that by the Schwarz inequality and the triangle inequality one obtains [AS72]

$$|\gamma(f,g)|^2 \leq (f,f)_S \ (g,g)_S \ , \tag{3.13}$$

which is the complex version of (2.21).

It is remarkably easy to characterize pure, quasi-free states in this scheme. Namely, denote by $\mathscr{K}_S$ the Hilbert space completion of $\mathscr{K}$ by $(\cdot,\cdot)_S$. On $\mathscr{K}_S$ we have an operator $\hat{S}$ satisfying $(f, \hat{S}g)_S = S(f,g)$. The state ω_S is a pure quasi-free state if and only if $\hat{S}$ is a basis projection on $\mathscr{K}_S$ [AS72].

3.2 The spacetime and the field

As already noted, Robertson-Walker spacetimes are homogeneous and isotropic solutions to the Einstein equations. They are globally hyperbolic Lorentzian manifolds with topology $\mathcal{M}^\varepsilon = \mathbb{R} \times \Sigma^\varepsilon$, where $\varepsilon = 0, +1, -1$ discriminates three types of spacelike hypersurfaces. The Cauchy surfaces Σ^ε are homogeneous Riemannian manifolds with constant curvature of sign ε. The homogeneous and isotropic spacetimes can be endowed with the Robertson-Walker metrics

$$ds^2 = dt^2 - \mathrm{a}(t)^2 \left[\frac{dr^2}{1-\varepsilon r^2} + r^2 \left(d\theta^2 + \sin^2\theta \ d\varphi^2 \right) \right] \ , \tag{3.14}$$

where the coordinates cover the ranges $r \in [0,\infty)$, $\theta \in [0,\pi]$, $\varphi \in [0, 2\pi]$ for $\varepsilon = 0, -1$ and $r \in [0,1]$ for $\varepsilon = +1$. The function $\mathrm{a}(t)$ is a strictly positive, smooth function describing the expansion of the universe, and $H(t) = \frac{\dot{\mathrm{a}}(t)}{\mathrm{a}(t)}$ is the Hubble parameter.

The induced metric on the Cauchy surfaces can be written as

$$ds^2 = dt^2 - \mathrm{a}(t)^2 \mathfrak{s}^{\varepsilon}_{ij} dx^i dx^j \ , \tag{3.15}$$

where we wrote the induced metric on the Cauchy surface as $\mathfrak{h}^{\varepsilon}_{ij}(t) = \mathrm{a}(t)^2 \mathfrak{s}^{\varepsilon}_{ij}$. Note that the metric $\mathfrak{h}_{ij}$ is time-dependent while $\mathfrak{s}_{ij}$ is not. We use Σ to denote the manifold with metric $\mathfrak{s}_{ij}$, while Σ_t is endowed with the metric $\mathfrak{h}_{ij}$. The future directed normal fields of all the hypersurfaces Σ^{ε} are given by $n^{\mu} = (1, 0, 0, 0)$. These fields are geodesic, i.e., $n^{\mu} \nabla_{\mu} n^{\nu} = 0$.

It is convenient to regard the Cauchy surfaces Σ^{ε} as being embedded in $\mathbb{R}^4$ by

$$\Sigma^0 = \left\{ x \in \mathbb{R}^4 : x^0 = 0 \right\} , \tag{3.16}$$

$$\Sigma^+ = \left\{ x \in \mathbb{R}^4 : (x^0)^2 + \sum_{i=1}^{3} (x^i)^2 = 1 \right\} , \tag{3.17}$$

$$\Sigma^- = \left\{ x \in \mathbb{R}^4 : (x^0)^2 - \sum_{i=1}^{3} (x^i)^2 = 1 \ , x^0 > 0 \right\} . \tag{3.18}$$

Generally speaking, one calls the spacetime $\mathcal{M}^+$ a closed universe since Σ^+ is compact. It is also customary to call $\mathcal{M}^-$ and $\mathcal{M}^0$ open and flat universes, respectively. Each of the Cauchy surfaces Σ^{ε} is a homogeneous surface for a different symmetry group $\boldsymbol{G}^{\varepsilon}$. In detail, these are the groups: $\boldsymbol{G}^0 = \boldsymbol{E}(3)$, the Euclidean group; $\boldsymbol{G}^+ = \boldsymbol{SO}(4)$, the rotation Group; and $\boldsymbol{G}^- = \mathcal{L}^{\uparrow}_{+}(4)$, the Lorentz group.

The field equation

In Robertson-Walker spacetimes the Klein-Gordon equation (2.2) becomes

$$\frac{\partial^2}{\partial t^2}\phi(t, \mathbf{x}) + 3H(t)\frac{\partial}{\partial t}\phi(t, \mathbf{x}) + (-\Delta_{\mathfrak{h}} + m^2)\phi(t, \mathbf{x}) = 0 \ , \tag{3.19}$$

where $\Delta_{\mathfrak{h}}$ denotes the Laplacian on Σ^{ε}_t. If one assumes that the field modes $u_{\mathbf{k}}(x) = \overline{T}_{\mathrm{k}}(t) Y_{\mathbf{k}}(\mathbf{x})$ and their complex conjugates form a complete orthonormal basis, the general solution of the Klein-Gordon equation can be written as

$$\phi(t, \mathbf{x}) = \int \mathrm{d}\mathbf{k} \left[\overline{T}_{\mathrm{k}}(t) Y_{\mathbf{k}}(\mathbf{x}) a(\mathbf{k}) + T_{\mathrm{k}}(t) \overline{Y}_{\mathbf{k}}(\mathbf{x}) a(\mathbf{k})^* \right] \ . \tag{3.20}$$

We think of $a(\mathbf{k}), a(\mathbf{k})^*$ as arbitrary complex coefficients with no reference to particles. This decomposition of the field is valid on all types of Robertson-Walker spacetimes if one defines the measure $\mathrm{d}\mathbf{k}$ accordingly. Our notation is as follows:

$$\varepsilon = 0 \quad : \qquad \int \mathrm{d}\mathbf{k} := \int_{\mathbb{R}^3} d^3\mathbf{k} \ , \qquad \mathbf{k} := (k_1, k_2, k_3) \in \mathbb{R}^3, \ \mathrm{k} := |\mathbf{k}| \ , \tag{3.21a}$$

$$\varepsilon = +1 : \qquad \int \mathrm{d}\mathbf{k} := \sum_{\mathrm{k}=0}^{\infty} \sum_{l=0}^{\mathrm{k}} \sum_{m=-l}^{l} , \qquad \mathbf{k} := (\mathrm{k}, l, m) \in \mathbb{N} \times \mathbb{N} \times \mathbb{Z} \ , \tag{3.21b}$$

$$\varepsilon = -1 : \qquad \int \mathrm{d}\mathbf{k} := \int_{\mathbb{R}^3} d^3\mathbf{k} \ , \qquad \mathbf{k} := (k_1, k_2, k_3) \in \mathbb{R}^3, \ \mathrm{k} := |\mathbf{k}| \ . \tag{3.21c}$$

Note the subtle difference in notation between the absolute value of the three-momentum, $\mathrm{k} := |\mathbf{k}|$, and the four-momentum $k := (k_0, k_1, k_2, k_3) = (k_0, \mathbf{k})$. The functions $T_{\mathrm{k}}(t)$ depend on k and the functions $Y_{\mathbf{k}}(\mathbf{x})$ depend on $\mathbf{k}$.

Homogeneous, isotropic, quasi-free states

The groups $\boldsymbol{G}^{\varepsilon}$, act as isometry groups on the manifolds $\mathcal{M}^{\varepsilon} := \mathbb{R} \times \Sigma^{\varepsilon}$ by $\mathrm{g}(t, \mathbf{x}) = (t, \mathrm{g}\mathbf{x})$, $\mathrm{g} \in \boldsymbol{G}^{\varepsilon}$. It follows that they must commute with the fundamental solution E and thus act as a group of transformations on the phase space. In turn, this defines a group of (Bogoliubov) automorphisms $\{\alpha_{\mathrm{g}}\}$ on the Weyl algebra via

$$\alpha_{\mathrm{g}}(W(f)) := W(\mathrm{g}f) \tag{3.22}$$

for $\mathrm{g} \in \boldsymbol{G}^{\varepsilon}$. Now, we say that a state ω is homogeneous and isotropic if $\omega \circ \alpha_{\mathrm{g}} = \omega$, $\mathrm{g} \in \boldsymbol{G}^{\varepsilon}$. Since a quasi-free state ω_S is, by definition, uniquely determined by its two-point distribution $S(f_1, f_2)$, this translates to the necessary and sufficient condition

$$S(\mathrm{g}f_1, \mathrm{g}f_2) = S(f_1, f_2) \tag{3.23}$$

for all $\mathrm{g} \in \boldsymbol{G}^{\varepsilon}$. The $\boldsymbol{G}$-invariance of the two-point distribution is analyzed in [LR90] by passing to the phase space $(\hat{\mathscr{M}}, \hat{\sigma})$ of initial data for $\phi(x)$ at time t, where

$$\hat{\mathscr{M}} := \{(u, \mathrm{a}(t)^3 p), u, p \in \mathscr{D}(\Sigma, \mathbb{R})\} \tag{3.24}$$

and the symplectic form is a variant of (2.16):

$$\hat{\sigma}(F_1, F_2) := \mathrm{a}(t)^3 \int_{\Sigma} \mathrm{d}\mathbf{x} \, (p_1 u_2 - u_1 p_2) \tag{3.25}$$

for $F_i := (u_i, \mathrm{a}(t)^3 p_i) \in \hat{\mathscr{M}}$, $i = 1, 2$, where $\mathrm{d}\mathbf{x} = d^3x\sqrt{|\mathfrak{s}|}$. Please note that $\hat{\sigma}$ is defined using the measure derived from $\mathfrak{s}_{ij}$ and not from $\mathfrak{h}_{ij}$.

By introducing suitable topologies on $\hat{\mathscr{M}}$, one finds that it is sufficient to compute the commutants of the unitary representations U^ε of $\boldsymbol{G}^\varepsilon$ on $\mathrm{L}^2(\Sigma)$ given by $U^\varepsilon_{\mathrm{g}} f := f \circ \mathrm{g}^{-1}$, $f \in \mathscr{D}(\Sigma)$ [LR90]. The representations U^ε are decomposed into irreducible representations by (generalized analogues to) Fourier transforms

$$\tilde{f}(\mathbf{k}) := \int \mathrm{d}\mathbf{x}\ \overline{Y}_{\mathbf{k}}(\mathbf{x}) f(\mathbf{x}) \tag{3.26}$$

for $f \in \mathrm{L}^2(\Sigma)$. In each case, the Fourier transform is a unitary operator from $\mathrm{L}^2(\Sigma^\varepsilon)$ to $\mathrm{L}^2(\widetilde{\Sigma}^\varepsilon)$, where $\widetilde{\Sigma}^\varepsilon$ denotes the momentum space associated to Σ^ε. And, again in each case, a bounded operator on $\mathrm{L}^2(\Sigma^\varepsilon)$ commuting with U^ε corresponds on $\mathrm{L}^2(\Sigma^\varepsilon)$ to a multiplication by a bounded function of k.

The functions $Y_{\mathbf{k}}(\mathbf{x})$ constitute an orthonormal basis of eigenfunctions of the Laplacian $\Delta_{\mathfrak{s}}$ in $\mathrm{L}^2(\Sigma)$ (see below for the precise forms). The inverse Fourier transform is given by

$$f(\mathbf{x}) = \int \mathrm{d}\mathbf{k}\ Y_{\mathbf{k}}(\mathbf{x}) \tilde{f}(\mathbf{k}) \tag{3.27}$$

and one has the usual completeness relations

$$\int \mathrm{d}\mathbf{k}\ Y_{\mathbf{k}}(\mathbf{x}) \overline{Y}_{\mathbf{k}}(\mathbf{x}') = \delta(\mathbf{x}, \mathbf{x}')\ , \tag{3.28}$$

$$\int \mathrm{d}\mathbf{x}\ Y_{\mathbf{k}}(\mathbf{x}) \overline{Y}_{\mathbf{k}'}(\mathbf{x}) = \delta(\mathbf{k}, \mathbf{k}')\ . \tag{3.29}$$

The $\delta(\mathbf{k}, \mathbf{k}')$-distribution is to be taken with respect to the measures $\mathrm{d}\mathbf{k}$ defined in (3.21):

$$\int \mathrm{d}\mathbf{k}' f(\mathbf{k}') \delta(\mathbf{k}, \mathbf{k}') = f(\mathbf{k})\ . \tag{3.30}$$

Spatial mode functions

We give a brief account of the functions $Y_{\mathbf{k}}(\mathbf{x})$ in each of the three types of Robertson-Walker spaces. What is needed is a direct sum or direct integral decomposition of the space $\mathrm{L}^2(\Sigma^\varepsilon)$ in terms of eigenfunctions of the Laplacian $\Delta_{\mathfrak{s}}$, i.e.,

$$\Delta_{\mathfrak{s}} Y_{\mathbf{k}}(\mathbf{x}) = -E(\mathrm{k}) Y_{\mathbf{k}}(\mathbf{x})\ . \tag{3.31}$$

In each case, the decomposition is obtained by different means, but it exists and allows to treat, to a great extent, the solutions in the different types of Robertson-Walker spacetimes on an equal footing [LR90].

[$\varepsilon = 0$]: In the flat case we have $\Delta_{\mathfrak{h}} = \frac{1}{\mathrm{a}^2}\Delta_{\mathfrak{s}}$. Thus, it follows that $\Delta_{\mathfrak{s}} Y_{\mathbf{k}}(\mathbf{x}) = -\mathrm{k}^2 Y_{\mathbf{k}}(\mathbf{x})$ and that the generalized eigenvectors $Y_{\mathbf{k}}(\mathbf{x})$ are independent of t. The eigenvectors and their negative eigenvalues are given by

$$Y_{\mathbf{k}}(\mathbf{x}) = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{\mathrm{i}\mathbf{k}\mathbf{x}} \ , \qquad\qquad E(\mathrm{k}) := \mathrm{k}^2 \ . \tag{3.32}$$

The direct integral decomposition amounts to the ordinary Fourier transform. Note the useful relations $\overline{Y_{\mathbf{k}}(\mathbf{x})} = Y_{-\mathbf{k}}(\mathbf{x})$ and $|Y_{\mathbf{k}}(\mathbf{x})|^2 = \frac{1}{(2\pi)^3}$.

[$\varepsilon = +1$]: For the closed universe, the solutions $Y_{\mathbf{k}}(\mathbf{x})$ are the spherical harmonics

$$Y_{\mathbf{k}}(\psi, \vartheta, \varphi) = A_{\mathrm{k}l}\ \Pi^{+}_{\mathrm{k}l}(\psi)\ Y_{l,m}(\vartheta, \varphi) \ , \qquad\qquad E(\mathrm{k}) := \mathrm{k}(\mathrm{k}+2) \ , \tag{3.33}$$

($\mathrm{k} = 0, 1, \ldots;\ l = 0, 1, \ldots, k;\ m = -l, -l+1, \ldots, l$), where the $Y_{l,m}$ are the harmonics on the 2-sphere, the $\Pi^{+}_{\mathrm{k}l}$ are real polynomials in $\sin\psi$ and $\cos\psi$, and the $A_{\mathrm{k}l}$ are real normalization constants. One has a direct sum decomposition $L^2(\Sigma^+) = \bigoplus_{\mathrm{k}=0}^{\infty} \mathcal{H}_{\mathrm{k}}$, where $\mathcal{H}_{\mathrm{k}}$ denotes the span of $Y_{\mathrm{k},l,m}$ as l and m vary.

[$\varepsilon = -1$]: In the open universe the Cauchy surface Σ^- is regarded as being embedded in $\mathbb{M}$, $\xi = (1, \boldsymbol{\xi}) \in \mathbb{M}$ and $x \cdot \xi$ is the Minkowski scalar product. A set of generalized eigenvectors are

$$Y_{\mathbf{k}}(x) = \frac{1}{(2\pi)^{\frac{3}{2}}} (x \cdot \xi)^{-1+\mathrm{i}\mathrm{k}} \ , \qquad\qquad E(\mathrm{k}) := \mathrm{k}^2 + 1 \ , \tag{3.34}$$

where $\mathbf{k} = \mathrm{k}\boldsymbol{\xi} \in \mathbb{R}^3$. Here, the Fourier transform is a map with values in $\mathrm{L}^2(\mathrm{S}^2, d\Omega)$, where S^2 is the two-sphere embedded in $\mathbb{R}^3$, i.e., a function on the set of horospheres, in the language of [GGV66].

Time-dependence

The time-dependent function $T_{\mathrm{k}}(t)$, which appears in (3.20), is required to be a solution to the differential equation

$$\ddot{T}_{\mathrm{k}}(t) + 3H(t)\dot{T}_{\mathrm{k}}(t) + \omega^2_{\mathrm{k}}(t) T_{\mathrm{k}}(t) = 0 \ , \tag{3.35}$$

where the frequencies $\omega_{\mathrm{k}}(t)$ are given by

$$\omega^2_{\mathrm{k}}(t) := \frac{E(\mathrm{k})}{\mathrm{a}(t)^2} + \mathrm{m}^2 \tag{3.36}$$

and, additionally, to satisfy the condition

$$\overline{T}_{\mathrm{k}}(t)\dot{T}_{\mathrm{k}}(t) - T_{\mathrm{k}}(t)\dot{\overline{T}}_{\mathrm{k}}(t) = \frac{\mathrm{i}}{\mathrm{a}(t)^3} \ . \tag{3.37}$$

The explicit form of $E(\mathrm{k})$ in each type of Robertson-Walker spacetime has been given in the last section. The condition (3.37), which amounts to the Wronskian, determines the commutation relations of the $a(\mathbf{k}), a(\mathbf{k})^*$ [HNS84, PF74].

Equation (3.35) is an ordinary, homogeneous, linear differential equation with variable coefficients. In case of a static spacetime it has the explicit solutions

$$T_{\mathrm{k}}(t) = \frac{1}{\sqrt{2\mathrm{a}^3\omega_{\mathrm{k}}}}\mathrm{e}^{-\mathrm{i}\omega_{\mathrm{k}}t} \ . \tag{3.38}$$

In the general case it has a fundamental system $T_{\mathrm{k}}(t), \overline{T}_{\mathrm{k}}(t)$ of solutions, which cannot be calculated explicitly.

Adiabatic vacuum states

The only freedom one has in the construction of pure, homogeneous, isotropic, quasi-free states is the choice of initial data for the function $T_{\mathrm{k}}(t)$. This choice can be made on physical grounds. For example, one can chose initial values such that the resulting states, in a certain sense, minimize particle creation in an expanding universe and reduce to the known particle notion in the static case. Then, one obtains the so-called adiabatic vacuum states [Par69].

In [LR90] the former definition of adiabatic vacuum states was put on a firm basis. The adiabatic vacuum states were redefined by fixing the large k behaviour of $T_{\mathrm{k}}(t)$ and $\dot{T}_{\mathrm{k}}(t)$ such that the resulting states adhered the principle of local definiteness [HNS84], which, roughly, requires that the the set of expectation values measurable in a bounded region $\mathcal{O}$ of the spacetime in a GNS representation of a state ω should not depend on the state ω. This rules out inequivalent representations of the local algebra of bounded observables $\mathfrak{A}(\mathcal{O})$ arising from different global states, which would be considered a pathology. For a precise definition and discussion of the principle of local definiteness and other related notions see [Ver94].

One can obtain iterative solutions $T^n_{\mathrm{k}}(t)$ of (3.35) and hereby the adiabatic vacuum states [Par69, LR90], by using a WKB-type ansatz

$$T_{\mathrm{k}}(t) = \frac{1}{\left(2a(t)^3\Omega_{\mathrm{k}}(t)\right)^{1/2}} \exp\left(\mathrm{i}\int_{t_0}^{t} dt\ \Omega_{\mathrm{k}}(t)\right) \tag{3.39}$$

with yet undetermined positive functions $\Omega_{\mathrm{k}}(t)$. This ansatz satisfies the normalization, and it satisfies (3.35) if

$$\Omega^2_{\mathrm{k}} = \omega^2_{\mathrm{k}} - \frac{3}{4}\left(\frac{\dot{\mathrm{a}}}{\mathrm{a}}\right)^2 - \frac{3}{2}\frac{\ddot{\mathrm{a}}}{\mathrm{a}} + \frac{3}{4}\left(\frac{\dot{\Omega}_{\mathrm{k}}}{\Omega_{\mathrm{k}}}\right)^2 - \frac{1}{2}\frac{\ddot{\Omega}_{\mathrm{k}}}{\Omega_{\mathrm{k}}} \ . \tag{3.40}$$

Now start with an iteration

$$\left(\Omega_{\mathrm{k}}^{(0)}\right)^2 = \omega_{\mathrm{k}}^2 \ , \tag{3.41}$$

$$\left(\Omega_{\mathrm{k}}^{(n+1)}\right)^2 = \omega_{\mathrm{k}}^2 - \frac{3}{4}\left(\frac{\dot{\mathrm{a}}}{\mathrm{a}}\right)^2 - \frac{3}{2}\frac{\ddot{\mathrm{a}}}{\mathrm{a}} + \frac{3}{4}\left(\frac{\dot{\Omega}_{\mathrm{k}}^{(n)}}{\Omega_{\mathrm{k}}^{(n)}}\right)^2 - \frac{1}{2}\frac{\ddot{\Omega}_{\mathrm{k}}^{(n)}}{\Omega_{\mathrm{k}}^{(n)}} \ . \tag{3.42}$$

The iteration procedure breaks down when we obtain a negative value for $\left(\Omega_k^{(n+1)}\right)^2$. This does not happen if one restricts to a time interval, $t \in I$, where $I \in \mathbb{R}$ is finite, and, in addition, k is chosen sufficiently large, $\mathrm{k} \geq \mathrm{k}_{\mathrm{min}}$ [LR90]. Then, one defines the for $t_0, t \in I$ the function

$$W_{\mathrm{k}}^{(n)}(t) = \frac{1}{\left(2a(t)^3\Omega_{\mathrm{k}}^{(n)}(t)\right)^{1/2}} \exp\left(i\int_{t_0}^{t} dt\ \Omega_k^{(n)}(t)\right) \ . \tag{3.43}$$

An adiabatic vacuum state of order n is the pure, quasi-free state obtained as the exact solution of (3.35) with the initial conditions

$$T_{\mathrm{k}}(t) = W_{\mathrm{k}}^{(n)}(t) \ , \qquad \dot{T}_{\mathrm{k}}(t) = \dot{W}_{\mathrm{k}}^{(n)}(t) \ . \tag{3.44}$$

The adiabatic vacuum states depend on several quantities involved in their definition. First, they depend on the initial time t used for the initial values in (3.44). This has no effect on the adiabatic vacuum state, as it amounts to common phase change of the initial conditions. Second, they depend on the extrapolation of $\Omega^{(n)}$ to small k, which is always possible in a continuous manner, and amounts to some Bogoliubov transformation on the state, not affecting the large k behaviour. Of course, they depend also on the order of iteration, n.

It has been shown in [Jun96, Jun02] that adiabatic vacuum states of infinite order are Hadamard states. This fact is of indirect importance for our construction as is is used in [Olb07a] to prove the Hadamard property of the states of low energy, and we base our proof of Hadamard property on the latter fact. The notion of adiabatic vacuum states was extended to more general spacetimes by the usage of Sobolev wavefront sets in [JS02].

3.3 The two-point distribution

The two-point distribution of a homogeneous, isotropic, quasi-free state can be characterized by different means. For example, in [LR90] it is given in a form that takes data on the surface Σ. So, let $F_i := (u_i, \mathrm{a}(t)^3 p_i) \in \hat{\mathscr{M}}$ be a pair of initial values on the phase space associated to Σ.

Theorem 3.1 ([LR90]) *The homogeneous and isotropic states on Robertson-Walker spacetimes have two-point distributions of the form*

$$\omega^{(2)}(F, F') := \int \mathrm{d}\mathbf{k} \left\langle \tilde{F}(\mathbf{k}), S(\mathrm{k})\tilde{F}'(\mathbf{k}) \right\rangle \ , \tag{3.45}$$

where

$$\left\langle \tilde{F}(\mathbf{k}), S(\mathrm{k})\tilde{F}'(\mathbf{k}) \right\rangle := \sum_{i,j=0}^{1} \bar{\tilde{F}}_i(\mathbf{k}) S_{ij}(\mathrm{k}) \tilde{F}'_j(\mathbf{k}) \ . \tag{3.46}$$

Here $\mathrm{k} \mapsto S_{ij}(\mathrm{k})$ *is measurable and polynomially bounded. For the matrix* $S(\mathrm{k})$ *it holds almost everywhere in* k *that*

$$S_{01}(\mathrm{k}) - S_{10}(\mathrm{k}) = \mathrm{i} \tag{3.47a}$$

$$S_{01}(\mathrm{k}) = \overline{S}_{10}(\mathrm{k}) \tag{3.47b}$$

$$S_{00}(\mathrm{k}) \geq 0 \tag{3.47c}$$

$$S_{00}(\mathrm{k}) S_{11}(\mathrm{k}) \geq |S_{01}(\mathrm{k})|^2 \ . \tag{3.47d}$$

Obviously equations (3.47c) implement (3.47c) the positivity of the state (compare to (2.21)). We remark that the two-point distributions depend only on the magnitude k of the three-momentum $\mathbf{k}$ because of the symmetry of the states. Exploiting these relations, it is possible to write $S_{01}(\mathrm{k}) = S_{01}^{\Re}(\mathrm{k}) + \frac{\mathrm{i}}{2}$. So, with $\mathbb{J} = \left(\begin{smallmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{smallmatrix}\right)$ the matrix $S(\mathrm{k})$ can be written as

$$S(\mathrm{k}) = S + \frac{\mathrm{i}}{2}\mathbb{J} \ , \tag{3.48}$$

where we introduced

$$S := \begin{pmatrix} S_{00} & S_{01}^{\Re} \\ S_{01}^{\Re} & S_{11} \end{pmatrix} \ . \tag{3.49}$$

We distinguish the original matrix $S(\mathrm{k})$ and its real part S by omitting the k-dependence in the latter. This will cause no trouble since, from now on, we will almost exclusively deal with S. We remark that equation (3.47d) becomes

$$[S] \geq \frac{1}{4} \ , \tag{3.50}$$

where $[S] = \det S$. Equation (3.50) resembles a generalized uncertainty relation for the covariance matrix of a state in quantum statistical mechanics. States of minimum uncertainty are pure states, which satisfy $[S] = \frac{1}{4}$.

The two-point distribution of pure, quasi-free states is given by (3.45) with

$$S(\mathrm{k}) := \begin{pmatrix} |p(\mathrm{k})|^2 & -q(\mathrm{k})\overline{p(\mathrm{k})} \\ -\overline{q(\mathrm{k})}p(\mathrm{k}) & |q(\mathrm{k})|^2 \end{pmatrix} \ , \tag{3.51}$$

where $p(\mathrm{k})$ and $q(\mathrm{k})$ are (essentially polynomially bounded and measurable) complex-valued functions satisfying

$$\overline{q(\mathrm{k})}p(\mathrm{k}) - q(\mathrm{k})\overline{p(\mathrm{k})} = -\mathrm{i} \ . \tag{3.52}$$

The functions $p(\mathrm{k})$ and $q(\mathrm{k})$ are proportional to the initial data of $T_{\mathrm{k}}(t)$ [Jun96]:

$$S(\mathrm{k}) = \begin{pmatrix} \mathrm{a}^6\dot{\overline{T}}_{\mathrm{k}}\dot{T}_{\mathrm{k}} & -\mathrm{a}^3\dot{\overline{T}}_{\mathrm{k}}T_{\mathrm{k}} \\ -\mathrm{a}^3\overline{T}_{\mathrm{k}}\dot{T}_{\mathrm{k}} & \overline{T}_{\mathrm{k}}T_{\mathrm{k}} \end{pmatrix} \ .$$

The fundamental solution

For the calculation of the explicit four-smeared two-point distribution of a quasi-free state we will need the following characterization of the fundamental solution E (see [LR90]). First, define the generalized function $G(x,y)$ by

$$G(x,y) := \int \mathrm{d}\mathbf{k}\ G_{\mathrm{k}}(x^0,y^0)Y_{\mathbf{k}}(\mathbf{x})\overline{Y}_{\mathbf{k}}(\mathbf{y}) \ , \tag{3.53}$$

$$G_{\mathrm{k}}(x^0,y^0) := \mathrm{i}(T_{\mathrm{k}}(x^0)\overline{T}_{\mathrm{k}}(y^0) - \overline{T}_{\mathrm{k}}(x^0)T_{\mathrm{k}}(y^0)) \ . \tag{3.54}$$

Then the fundamental solution $E : \mathscr{D}(\mathcal{M}) \to \mathscr{E}(\mathcal{M})$ can be written as

$$(Ef)(x^0,\mathbf{x}) := -G(x,f) := \int dy^0 \int \mathrm{d}\mathbf{k}\ Y_{\mathbf{k}}(\mathbf{x})G_{\mathrm{k}}(x^0,y^0)\check{f}(y^0,\mathbf{k}) \ , \tag{3.55}$$

where

$$\check{f}(y^0,\mathbf{k}) := \mathrm{a}(y^0)^3 \int d^3y \sqrt{|\mathfrak{s}|}\ \overline{Y}_{\mathbf{k}}(\mathbf{y})f(y^0,\mathbf{y}) \ . \tag{3.56}$$

The kernel $G_{\mathrm{k}}(\cdot,y^0)$ satisfies for each fixed y^0 equation (3.35) (by linearity) with initial conditions

$$G_{\mathrm{k}}(y^0,y^0) = \mathrm{i}(T_{\mathrm{k}}(y^0)\overline{T}_{\mathrm{k}}(y^0) - \overline{T}_{\mathrm{k}}(y^0)T_{\mathrm{k}}(y^0)) = 0 \ , \tag{3.57}$$

$$\dot{G}_{\mathrm{k}}(y^0,y^0) = \mathrm{i}(\dot{T}_{\mathrm{k}}(y^0)\overline{T}_{\mathrm{k}}(y^0) - \dot{\overline{T}}_{\mathrm{k}}(y^0)T_{\mathrm{k}}(y^0)) = -\frac{1}{\mathrm{a}(y^0)^3} \ . \tag{3.58}$$

This shows that $G_{\mathrm{k}}(x^0,y^0)$ is independent of the particular solution $T_{\mathrm{k}}(t)$ used in equation (3.54).

3.3.1 Four-smeared two-point distribution

As a first step to our construction, we need the explicit form of the two-point distribution $S(f,g)$ of a homogeneous, isotropic, quasi-free state in terms of the real matrix S from (3.49) and the solutions to equation (3.35). We prove the following lemma.

Lemma 3.2 *Let ω be a quasi-free, homogeneous, isotropic state of the Klein-Gordon field in a Robertson-Walker spacetime $\mathcal{M}$. Then the two-point distribution of ω is given by*

$$S(f,g) = \int d\mu(x) \int d\mu(x')\ \bar{f}(x) g(x')\ \omega^{(2)}(x,x') \tag{3.59}$$

with $d\mu(x) := \sqrt{[\mathfrak{g}]} d^4x$, where

$$\omega^{(2)}(x,x') := \int \mathrm{d}\mathbf{k}\ Y_{\mathbf{k}}(\mathbf{x}) \overline{Y}_{\mathbf{k}}(\mathbf{x}') \tag{3.60}$$
$$\times \left[T_{\mathrm{k}}(t) \overline{T}_{\mathrm{k}}(t') \left(b_1 - \frac{1}{2} \right) + T_{\mathrm{k}}(t) T_{\mathrm{k}}(t') \cdot b_2 + \overline{T}_{\mathrm{k}}(t) \overline{T}_{\mathrm{k}}(t') \cdot \bar{b}_2 + \overline{T}_{\mathrm{k}}(t) T_{\mathrm{k}}(t') \left(b_1 + \frac{1}{2} \right) \right]$$

and

$$b_1 := S_{00} |T_{\mathrm{k}}(t_0)|^2 + \mathrm{a}(t_0)^6 S_{11} |\dot{T}_{\mathrm{k}}(t_0)|^2 + \left(\overline{T}_{\mathrm{k}}(t_0) \dot{T}_{\mathrm{k}}(t_0) + T_{\mathrm{k}}(t_0) \dot{\overline{T}}_{\mathrm{k}}(t_0) \right) \mathrm{a}(t_0)^3 S_{01}^{\Re} \ , \tag{3.61a}$$

$$b_2 := -S_{00} \overline{T}_{\mathrm{k}}^2(t_0) - \mathrm{a}(t_0)^6 S_{11} \dot{\overline{T}}_{\mathrm{k}}^2(t_0) - 2 \overline{T}_{\mathrm{k}}(t_0) \dot{\overline{T}}_{\mathrm{k}}(t_0) \mathrm{a}(t_0)^3 S_{01}^{\Re} \ . \tag{3.61b}$$

Proof. In order obtain this formula for the two-point distribution, we need to calculate the two-point distribution of a homogeneous, isotropic, quasi-free state (3.45), using the initial values $F, H \in \mathscr{M}$ defined by

$$F := \begin{pmatrix} \rho_0 E f \\ \mathrm{a}(t_0)^3 \rho_1 E f \end{pmatrix} \ , \qquad\qquad H := \begin{pmatrix} \rho_0 E h \\ \mathrm{a}(t_0)^3 \rho_1 E h \end{pmatrix} \tag{3.62}$$

on a Cauchy surface at time t_0. First, we need some Fourier transforms. Using equations (3.26), (3.29) and the abbreviated notation

$$\rho_0 G_{\mathrm{k}}(x^0, y^0) := G_{\mathrm{k}}(t_0, y^0) \ , \tag{3.63}$$
$$\rho_1 G_{\mathrm{k}}(x^0, y^0) := \dot{G}_{\mathrm{k}}(t_0, y^0) \tag{3.64}$$

one obtains

$$\widetilde{\rho_0 E f}(\mathbf{k}) = \int dy^0\ G_{\mathrm{k}}(t_0, y^0) \check{f}(y^0, \mathbf{k}) \ , \tag{3.65}$$

$$\overline{\widetilde{\rho_0 E f}}(\mathbf{k}) = \int dy^0\ \overline{G}_{\mathrm{k}}(t_0, y^0) \bar{\check{f}}(y^0, \mathbf{y}) \ , \tag{3.66}$$

$$\widetilde{\rho_1 E f}(\mathbf{k}) = \int dy^0\ \dot{G}_{\mathrm{k}}(t_0, y^0) \check{f}(y^0, \mathbf{k}) \ , \tag{3.67}$$

$$\overline{\widetilde{\rho_1 E f}}(\mathbf{k}) = \int dy^0\ \dot{\overline{G}}_{\mathrm{k}}(t_0, y^0) \bar{\check{f}}(y^0, \mathbf{y}) \ . \tag{3.68}$$

The Fourier transform of $\mathrm{a}(t_0)^3\rho_1 Ef$ is simply $\mathrm{a}(t_0)^3\widetilde{\rho_1 Ef}$. Using this and (3.62) we can write the integrand of the two-point distribution (3.45) as

$$\left\langle \tilde{F}(\mathbf{k}), S(\mathrm{k})\tilde{H}(\mathbf{k})\right\rangle = \sum_{i,j=0}^{1} \bar{\tilde{F}}_i(\mathbf{k})S_{ij}(\mathrm{k})\tilde{H}_j(\mathbf{k}) \tag{3.69}$$

$$\begin{aligned} &= \overline{\widetilde{\rho_0 Ef}}(\mathbf{k})S_{00}(\mathrm{k})\widetilde{\rho_0 Eh}(\mathbf{k}) + \mathrm{a}(t_0)^3\overline{\widetilde{\rho_0 Ef}}(\mathbf{k})S_{01}(\mathrm{k})\widetilde{\rho_1 Eh}(\mathbf{k}) \\ &\quad + \mathrm{a}(t_0)^3\overline{\widetilde{\rho_1 Ef}}(\mathbf{k})S_{10}(\mathrm{k})\widetilde{\rho_0 Eh}(\mathbf{k}) + \mathrm{a}(t_0)^6\overline{\widetilde{\rho_1 Ef}}(\mathbf{k})S_{11}(\mathrm{k})\widetilde{\rho_1 Eh}(\mathbf{k}) \end{aligned} \tag{3.70}$$

$$\begin{aligned} &= \int d\mu(y)\int d\mu(y')\bar{f}(y^0,\mathbf{y})h(y'^0,\mathbf{y}')Y_{\mathbf{k}}(\mathbf{y})\overline{Y}_{\mathbf{k}}(\mathbf{y}')\times \\ &\Big[\overline{G}_{\mathrm{k}}(t_0,y^0)S_{00}(\mathrm{k})G_{\mathrm{k}}(t_0,y'^0) + \mathrm{a}(t_0)^3\overline{G}_{\mathrm{k}}(t_0,y^0)S_{01}(\mathrm{k})\dot{G}_{\mathrm{k}}(t_0,y'^0) \\ &\quad + \mathrm{a}(t_0)^3\dot{\overline{G}}_{\mathrm{k}}(t_0,y^0)S_{10}(\mathrm{k})G_{\mathrm{k}}(t_0,y'^0) + \mathrm{a}(t_0)^6\dot{\overline{G}}_{\mathrm{k}}(t_0,y^0)S_{11}(\mathrm{k})\dot{G}_{\mathrm{k}}(t_0,y'^0)\Big] \ , \end{aligned} \tag{3.71}$$

where $d\mu(y) := \sqrt{|\mathfrak{g}|}d^4y = \mathrm{a}(y^0)^3\sqrt{|\mathfrak{s}|}dy^0d^3y$. We can now write the two-point distribution as

$$S(f,h) = \int \mathrm{d}\mathbf{k}\left\langle \tilde{F}(\mathbf{k}), S(\mathrm{k})\tilde{H}(\mathbf{k})\right\rangle \tag{3.72}$$

$$= \int d\mu(y)\int d\mu(y')\ \bar{f}(y)h(y')\ \omega^{(2)}(y,y') \tag{3.73}$$

with

$$\begin{aligned} \omega^{(2)}(y,y') &:= \int \mathrm{d}\mathbf{k}\ Y_{\mathbf{k}}(\mathbf{y})\overline{Y}_{\mathbf{k}}(\mathbf{y}') \\ &\times\Big[\overline{G}_{\mathrm{k}}(t_0,y^0)G_{\mathrm{k}}(t_0,y'^0)S_{00}(\mathrm{k}) + \overline{G}_{\mathrm{k}}(t_0,y^0)\dot{G}_{\mathrm{k}}(t_0,y'^0)\mathrm{a}(t_0)^3S_{01}(\mathrm{k}) \\ &\quad + \dot{\overline{G}}_{\mathrm{k}}(t_0,y^0)G_{\mathrm{k}}(t_0,y'^0)\mathrm{a}(t_0)^3S_{10}(\mathrm{k}) + \dot{\overline{G}}_{\mathrm{k}}(t_0,y^0)\dot{G}_{\mathrm{k}}(t_0,y'^0)\mathrm{a}(t_0)^6S_{11}(\mathrm{k})\Big] \ . \end{aligned} \tag{3.74}$$

We need to calculate the quantity in the square brackets. From the definition (3.54) of $G_{\mathrm{k}}(x^0,y^0)$ we have

$$G_{\mathrm{k}}(t_0,y^0) := \mathrm{i}\left(T_{\mathrm{k}}(t_0)\overline{T}_{\mathrm{k}}(y^0) - \overline{T}_{\mathrm{k}}(t_0)T_{\mathrm{k}}(y^0)\right) \ . \tag{3.75}$$

In the following we use the abbreviated notation

$$G := G_{\mathrm{k}}(t_0,y^0)\ , \qquad G' := G_{\mathrm{k}}(t_0,y'^0)\ , \tag{3.76}$$

$$\dot{G} := \partial_{t_0}G_{\mathrm{k}}(t_0,y^0)\ , \qquad \dot{G}' := \partial_{t_0}G_{\mathrm{k}}(t_0,y'^0)\ , \tag{3.77}$$

and

$$T_0 := T_{\mathrm{k}}(t_0)\ , \qquad T := T_{\mathrm{k}}(y^0)\ , \qquad T' := T_{\mathrm{k}}(y'^0)\ . \tag{3.78}$$

Note that

$$G = \mathrm{i}(T_0\overline{T} - \overline{T}_0 T) \;, \qquad G' = \mathrm{i}(T_0\overline{T'} - \overline{T}_0 T') \;, \tag{3.79}$$

$$\dot{G} = \mathrm{i}(\dot{T}_0\overline{T} - \dot{\overline{T}}_0 T) \;, \qquad \dot{G}' = \mathrm{i}(\dot{T}_0\overline{T'} - \dot{\overline{T}}_0 T') \;. \tag{3.80}$$

This gives the intermediate results

$$\overline{G}G' = |T_0|^2 T\overline{T'} - \overline{T}_0^2 TT' - T_0^2\overline{TT'} + |T_0|^2\overline{T}T' \;, \tag{3.81}$$

$$\dot{\overline{G}}\dot{G}' = |\dot{T}_0|^2 T\overline{T'} - \dot{\overline{T}}_0^2 TT' obtain - \dot{T}_0^2\overline{TT'} + |\dot{T}_0|^2\overline{T}T' \;, \tag{3.82}$$

$$\dot{\overline{G}}G' = T_0\dot{\overline{T}}_0 T\overline{T'} - \overline{T}_0\dot{\overline{T}}_0 TT' - T_0\dot{T}_0\overline{TT'} + \overline{T}_0\dot{T}_0\overline{T}T' \;, \tag{3.83}$$

$$\overline{G}\dot{G}' = \dot{T}_0\overline{T}_0 T\overline{T'} - \overline{T}_0\dot{\overline{T}}_0 TT' - T_0\dot{T}_0\overline{TT'} + \dot{\overline{T}}_0 T_0\overline{T}T' \;. \tag{3.84}$$

Making use of $S_{01} = S_{01}^{\Re} + \frac{\mathrm{i}}{2}$ and $S_{10} = S_{01}^{\Re} - \frac{\mathrm{i}}{2}$ we finally arrive at

$$\begin{aligned}
[\dots] = {} & T\overline{T'}\left[S_{00}|T_0|^2 + \mathrm{a}^6 S_{11}|\dot{T}_0|^2 + (\overline{T}_0\dot{T}_0 + T_0\dot{\overline{T}}_0)\mathrm{a}^3 S_{01}^{\Re} - \frac{1}{2}\right] \\
& + TT'\left[-S_{00}\overline{T}_0^2 - \mathrm{a}^6 S_{11}\dot{\overline{T}}_0^2 - 2\overline{T}_0\dot{\overline{T}}_0\mathrm{a}^3 S_{01}^{\Re}\right] \\
& + \overline{TT'}\left[-S_{00}T_0^2 - \mathrm{a}^6 S_{11}\dot{T}_0^2 - 2T_0\dot{T}_0\mathrm{a}^3 S_{01}^{\Re}\right] \\
& + \overline{T}T'\left[S_{00}|T_0|^2 + \mathrm{a}^6 S_{11}|\dot{T}_0|^2 + (\overline{T}_0\dot{T}_0 + T_0\dot{\overline{T}}_0)\mathrm{a}^3 S_{01}^{\Re} + \frac{1}{2}\right] \;,
\end{aligned} \tag{3.85}$$

which gives the lemma. □

4 Quantum energy inequalities

This chapter starts with a brief overview of quantum energy inequalities and their interpretation as stability conditions. Then, we quote the worldline quantum inequality of Fewster [Few00], which we will use as the basis of our construction of almost equilibrium states. Afterwards, we give an explicit expression for the worldline averaged stress-energy in Robertson-Walker spacetimes in a form that is suitable for the minimization procedure to be accomplished in chapter 5.

4.1 A brief review

The geometry of spacetime is related to its matter content via Einstein's equation

$$R_{\mu\nu} - \frac{1}{2} R \, \mathfrak{g}_{\mu\nu} = -8\pi \boldsymbol{T}_{\mu\nu} \; . \tag{4.1}$$

Without restrictions on the stress-energy tensor there would be no restrictions on the metric, thus no clue on physically realizable solutions. Apart from covariant conservation of energy, $\nabla_\mu \boldsymbol{T}^{\mu\nu}$, the stress-energy tensor is believed to obey several more energy conditions, of which the most fundamental one is the weak energy condition (WEC). It says that

$$\boldsymbol{T}_{\mu\nu} u^\mu u^\nu \geq 0 \tag{4.2}$$

for timelike u^μ is satisfied by all forms of physically reasonable matter. Interpreting u^μ as the four velocity of an observer, it guarantees that all observers at all points in spacetime always measure nonnegative energy density.

The energy conditions are crucial ingredients in many important results concerning the behaviour of solutions to Einstein's equations. For instance, a result that requires energy conditions is the positivity of the asymptotic gravitational mass of isolated objects [SY79, LV81, Wit81]. This has implications on the stability of Minkowski spacetime. Furthermore, energy conditions ensure that entertaining phenomena like traversable wormholes and stargates in 'designer spacetimes', time machines, i.e., spacetimes with closed timelike curves, and warp drives are forbidden [FSW93, Haw92]. The WEC is also used in theorems, which prove that at a certain stage the formation of singularities becomes inevitable. These singularities are related to gravitational collapse [Pen65] as well as to an initial big bang [HE73]. Only recently, it was suggested that in inflationary cosmology an initial singularity may exists even if the energy conditions are violated

[BGV03]. Most important for us, energy conditions are necessary for the second law of thermodynamics to hold (see the discussion below).

As opposed to classical field theory, it is known that the weak energy condition is violated in quantum field theory. In fact, in any Wightman field the renormalized energy density may become arbitrarily negative at a spacetime point [EGJ65, Kuo97]. This may happen under very general assumptions and for free as well as interacting local quantum fields. Simple examples of states with negative energy density are given by certain superpositions of the vacuum state with a two-particle state [Pfe98, FHR02]. Besides this, there are also examples for negative energy densities that do not rely on the availability of particles, e.g., the Casimir effect or squeezed states of light (see references in [Fla97]).

Quantum inequalities were introduced originally in [For78], where it is argued that unconstrained negative energy fluxes $F = E/t$ can violate the second law of thermodynamics. However, all evidence tells us that the second law of thermodynamics holds on a macroscopic level. Quantum inequalities provide a mechanism that prevents the microscopical violations to survive on a macroscopic level. The argument goes as follows. An absorber is a quantum system that has an energy uncertainty $\Delta E \gtrsim t^{-1}$, where t is some timescale. The magnitude of change in its energy due to absorption of negative flux is of the order of $t|F|$. Hence, no macroscopic effects remain if the magnitude and duration of the negative energy flux is constrained by $|F| \lesssim t^{-2}$.

To constrain the negative energy that observers can measure it was suggested using the integral of the energy density over the worldline of a geodesic observer [Tip78] – a concept which led to the averaged weak energy condition (AWEC) $\int_{-\infty}^{\infty} d\tau \, \langle \boldsymbol{T}_{\mu\nu} u^\mu u^\nu \rangle \geq 0$, where u^μ is the observers four-velocity and τ is his proper time. This condition allows for the energy density to be pointwise negative as long as there is enough positive energy elsewhere on the worldline to compensate for this. A related condition is the averaged null energy condition (ANEC), which follows from integration along null geodesics [WY91]. Unfortunately, these conditions are violated easily for the vacuum state in certain spacetimes. It was then discovered [FR95] that introducing a sampling function into the AWEC integral successfully constrains the magnitude and duration of negative energy densities. The idea of averaging the renormalized stress-energy tensor over regions or curves in spacetime has been very fruitful since then and led to a variety of quantum weak energy inequalities of different types in different settings – see the reviews [Pfe98, Few05a].

An absolute quantum energy inequality (QEI) for the renormalized stress-energy tensor has the general form [FP06]

$$\int_{\mathcal{K}} d\mathcal{K} \, \langle : \boldsymbol{T}_{\mu\nu} : \rangle_\omega \, f^{\mu\nu} \geq -Q(f^{\mu\nu}) \, , \tag{4.3}$$

where the integral is taken over a region $\mathcal{K}$ of spacetime and the sampling tensor $f^{\mu\nu}$ belongs to the class of second rank contravariant tensor fields, possibly singularly sup-

ported on curves or surfaces in $\mathcal{K}$. Furthermore, Q is a positive, real-valued map on these tensors, and ω belongs to a class of states of the theory – usually the class of Hadamard states if curved spacetime is considered.

Most quantum energy inequalities are obtained by averaging with a sampling function $f(t)$ along the worldline of an observer,

$$\int_\gamma dt\ f(t) \left\langle : \boldsymbol{T}_{\mu\nu} : (t,t) \right\rangle_\omega u^\mu(t) u^\nu(t) \geq -Q(f)\ , \tag{4.4}$$

where u^μ denotes the four-velocity of the observer. Early quantum inequalities were derived for Lorentzian sampling functions $f_{t_0}(t) = t_0/\left(\pi(t^2+t_0^2)\right)$. To give an explicit example, for a free quantized scalar field in Minkowski spacetime it holds

$$\int_{-\infty}^{\infty} dt\ f_{t_0}(t) \left\langle : \boldsymbol{T}_{\mu\nu} : \right\rangle u^\mu u^\nu \geq -\frac{3}{32\pi^2 t_0^4}\ , \tag{4.5}$$

in the frame of an arbitrary inertial observer with proper time coordinate t for any state [FR95]. In the meantime, the class of admissible sampling functions has been extended to arbitrary smooth positive functions with sufficiently nice decay properties.

A simple configuration leading to violation of the AWEC and absolute QEIs is an observer at rest between uncharged, perfectly conducting plates. Then, the Casimir effect [Cas48] predicts negative vacuum energy for the quantized electromagnetic field measured by such an observer. In curved spacetimes a further difficulty is normal ordering of the stress-energy tensor. This problem is solved by difference QEIs, which are inequalities of the type

$$\int_\gamma dt\ f(t) \left[\left\langle \boldsymbol{T}_{\mu\nu}(\gamma(t)) \right\rangle_\omega - \left\langle \boldsymbol{T}_{\mu\nu}(\gamma(t)) \right\rangle_{\omega_0} \right] \gamma^\mu(t) \gamma^\nu(t) \geq -Q(f, \omega_0)\ , \tag{4.6}$$

where ω_0 is a reference state. Clearly, in the Fock representation of a Hadamard state ω_0 we would, by Wald's fourth axiom (see section 2.2.4), regain an absolute QEI. Difference QEIs have been proved on arbitrary globally hyperbolic spacetimes with general sampling functions on the class of Hadamard states. See below for a precise statement.

Sampling along timelike curves is not the only possibility to obtain energy inequalities. One can try sampling in a spacetime region or one may sample over a spatial region alone:

$$H(\xi, \Sigma) := \int_\Sigma d\mu(\mathbf{x}) f(\mathbf{x}) \left\langle : \boldsymbol{T}_{\mu\nu} : \right\rangle \xi^\mu \xi^\nu\ , \tag{4.7}$$

where ξ^μ is a vector field that is orthogonal to Σ and $f(\mathbf{x})$ has compact support on Σ. Only for a restricted class of theories, namely, conformal fields in two spacetime dimensions, spacelike sampled quantum inequalities have been derived [Fla97, Vol00]. Rather

it seems that compactly supported weighted averages over spacelike surfaces alone are generally unbounded below for dimensions $n \geq 3$ [FHR02]. Naively, this kind of objects could have been hoped to be prototypes of 'local Hamiltonians'. Interestingly, the integrals involved here resemble the integrals that were investigated some forty years ago in order to derive symmetry generating global charge operators from local currents (see [Völ77, Orz70, Req76]). In particular, these investigations suggest, that spacelike smearing alone of local currents, does not yield operators with sensible properties. In view of these problems with spacelike averaging, we adopt the viewpoint that the investigation of timelike averaged stress-energy tensor energy densities is more promising.

Let us make two more remarks. First, we note that there are quantum field theories which do not satisfy quantum inequalities. For example, the non-minimally coupled scalar fields violate the energy conditions already on the classical level and, as expected, their averaged energy density is unbounded below on the class of Hadamard states. Recently, Fewster and Osterbrink derived state dependent quantum inequalities for the fields with coupling $0 < \xi \leq \frac{1}{4}$ [FO08]. Second, the issue of quantum energy inequalities for interacting fields is not yet resolved, though, recently, some progress in this direction has been reported by Fewster and Bostelmann [FB].

4.1.1 Stability conditions

Quantum inequalities seem to be closely related to other stability conditions in quantum field theory, as has been pointed out by Fewster and Verch [FV03, Few05b]. On the microscopic level the microlocal spectrum condition (theorem 2.6) serves as a suitable stability condition. Now, theorem 4.1 states that quantum inequality exists for all states that satisfy the microlocal spectrum condition on arbitrary globally hyperbolic spacetimes. In [FV03] a macroscopic stability condition was related to the quantum inequalities. It was shown that on static spacetimes the existence of passive states (see below) follows from the existence of quantum weak energy inequalities. The circle is closed by noting that in [SV00] it was shown that the two-point distributions of passive states of (vector-valued) quantum fields in a stationary-spacetime satisfy the microlocal spectrum condition. Now, viewing quantum inequalities as mesoscopic stability conditions this relates stability conditions on three different scales.

Passivity

Let us briefly comment on the notion of passivity. A state on a C*-algebra $(\mathfrak{A}, \alpha_t)$ is called passive if and only if

$$\omega\left(U^* \frac{\delta}{\mathrm{i}}(U)\right) \geq 0 \tag{4.8}$$

for any $U \in \mathcal{U}(\mathfrak{A}) \cap D(\delta)$, where $\mathcal{U}_0$ denotes the unit-component of the group $\mathcal{U}(\mathfrak{A})$ of all unitary elements of $\mathfrak{A}$ and $D(\delta)$ is the set of all $A \in \mathfrak{A}$ for which the the generator

$$\delta(A) := \lim_{t\to 0} \frac{1}{t}(\alpha_t(A) - A) \tag{4.9}$$

exists [PW78, BR97]. For example, for bounded operators on the Hilbert space of a quantum mechanical system with Hamiltonian H, the generator amounts to a bounded symmetric derivation $\delta(A) = \mathrm{i}[H, A]$ (see the monograph [Sak91]). The notion of passivity was introduced in [PW78] as a precise mathematical formulation of the second law of thermodynamics, which says that systems at equilibrium are unable to perform mechanical work in cyclic processes. This justifies to call it a macroscopic stability condition. It is valid for infinite systems and is closely related to the KMS condition (see chapter 5) by the fact that KMS states and mixtures of KMS are passive. Under certain technical conditions ensuring that we deal with pure phases, the inverse statement, namely, that passive states are KMS states or ground states, is also true.

To date, there exists no formulation of passivity for non-stationary spacetimes. A direct implementation would require to replace the (strongly-continuous) group of automorphism α_t by a propagator family of automorphisms $\alpha_{t,s}$ (see the related discussion in section 2.2) and thus to deal with a time-dependent family of derivations δ_t. Such dynamical families are not well investigated with respect to (non)-equilibrium states – only two references are know to the present author. First, in [BMS02] certain states on Robertson-Walker spacetimes, which were obtained by 'transplantation' from de Sitter space, are proved to be locally passive in a certain sense. Second, in [Oji86] a general framework for the treatment of time-dependent non-equilibrium processes was proposed, which makes use of the propagator families and their generators. This (perturbative) scheme is equivalent the standard thermo field dynamics if and only if the states under consideration are equilibrium states and the dynamics is time-independent. This remark ends our digression on passivity.

4.2 A general worldline inequality

The classical energy-momentum tensor of the minimally coupled massive scalar field is given by

$$\boldsymbol{T}_{\mu\nu} = \nabla_\mu\phi\nabla_\nu\phi - \frac{1}{2}\mathfrak{g}_{\mu\nu}\left(\nabla^\sigma\phi\nabla_\sigma\phi + \mathrm{m}^2\phi^2\right) \tag{4.10}$$

The quantized and point split version of (4.10) is defined as follows [Few00, FS07]. For a smooth timelike curve $\gamma(t)$ in $\mathcal{M}$, where t is the proper time of the curve, denote by $\mathcal{U}$ a tubular neighborhood of γ. Choose an orthonormal frame $\{e^\mu_\alpha\}_{\alpha=0,1,2,3}$ in $\mathcal{U}$ so that $\mathfrak{g}^{\mu\nu} = \mathfrak{n}^{\alpha\beta}e^\mu_\alpha e^\nu_\beta$ and such that the restriction of e^μ_0 to γ equals the four-velocity of the curve, $e^\mu_0|_\gamma = \dot\gamma^\mu(t)$.

Suppose that the two-point distribution of ω_0 obeys the microlocal spectrum condition. Then one can define a distribution by

$$\left\langle \boldsymbol{T}_{\mu\nu'}\, v^\mu v^{\nu'} \right\rangle_{\omega_0}(t,t') := \frac{1}{2}\sum_{\alpha=0}^{3} \boldsymbol{\varphi}^* \left[\left(e^\mu_\alpha \nabla_\mu \otimes e^{\nu'}_\alpha \nabla_{\nu'} \right) \omega_0^{(2)}(x,x') \right] + \frac{1}{2}\mathrm{m}^2 \boldsymbol{\varphi}^* \left[(\mathbb{1}\otimes\mathbb{1})\, \omega_0^{(2)}(x,x') \right] \ . \tag{4.11}$$

Here $\boldsymbol{\varphi}^* : \mathcal{M}\times\mathcal{M} \to \mathbb{R}^2$ denotes the pull-back induced by the map $\boldsymbol{\varphi}(t,t') = (\gamma(t),\gamma(t'))$. That (4.11) is a well defined distribution on $\mathbb{R}^2$ is shown in [Few00]. Let $\mathfrak{A}$ be the algebra of observables of the minimally coupled scalar field of mass $\mathrm{m} \geq 0$ on a globally hyperbolic spacetime $(\mathcal{M}, \mathfrak{g}_{\mu\nu})$ with dimension $n \geq 2$. Let, furthermore, $\gamma : \mathbb{R} \to \mathcal{M}$ be a smooth timelike curve. Then the following theorem holds.

Theorem 4.1 ([Few00]) *Let ω and ω_0 be states on $\mathfrak{A}(\mathcal{M}, \mathfrak{g}_{\mu\nu})$ with globally Hadamard two-point distributions and define the normal ordered energy density relative to ω_0 by*

$$\langle : \boldsymbol{T} : \rangle_\omega := \langle \boldsymbol{T} \rangle_\omega - \langle \boldsymbol{T} \rangle_{\omega_0} \ . \tag{4.12}$$

Then $\langle : \boldsymbol{T} : \rangle_\omega$ is smooth, and the quantum inequality

$$\int_\gamma dt\ f(t)^2 \langle : \boldsymbol{T} : \rangle_\omega (t,t) \geq -\int_0^\infty \frac{d\lambda}{\pi} \big[(f \otimes \widetilde{f})\, \langle \boldsymbol{T} \rangle_{\omega_0} \big](-\lambda,\lambda) \tag{4.13}$$

holds for all real-valued $f \in \mathscr{D}(\mathbb{R})$, and the right hand side is convergent for all such f.

4.2.1 Stress-energy in Robertson-Walker spacetimes

As a necessary prerequisite for the construction the almost equilibrium states we need the explicit form of the left hand side of (4.13) in Robertson-Walker spacetimes; This will be part of our free energy functional to be defined in chapter 5. We state the result as a lemma.

Lemma 4.2 *Let $\boldsymbol{T}_{\mu\nu}$ be the stress-energy tensor of real, linear, scalar field in Robertson-Walker spacetimes and let ω, ω_0 two homogeneous, isotropic states. Furthermore, let $f \in \mathscr{D}(\mathcal{M})$ and γ be the worldline of an isotropic observer. Then,*

$$\int \mathrm{d}t\ f(t)^2 \left(\langle \boldsymbol{T} \rangle_\omega (t,t) - \langle \boldsymbol{T} \rangle_{\omega_0} (t,t) \right) = \int d\mu(\mathbf{k})^\varepsilon \int dt\ f(t)^2 \left(\boldsymbol{\rho}_{\mathrm{k}}(t) - \boldsymbol{\rho}_{\mathrm{k},0}(t) \right) \ , \tag{4.14}$$

where

$$\boldsymbol{\rho}_{\mathrm{k}}(t) := b_1(S) \left(|\dot{T}_{\mathrm{k}}(t)|^2 + \omega_{\mathrm{k}}^2 |T_{\mathrm{k}}(t)|^2 \right) + \Re \left\{ b_2(S) \left(\dot{T}_{\mathrm{k}}(t)^2 + \omega_{\mathrm{k}}^2 T_{\mathrm{k}}(t)^2 \right) \right\} \ , \tag{4.15}$$

and the coefficients b_1, b_2 are defined in (3.61a). *The energy density $\boldsymbol{\rho}_{\mathrm{k},0}(t)$ is defined analogously. The measures $d\mu(\mathbf{k})^{\varepsilon}$ differ by constants from the measures* $\mathrm{d}\mathbf{k}$ *defined in 3.21:*

$$d\mu(\mathbf{k})^0 := \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3} , \qquad d\mu(\mathbf{k})^+ := \frac{\mathrm{d}\mathbf{k}}{V_{\Sigma^+}} , \qquad d\mu(\mathbf{k})^- := \frac{\mathrm{d}\mathbf{k}}{2\pi^2} . \tag{4.16}$$

Proof. The stress-energy tensor of the Klein-Gordon field (2.2) is given by equation (4.10). In order to calculate the left hand side of (4.14) we have to consider the point-split expression

$$\begin{aligned} &\int dt\ f(t)^2 \left[\langle \boldsymbol{T}_{00} \rangle_{\omega} (t,t) - \langle \boldsymbol{T}_{00} \rangle_{\omega_0} (t,t) \right] \\ &\qquad = \int dt\ f(t)^2 \lim_{t' \to t} \left(\frac{1}{2} \nabla_0 \nabla'_0 - \frac{1}{2} \sum_{\mu,\nu=1}^{3} \mathfrak{g}^{\mu\nu} \nabla_\mu \nabla'_\nu - \frac{1}{2}\, \mathrm{m}^2 \right) \boldsymbol{F}(x,x') \Big|_{\substack{x=\gamma(t) \\ x'=\gamma(t')}} , \end{aligned} \tag{4.17}$$

where

$$\boldsymbol{F}(x,x') := \omega^{(2)}(x,x') - \omega_0^{(2)}(x,x') \tag{4.18}$$

and the two-point distribution $\omega^{(2)}(x,x')$ is given in lemma 3.2. We need the limits $x' \to x$ of the involved derivatives of the functional $\boldsymbol{F}(x,x')$. For the restricted case of pure states, this calculation has been performed in [Olb07b]. See also [PF74] for similar results. In section 5.5 we will see that the limiting case of pure states amounts to the values $b_2 = 0$ and $b_1 = \frac{1}{2}$.

The difference $\boldsymbol{F}(x,x')$ is a smooth function if ω and ω_0 are Hadamard states. In that case, the coincidence limit $x \to x'$ is well defined. The derivatives involved in the energy momentum tensor and which have to be calculated for each of the three cases $\varepsilon = 0, 1, -1$ are

$$\lim_{x' \to x} \boldsymbol{F}(x,x') , \qquad \lim_{x' \to x} \nabla_0 \nabla'_0 \boldsymbol{F}(x,x') , \qquad \lim_{x' \to x} \sum_{\mu,\nu=1}^{3} \mathfrak{g}^{\mu\nu} \nabla_\mu \nabla'_\nu \boldsymbol{F}(x,x') . \tag{4.19}$$

With the convention that latin indices are summed from 1 to 3 we can simplify the spatial derivative as

$$\sum_{\mu,\nu=1}^{3} \mathfrak{g}^{\mu\nu} \nabla_\mu \nabla'_\nu = \mathfrak{h}^{ij} \nabla_i \nabla'_j = \frac{1}{\mathrm{a}^2} \mathfrak{s}^{ij} \nabla_i \nabla'_j . \tag{4.20}$$

Besides that, we simplify the notation by introducing ellipsis for the second summand, which always looks like the first except that it belongs to the state ω_0.

[$\varepsilon = 0$]: This is, as expected, the simplest case. The modulus $|Y_{\mathbf{k}}(\mathbf{x})|^2 = \frac{1}{(2\pi)^3}$ of the spatial solutions is independent of $\mathbf{x}$. Thus, we can calculate directly

$$\lim_{x'\to x} \boldsymbol{F}(x,x') = \int \mathrm{d}\mathbf{k}\ |Y_{\mathbf{k}}(\mathbf{x})|^2 \Big[|T_{\mathrm{k}}(x^0)|^2 \left(b_1 + \frac{1}{2}\right) + T_{\mathrm{k}}(x^0)^2 \cdot b_2 \tag{4.21}$$
$$+ \overline{T}_{\mathrm{k}}(x^0)^2 \cdot \bar{b}_2 + |T_{\mathrm{k}}(x^0)|^2 \left(b_1 - \frac{1}{2}\right) \Big] - \dots$$
$$= \frac{1}{(2\pi)^3} \int \mathrm{d}\mathbf{k} \left[2|T_{\mathrm{k}}(x^0)|^2 \cdot b_1 + 2\Re\left\{ T_{\mathrm{k}}(x^0)^2 \cdot b_2 \right\} \right] - \dots \tag{4.22}$$
$$= 2 \int d\mu(\mathbf{k}) \left[|T_{\mathrm{k}}(x^0)|^2 \cdot b_1 + \Re\left\{ T_{\mathrm{k}}(x^0)^2 \cdot b_2 \right\} \right] - \dots\ , \tag{4.23}$$

where we defined the measure $d\mu(\mathbf{k}) = \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}$. Similarly we obtain for the term involving time derivatives

$$\lim_{x'\to x} \nabla_0 \nabla'_0 \boldsymbol{F}(x,x') = 2 \int d\mu(\mathbf{k}) \left[|\dot{T}_{\mathrm{k}}(x^0)|^2 \cdot b_1 + \Re\left\{ \dot{T}_{\mathrm{k}}(x^0)^2 \cdot b_2 \right\} \right] - \dots\ . \tag{4.24}$$

The third object involves spatial derivatives. Is is calculated with the aid of (4.20) as

$$\lim_{x'\to x} \sum_{\mu,\nu=1}^{3} \mathfrak{g}^{\mu\nu} \nabla_\mu \nabla'_\nu \boldsymbol{F}(x,x') = \frac{1}{\mathrm{a}(x^0)^2} \lim_{x'\to x} \mathfrak{s}^{ij} \nabla_i \nabla'_j \boldsymbol{F}(x,x') \tag{4.25}$$
$$= \frac{1}{\mathrm{a}(x^0)^2} \int \mathrm{d}\mathbf{k}\ \mathfrak{s}^{ij} \nabla_i Y_{\mathbf{k}}(\mathbf{x}) \nabla'_j \overline{Y}_{\mathbf{k}}(\mathbf{x}') \left[2|T_{\mathrm{k}}(x^0)|^2 \cdot b_1 + 2\Re\left\{ T_{\mathrm{k}}(x^0)^2 \cdot b_2 \right\} \right] - \dots \tag{4.26}$$
$$= \frac{1}{(2\pi)^3} \int \mathrm{d}\mathbf{k}\ \frac{E(\mathrm{k})}{\mathrm{a}(x^0)^2} \left[2|T_{\mathrm{k}}(x^0)|^2 \cdot b_1 + 2\Re\left\{ T_{\mathrm{k}}(x^0)^2 \cdot b_2 \right\} \right] - \dots \tag{4.27}$$
$$= 2 \int d\mu(\mathbf{k}) \frac{E(\mathrm{k})}{\mathrm{a}(x^0)^2} \left[|T_{\mathrm{k}}(x^0)|^2 \cdot b_1 + \Re\left\{ T_{\mathrm{k}}(x^0)^2 \cdot b_2 \right\} \right] - \dots\ . \tag{4.28}$$

Here we used that $\mathfrak{s}^{ij} \nabla_i Y_{\mathbf{k}}(\mathbf{x}) \nabla_j \overline{Y}_{\mathbf{k}}(\mathbf{x}) = \frac{1}{(2\pi)^3} \cdot E(\mathrm{k})$, which follows directly from (3.32).

[$\varepsilon = +1$]: In this case we have to work a little more. The states under consideration are assumed to be homogeneous. Thus, the quantities $\lim_{x'\to x} \boldsymbol{F}(x,x')$ and $\lim_{x'\to x} \nabla_0 \nabla'_0 \boldsymbol{F}(x,x')$ cannot depend on the spatial coordinates $\mathbf{x}$ and $\mathbf{x}'$. By the com-

pactness of Σ^+, we can carry out the limiting procedure, integrate over Σ^+ using the measure $\mathrm{d}\mathbf{x}$ and divide by the volume V_{Σ^+}. This gives

$$\lim_{x'\to x} \boldsymbol{F}(x,x') = \frac{1}{V_{\Sigma^+}} \int\limits_{\Sigma^+} \mathrm{d}\mathbf{x} \lim_{x'\to x} \boldsymbol{F}(x,x') \tag{4.29}$$

$$= \frac{1}{V_{\Sigma^+}} \int \mathrm{d}\mathbf{k} \int\limits_{\Sigma^+} \mathrm{d}\mathbf{x}\ |Y_{\mathbf{k}}(\mathbf{x})|^2 \big[|T_{\mathrm{k}}(x^0)|^2 b_1 + T_{\mathrm{k}}(x^0)^2 b_2 \tag{4.30}$$

$$+ \overline{T}_{\mathrm{k}}(x^0)^2 \bar{b}_2 + |T_{\mathrm{k}}(x^0)|^2 b_1 \big] - \dots$$

$$= \frac{1}{V_{\Sigma^+}} \int \mathrm{d}\mathbf{k}\ \delta(\mathbf{k},\mathbf{k}) \left[2|T_{\mathrm{k}}(x^0)|^2 b_1 + 2\Re\left\{ T_{\mathrm{k}}(x^0)^2 b_2 \right\} \right] - \dots \tag{4.31}$$

$$= 2 \int d\mu(\mathbf{k}) \left[|T_{\mathrm{k}}(x^0)|^2 b_1 + \Re\left\{ T_{\mathrm{k}}(x^0)^2 b_2 \right\} \right] - \dots\ , \tag{4.32}$$

where we used (3.29) and defined the measure $d\mu(\mathbf{k}) = \frac{\mathrm{d}\mathbf{k}}{V_{\Sigma^+}}$. Again, after taking the time derivatives, we can perform the same calculation as before:

$$\lim_{x'\to x} \nabla_0 \nabla'_0 \boldsymbol{F}(x,x') = 2 \int d\mu(\mathbf{k}) \left[|\dot{T}_{\mathrm{k}}(x^0)|^2 b_1 + \Re\left\{ \dot{T}_{\mathrm{k}}(x^0)^2 b_2 \right\} \right] - \dots\ . \tag{4.33}$$

The spatial part gives the preliminary expression

$$\lim_{x'\to x} \sum_{\mu,\nu=1}^{3} \mathfrak{g}^{\mu\nu} \nabla_\mu \nabla'_\nu \boldsymbol{F}(x,x') = \frac{1}{V_{\Sigma^+}} \int\limits_{\Sigma} \mathrm{d}\mathbf{x} \frac{1}{\mathrm{a}^2(x^0)} \lim_{x'\to x} \mathfrak{s}^{ij} \nabla_i \nabla'_j \boldsymbol{F}(x,x') \tag{4.34}$$

$$= \frac{1}{\mathrm{a}(x^0)^2} \frac{1}{V_{\Sigma^+}} \int\limits_{\Sigma^+} \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{k}\ \lim_{x'\to x} \mathfrak{s}^{ij}\ \nabla_i Y_{\mathbf{k}}(\mathbf{x})\ \nabla'_j \overline{Y}_{\mathbf{k}}(\mathbf{x}') \tag{4.35}$$

$$\times \left[T_{\mathrm{k}}(x^0) \overline{T}_{\mathrm{k}}(x'^0) \left(b_1 + \frac{1}{2} \right) + T_{\mathrm{k}}(x^0) T_{\mathrm{k}}(x'^0) b_2 \right.$$

$$\left. + \overline{T}_{\mathrm{k}}(x^0) \overline{T}_{\mathrm{k}}(x'^0) \bar{b}_2 + \overline{T}_{\mathrm{k}}(x^0) T_{\mathrm{k}}(x'^0) \left(b_1 - \frac{1}{2} \right) \right] - \dots$$

$$= \frac{1}{\mathrm{a}(x^0)^2} \frac{1}{V_{\Sigma^+}} \int \mathrm{d}\mathbf{k} \int\limits_{\Sigma^+} \mathrm{d}\mathbf{x}\ \mathfrak{s}^{ij}\ \nabla_i Y_{\mathbf{k}}(\mathbf{x}) \nabla_j\ \overline{Y}_{\mathbf{k}}(\mathbf{x}) \tag{4.36}$$

$$\times \left[|T_{\mathrm{k}}(x^0)|^2 b_1 + T_{\mathrm{k}}(x^0)^2 b_2 + \overline{T}_{\mathrm{k}}(x^0)^2 \bar{b}_2 + |T_{\mathrm{k}}(x^0)|^2 b_1 \right] - \dots\ .$$

Since Σ^+ is compact without boundary, we can perform a partial integration [Tay96] using

$$\int\limits_{\Sigma^+} \mathrm{d}\mathbf{x}\ \mathfrak{s}^{ij}\ \nabla_j Y_{\mathbf{k}}(\mathbf{x})\ \nabla_i \overline{Y}_{\mathbf{k}}(\mathbf{x}) = - \int\limits_{\Sigma^+} \mathrm{d}\mathbf{x}\ \Delta Y_{\mathbf{k}}(\mathbf{x})\ \overline{Y}_{\mathbf{k}}(\mathbf{x})\ . \tag{4.37}$$

Furthermore, since $\Delta_{\mathfrak{s}} Y_{\mathbf{k}}(\mathbf{x}) = -E(\mathrm{k}) Y_{\mathbf{k}}(\mathbf{x})$, it follows that

$$= \frac{1}{V_{\Sigma^+}} \int \mathrm{d}\mathbf{k} \int\limits_{\Sigma^+} \mathrm{d}\mathbf{x}\ |Y_{\mathbf{k}}(\mathbf{x})|^2 \frac{E(\mathrm{k})}{\mathrm{a}(x^0)^2} \left[2|T_{\mathrm{k}}(x^0)|^2 b_1 + 2\Re\left\{ T_{\mathrm{k}}(x^0)^2 b_2 \right\} \right] - \dots \tag{4.38}$$

$$= \frac{1}{V_{\Sigma^+}} \int \mathrm{d}\mathbf{k}\ \delta(\mathbf{k},\mathbf{k}) \frac{E(\mathrm{k})}{\mathrm{a}(x^0)^2} \left[2|T_{\mathrm{k}}(x^0)|^2 b_1 + 2\Re\left\{ T_{\mathrm{k}}(x^0)^2 b_2 \right\} \right] - \dots \tag{4.39}$$

$$= 2 \int d\mu(\mathbf{k}) \frac{E(\mathrm{k})}{\mathrm{a}(x^0)^2} \left[|T_{\mathrm{k}}(x^0)|^2 b_1 + \Re\left\{ T_{\mathrm{k}}(x^0)^2 b_2 \right\} \right] - \dots\ . \tag{4.40}$$

[$\varepsilon = -1$]: In this case one uses techniques from the harmonic analysis of hyperbolic spaces with negative constant curvature, also called Lobachevskian spaces [GGV66]. In order to find a direct integral representation of the isometry group $\boldsymbol{G}^-$, one embeds Σ^- as a three-dimensional hyperboloid with coordinates $\mathbf{x} = (x_1, x_2, x_3)$ into the four-dimensional Minkowski spacetime $(\mathbb{M}, \mathfrak{n}_{\mu\nu})$ by means of the map $\iota : \mathbb{R}^3 \to \mathbb{M}, \mathbf{x} \mapsto (\sqrt{1+\mathbf{x}^2}, \mathbf{x})$. One can calculate the metric on Σ^- as the pullback $\mathfrak{g}_{\mu\nu} = \iota^* \mathfrak{n}_{\mu\nu}$, which gives

$$\mathfrak{h}_{ij}(\mathbf{x}) = \delta_{ij} - \frac{x^i x^j}{1+\mathbf{x}^2} \qquad \Leftrightarrow \qquad \mathfrak{h}^{ij}(\mathbf{x}) = \delta_{ij} + x_i x_j\ . \tag{4.41}$$

Now, define a normalized momentum by $\xi := \mathbf{k}/\mathrm{k}$ and write for each k the Fourier transform of a function $h \in \mathscr{D}(\Sigma^-)$ as

$$\tilde{h}_{\mathrm{k}}(\boldsymbol{\xi}) := \int \mathrm{d}\mathbf{x}\ Y_{\mathrm{k}\boldsymbol{\xi}}(\mathbf{x}) h(\mathbf{x})\ , \tag{4.42}$$

where $Y_{\mathbf{k}}(\mathbf{x})$ are eigenfunctions of the Laplace operator given by (3.34). This Fourier transform is a map with values in $\mathrm{L}^2(\mathrm{S}^2, d\Omega)$, where S^2 is the two-sphere embedded in $\mathbb{R}^3$ and $d\Omega$ denotes the induced measure on S^2. The Lorentz transformations $\mathrm{g} : f(x) \mapsto f(x\mathrm{g})$ on the functions $f(x)$ correspond to operators

$$U_{\mathrm{k}}(\mathrm{g}) \tilde{h}_{\mathrm{k}} = \left(\widetilde{U(\mathrm{g}) h} \right)_{\mathrm{k}}\ . \tag{4.43}$$

Let g_x be the Lorentz transformation that maps $(\sqrt{1+\mathbf{x}}, \mathbf{x})$ to $(1,0,0,0)$. Then by the unitarity of $U_{\mathrm{k}}(\mathrm{g})$

$$|Y_{\mathbf{k}}(\mathbf{x})|^2 = \frac{1}{(2\pi)^3} \int d\Omega(\boldsymbol{\xi})\, (x \cdot \xi)^{-2} \tag{4.44}$$

$$= \frac{1}{(2\pi)^3} \int d\Omega(\boldsymbol{\xi}) \left(x \cdot \mathrm{g}_x^{-1} \xi \right)^{-2} \tag{4.45}$$

$$= \frac{1}{(2\pi)^3} \int d\Omega(\boldsymbol{\xi}) \left(\mathrm{g}_x x \cdot \xi \right)^{-2} \tag{4.46}$$

$$= \frac{1}{(2\pi)^3} \int d\Omega(\boldsymbol{\xi}) = \frac{4\pi}{(2\pi)^3}\ . \tag{4.47}$$

Again, as for $\varepsilon = 0$, the modulus of $Y_{\mathbf{k}}(\mathbf{x})$ is a constant. Using this, we obtain

$$\begin{aligned}\lim_{x'\to x} \boldsymbol{F}(x,x') &= \int \mathrm{d}\mathbf{k}\ |Y_{\mathbf{k}}(\mathbf{x})|^2 \qquad (4.48)\\ &\quad\times\left[|T_{\mathrm{k}}(x^0)|^2\left(b_1+\frac{1}{2}\right)+T_{\mathrm{k}}(x^0)^2 b_2\right.\\ &\quad\left.+\overline{T}_{\mathrm{k}}(x^0)^2\bar{b}_2+|T_{\mathrm{k}}(x^0)|^2\left(b_1-\frac{1}{2}\right)\right]-\dots\\ &= \frac{4\pi}{(2\pi)^3}\int \mathrm{d}\mathbf{k}\left[2|T_{\mathrm{k}}(x^0)|^2+2\Re\left\{T_{\mathrm{k}}(x^0)^2 b_2\right\}\right]-\dots \qquad (4.49)\\ &= 2\int d\mu(\mathbf{k})\left[|T_{\mathrm{k}}(x^0)|^2+\Re\left\{T_{\mathrm{k}}(x^0)^2 b_2\right\}\right]-\dots\ , \qquad (4.50)\end{aligned}$$

where $d\mu(\mathbf{k}) = \frac{\mathrm{d}\mathbf{k}}{2\pi^2}$. Similarly, one finds

$$\lim_{x'\to x}\nabla_0\nabla_0'\boldsymbol{F}(x,x') = 2\int d\mu(\mathbf{k})\left[|\dot{T}_{\mathrm{k}}(x^0)|^2+\Re\left\{\dot{T}_{\mathrm{k}}(x^0)^2 b_2\right\}\right]-\dots\ . \qquad (4.51)$$

Finally, since $\mathfrak{s}^{ij}\nabla_i Y_{\mathbf{k}}(\mathbf{x})\nabla_j'\overline{Y}_{\mathbf{k}}(\mathbf{x}') = (1+\mathrm{k}^2)|Y_{\mathbf{k}}(\mathbf{x})| = E(\mathrm{k})|Y_{\mathbf{k}}(\mathbf{x})|$ we obtain by

$$Y_{\mathbf{k}}(x) = \frac{1}{(2\pi)^{\frac{3}{2}}}\left(x^0-\frac{\mathbf{x}\cdot\boldsymbol{\xi}}{\mathrm{k}}\right)^{-1+\mathrm{ik}} \qquad (4.52)$$

(see (3.34)) for the spatial derivatives the expression

$$\begin{aligned}&\lim_{x'\to x}\sum_{\mu,\nu=1}^{3}\mathfrak{g}^{\mu\nu}\nabla_\mu\nabla_\nu'\boldsymbol{F}(x,x') = \frac{1}{\mathrm{a}^2(x^0)}\lim_{x'\to x}\mathfrak{s}^{ij}\nabla_i\nabla_j'\boldsymbol{F}(x,x') \qquad (4.53)\\ &= \frac{1}{\mathrm{a}(x^0)^2}\int \mathrm{d}\mathbf{k}\ \mathfrak{s}^{ij}\nabla_i Y_{\mathbf{k}}(\mathbf{x})\nabla_j'\overline{Y}_{\mathbf{k}}(\mathbf{x}')\left[2|T_{\mathrm{k}}(x^0)|^2+2\Re\left\{T_{\mathrm{k}}(x^0)^2 b_2\right\}\right]-\dots \qquad (4.54)\\ &= \frac{1}{(2\pi)^3}\int \mathrm{d}\mathbf{k}\ \frac{E(\mathrm{k})}{\mathrm{a}(x^0)^2}\left[2|T_{\mathrm{k}}(x^0)|^2 b_1+2\Re\left\{T_{\mathrm{k}}(x^0)^2 b_2\right\}\right]-\dots \qquad (4.55)\\ &= 2\int d\mu(\mathbf{k})\frac{E(\mathrm{k})}{\mathrm{a}^2(x^0)}\left[|T_{\mathrm{k}}(x^0)|^2 b_1+\Re\left\{T_{\mathrm{k}}(x^0)^2 b_2\right\}\right]-\dots\ . \qquad (4.56)\end{aligned}$$

Putting all this together gives the desired result. □

A better parametrization

For the actual minimization, it will be convenient to parametrize the averaged stress-energy by the components of the two-point matrix S. For this, note that

$$\int dt\ f(t)^2\boldsymbol{\rho}_k(t) = b_1(S)c_1(T_{\mathrm{k}},f)+\Re\left\{b_2(S)c_2(T_{\mathrm{k}},f)\right\}\ , \qquad (4.57)$$

where we have defined

$$c_1(T_{\rm k}, f) := \int dt\ f(t)^2 \left(|\dot{T}_{\rm k}(t)|^2 + \omega_{\rm k}^2 |T_{\rm k}(t)|^2 \right) \ , \tag{4.58a}$$

$$c_2(T_{\rm k}, f) := \int dt\ f(t)^2 \left(\dot{T}_{\rm k}(t)^2 + \omega_{\rm k}^2 T_{\rm k}(t)^2 \right) \ . \tag{4.58b}$$

Our definition of the quantities $c_1(T_{\rm k}, f)$ and $c_2(T_{\rm k}, f)$ differ from the one in [Olb07a] by a factor of 2. Now, inserting b_1 and b_2 we can write

$$\int dt\ f(t)^2 \boldsymbol{\rho}_k(t) = S_{00}\ d_1(T_{\rm k}, f) + {\rm a}^6 S_{11}\ d_2(T_{\rm k}, f) + {\rm a}^3 S_{01}^{\Re}\ d_3(T_{\rm k}, f) \ , \tag{4.59}$$

where

$$d_1(T_{\rm k}, f) := |T_{\rm k}(t_0)|^2 c_1(T_{\rm k}, f) - \Re \left\{ \overline{T}_{\rm k}^2(t_0) c_2(T_{\rm k}, f) \right\} \ , \tag{4.60a}$$

$$d_2(T_{\rm k}, f) := |\dot{T}_{\rm k}(t_0)|^2 c_1(T_{\rm k}, f) - \Re \left\{ \dot{\overline{T}}_{\rm k}^2(t_0) c_2(T_{\rm k}, f) \right\} \ , \tag{4.60b}$$

$$d_3(T_{\rm k}, f) := \left(\overline{T}_{\rm k}(t_0) \dot{T}_{\rm k}(t_0) + T_{\rm k}(t_0) \dot{\overline{T}}_{\rm k}(t_0) \right) c_1(T_{\rm k}, f) - \Re \left\{ 2 \overline{T}_{\rm k}(t_0) \dot{\overline{T}}_{\rm k}(t_0) c_2(T_{\rm k}, f) \right\} \ . \tag{4.60c}$$

5 Almost equilibrium states

In this section we tackle the construction the almost equilibrium states. First, we explain the basic ideas behind the procedure and the definition of the free energy functional associated to the states of interest. Then, we calculate the entropy, which is the part of the free energy, that cannot be inferred from the quantum energy inequalities discussed in the last chapter. This is followed by the actual minimization and the definition of the almost equilibrium states. In the last section we prove that the almost equilibrium states are indeed Hadamard states.

5.1 KMS states

Consider a finite quantum system that is described by an algebra of observables $\mathfrak{A}$. A general state ω on $\mathfrak{A}$ is described by a density matrix ρ and the expectation value of an observable $A \in \mathfrak{A}$ is given by

$$\omega(A) = \mathrm{Tr}(\rho A) \tag{5.1}$$

Now, a state ω on $\mathfrak{A}$ is a thermal equilibrium state at inverse temperature $\beta \in \mathbb{R}$ if it is a Gibbs state. A Gibbs state is given by a density matrix of the form

$$\rho_{\beta H} := \frac{\mathrm{e}^{-\beta H}}{\mathrm{Tr}(\mathrm{e}^{-\beta H})} \ , \tag{5.2}$$

where $H = H^*$ is a self-adjoint operator (the free Hamiltonian) and $\mathrm{e}^{-\beta H}$ is a trace class operator, which means that $\mathrm{Tr}(e^{-\beta H}) \leq \infty$. The trace class property of $\mathrm{e}^{-\beta H}$ is guaranteed for finite volume systems by the properties of H in that case [Haa96]. A simple calculation using the cyclic invariance of the trace, $\mathrm{Tr}(ABC) = \mathrm{Tr}(CAB)$, shows that Gibbs states formally satisfy the relation

$$\omega(AB) = \omega(B\alpha_{\mathrm{i}\beta}(A)) \ , \tag{5.3}$$

for all $A, B \in \mathfrak{A}$, where the automorphism

$$\alpha_t(A) := \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH} \tag{5.4}$$

describes the free time evolution of an observable $A \in \mathfrak{A}$. Equation (5.3) gives the combinatorics inherent to thermal equilibrium states of finite as well as infinite quantum systems.

Now, consider a state ω_ρ that is described by a density matrix ρ and define the entropy of ω_ρ by the von Neumann entropy functional

$$\mathcal{S}(\omega_\rho) := -\operatorname{Tr}(\rho \ln \rho) \ , \tag{5.5}$$

where we understand that $x \ln x = 0$ at $x = 0$. If one defines the free energy of the state ω_ρ by

$$\mathcal{F}(\omega_\rho) := \omega_\rho(H) - \frac{1}{\beta}\mathcal{S}(\omega_\rho) \ , \tag{5.6}$$

then the Gibbs state is the unique state that minimizes the free energy $\mathcal{F}(\omega_\rho)$. Equivalently, the Gibbs state maximizes the entropy at fixed energy [BR97, Weh78].

A necessary condition for Gibbs states to be well defined is that H has a purely discrete spectrum bounded from below (We consider only positive temperature states: $\beta > 0$). For infinite systems, Gibbs states are ill defined because $\operatorname{Tr}(e^{-\beta H}) = \infty$. Nonetheless, a generalized definition of thermal equilibrium states exists for infinite systems, namely, the notion of KMS states. The above notion of a Gibbs state implies a characterization in terms of analytic functions $F_{A,B}$ for any pair $A, B \in \mathfrak{A}$, that satisfy certain boundary conditions, provided that the Hamiltonian H is bounded below and $\mathrm{e}^{-\beta H/2}$ is of trace class (see, e.g., [Emc72, Weh78]). That this characterization survives the thermodynamical limit and thus can be used for the definition of equilibrium states in the general case has been shown in [HHW67]. Since then, many applications have shown that KMS states indeed describe thermal equilibrium.

We come to the definition of KMS states. Consider a C*-dynamical system $(\mathfrak{A}, \alpha_t)$.

Definition 5.1 (KMS state) Let $\beta > 0$ denote the inverse temperature. A state ω_β is called a β-KMS state if for all $A, B \in \mathfrak{A}$ there is a function $F_{A,B}(t) : C_\beta \to \mathbb{C}$ which is analytic in the strip $C_\beta := \{z \in \mathbb{C} : 0 < \Im z < \beta\}$, bounded and continuous on its closure $\overline{C}_\beta$, and satisfies the boundary conditions

$$F_{A,B}(t) = \omega_\beta(A\alpha_t(B)), \qquad F_{A,B}(t + \mathrm{i}\beta) = \omega_\beta(\alpha_t(B)A) \ . \tag{5.7}$$

Of course, on a non-stationary spacetime there exists no global C*-dynamical system. Thus, no global KMS state can exist in that spacetimes. We remark that a relativistic KMS condition has been defined in [BB94].

5.2 Almost equilibrium states

As noted in chapter 4, it is well known that in non-stationary spacetimes there is no global generator of time-translations. The standard Hamiltonian – the integral of the energy density over the Cauchy surface – is not conserved. Even worse, the energy density is not bounded-below at a spacetime point, and spatially averaged energy densities

are ill defined for dimensions $n > 2$. An energy quantity which is unbounded below, poses serious problems regarding the existence of equilibrium states. However, as we have also seen, there exists a quantum inequality that gives lower bounds on the difference of energy densities of Hadamard states averaged along the worldline of an observer in any globally hyperbolic spacetime. Thus, one can expect to find ground states with respect to this kind of energy. Indeed, in [Olb07a] states with this property so-called states of low energy, were constructed (see section 5.5). However, states of low energy are pure states; consequently, they do not describe systems in thermal equilibrium. They are merely ground states of a class of almost equilibrium states, as we will show in this chapter.

Our guiding idea for the construction of the almost equilibrium states is to define a sensible free energy functional $\mathcal{F}(\omega)$ on the class of homogeneous, isotropic, quasi-free states that is based on the quantum inequality stated in theorem 4.13. We write this functional exclusively in terms of the two-point matrix (3.49). Subsequently, we minimize this functional with respect to the components of (3.49).

Suppose that we can define a sensible free energy functional $\mathcal{F}(\omega)$, where we replace the energy expectation value $\omega_\rho(H)$ present in (5.6) by the worldline averaged expectation value of the (renormalized) stress-energy tensor,

$$\omega(H_f) := \int_\gamma dt\ f(t)^2 \left\langle : \boldsymbol{T} : \right\rangle_\omega (t,t)\ , \tag{5.8}$$

for some real-valued $f \in \mathscr{D}(\mathbb{R})$. Additionally, we assume that γ is the worldline of an isotropic observer. To remind the reader, an isotropic observer moves along a timelike geodesic with tangent vector orthogonal to the homogeneous spacelike surfaces. For such an observer, the spacetime looks spatially isotropic at any instant of time. Note also that $\mathcal{F}(\omega)$ is actually a free energy density rather than a free energy and, at this stage, it is unclear how to define the entropy $\mathcal{S}(\omega)$.

The minimization of $\mathcal{F}(\omega)$ means the following. We consider the class of homogeneous, isotropic, quasi-free states. All such states are completely determined by their two-point distributions (3.60). Within this class we look for a distinguished state $\omega_{\beta,f}$ such that for any other state ω in the same class the free energy is larger, i.e.,

$$\mathcal{F}(\omega) - \mathcal{F}(\omega_{\beta,f}) \geq 0\ . \tag{5.9}$$

In the rest of this chapter we will show that such a state $\omega_{\beta,f}$ exists and is uniquely determined by its two-point distribution. Furthermore, we show that the two-point distribution of the state $\omega_{\beta,f}$ satisfies the Hadamard condition. This latter step is crucial for the whole construction by the following argument.

The difference of the energy densities involved in the left hand side of (5.9) is

$$\omega(H_f) - \omega_{\beta,f}(H_f)) = \int_\gamma dt\ f(t)^2 \left(\langle \boldsymbol{T} \rangle_\omega (t,t) - \langle \boldsymbol{T} \rangle_{\omega_{\beta,f}} (t,t) \right)\ . \tag{5.10}$$

Provided that the states ω and $\omega_{\beta,f}$ satisfy the Hadamard condition and $\dim \mathcal{M} \geq 2$, the integral on the right hand side of (5.10) is well defined and bounded from below as we know from theorem (4.13). At this stage, it is, as a matter of fact, not known if the state that eventually minimizes this functional is a Hadamard state. So, the initial ansatz is justified afterwards by proving that the resulting state $\omega_{\beta,f}$ is indeed a Hadamard state.

The integral on the right hand side of (5.10) has the form given in lemma 4.2. It is a difference of integrals of the energy density $\boldsymbol{\rho}_{\mathrm{k}}$ for each mode $\mathbf{k}$. Note that this mode decomposition of the energy is due to the symmetry of the spacelike surfaces in Robertson-Walker spacetimes and familiar from standard quantum field theory, which, after all, can be viewed as a theory of infinitely many, independent, harmonic oscillators. We infer from this observation that, when looking for the minimum of the averaged energy density, we can confine ourselves to a single mode $\mathbf{k}$. Put differently, we can minimize the integrand instead of the integral to obtain the overall minimum. In order to utilize this principle for the free energy, we write

$$\mathcal{F}(\omega) := \int d\mu(\mathbf{k}) \mathcal{F}_{\mathbf{k}} \ , \tag{5.11}$$

where we have defined the free energy of a single mode by

$$\mathcal{F}_{\mathbf{k}} := \int_{\gamma} dt \ f(t)^2 \boldsymbol{\rho}_{\mathrm{k}}(t) - \frac{1}{\beta} \mathcal{S}_{\mathbf{k}}(\omega) \ . \tag{5.12}$$

We have yet to define the entropy $\mathcal{S}_{\mathbf{k}}$. Since each mode $\mathbf{k}$ can be considered as an independent quantum system with one degree of freedom, it is natural to ascribe an entropy given by the von Neumann entropy functional (5.5) to it. Then, $\mathcal{S}_{\mathbf{k}}$ is completely characterized by the density matrix one ascribes to the single-mode system. Since we want our states to exhibit thermal behavior, we take our modes to be Gibbs equilibrium states. This means, we consider density matrices

$$\rho_{\beta K} := \frac{\mathrm{e}^{-\beta K}}{\mathrm{Tr}(e^{-\beta K})} \ , \tag{5.13}$$

where we assume that K is a positive definite, quadratic form that is not diagonalized from the outset. The latter point is important, since, such a form is determined by three real parameters, just as the two-point distribution (3.49) of a quasi-free state.

The further course of action will be as follows. In lemma 5.2 we state the generating functional of KMS states with respect to the evolution generated by K. Then (by equation (5.54)) we obtain a one-to-one correspondence between the generator K and the two-point matrix S. This relation is used to express the free energy $\mathcal{F}_{\mathbf{k}}$ in terms of S_{11}, S_{22}, and $[S]$, which then allows to minimize with respect to these variables. The result of the minimization will be a uniquely determined state of inverse temperature β associated to the sampling function $f(t)$.

5.3 The entropy

For the entropy of a mode $\mathbf{k}$, we use the von Neumann entropy associated to the Gibbs state with density matrix $\rho_{\beta K}$:

$$\mathcal{S}_{\mathbf{k}}(\omega_{\rho_{\beta K}}) = -\operatorname{Tr}(\rho_{\beta K} \ln \rho_{\beta K}) \ , \tag{5.14}$$

where we have defined a positive definite, real quadratic form for the position and momentum operators (q, p) by

$$K(q,p) := K_{00}q^2 + K_{01}(qp+pq) + K_{11}p^2 = \begin{pmatrix} q \\ p \end{pmatrix}^{\intercal} \cdot \begin{pmatrix} K_{00} & K_{01} \\ K_{01} & K_{11} \end{pmatrix} \cdot \begin{pmatrix} q \\ p \end{pmatrix} \ . \tag{5.15}$$

In order to calculate the entropy we use canonical diagonalization of K. This is possible for any positive definite quadratic form on the phase space.

Canonical diagonalization of K

The canonical diagonalization of a quadratic Hamiltonian is a well investigated technique (for general results see, e.g., [MQ71, BG79]). We consider the simple case of linear transformation matrices M for the coordinates q, p that are canonical, which means

$$M^{\intercal}\mathbb{J}M = \mathbb{J} \ , \qquad\qquad \mathbb{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \ . \tag{5.16}$$

The eigenvalues of the matrix

$$\mathbb{J}K = \begin{pmatrix} K_{01} & K_{11} \\ -K_{00} & -K_{01} \end{pmatrix} \tag{5.17}$$

are $\pm \mathrm{i}\sqrt{[K]}$. It turns out that in this model $\Omega := 2\sqrt{[K]}$ plays the role of the oscillator frequency. The eigenvectors $\mathbf{v} = \mathbf{m}_1 + \mathrm{i}\mathbf{m}_2$ and $\overline{\mathbf{v}} = \mathbf{m}_1 - \mathrm{i}\mathbf{m}_2$ are

$$\mathbf{v} = y\left[\begin{pmatrix} K_{11} \\ -K_{01} \end{pmatrix} + \mathrm{i}\begin{pmatrix} 0 \\ \sqrt{[K]} \end{pmatrix}\right] \ , \qquad \overline{\mathbf{v}} = y\left[\begin{pmatrix} K_{11} \\ -K_{01} \end{pmatrix} - \mathrm{i}\begin{pmatrix} 0 \\ \sqrt{[K]} \end{pmatrix}\right] \ , \tag{5.18}$$

which defines the vectors $\mathbf{m}_1, \mathbf{m}_2$ needed for the transformation matrix $M = (\mathbf{m}_1, \mathbf{m}_2)$:

$$M = y\begin{pmatrix} K_{11} & 0 \\ -K_{01} & \sqrt{[K]} \end{pmatrix} \ . \tag{5.19}$$

The normalization constant y is fixed by the condition $\mathbf{m}_i^{\intercal}\mathbb{J}\mathbf{m}_j = \mathbb{J}_{ij}$, which gives

$$y = \pm\frac{1}{\sqrt{K_{11}\sqrt{[K]}}} \ , \tag{5.20}$$

so that

$$M = \pm \frac{1}{\sqrt{K_{11}\sqrt{[K]}}} \begin{pmatrix} K_{11} & 0 \\ -K_{01} & \sqrt{[K]} \end{pmatrix} . \tag{5.21}$$

This M diagonalizes the quadratic form K by

$$M^{\intercal} K M = \begin{pmatrix} \sqrt{[K]} & 0 \\ 0 & \sqrt{[K]} \end{pmatrix} . \tag{5.22}$$

The new coordinates are given by

$$Q = \frac{1}{\sqrt{K_{11}\sqrt{[K]}}} \begin{pmatrix} K_{11} \\ -K_{01} \end{pmatrix}^{\intercal} \begin{pmatrix} p \\ -q \end{pmatrix} = \frac{K_{11}p + K_{01}q}{\sqrt{K_{11}\sqrt{[K]}}} , \tag{5.23}$$

$$P = -\frac{1}{\sqrt{K_{11}\sqrt{[K]}}} \begin{pmatrix} 0 \\ \sqrt{[K]} \end{pmatrix}^{\intercal} \begin{pmatrix} p \\ -q \end{pmatrix} = \frac{\sqrt{[K]}q}{\sqrt{K_{11}\sqrt{[K]}}} . \tag{5.24}$$

If we define the frequency $\Omega := 2\sqrt{[K]}$ then the diagonalized matrix reads $\frac{1}{2}\left(\begin{smallmatrix} \Omega & 0 \\ 0 & \Omega \end{smallmatrix}\right)$. However there is still some freedom left in the choice of the coordinates. We can perform a simultaneous transformation $q' := yQ$ and $p' := y^{-1}P$ in order to gain a more suitable form of the matrix. Choosing $y = \sqrt{\Omega}$ leads to

$$K = \frac{1}{2} \begin{pmatrix} \Omega^2 & 0 \\ 0 & 1 \end{pmatrix} . \tag{5.25}$$

We conclude that choosing appropriate coordinates (q', p') is is possible to diagonalize the 'Hamiltonian' matrix K and write it in the standard harmonic oscillator form

$$K(q', p') = \frac{1}{2}(\Omega^2 q'^2 + p'^2) . \tag{5.26}$$

Therefore, for all basis-independent quantities, we can use standard results from the the theory of the one dimensional, harmonic oscillator with frequency Ω. For example the eigenvalues of the system are

$$K_n = \left(n + \frac{1}{2}\right) 2\sqrt{[K]} , \tag{5.27}$$

and the partition function is (see, e.g., [Rei87])

$$Z := \mathrm{Tr}(e^{-\beta K}) = \frac{e^{-\beta\sqrt{[K]}}}{1 - e^{-2\beta\sqrt{[K]}}} = \frac{1}{2\sinh\left(\beta\sqrt{[K]}\right)} . \tag{5.28}$$

From the partition function Z one obtains the entropy as

$$\mathcal{S}_{\mathbf{k}}(\omega_{\rho_{\beta K}}) = -\ln\left(1 - e^{-2\beta\sqrt{[K]}}\right) + 2\beta\sqrt{[K]}\frac{e^{-2\beta\sqrt{[K]}}}{1 - e^{-2\beta\sqrt{[K]}}} . \tag{5.29}$$

5.3.1 The generator of KMS states

Now we know the entropy $\mathcal{S}_{\mathbf{k}}(\omega_{\rho_{\beta K}})$ of the modes in terms of the Hamiltonian matrix K. Note, that the expression (5.29) involves only the the determinant of K. Next, as we want to characterize states by their two-point distribution, we need the correspondence between the matrices K and S. For this, we characterize the KMS states on a Weyl algebra with respect to the time-evolution generated by K. The result, which is stated in the following lemma, generalizes a result of [NT93].

Lemma 5.2 *Let $\mathfrak{A}$ be the Weyl algebra generated by the exponentials of the position and momentum operators and let the time evolution be generated by a positive Hermitian form K, with $[K] := \det K \neq 0$ on the phase space elements $\mathbf{z} \in \mathbb{R}^2$. Then, the generator of a KMS state associated to the inverse temperature $\beta > 0$ on $\mathfrak{A}$ is given by*

$$\omega(W(\mathbf{z})) = \mathrm{e}^{-\frac{1}{4}\sqrt{[K]}\ \mathbf{z}^{\intercal}K^{-1}\mathbf{z}\ \coth\left(\sqrt{[K]}\beta\right)}. \tag{5.30}$$

Proof. To prove this, we consider the exponentiated one-dimensional Heisenberg *-algebra generated by q and p, which are subject to the commutation relations

$$[q, p] = \mathrm{i}\ , \tag{5.31}$$
$$[q, q] = 0 = [p, p]\ , \tag{5.32}$$

and invariant under involution, $q^* = q$, $p^* = p$. The Weyl operators are given by

$$W(\mathbf{z}) := \mathrm{e}^{-\mathrm{i}(z_1 q + z_2 p)}\ , \tag{5.33}$$

where $\mathbf{z} = (z_1, z_2) \in \mathbb{R}^2$. We define a symplectic form σ by

$$\sigma(\mathbf{z}, \mathbf{z}') = z_1 z_2' - z_2 z_1'\ . \tag{5.34}$$

The Weyl operators $W(z)$, which generate the algebra $\mathfrak{W}$, satisfy the Weyl relations

$$W(\mathbf{z})^* = W(-\mathbf{z})\ , \tag{5.35}$$
$$W(\mathbf{z})W(\mathbf{z}') = \mathrm{e}^{-\frac{\mathrm{i}}{2}\sigma(\mathbf{z},\mathbf{z}')}W(\mathbf{z} + \mathbf{z}')\ . \tag{5.36}$$

A state ω is, as usual, defined as a positive, linear, normalized functional on $\mathfrak{W}$. By the GNS theorem we have a representation π_ω and a representation space $\mathcal{H}_\omega$ with vectors $|\mathbf{z}\rangle = W(\mathbf{z})|0\rangle$ and $|0\rangle$ being the cyclic vector of $\mathcal{H}_\omega$. A state ω on $\mathfrak{W}$ is determined by its action on the Weyl operators

$$f(\mathbf{z}) := \omega(W(\mathbf{z})) = \langle 0, W(\mathbf{z})0\rangle\ . \tag{5.37}$$

The scalar product of two arbitrary vectors is given by

$$\langle \mathbf{z}', \mathbf{z}\rangle = \langle W(\mathbf{z}')0, W(\mathbf{z})0\rangle = \mathrm{e}^{\frac{\mathrm{i}}{2}\sigma(\mathbf{z}',\mathbf{z})}f(\mathbf{z} - \mathbf{z}')\ . \tag{5.38}$$

The time automorphisms α_t over $\mathfrak{W}$ correspond to symplectic transformation matrices B_t on the phase space. The KMS condition (5.7) together with the Weyl relations yields

$$\mathrm{e}^{-\frac{\mathrm{i}}{2}\sigma(\mathbf{z},\mathbf{z}')} f(\mathbf{z}+\mathbf{z}') = \mathrm{e}^{-\frac{\mathrm{i}}{2}\sigma(\mathbf{z}',B_{\mathrm{i}\beta}\mathbf{z})} f(B_{\mathrm{i}\beta}\mathbf{z}+\mathbf{z}') \ . \tag{5.39}$$

If $\mathbf{z}' = -\mathbf{z}$ this simplifies to (Note that $f(0) = 1$):

$$1 = \mathrm{e}^{\frac{\mathrm{i}}{2}\sigma(\mathbf{z},B_{\mathrm{i}\beta}\mathbf{z})} f((B_{\mathrm{i}\beta}-\mathbb{1})\mathbf{z}) \tag{5.40}$$

$$f((B_{\mathrm{i}\beta}-\mathbb{1})\mathbf{z}) = \mathrm{e}^{-\frac{\mathrm{i}}{2}\sigma(\mathbf{z},B_{\mathrm{i}\beta}\mathbf{z})} \ . \tag{5.41}$$

Since for invertible $(B_{\mathrm{i}\beta}-\mathbb{1})$ we have

$$\mathrm{e}^{-\frac{\mathrm{i}}{2}\sigma(\mathbf{z},B_{\mathrm{i}\beta}\mathbf{z})} = \mathrm{e}^{-\frac{\mathrm{i}}{2}\left(\sigma\left(\frac{1}{B_{\mathrm{i}\beta}-\mathbb{1}}(B_{\mathrm{i}\beta}-\mathbb{1})\mathbf{z},(B_{\mathrm{i}\beta}-\mathbb{1})\mathbf{z}\right)\right)} \ , \tag{5.42}$$

a transformation $(B_{\mathrm{i}\beta}-\mathbb{1})\mathbf{z} \to \mathbf{z}$ gives

$$f(\mathbf{z}) = \mathrm{e}^{-\frac{\mathrm{i}}{2}\sigma\left(\frac{1}{B_{\mathrm{i}\beta}-\mathbb{1}}\mathbf{z},\mathbf{z}\right)} \ . \tag{5.43}$$

Next, we tackle the relation between the matrices K and S. The time evolution generated by K is given by

$$\alpha_t(W(z)) = \mathrm{e}^{-\mathrm{i}Kt}\mathrm{e}^{\mathrm{i}(z_1 q+z_2 p)}\mathrm{e}^{\mathrm{i}Kt} = \mathrm{e}^{\mathrm{i}(z_1(t)q+z_2(t)p)} \ . \tag{5.44}$$

The time evolution of $\mathbf{z}(t)$ is given by the Heisenberg equation $\dot{\mathbf{z}} = \mathrm{i}[K,\mathbf{z}]$. The commutators $[K,q]$ and $[K,p]$ can be calculated by (5.31) and the identity $[A,BC] = [A,B]C + B[A,C]$. The Heisenberg equation gives the system of differential equations

$$\begin{pmatrix}\dot{z}_1\\ \dot{z}_2\end{pmatrix} = \begin{pmatrix}2K_{01} & -2K_{00}\\ 2K_{11} & -2K_{01}\end{pmatrix}\cdot\begin{pmatrix}z_1\\ z_2\end{pmatrix} \ . \tag{5.45}$$

We introduce the frequency

$$\Omega := 2\sqrt{[K]} \ , \tag{5.46}$$

where $[K] := K_{00}K_{11} - K_{01}^2$ is the determinant of the matrix K. Furthermore, we set

$$\kappa_{01} := \frac{K_{01}}{\sqrt{[K]}} \ , \qquad \kappa_{00} := \frac{K_{00}}{\sqrt{[K]}} \ , \qquad \kappa_{11} := \frac{K_{11}}{\sqrt{[K]}} \ . \tag{5.47}$$

Then, the time evolution can be written as

$$\mathbf{z}(t) = B_t\mathbf{z}(0) \ , \tag{5.48}$$

where

$$B_t := \begin{pmatrix}\cos(\Omega t)+\kappa_{01}\sin(\Omega t) & -\kappa_{00}\sin(\Omega t)\\ \kappa_{11}\sin(\Omega t) & \cos(\Omega t)-\kappa_{01}\sin(\Omega t)\end{pmatrix} \ . \tag{5.49}$$

The matrix B_t generalizes the usual harmonic oscillator evolution matrix. To implement the KMS condition we complexify time, $t \to \mathrm{i}\beta$, and since $\sin(\mathrm{i}\beta) = \mathrm{i}\sinh(\beta)$ and $\cos(\mathrm{i}\beta) = \cosh(\beta)$, we obtain

$$B_{\mathrm{i}\beta} = \begin{pmatrix} \cosh(\Omega\beta) + \mathrm{i}\,\kappa_{01}\sinh(\Omega\beta) & -\mathrm{i}\,\kappa_{00}\sinh(\Omega\beta) \\ \mathrm{i}\,\kappa_{11}\sinh(\Omega\beta) & \cosh(\Omega\beta) - \mathrm{i}\,\kappa_{01}\sinh(\Omega\beta) \end{pmatrix} . \tag{5.50}$$

The matrix $(B_{\mathrm{i}\beta} - \mathbb{1})$ is invertible for $[K]\,, \beta \neq 0$ (note that $\coth\left(\frac{x}{2}\right) = \frac{\sinh(x)}{\cosh(x)-1}$)

$$(B_{\mathrm{i}\beta} - \mathbb{1})^{-1} = -\frac{1}{2}\begin{pmatrix} 1 - \mathrm{i}\,\kappa_{01}\coth\left(\frac{\Omega\beta}{2}\right) & \mathrm{i}\,\kappa_{00}\coth\left(\frac{\Omega\beta}{2}\right) \\ -\mathrm{i}\,\kappa_{11}\coth\left(\frac{\Omega\beta}{2}\right) & 1 + \mathrm{i}\,\kappa_{01}\coth\left(\frac{\Omega\beta}{2}\right) \end{pmatrix} , \tag{5.51}$$

and thus we find

$$\sigma\left(\frac{1}{B_{\mathrm{i}\beta} - \mathbb{1}}\mathbf{z}, \mathbf{z}\right) = -\frac{\mathrm{i}}{2}\frac{1}{\sqrt{[K]}}\begin{pmatrix} z_1 \\ z_2 \end{pmatrix}^{\intercal}\begin{pmatrix} K_{11} & -K_{01} \\ -K_{01} & K_{00} \end{pmatrix}\begin{pmatrix} z_1 \\ z_2 \end{pmatrix}\coth\left(\sqrt{[K]}\beta\right) . \tag{5.52}$$

So we have found the generator

$$f(\mathbf{z}) = \mathrm{e}^{-\frac{1}{4}\sqrt{[K]}\ \mathbf{z}^{\intercal}K^{-1}\mathbf{z}\ \coth\left(\sqrt{[K]}\beta\right)} . \tag{5.53}$$

This proves lemma 5.2. □

Defining the quadratic form $S(\mathbf{z}, \mathbf{z}) := \frac{1}{2}(\mathbf{z}^{\intercal}S\mathbf{z})$ and remembering that the generator of a quasi-free state is given by $f(\mathbf{z}) = \mathrm{e}^{-\frac{1}{2}S(\mathbf{z},\mathbf{z})}$ we infer that

$$\begin{pmatrix} S_{00} & S_{01}^{\Re} \\ S_{01}^{\Re} & S_{11} \end{pmatrix} = \frac{1}{2\sqrt{[K]}}\coth\left(\beta\sqrt{[K]}\right)\begin{pmatrix} K_{11} & -K_{01} \\ -K_{01} & K_{00} \end{pmatrix} . \tag{5.54}$$

Inverting (5.54) gives

$$\begin{pmatrix} K_{00} & K_{01} \\ K_{01} & K_{11} \end{pmatrix} = \frac{1}{\beta\sqrt{[S]}}\operatorname{Arcoth}(2\sqrt{[S]})\begin{pmatrix} S_{11} & -S_{01}^{\Re} \\ -S_{01}^{\Re} & S_{00} \end{pmatrix} . \tag{5.55}$$

The determinants of K and S are related by

$$\sqrt{[K]} = \frac{1}{\beta}\operatorname{Arcoth}(2\sqrt{[S]}) , \qquad \sqrt{[S]} = \frac{1}{2}\coth(\beta\sqrt{[K]}) . \tag{5.56}$$

Thus, we can write the entropy per mode as

$$\mathcal{S}_{\mathbf{k}}(\omega_{\rho_{\beta K}}) = -\ln\left(1 - \mathrm{e}^{-2\operatorname{Arcoth}(2\sqrt{[S]})}\right) + 2\operatorname{Arcoth}(2\sqrt{[S]})\frac{\mathrm{e}^{-2\operatorname{Arcoth}(2\sqrt{[S]})}}{1 - \mathrm{e}^{-2\operatorname{Arcoth}(2\sqrt{[S]})}} \tag{5.57}$$

$$= 2\sqrt{[S]}\operatorname{Arcoth}(2\sqrt{[S]}) + \frac{1}{2}\ln\left(\frac{4\,[S] - 1}{4}\right) , \tag{5.58}$$

where, for the second line, we used that $\operatorname{Arcoth}(y) = \frac{1}{2}\ln\left(\frac{y+1}{y-1}\right)$ and thus $\mathrm{e}^{-2\operatorname{Arcoth}(4y)} = \frac{4y+1}{4y-1}$.

5.4 Minimization of the free energy

Using the energy density (4.59) and the entropy formula (5.58) we can write the free energy functional $\mathcal{F}_{\mathbf{k}}$ exclusively in terms of the two-point matrix (3.49).

$$\begin{aligned}\mathcal{F}_{\mathbf{k}} := S_{00}d_1(T_{\mathrm{k}},f) + \mathrm{a}^6 S_{11}d_2(T_{\mathrm{k}},f) \pm \mathrm{a}^3\sqrt{S_{00}S_{11}-[S]}\,d_3(T_{\mathrm{k}},f) \\ -\frac{1}{\beta}\left[2\sqrt{[S]}\,\mathrm{Arcoth}(2\sqrt{[S]}) + \frac{1}{2}\ln\left(\frac{4\,[S]-1}{4}\right)\right]\ ,\end{aligned} \tag{5.59}$$

where we used $[S] := S_{00}S_{11} - (S_{01}^{\Re})^2$ to eliminate $S_{01}^{\Re}$ in favour of the determinant $[S]$. The remaining task is a simple exercise, namely, the minimization of this expression. A necessary condition for the minimization of $\mathcal{F}_{\mathbf{k}}$ is that we have a critical point, i.e., the gradient of the function vanishes:

$$\nabla_{(S_{00},S_{11},[S])}\mathcal{F}_{\mathbf{k}} \stackrel{!}{=} 0\ . \tag{5.60}$$

This amounts to the equations

$$d_1(T_{\mathrm{k}},f) + \frac{\mathrm{a}(t_0)^3 d_3(T_{\mathrm{k}},f)}{2}\frac{S_{11}}{\sqrt{S_{00}S_{11}-[S]}} = 0\ , \tag{5.61}$$

$$d_2(T_{\mathrm{k}},f) + \frac{d_3(T_{\mathrm{k}},f)}{2\mathrm{a}(t_0)^3}\frac{S_{00}}{\sqrt{S_{00}S_{11}-[S]}} = 0\ , \tag{5.62}$$

$$-\frac{1}{\beta\sqrt{[S]}}\,\mathrm{Arcoth}(2\sqrt{[S]}) \pm \frac{\mathrm{a}(t_0)^3 d_3(T_{\mathrm{k}},f)}{2}\frac{1}{\sqrt{S_{00}S_{11}-[S]}} = 0\ , \tag{5.63}$$

where the coefficients $d_i(T,f)$ are given by (4.60). Multiplying (5.61) by (5.62) we obtain

$$\sqrt{S_{00}S_{11}-[S]} = \frac{|d_3|}{\sqrt{4d_1d_2-d_3^2}}\sqrt{[S]}\ . \tag{5.64}$$

Using this, and assuming $\beta > 0$, the critical point is obtained from (5.63) as

$$\sqrt{[S]} = \frac{1}{2}\coth\left(\frac{\beta}{2}\mathrm{a}(t)^3\sqrt{4d_1d_2-d_3^2}\right)\ , \tag{5.65}$$

where we omitted the combination of signs from (5.63) and $d_3/|d_3|$ giving no solution for $\beta > 0$. So, given a sampling function $f(t)$ there is for every $\beta > 0$ a unique solution to equation (5.65) and thus a unique minimum of the free energy functional $\mathcal{F}(\omega_{\rho_{\beta K}})$ given in (5.59). We state this result as a theorem.

Theorem 5.3 *Consider the Weyl algebra $\mathfrak{A}$ of the minimally coupled Klein-Gordon field in a Robertson-Walker spacetime. Define the free energy of a homogeneous, isotropic, quasi-free state ω on $\mathfrak{A}$ by*

$$\mathcal{F}(\omega) := \int d\mu(\mathbf{k})\mathcal{F}_{\mathbf{k}}\ , \tag{5.66}$$

where

$$\mathcal{F}_{\mathbf{k}} := \int_{\gamma} dt\ f(t)^2 \boldsymbol{\rho}_{\mathrm{k}}(t) - \frac{1}{\beta}\mathcal{S}_{\mathbf{k}}(\omega)\ . \tag{5.67}$$

and $\boldsymbol{\rho}_{\mathrm{k}}$ is the energy density of a mode. Averaging takes place along a timelike curve γ with a sampling function $f \in \mathscr{D}(\mathbb{R})$, and each mode is assigned the von Neumann entropy $\mathcal{S}_{\mathbf{k}}(\omega)$. Then, for every $\beta > 0$ and every function f, there is a unique state $\omega_{\beta,f}$ that minimizes $\mathcal{F}(\omega)$. This state is determined by

$$\sqrt{[S]} = \frac{1}{2}\coth\left(\frac{\beta}{2}\mathrm{a}(t)^3\sqrt{4d_1(T_{\mathrm{k}},f)d_2(T_{\mathrm{k}},f) - d_3^2(T_{\mathrm{k}},f)}\right) \tag{5.68}$$

supplemented by equations (5.61)*, and* (5.62)*, where T_{k} is an arbitrary solution to* (3.35) *satisfying* (3.37)*. We refer to $\omega_{\beta,f}$ as an almost equilibrium state of inverse temperature β associated to f.*

The almost equilibrium states are parametrized by arbitrary solutions $T_{\mathrm{k}}(t)$ of the time-dependent part of the Klein-Gordon equation. As we will see in the next section, they resemble equilibrium states in Minkowski space if one uses the states of low energy for the parametrization.

5.5 Hadamard property

In this section, we prove that the two-point distribution of the almost equilibrium states satisfies the Hadamard condition. This is of twofold importance. First, it is a necessary condition to make our ansatz meaningful, as otherwise the energy difference involved in the free energy (5.10) is not bounded below and our formal result remains formal. Second, it proves that the almost equilibrium states can be considered as physical states in the sense we described in chapter 2.

We are in the fortunate situation that we can base our proof on previous related work [Jun96, JS02, Olb07a, Olb07b]. It was shown in [Olb07a] that the states of low energy are Hadamard states. The proof used the fact that for large momenta k and large iteration order n the difference of the two-point distributions of the states of low energy and the adiabatic vacuum states converges to zero. Thus, the two-point distributions differ only by a smooth function. Since adiabatic vacuum states of infinite order are Hadamard states [Jun96, Jun02], this proves the Hadamard property of the states of low energy. Along the same line of reasoning, we show that the two-point distributions of the almost equilibrium states and of the states of low energy also differ only by a smooth function. The calculations are simplified a great deal, due to the fact that the states of low energy are the natural ground states associated to the almost equilibrium states.

Parametrization by states of low energy

Let us first introduce the states of low energy [Olb07a]. Consider the Weyl algebra $\mathfrak{A}$ of the free Klein-Gordon field over a Robertson-Walker spacetime $(\mathcal{M}, \mathfrak{g}_{\mu\nu})$ and $f(t) \in \mathscr{D}(\mathbb{R})$. In the set of homogeneous, isotropic, pure quasi-free states on $\mathfrak{A}$, there is a state $\omega_{\infty,f}$ for which the averaged energy density

$$\omega(H_f) = \int\limits_{\gamma} dt\ f(t)^2 \left\langle : \boldsymbol{T} : \right\rangle_{\omega} (t) \tag{5.69}$$

is minimal. The averaging is understood along the path of an isotropic observer. This state is given by the two-point distribution

$$\omega^{(2)}_{\infty,f}(x, x') = \int \mathrm{d}\mathbf{k}\ Y_{\mathbf{k}}(\mathbf{x}) \overline{Y}_{\mathbf{k}}(\mathbf{x}')\, \overline{L}_{\mathrm{k}}(t) L_{\mathrm{k}}(t') \tag{5.70}$$

with

$$L_{\mathrm{k}}(t) = \lambda T_{\mathrm{k}}(t) + \mu \overline{T}_{\mathrm{k}}(t), \tag{5.71}$$

where T_{k} is an arbitrary solution of the differential equation (3.35) fulfilling the continuity condition (3.37) and λ, μ are given by the equations

$$\lambda = \exp(i\alpha) \sqrt{\frac{c_1}{2\sqrt{c_1^2 - |c_2|^2}} + \frac{1}{2}}\ , \qquad \mu = \sqrt{\frac{c_1}{2\sqrt{c_1^2 - |c_2|^2}} - \frac{1}{2}}\ . \tag{5.72}$$

The coefficients $c_1 = c_1(T_{\mathrm{k}}, f)$ and $c_2 = c_2(T_{\mathrm{k}}, f)$, up to a factor of 2, are defined in equation (4.58). Setting $T_{\mathrm{k}} = L_{\mathrm{k}}$, it follows that a state given by L_{k} is a state of low energy if and only if it satisfies $c_2(L_{\mathrm{k}}, f) = 0$.

For the proof of the Hadamard property, and presumably for most other purposes, the expression (5.68) defining almost equilibrium states is simplified considerably by using the states of low energy for the parametrization. So, we plug in a state of low energy $L_{\mathrm{k}}(t)$ into (5.65). Note that the squared modulus of (3.37), is given by the useful relation

$$4|T|^2|\dot{T}|^2 - \left(\overline{T}\dot{T} + T\dot{\overline{T}}\right)^2 = |\overline{T}\dot{T} - T\dot{\overline{T}}|^2 = \frac{1}{\mathrm{a}^6}\ , \tag{5.73}$$

which turns up several times in the calculations. Plugging in the states of low energy into the expression $4d_1d_2 - d_3$ gives, due to $c_2(L_{\mathrm{k}}(t), f) = 0$ in equation (4.60),

$$4d_1d_2 - d_3^2 = 4|L_{\mathrm{k}}(t_0)|^2|\dot{L}_{\mathrm{k}}(t_0)|^2 c_1^2(L_{\mathrm{k}}, f) - \left(\overline{L}_{\mathrm{k}}(t_0)\dot{L}_{\mathrm{k}}(t_0) + L_{\mathrm{k}}(t_0)\dot{\overline{L}}_{\mathrm{k}}(t_0)\right)^2 c_1^2(L_{\mathrm{k}}, f) \tag{5.74}$$

$$= \frac{1}{\mathrm{a}(t_0)^6} c_1^2(L_{\mathrm{k}}, f)\ . \tag{5.75}$$

Using this, equation (5.65) becomes

$$\sqrt{[S]} = \frac{1}{2}\coth\left(\frac{\beta}{2}\, c_1(L_\mathrm{k}, f)\right) \ . \tag{5.76}$$

Solving for S_{00} and S_{11} at the minimum of the free energy gives

$$S_{11} = \frac{2|d_1|}{\mathrm{a}^3\sqrt{4d_1d_2 - d_3^2}}\sqrt{[S]} \ , \tag{5.77}$$

$$S_{00} = \frac{2\mathrm{a}^3|d_2|}{\sqrt{4d_1d_2 - d_3^2}}\sqrt{[S]} \ , \tag{5.78}$$

where d_1 and d_2 have the same sign. Noting that d_1 and d_2 are always positive for states of low energy, this reduces to

$$S_{11} = 2|L_\mathrm{k}(t_0)|^2\sqrt{[S]} \ , \tag{5.79}$$

$$S_{00} = 2\mathrm{a}(t_0)^6|\dot{L}_\mathrm{k}(t_0)|^2\sqrt{[S]} \tag{5.80}$$

for the almost equilibrium states.

Now, we calculate the coefficients b_1 and b_2. We can use the expressions for S_{00} and S_{11} to find an expression of $S_{01}^\Re$ from $[S] = S_{00}S_{11} - (S_{01}^\Re)^2$:

$$S_{01}^\Re = \pm\sqrt{4\mathrm{a}(t_0)^6|L_\mathrm{k}(t_0)|^2|\dot{L}_\mathrm{k}(t_0)|^2 - 1}\cdot\sqrt{[S]} \ . \tag{5.81}$$

On the other hand we know that with the normalization (3.37) we have equation (5.73) giving

$$\mathrm{a}(t_0)^3\left(\overline{L}_\mathrm{k}(t_0)\dot{L}_\mathrm{k}(t_0) + L_\mathrm{k}(t_0)\dot{\overline{L}}_\mathrm{k}(t_0)\right) = \pm\sqrt{4\mathrm{a}(t_0)^6|L_\mathrm{k}(t_0)|^2|\dot{L}_\mathrm{k}(t_0)|^2 - 1} \ . \tag{5.82}$$

Each of the last two equations has two possible signs. If the signs adjust such that their product is negative we can write

$$b_1 = S_{00}|L_\mathrm{k}(t_0)|^2 + \mathrm{a}(t_0)^6S_{11}|\dot{L}_\mathrm{k}(t_0)|^2 + \left(\overline{L}_\mathrm{k}(t_0)\dot{L}_\mathrm{k}(t_0) + L_\mathrm{k}(t_0)\dot{\overline{L}}_\mathrm{k}(t_0)\right)\mathrm{a}(t_0)^3S_{01}^\Re \tag{5.83}$$

$$= 4\mathrm{a}(t_0)^6|L_\mathrm{k}(t_0)|^2|\dot{L}_\mathrm{k}(t_0)|^2\sqrt{[S]} - \left(4\mathrm{a}(t_0)^6|L_\mathrm{k}(t_0)|^2|\dot{L}_\mathrm{k}(t_0)|^2 - 1\right)\sqrt{[S]} \tag{5.84}$$

$$= \sqrt{[S]} \ . \tag{5.85}$$

Assuming the same adjustment of signs as before, we have an alternative expression for $S_{01}^\Re$, namely

$$S_{01}^\Re = -\mathrm{a}(t_0)^3\left(\overline{L}_\mathrm{k}(t_0)\dot{L}_\mathrm{k}(t_0) + L_\mathrm{k}(t_0)\dot{\overline{L}}_\mathrm{k}(t_0)\right)\sqrt{[S]} \ , \tag{5.86}$$

which inserted into b_2 gives

$$b_2 = -S_{00}\overline{L}_{\mathrm{k}}^2(t_0) - \mathrm{a}(t_0)^6 S_{11}\dot{\overline{L}}_{\mathrm{k}}^2(t_0) - 2\overline{L}_{\mathrm{k}}(t_0)\dot{\overline{L}}_{\mathrm{k}}(t_0)\mathrm{a}(t_0)^3 S_{01}^{\Re} \tag{5.87}$$

$$= 2\mathrm{a}(t_0)^6\sqrt{[S]}\Big[|\dot{L}_{\mathrm{k}}(t_0)|^2\overline{L}_{\mathrm{k}}^2(t_0) - |L_{\mathrm{k}}(t_0)|^2\dot{\overline{L}}_{\mathrm{k}}^2(t_0) \tag{5.88}$$

$$+ \overline{L}_{\mathrm{k}}(t_0)\dot{\overline{L}}_{\mathrm{k}}(t_0)\left(\overline{L}_{\mathrm{k}}(t_0)\dot{L}_{\mathrm{k}}(t_0) + L_{\mathrm{k}}(t_0)\dot{\overline{L}}_{\mathrm{k}}(t_0)\right)\Big] \tag{5.89}$$

$$= 0\ . \tag{5.90}$$

5.5.1 Almost equilibrium states are Hadamard states

Now we are prepared to prove that our construction indeed yields Hadamard states.

Proposition 5.4 *The two-point distribution of an almost equilibrium state $\omega_{\beta,f}$ satisfies the Hadamard condition.*

Proof. The strategy for the proof is the following. We show that that the difference of the two-point distributions, i.e., $(\omega^{(2)}_{\beta,f} - \omega^{(2)}_{\infty,f})(x,x')$, is a smooth function and thus the singular parts of $\omega_{\beta,f}$ and $\omega_{\infty,f}$ coincide. As indicated in section 2.2.4 an implicit infrared cutoff for the relevant integrals can be assumed, i.e., we have only to care for the large k behaviour. (For the closed case $\varepsilon = +1$ no such assumption is needed.) Since the states of low energy $\omega_{\infty,f}$ are known to have a Hadamard singularity structure, this proves the same for the almost equilibrium states $\omega_{\beta,f}$.

We have shown that $b_1 = \sqrt{[S]}$ and $b_2 = 0$. Hence,

$$\left(\omega^{(2)}_{\beta,f} - \omega^{(2)}_{\infty,f}\right)(x,x') = \int \mathrm{d}\mathbf{k}\ Y_{\mathbf{k}}(\mathbf{x})\overline{Y}_{\mathbf{k}}(\mathbf{x}')\frac{L_{\mathrm{k}}(x^0)\overline{L}_{\mathrm{k}}(x'^0) + \overline{L}_{\mathrm{k}}(x^0)L_{\mathrm{k}}(x'^0)}{\mathrm{e}^{\beta c_1(L_{\mathrm{k}},f)} - 1}\ . \tag{5.91}$$

In [LR90] the following estimates for the growth of $Y_{\mathbf{k}}(\mathbf{x})$ and $T_{\mathrm{k}}(t)$ and their derivatives for large k are given (α is a multi-index, $j \in \mathbb{N}$):

$$|\mathrm{D}^{\alpha}_{\mathbf{x}}Y_{\mathbf{k}}(\mathbf{x})| = O(k^{|\alpha|+2})\ , \tag{5.92}$$

and

$$\mathrm{D}^j_t L_{\mathrm{k}}(t) = O(k^{j-\frac{1}{2}})\ . \tag{5.93}$$

Using this, we can then estimate the growth of the following expression

$$\sup\left|\mathrm{D}^{\nu}_{(x,x')}\left[Y_{\mathbf{k}}(\mathbf{x})\overline{Y}_{\mathbf{k}}(\mathbf{x}')\left(L_{\mathrm{k}}(t)\overline{L}_{\mathrm{k}}(t') + \overline{L}_{\mathrm{k}}(t)L_{\mathrm{k}}(t')\right)\right]\right| \tag{5.94}$$

$$= \sup\left|\mathrm{D}^{|\sigma|}_{\mathbf{x}}Y_{\mathbf{k}}(\mathbf{x})\ \mathrm{D}^{|\sigma'|}_{\mathbf{x}'}\overline{Y}_{\mathbf{k}}(\mathbf{x}')\left(\mathrm{D}^j_t L_{\mathrm{k}}(t)\ \mathrm{D}^{j'}_{t'}\overline{L}_{\mathrm{k}}(t') + \mathrm{D}^j_t\overline{L}_{\mathrm{k}}(t)\ \mathrm{D}^{j'}_{t'}L_{\mathrm{k}}(t')\right)\right| \tag{5.95}$$

$$\leq \left|\mathrm{D}^{|\sigma|}_{\mathbf{x}}Y_{\mathbf{k}}(\mathbf{x})\right|\left|\mathrm{D}^{|\sigma'|}_{\mathbf{x}'}\overline{Y}_{\mathbf{k}}(\mathbf{x}')\right|\left(\left|\mathrm{D}^j_t L_{\mathrm{k}}(t)\right|\left|\mathrm{D}^{j'}_{t'}\overline{L}_{\mathrm{k}}(t')\right| + \left|\mathrm{D}^j_t\overline{L}_{\mathrm{k}}(t)\right|\left|\mathrm{D}^{j'}_{t'}L_{\mathrm{k}}(t')\right|\right) \tag{5.96}$$

$$= O(k^{3+|\nu|})\ , \tag{5.97}$$

where $|\nu| = |\alpha| + |\alpha'|$ and $\alpha = |\sigma| + j$, $\alpha' = |\sigma'| + j'$. We also need an estimate for the growth of $c_1(\mathrm{k}) := c_1(T_\mathrm{k}, f)$. In [Olb07b] it has been shown that the k-dependence of $c_1(T_\mathrm{k}, f)$ for large k is such that there exist constants $a_1, a_2 > 0$ with

$$a_1(1 + \mathrm{k}) \leq c_1(\mathrm{k}) \leq a_2(1 + \mathrm{k}) \ . \tag{5.98}$$

Thus, the factor $\frac{1}{\mathrm{e}^{\beta c_1(L_\mathrm{k}, f)} - 1}$, which vanishes faster than any polynomial, makes the integral

$$\mathrm{D}^\alpha_{(x,x')}(\omega^{(2)} - \omega^{(2)}_{\infty,f})(x, x') \tag{5.99}$$

$$= \int \mathrm{d}\mathbf{k} \ \mathrm{D}^\alpha_{(x,x')} \left\{ Y_\mathbf{k}(\mathbf{x}) \overline{Y}_\mathbf{k}(\mathbf{x}') \frac{L_\mathrm{k}(t) \overline{L}_\mathrm{k}(t') + \overline{L}_\mathrm{k}(t) L_\mathrm{k}(t')}{\mathrm{e}^{\beta c_1(L_\mathrm{k}, f)} - 1} \right\} \tag{5.100}$$

converge absolutely. This proves that the two-point difference (5.91) is a smooth function which in turn proves the Hadamard property of $\omega^{(2)}_{\beta,f}(x, x')$. □

6 Summary and Outlook

The present thesis is the successful accomplishment of a natural task suggested by recent results in quantum field theory in curved spacetimes. In [Olb07a] ground states, so-called states of low energy, for the worldline averaged, renormalized stress-energy tensor of the Klein-Gordon field in Robertson-Walker spacetimes were constructed. They are obtained by minimizing the averaged energy density that an isotropic observer measures in a pure, homogeneous, isotropic, quasi-free state. The states of low energy depend on the sampling function used in the averaging procedure.

In this thesis we constructed, in the same setting, a family of states that we consider as almost equilibrium states to the inverse temperature β. The almost equilibrium states are obtained by a suitable application of the principle of minimal free energy – a cornerstone of statistical mechanics. More precisely, we defined a free energy functional on the homogeneous, isotropic, quasi-free states of the Klein-Gordon field, where the 'inner energy' was constructed from the worldline averaged stress-energy tensor since that quantity is known to be lower bounded on the class of Hadamard states by a quantum energy inequality [Few00]. We showed how this energy can be written in terms of the same parameters that determine the two-point distribution of a homogeneous, isotropic, quasi-free state. Viewing each mode of the quantum field as a quantum system with one degree of freedom, we assigned to the modes the usual von Neumann entropy. An essential point of the whole construction was the determination of the entropy of such a system in terms of the two-point distribution. This was accomplished by calculating the generator of a KMS state on the Weyl algebra of a system with a single degree of freedom. By subsequent minimization of the free energy, we obtained an explicit expression for the two-point distribution of a family of states, determined, again, by the sampling function of the averaging procedure and the inverse temperature β. Finally, we showed that the two-point distributions of the almost equilibrium states satisfy the Hadamard condition. The latter step is a vital part of the construction as otherwise the utilized quantum inequality would not guarantee the existence of a finite lower bound for the averaged stress-energy.

The formulation of quantum field theory in curved spacetimes disentangles the construction of the quantum algebra from the construction of the quantum states. It is well known how to construct the algebra of a linear quantum field in a globally hyperbolic spacetime. The construction of physically meaningful states, however, is less straightforward. With decreasing symmetry properties of the underlying spacetime it becomes increasingly complicated to single out such states or rather classes of them. Regarding timelike symmetries, the step from stationary to non-stationary spacetimes is the biggest

one. It brings along unitarily inequivalent representations of the algebra of observables and makes the concept of a conserved Hamiltonian that generates global time evolution useless. In view of this situation, it is important to watch for other notions of energy that may be more meaningful. We advocate that such a notion is provided by the averaged energy densities used in the quantum energy inequalities.

The almost equilibrium states defined here are, to date, the sole example of explicitly constructed (global) Hadamard states with thermal properties on a non-stationary spacetime. For quantum fields in a non-stationary spacetime it is not reasonable to expect the existence of true equilibrium states with definite temperature $1/\beta$ since the influence of tidal forces will always destroy such property. We claim that the almost equilibrium states are reasonably defined approximations to equilibrium, and that they provide an interesting starting point for future investigations. Due to the setting, namely, quantum fields in cosmological spacetimes, they might provide a class of states useful in the inflationary scenario and the analysis of the cosmic microwave background.

Like the states of low energy, the two-point distribution of an almost equilibrium state involves a sampling function $f(t) \in \mathscr{D}(\mathbb{R})$. The function $f(t)$ describes the measurement of energy by an isotropic observer. This function introduces some freedom in the construction which may be used to design states with desired properties. This might be useful with respect to models of the early universe.

Admittedly, our construction of almost equilibrium states makes heavy use of the mode decomposition, which is available in Robertson-Walker spacetimes because of the underlying symmetries. In general, there is no satisfactory mode decomposition on an arbitrary non-stationary spacetime, and thus there is no direct route for a generalization of our method.

Quantum energy inequalities, which play a major role in our construction, are among a family of interconnected criteria for dynamical stability of quantum systems [FV03]. In [SV08], a link between local thermal equilibrium states of a linear scalar field on a curved spacetime and quantum energy inequalities was alluded. It was proved that the existence of a linear scalar quantum field fulfilling some local thermal condition, in the sense of [BOR02], implies a quantum energy inequality for these states. However, no states are known that fulfill the hypothesis of the paper. Due to our construction, which, starts with a quantum inequality rather than to derive one, it might turn out that the almost equilibrium states provide examples for local thermal equilibrium states (see below).

Among the mentioned stability criteria for quantum systems there is passivity, which has not been generalized to non-stationary spacetimes so far. It is known that KMS states and mixtures of KMS states are passive. It might be worth considering, whether almost equilibrium states (and mixtures of almost equilibrium states) are 'almost passive' in a sense to be specified. Such a notion of passivity should be able to measure the amount of mechanical work that can be performed, owing to the present tidal forces, by a system in a cyclic process in a non-stationary spacetime.

Local thermal equilibrium states

The compact support of the sampling function $f(t)$ introduces intrinsically a kind of localization in time and, by taking the associated closed double cone, a localization in spacetime into the almost equilibrium states. An open question for future investigations might be how almost equilibrium states are connected to other notions of local thermal equilibrium. The most interesting states would be the local thermal equilibrium (LTE) states in the sense of Buchholz, Ojima, and Roos in [BOR02]. This approach gives a precise meaning to the saying that by a local measurement one cannot distinguish between local and global equilibrium states. This abstract idea is implemented in field theory by the following procedure. First, one chooses a set of global thermal equilibrium states, e.g., mixtures of KMS states in different inertial systems. Then, for a point x, one chooses a certain set $\mathcal{S}_x$ of reference observables. A state ω is called $\mathcal{S}_x$-thermal if its expectations values for all observables in $\mathcal{S}_x$ coincide with the expectation values for some global thermal equilibrium state ω_x. Thus, as long as one considers observables from $\mathcal{S}_x$ it is impossible to distinguish between the local state ω and the global thermal equilibrium state ω_x. Of course, nothing is said or assumed about the expectation values of other observables. Thus, in general, ω does not coincide with the global state ω_x. The spaces $\mathcal{S}_x$ are chosen as the linear spaces generated by the balanced derivatives of the Wick-square $:\phi^2:(x)$. Balanced derivatives are defined in [BOR02] as

$$\eth_{\boldsymbol{\mu}} :\phi^2:(x) = \lim_{\zeta\to 0} \left[\phi(x+\zeta)\phi(x-\zeta) - \omega_0(\phi(x+\zeta)\phi(x-\zeta))\mathbb{1}\right] \ , \tag{6.1}$$

where $\eth_{\boldsymbol{\mu}} = \partial_{\zeta^{\mu_1}} \dots \partial_{\zeta^{\mu_n}}$ with the multi-index $\boldsymbol{\mu} := (\mu_1, \dots, \mu_n) \in \mathbb{N}^n$ and ω_0 is the vacuum state. Here, one takes the limit along spacelike directions $\zeta \in \mathbb{M}$ in Minkowski spacetime, so that $\phi(x+\zeta)\phi(x-\zeta)$ is well defined as a quadratic form [Bos00]. Now, with this approach one calculates for the Wick-square, which corresponds to the balanced derivative of zero-th order, of the massless field in Minkowski space

$$\omega^{\beta e}(:\phi:(x)) = \frac{1}{12\beta^2} \ . \tag{6.2}$$

independently of x, where e is an orthonormal tetrad defining the Lorentz frame of the KMS state (see the relativistic KMS condition [BB94]). This is interpreted as an indication that the the Wick-square serves as a scalar thermometer.

It is natural to ask for the Wick-square of an almost equilibrium state and if there is a similar interpretation as thermometer. Hereby, one has to resolve an ambiguity in the definition the Wick-square since one has to choose a ground state. By construction, it is natural to choose the states of low energy for this purpose. But, by the method of locally covariant quantum fields [BFV03], one could also choose the Minkowski vacuum. The latter procedure should be viable by the generalization of LTE states for curved spacetimes that is proposed [SV08].

To the very end, let us make some speculative remarks regarding the former procedure. We use use the states of low energy for the parametrization and as the ground

state. For simplicity, we consider flat Robertson-Walker spacetimes. By some formal manipulations, one easily, obtains the expression

$$\lim_{\zeta\to 0}\left(\omega^{(2)}_{\beta,f}-\omega^{(2)}_{\infty,f}\right)(x+\zeta,x-\zeta)=\frac{1}{(2\pi)^3}\int \mathrm{d}\mathbf{k}\,\frac{2|L_{\mathrm{k}}(x^0)|^2}{\mathrm{e}^{\beta c_1(L_k,f)}-1}\,. \tag{6.3}$$

Note that this expression bears a strong resemblance to its Minkowski spacetime counterpart. In that case by equation (3.38) we have $2|L_{\mathrm{k}}(x^0)|^2=\frac{1}{\omega_{\mathrm{k}}}$ and $c_1(L_k,f)=\omega_{\mathrm{k}}$ provided that $\int f(t)^2dt=1$. We learn from this that $c_1(T_{\mathrm{k}},f)$ possibly plays the role of a generalized frequency. In order to proceed into the direction of LTE states on needs estimates on $c_1(L_k,f)$. Such estimates may, e.g, lead to the interpretation that the almost equilibrium states are a mixture of LTE states with a range of temperatures $a(f)<\beta<b(f)$.

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Acknowledgements

I am deeply grateful to my supervisor Prof. Klaus Fredenhagen for initiating and caring for this project; I thank him for the offered trust and the kind hospitality in his working group.

I am also grateful to Nicola Pinamonti for many useful discussions on the subject and critical reading of the manuscript. It helped a lot.

Furthermore, I have to thank Prof. Hans-Jürgen Seifert for his amiableness, which made life much easier in the past years.

And, of course, I thank all friends and colleagues, past and present, at the AQFT group, the II. Institute for Theoretical Physics, DESY, and elsewhere.

Finally, I thank my parents for still supporting me, as always, in every respect, as much as they can, in whatever I do. We have come long way in one generation. The honor belongs to you.

Financial support of the Emmy-Noether Projekt "Hawking-Strahlung Schwarzer Löcher" and of the Graduiertenkolleg "Zukünftige Entwicklungen in der Teilchenphysik" is gratefully acknowledged.