Local Thermal Equilibrium on Curved Spacetimes and Linear Cosmological Perturbation Theory

Der Fakultät für Physik und Geowissenschaften
der Universität Leipzig
eingereichte

D I S S E R T A T I O N

zur Erlangung des akademischen Grades

DOCTOR RERUM NATURALIUM
(Dr. rer. nat.)

vorgelegt

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geboren am 23.03.1983 in Bielefeld (Deutschland)

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Tag der Verleihung: 17.06.2013

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Bibliographische Beschreibung

Eltzner, Benjamin
Local Thermal Equilibrium on Curved Spacetimes and Linear Cosmological Perturbation Theory
Universität Leipzig, Dissertation
154 S., 52 Lit., 4 Abb.

Referat: In dieser Arbeit wird die von Schlemmer eingeführte Erweiterung des Kriteriums für lokales thermisches Gleichgewicht in Quantenfeldtheorien von Buchholz, Ojima und Roos auf gekrümmte Raumzeiten untersucht. Dabei werden verschiedene Probleme identifiziert und insbesondere die bereits von Schlemmer gezeigte Instabilität unter Zeitentwicklung untersucht. Es wird eine alternative Herangehensweise an lokales thermisches Gleichgewicht in Quantenfeldtheorien auf gekrümmten Raumzeiten vorgestellt und deren Probleme diskutiert. Es wird dann eine Untersuchung des dynamischen Systems der linearen Feld- und Metrikstörungen im üblichen Inflationsmodell mit Blick auf Uneindeutigkeit der Quantisierung durchgeführt. Zuletzt werden die Temperaturfluktuationen der kosmischen Hintergrundstrahlung auf Kompatibilität mit lokalem thermalem Gleichgewicht überprüft.

Contents

1. Introduction

The description of the very early stages of development of the universe is an intricate problem in theoretical physics. Due to the expansion of the universe it is clear that general relativity is necessary to describe spacetime, while the very high energy density in the early universe calls for a description of matter in terms of quantum field theory. The field of cosmology has therefore been and continues to be a major source of progress in the development of quantum field theory on curved spacetimes as a theoretical tool.

Since the discoveries of some peculiar effects, most prominently the Hawking and Unruh effects and cosmological particle creation it has been clear that quantum field theory on curved spacetime yields genuinely new results in comparison to standard quantum field theory on flat spacetime. On a theoretical level however also genuinely new problems arise. In standard quantum field theory a wealth of states with well understood physical meaning has been characterised. This is linked to two circumstances which are absent in quantum field theory on curved spacetime. Firstly, there is a unique Poincaré invariant state called the vacuum and secondly the states in the vacuum Fock space can be understood in terms of a well defined particle interpretation. In quantum field theory on curved spacetimes no Poincaré symmetry exists and the effect of cosmological particle creation shows that particle number is no longer a concept strictly linked to a state, which makes particle interpretation on general spacetimes ambiguous as a whole.

In standard quantum field theory a treatment of quantum fields and states in terms of the vacuum Fock space is common. However, limitations of the Fock space formalism become apparent not only on curved spacetimes, but also in the context of thermodynamics. The theoretical framework of statistical physics derives macroscopic thermodynamics from the underlying microscopic theory and has been very successful in doing so. However, the attempt to reconcile statistical physics with quantum field theory leads to a problem. The principal object defining a state in terms of statistical physics is the density matrix which is a well defined object on a quantum mechanical Hilbert space of countable dimension and thus for quantum systems in a finite volume. Thermal equilibrium is described by Gibbs density matrices which act on the vacuum Fock space for a quantum field theory. Taking the thermodynamic limit of infinite volume causes the trace of Gibbs density matrices to diverge which means that the thermodynamic limit does not lead to a well defined state in the vacuum Fock space.

The simplest cosmological models that are usually taken as a starting point for cosmological investigations are the Friedmann-Robertson-Walker spacetimes, where the basic models are simply fluid dynamical and the thermodynamical models. As the energy density in the early universe is very high, a high temperature is to be expected and therefore a treatment of matter in terms of thermal quantum field theory seems to be in order. Because of this the theoretical treatment of cosmology is also afflicted by the limitations of the vacuum Fock space formalism of quantum field theory.

Standard treatments of the cosmology of the very early universe circumvent the obstacles outlined above by following a rather heuristic and ad hoc procedure. The problem of thermal quantum field theory is usually avoided altogether and a Hilbert space treatment is applied without a proper definition of its context. The present work will take a different route by sticking to a clear mathematical framework and using mathematical tools designed specifically for the treatment of thermal quantum field theory in curved spacetimes. In the course of this investigation the fitness of these tools for the treatment of physical problems as well as the validity of certain standard procedures applied in the standard literature on cosmology of the very early universe will be reflected.

To overcome the limitations of the vacuum Fock space approach to quantum field theory the algebraic approach to quantum field theory has turned out to be successful. In this context the fundamental objects of interest are not field operators and density matrices on a Fock space but an abstract algebra of observables and states on this algebra, which are given by positive normalised functionals. There is a well defined connection between the algebraic treatment and the vacuum Fock space picture, in the case of Minkowski spacetime. In this sense algebraic quantum field theory can be seen to embody the standard approach to quantum field theory. However, algebraic quantum field theory goes considerably beyond the vacuum Fock space approach in that thermodynamic equilibrium states in the thermodynamic limit are included in the extended set of states on the algebra of observables. It also shows that the vacuum Fock space is in no way unique. For any state on the algebra there is a Hilbert space representation where the state is represented as a cyclic vector and for many states the Hilbert space of this representation is a Fock space.

On the other hand the large state space in algebraic quantum field theory leads from the problem of a scarcity of states to the opposite problem of an excess of states. Many states that are valid from the algebraic point of view can be regarded as unphysical for various reasons. Some states do not even admit n-point functions while the n-point functions of others have unacceptable singularity structure. The investigation of suitable restrictions for physically acceptable states is therefore an ongoing endeavour. A related question, especially for quantum field theories on curved spacetimes, is the question of physical interpretation and classification of states. The present work will be heavily concerned with this question, especially with the identification of suitable thermal states on curved spacetimes.

States of thermodynamic equilibrium in Minkowski spacetime are defined by a certain transformation behaviour of expectation values under time translation, the KMS condition. For the KMS condition to be well defined, the time translations must induce a one-parameter group of automorphisms on the algebra of observables which is the case if and only if they are a symmetry of the field theory. This is generically the case if they are a one-parameter group of isometries of spacetime, which holds true for static spacetimes. For quantum field theories on non-stationary spacetimes, time translations do not generically induce automorphisms on the algebra of observables which implies that KMS states cannot generically be defined.

The universe is known to expand, which means that spacetimes in cosmological models are non-stationary. Therefore, the impossibility to define KMS states on these spacetimes is relevant to the present work. As an illustration why global thermal equilibrium states cannot be expected to exist in an expanding spacetime, one may consider a universe filled with electromagnetic radiation with a black body intensity spectrum. The expansion of spacetime causes a redshift of the radiation, which implies a change of temperature linked to the black body spectrum. A similar effect is to be expected in the quantum treatment, which means that a thermal equilibrium state with the same temperature in the whole spacetime is no appropriate model for an expanding universe.

Therefore, a concept of thermality is needed which implements the possibility of different temperature at different spacetime points. A concept of local thermal equilibrium states, which are designed to be as similar as possible to KMS states while allowing temperature to vary in spacetime has been developed for Minkowski spacetime by [11]. The class of states identified in that work were dubbed local thermal equilibrium, or LTE, states. A straight forward generalisation of this class of states to general spacetimes has been proposed in [40] and [13] and worked out in more detail in [42]. The states described in those works are conventionally called extrinsic LTE states and some interesting results could be achieved for these states, e.g. in [43], where they were shown to satisfy quantum energy inequalities.

The present work will investigate extrinsic LTE states and the LTE concept in general in the context of cosmology of the early universe. The cosmological model treated here sticks close to the derivation of the temperature perturbations in the cosmic microwave background via cosmological perturbation theory. The temperature fluctuations of the cosmic microwave background are derived from the quantum state of perturbations during inflation and the fact that the observed spectrum fits the observations well is regarded as a major confirmation of the concept of inflation.

This model appears to be an ideal test case for thermal quantum field theory on curved spacetime and especially LTE because on the one hand it is rather simple such that a scalar field model suffices for the most part and on the other hand it leads to a non-trivial thermal state which offers the possibility to test the descriptive power of concepts of local thermality.

The investigation of the LTE concept in the present work will not be limited to the cosmological scenario but some additional questions will be considered. Especially the question whether the extrinsic LTE concept is applicable to spacetimes with a different topology of the space-like hypersurface is investigated.

Another topic the present work will make contact with is the work on "superstatistics" (e.g. [2]) in statistical mechanics where seemingly non-standard statistics emerging from a mixture of thermodynamic equilibrium states with different temperatures are investigated. As such mixtures of thermal equilibrium states occur very naturally in quantum theory, it seems that quantum theory provides a motivation for an in depth investigation of superstatistics. The interpretation of thermal observables as random fields which is common in cosmological perturbation theory as well as superstatistics is also natural for LTE states and will therefore be implemented in the present work. The question whether there is a prescription to decide if the statistics given for some model stem from a mixture of states with generic Bose or Fermi statistics translates to the question of identifying mixtures of KMS states in quantum field theory. Having such a method would be very valuable especially for the treatment of thermal quantum field theory on curved spacetimes. Therefore, this question will be addressed in the present work.

All the investigations on the topic of LTE states in the present work are related to the question of the connection between microscopic and macroscopic observables in thermal quantum field theory as an overarching topic. The extrinsic LTE condition contains a macroscopic interpretation of microscopic observables which will be investigated in the present work. The general difficulty of identifying a suitable connection between microobservables and macroobservables implies a considerable obstacle for alternatives to the extrinsic LTE concept. This point will be briefly discussed.

The present work is organised in three chapters. In Chapter 2 the necessary technical background for the following work is assembled. It does not contain significant original work, however the presentation is in many cases adapted to the requirements of the present work. Chapter 3 contains a discussion of the LTE concept, the focus lying on the extrinsic LTE condition for curved spacetimes. Several models are investigated and some considerations towards an extension or alternative to the extrinsic LTE concept are proposed. In chapter 4, the last major chapter parts of cosmological perturbation theory are discussed from a technical point of view and also in the light of the LTE concept. The work closes with conclusions and outlook. Some rather technical proofs are deferred to appendix A.

It is customary to use the first person plural in scientific works, even those written by a single author. The present work will conform with this tradition, however a brief reflection on the implication seems in order. The plural should not be mistaken as a *pluralis auctoris* that is meant to imply agreement with the reader. Instead, by using the plural, I wish to acknowledge first the work of others, on which my work is founded and without which it would have been impossible, and second the discussions with and creative input by many other researchers, without which many of the ideas in this work might never had fallen into place. In summary, the use of "we" should be understood as a reference to the inherently collective character of scientific research.

2. Technical Background

This chapter contains a description of the technical background on which this work is founded. We will start with the construction of the free scalar quantum field theory on a general globally hyperbolic spacetime. Relying on the principles of algebraic quantum field theory we will especially focus on the locally covariant framework for quantum field theory and local observables. A brief discussion of quantum states and state spaces will be conducted and it will be explained how they fit into the general covariant framework.

Next we will explain the concept of local thermal equilibrium states in flat spacetime. The subsequent description of the concept of local thermality developed for cosmological spacetimes will be complemented by a reflection on the local covariance principle.

The last part of this chapter constitutes an introduction to the formalism of cosmological perturbation theory. As this formalism is a highly developed technical tool that must be properly introduced to render even the notation of this work understandable, it is inevitable that the corresponding section is rather lengthy while not containing original results. We use units where $\hbar = c = k_B = 1$.

2.1. The Free Scalar Field on a Globally Hyperbolic Spacetime

2.1.1. Construction of the Scalar Field

Our treatment in this section is generic and contains no new results. We follow especially closely the treatment in [42] as we work in the same basic setting. We consider a spacetime described by a four-dimensional, smooth and oriented semi-Riemannian manifold $(\mathcal{M}, g)$ where the metric tensor g has the so-called Lorentzian signature $(+ - --)$. As the existence of other connected components does not influence the physics in one connected component we assume for simplicity that the spacetime be connected. As usual, all curvature quantities will be the ones derived from the unique Levi-Civita connection. We furthermore define

$$R^{\rho}{}_{\lambda\mu\nu} = \partial_{\mu}\Gamma^{\rho}_{\nu\lambda} + \Gamma^{\rho}_{\mu\tau}\Gamma^{\tau}_{\lambda\nu} - \partial_{\nu}\Gamma^{\rho}_{\mu\lambda} - \Gamma^{\rho}_{\nu\tau}\Gamma^{\tau}_{\lambda\mu}$$

$$R_{\mu\nu} = R^{\lambda}{}_{\mu\lambda\nu},$$

where Γ are the usual Christoffel symbols of the Levi-Civita connection. Our sign conventions corresponds to $(-++)$ according to the scheme of [30] which implies the following signs in the Klein-Gordon operator and the Einstein equation.

$$P_{m,\xi} = \Box + m^2 - \xi R = g^{\mu\nu}\nabla_{\mu}\nabla_{\nu} + m^2 - \xi R$$

$$G_{\mu\nu} = 8\pi T_{\mu\nu}.$$

To have a unique notion of future and past, the spacetime is furthermore required to be time oriented.

Definition 2.1.1.
A Lorentzian manifold $(\mathcal{M}, g)$ is called **time orientable** if there exists a globally defined smooth time-like vector field t^{μ}, i.e. $\forall p \in \mathcal{M}: \; g(p)(t,t) = g_{\mu\nu}(p)t^{\mu}(p)t^{\nu}(p) > 0$. A time-like vector $v \in T_p\mathcal{M}$ is called **future oriented** if $g(p)(t,v) > 0$.

In order for the Cauchy problem to be well-posed we require the spacetime to be globally hyperbolic.

Definition 2.1.2.

- A smooth curve $c : \mathbb{R} \supset I \to \mathcal{M}$ is called a **causal curve** if $\forall s \in I$: $g(c(s))(\dot{c}(s), \dot{c}(s)) \geq 0$.
- A point $p \in \mathcal{M}$ is called an **endpoint** of the curve c if for every neighbourhood U of p there exists an s_0 such that $c(s) \in U$ either for all $s > s_0$ or for all $s < s_0$.
- A causal curve is called **inextendible** if it has no endpoint.
- A hypersurface $\Sigma \subset \mathcal{M}$ is called a **Cauchy surface** if it is intersected exactly once by every inextendible causal curve.
- A spacetime $(\mathcal{M}, g)$ is called **globally hyperbolic** if it contains a Cauchy surface. It is then time orientable and diffeomorphic to $\Sigma \times \mathbb{R}$ as shown in [3].

From the requirement that the spacetime be globally hyperbolic it follows from Leray's theorem (e.g. [1]) that there are uniquely determined distributional advanced and retarded fundamental solutions $E^{\pm}$ to the Klein-Gordon operator $P_{m,\xi} = \Box + m^2 - \xi R$ with $m, \xi \in \mathbb{R}_0^+$.

$$\forall f \in C_0^\infty(\mathcal{M}) : \quad P_{m,\xi} E^{\pm} f = E^{\pm} P_{m,\xi} f = f$$

$$\mathrm{supp}(E^{\pm} f) \subset J^{\pm}(\mathrm{supp}(f))$$

From these advanced and retarded fundamental solutions we can derive the antisymmetric fundamental solution $E = E^+ - E^-$, sometimes called the "commutator function", which is needed to axiomatise the scalar field. This distribution can be interpreted as an antisymmetric bilinear form on C_0^∞ in the usual way

$$E(f, g) := \int_{\mathcal{M}} f(x)(Eg)(x) d_g x$$

where $d_g x$ denotes the volume element corresponding to g. By definition E obviously is a distributional bisolution to the Klein-Gordon equation

$$\forall f \in C_0^\infty(\mathcal{M}) : \quad P_{m,\xi} E f = E P_{m,\xi} f = 0$$

which implies $E(f, P_{m,\xi} g) = E(P_{m,\xi} f, g) = 0$.

Now we can define what we mean by a free scalar quantum field on a globally hyperbolic spacetime.

Definition 2.1.3.
For $f \in C_0^\infty(\mathcal{M})$ the symbols $\phi(f)$ with the following properties

- **Linearity:** $\forall f, g \in C_0^\infty(\mathcal{M}), \alpha \in \mathbb{C} : \quad \phi(\alpha f + g) = \alpha\phi(f) + \phi(g)$
- **Hermiticity:** $\phi(f)^* = \phi(\overline{f})$
- **Klein-Gordon equation:** $\phi(P_{m,\xi} f) = 0$
- **Commutation relations:** $[\phi(f), \phi(g)] = -iE(f, g)\mathbb{1}$

together with the identity generate a unital *-algebra $\mathcal{A}(\mathcal{M}, g)$ over $\mathbb{C}$. In this context the symbol ϕ is called a free scalar quantum field.

We will not concern ourselves with the construction of a Hilbert space as is done in [49] thus the $\phi(f)$ are up to now formal symbols that are not yet given any mathematical or physical meaning.

2.1.2. Algebra of Wick Products

To give mathematical meaning to the symbols $\phi(f)$ it is customary to define some topological *-algebra, the Hermitian elements of which can be interpreted as observables. An algebra which is often considered is the Weyl algebra described in [49], which can be interpreted as generated by exponentials of the $\phi(f)$, the so called Weyl symbols. This algebra has the additional property that it is a C^*-algebra which allows the application of highly developed formalism.

We will however need an algebra whose elements are closer to the concept of n-point functions, as such observables turn out to fit for the description of local thermality. To make precise the type of objects that should comprise our algebra we must take a detour and look for states in which we can define appropriately regularised n-point functions. To permit such an investigation it is useful to start from the unital *-algebra $\mathcal{A}(\mathcal{M}, g)$ generated by the symbols $\phi(f)$ and the identity as defined above. Compared to the Weyl algebra this algebra has the drawback that Hilbert space representatives of the $\phi(f)$ are usually unbounded and one has no preferred choice of topology. We will see that the algebra we are looking for is an enlargement of $\mathcal{A}(\mathcal{M}, g)$.

Definition 2.1.4.
A continuous linear functional $\omega : \mathcal{A}(\mathcal{M}, g) \to \mathbb{C}$ on a topological *-algebra $\mathcal{A}(\mathcal{M}, g)$ is called a **state** if it fulfils

- **Normalisation:** $\omega(\mathbb{1}) = 1$
- **Positivity:** $\forall A \in \mathcal{A}(\mathcal{M}, g) : \quad \omega(A^* A) \geq 0$

If no topology is chosen, the continuity requirement is dropped.

For later use we remark the following connection between states and representations of the algebra.

Theorem 2.1.5. *(GNS construction)*
*Let $\mathcal{A}(\mathcal{M}, g)$ be a *-algebra and $\omega : \mathcal{A}(\mathcal{M}, g) \to \mathbb{C}$ a state. Then there is a Hilbert space $\mathcal{H}_\omega$, a representation $\pi_\omega : \mathcal{A}(\mathcal{M}, g) \to (\mathcal{H}_\omega)$ (where $\mathscr{L}(\mathcal{H}_\omega)$ denotes the linear operators on $\mathcal{H}_\omega$) and a vector $|\Psi_\omega\rangle \in \mathcal{H}_\omega$ such that*

$$\forall\, A \in \mathcal{A}(\mathcal{M}, g) :\ \omega(A) = \langle \Psi_\omega |\, \pi_\omega(A)\, | \Psi_\omega \rangle \tag{2.1.1}$$

and $\{\pi_\omega(A)\, |\Psi_\omega\rangle\, | A \in \mathcal{A}(\mathcal{M}, g)\}$ is a dense subspace of $\mathcal{H}_\omega$, i.e. $|\Psi_\omega\rangle$ is cyclic.

For any second triple $(\mathcal{H}'_\omega, \pi'_\omega, |\Psi'_\omega\rangle)$ *fulfilling equation (2.1.1) there is an isometric isomorphism* $U : \mathcal{H}_\omega \to \mathcal{H}'_\omega$ *with*

$$\forall\, A \in \mathcal{A}(\mathcal{M}, g) : \; \pi'_\omega(A) = U \pi_\omega U^{-1} \tag{2.1.2}$$

$$|\Psi'_\omega\rangle = U\, |\Psi_\omega\rangle\, . \tag{2.1.3}$$

For definiteness we call two representations related by (2.1.2) and (2.1.3) strongly **unitarily equivalent** *while representations related only by (2.1.2) will simply be called unitarily equivalent.*

A state is uniquely determined by the set of its n-point functions

$$\mathscr{W}^\omega_n(f_1, \ldots, f_n) := \omega(\phi(f_1) \ldots \phi(f_n))$$

where these objects can in principle have unacceptable properties. The first restriction we therefore impose on states is that the n-point functions be distributions in all their arguments.

The next restriction is largely a matter of simplifying the treatment. From the commutation relation one sees that the part of the n-point functions that is antisymmetric under the transposition of arguments is fixed. The symmetric parts of the n-point functions can be understood in a very similar way to moments of a probability distribution. It is well known that the only types of probability distributions that are determined only by a finite number of non-vanishing cumulants are linear and Gaussian distributions. In the present work, we will mostly restrict to Gaussian states, also called quasifree states, with vanishing one-point function; these states are uniquely determined by their two-point functions.

The requirement that the two-point function be a bidistribution does not enforce a degree of regularity that is sufficient for our treatment. As we want to consider an algebra of appropriately regularised n-point functions we want to restrict to states with similar singularity structure. The singularity structure should be compatible with the one of the Minkowski vacuum. In a heuristic, physical sense the restriction we have in mind can be thought of as restricting the “short-distance” or “ultraviolet” behaviour of the two-point function. In a deeper sense it can be seen as a supplement for the spectrum condition that is implemented on Minkowski spacetime. On the mathematical level the condition can be linked to the microlocal description of singularities. This latter view is not suitable for the type of very explicit calculations aimed at in the present work, therefore we will stick to the older yet in our case more useful treatment of the singularity condition.

First we will need some additional geometric apparatus.

Definition 2.1.6.
For a point $x \in \mathcal{M}$ let $\exp_x : T_x\mathcal{M} \to \mathcal{M}$ be the exponential map. For any point there is a star-shaped neighbourhood on which $\exp_x$ is a diffeomorphism. Let $\tilde{N} \subset T_x\mathcal{M}$ star-shaped such that for all $y \in \tilde{N}$ the restriction $\exp_x|_{\tilde{N}}$ is a diffeomorphism. Then $N = \exp_x(\tilde{N})$ is called a **convex normal set** and for any two points from this set there is a unique geodesic connecting them.

A globally hyperbolic manifold is not in general a convex normal set but any point in any smooth semi-Riemannian manifold has a convex normal neighbourhood [32].

Definition 2.1.7.
Let $N \subset \mathcal{M}$ be a convex normal set and $x, y \in N$. Then

$$\sigma(x,y) := g(y)\left(\exp_y^{-1}(x), \exp_y^{-1}(x)\right) = g(x)\left(\exp_x^{-1}(y), \exp_x^{-1}(y)\right)$$

is called the **squared geodesic distance**.

The symmetry of σ stems from the definition of the exponential map, its smoothness (on $N \times N$) in both arguments is obvious from the smoothness of all functions involved in its definition. As our metric is Lorentzian σ will vanish if x and y are light-like related. To avoid problems connected to this fact, we define

$$\sigma_\varepsilon(x,y) := \sigma(x,y) + 2i\varepsilon\left(T(x) - T(y)\right) + \varepsilon^2$$

where T is a globally defined time function whose existence is guaranteed by the time orientability of $(\mathcal{M}, g)$.

Now we can introduce a distribution that characterises the singularity behaviour we want to restrict to

Definition 2.1.8.

- The **Hadamard parametrix** to order $k \in \mathbb{N}$ is given by

  $$\mathfrak{H}_{k,\varepsilon}(x,y) := \frac{v_{-1}(x,y)}{\sigma_\varepsilon(x,y)} + \frac{1}{L^2}\sum_{j=0}^{k} v_j(x,y)\left(\frac{\sigma(x,y)}{L^2}\right)^j \ln\left(\frac{-\sigma_\varepsilon(x,y)}{L^2}\right)$$

  where L is a free parameter defining a length scale and the $v_j(x,y)$ are given by the recursion

  $$2g^{\mu\nu}(\nabla_\mu\sigma)(\nabla_\nu v_{j+1}) + (\Box\sigma + 4j)v_{j+1} = \frac{-L^2}{\max(0,j)+1} P_{m,\xi} v_j$$

  with initial conditions $v_{-2}(x,y) = 0$ and $v_{-1}(x,x) = 1$.

- A state ω is called a **Hadamard state** if

  $$\forall\, N \subset \mathcal{M} \text{ convex normal, } k \in \mathbb{N} \quad \exists\, \mathfrak{R}_k^\omega \in C^k(N \times N) \quad \forall\, f, g \in C_0^\infty(N)$$

  $$\mathscr{W}_2^\omega(f,g) = \lim_{\varepsilon \to 0^+} \frac{1}{4\pi^2} \left(\mathfrak{H}_{k,\varepsilon}(f,g) + \mathfrak{R}_k^\omega(f,g)\right)$$

  where functions are interpreted as distributions in the usual way.

To define an enlarged algebra containing Wick products we refer to the definition of [9]. Taking the GNS representation corresponding to a Gaussian Hadamard state ω, we define

$$:\phi(f):_\omega = \pi_\omega(\phi(f))$$

$$:\phi(f_1)\dots\phi(f_{n+1}):_\omega = :\phi(f_1)\dots\phi(f_n):_\omega \pi_\omega(\phi(f_{n+1})) - \sum_{j=1}^{n} :\phi(f_1)\dots\widehat{\phi(f_j)}\dots\phi(f_{n+1}):_\omega \mathscr{W}_2^\omega(f_j, f_{n+1}). \quad (2.1.4)$$

It was shown in [9] that the ω-Wick monomials defined above can be interpreted as distributions of only one $f \in C_0^\infty$ by composing them with a map that "restricts to the diagonal" $x \mapsto (x, \dots x)$. The closures with respect to the respective Hilbert space topologies of *-algebras generated by the Wick monomials of different states were shown in [21] to be isomorphic, such that we get a state independent enlarged algebra $\mathcal{W}(\mathcal{M}, g) \supset \mathcal{A}(\mathcal{M}, g)$ to which all Gaussian Hadamard states carry over and which has a well defined topology.

As we will deal with some non-Gaussian states in the following, we would like to point out that it was shown in [39] that the truncated n-point distributions for non-Gaussian Hadamard states are smooth except for the two-point distribution. This implies that the singularity structure of all n-point distributions of a non-Gaussian Hadamard state is the same as for a Gaussian Hadamard state. This allows carrying over the definition of ω-Wick monomials to non-Gaussian Hadamard states, which finally means that all Hadamard states carry over to the enlarged algebra $\mathcal{W}(\mathcal{M}, g)$.

It is obvious that the definition of ω-Wick monomials essentially implies a renormalisation by subtraction of the n-point function of the reference Hadamard state ω. This renders the physical significance of these monomials rather questionable, as it is not clear in general which state should be picked for the renormalisation. Indeed in the special case of a spacetime that is Minkowski at early and late times but expands in between, it can be shown that the Minkowski vacuum of the early universe corresponds to a state with finite particle density in the late universe. This means that such a "state subtraction" renormalisation is not locally covariant as n-point functions of states are dependent on the whole spacetime. To characterise the physically significant elements of $\mathcal{W}(\mathcal{M}, g)$ we will introduce an additional covariance requirement.

2.1.3. Local Covariance Principle

The need for a requirement of general covariance on observables in quantum field theory on curved spacetime was first discussed in the context of the energy-momentum tensor by Wald [48]. In [21] a covariance requirement was proposed for Wick polynomials. A general framework for local covariance in quantum field theory was proposed in [10] using the language of category theory. As we will refer to this framework of local covariance in some detail, we will give the necessary definitions here. For a more detailed explanation and the definition of further structure, which we omit here, we refer to the original publication.

First we will define the categories that are needed in the following. We make use of the auxiliary definition

Definition 2.1.9.

- A subset $N \subset \mathcal{M}$ of an oriented, globally hyperbolic Lorentz manifold $(\mathcal{M}, g)$ is called **causally convex** if any causal curve $c : [a, b] \to \mathcal{M}$ with $c(a), c(b) \in N$ fulfils $\forall\, t \in [a, b] :\ c(t) \in N$.
- Two subsets $N_1, N_2 \subset \mathcal{M}$ of an oriented, globally hyperbolic Lorentz manifold $(\mathcal{M}, g)$ are called **causally separated** if there is no causal curve $c : [a, b] \to \mathcal{M}$ which intersects both of them.

Also we will in the following be interested in the algebra generated not only by the Wick products of the field ϕ but also of its covariant derivatives to arbitrary order. It is clear that the definition (2.1.4) can be extended to include derivatives in a straight forward manner. We will call the resulting topological *-algebra $\mathcal{W}^{\mathrm{d}}(\mathcal{M}, g)$. We will use the following categories:

$\mathfrak{Man}$:
$Obj(\mathfrak{Man})$: 4-dimensional, oriented, time oriented, globally hyperbolic Lorentz manifolds.
$Hom_{\mathfrak{Man}}$: orientation- and time-orientation-preserving isometric embeddings with causally convex image.

$\mathfrak{Test}$:
$Obj(\mathfrak{Test})$: $C_0^\infty(\mathcal{M})$ for all $(\mathcal{M}, g) \in Obj(\mathfrak{Man})$.
$Hom_{\mathfrak{Test}}$: push-forward maps for all $\psi \in Hom_{\mathfrak{Man}}$.

$\mathfrak{Alg}$:
: $Obj(\mathfrak{Alg})$: $\mathcal{W}^{\mathrm{d}}(\mathcal{M}, g)$ for all $(\mathcal{M}, g) \in Obj(\mathfrak{Man})$.
: $Hom_{\mathfrak{Alg}}$: injective, unit-preserving *-homomorphisms.

$\mathfrak{Sts}$:
: $Obj(\mathfrak{Sts})$: convex sets of states for all $\mathcal{W}^{\mathrm{d}}(\mathcal{M}, g) \in Obj(\mathfrak{Alg})$.
: $Hom_{\mathfrak{Sts}}$: positive maps which are duals to any $\alpha \in Hom_{\mathfrak{Alg}}$.

The composition of morphisms is always given by the usual composition of maps. The identity morphisms are obvious. Also there is a canonical covariant functor $T : \mathfrak{Man} \to \mathfrak{Test}$ associating to every manifold its corresponding test function space and to every isometric embedding the corresponding push-forward. Next we will define a number of category theoretical objects.

Definition 2.1.10.

- A covariant functor $Q : \mathfrak{Man} \to \mathfrak{Alg}$ is called a **locally covariant quantum field theory**.
- A locally covariant quantum field theory Q is called **causal**, if all pairs of morphisms $\psi_j \in Hom_{\mathfrak{Man}}((\mathcal{M}_j, g_j), (\mathcal{M}, g))$ $j \in \{1, 2\}$ with causally separated images fulfil

$$[(Q\psi_1)(Q(\mathcal{M}_1, g_1)), (Q\psi_2)(Q(\mathcal{M}_2, g_2))] = \{0\}$$

- A locally covariant quantum field theory Q fulfils the **time slice axiom** if for all $\psi \in Hom_{\mathfrak{Man}}((\mathcal{M}_1, g_1), (\mathcal{M}_2, g_2))$ with $\psi(\mathcal{M}_1)$ containing a Cauchy surface of $\mathcal{M}_2$ it holds

$$(Q\psi)(Q(\mathcal{M}_1, g_1)) = Q(\mathcal{M}_2, g_2)$$

- A natural transformation $\Phi : T \to Q$ is called a **locally covariant quantum field**.
- A contravariant functor $S : \mathfrak{Man} \to \mathfrak{Sts}$ is called a **locally contravariant state space**.

As we will use some results of [35] which are specific for locally covariant conformal quantum field theories, we will also review the differences in the definition here. First we need to clarify terminology.

Definition 2.1.11.

- Let $(\mathcal{M}_1, g_1)$ and $(\mathcal{M}_2, g_2)$ be globally hyperbolic spacetimes. A smooth injective map $\psi : \mathcal{M}_1 \to \mathcal{M}_2$ is called a **conformal embedding** if there is a map $\Omega : \psi(\mathcal{M}_1) \to \mathbb{R}^+$ called the conformal factor, such that $\psi_* g_1 = \Omega^{-2} g_2|_{\psi(\mathcal{M}_1)}$.

- Let $(\mathcal{M}_1, g_1)$ and $(\mathcal{M}_2, g_2)$ be globally hyperbolic spacetimes, $\psi : \mathcal{M}_1 \to \mathcal{M}_2$ a conformal embedding with conformal factor Ω, then $\psi_*^\lambda : C^\infty(\mathcal{M}_1) \to C^\infty(\mathcal{M}_2)$ defined by $\psi_*^\lambda(f) = \Omega^{-\lambda}\psi(f)$ is called the **λ-weighted push-forward** map.

Now we can define the modified categories

$\mathfrak{CMan}$:
Obj($\mathfrak{CMan}$): 4-dimensional, oriented, time oriented, globally hyperbolic Lorentz manifolds.
$Hom_{\mathfrak{CMan}}$: orientation- and time-orientation-preserving conformal embeddings with causally convex image.

$\mathfrak{Test}$:
$Obj(\mathfrak{Test}^\lambda)$: $C_0^\infty(\mathcal{M})$ for all $(\mathcal{M}, g) \in Obj(\mathfrak{Man})$.
$Hom_{\mathfrak{Test}^\lambda}$: λ-weighted push-forward maps for all $\psi \in Hom_{\mathfrak{Man}}$.

Obviously $\mathfrak{Man}$ is a subcategory of $\mathfrak{CMan}$. Also there are canonical covariant functors $T^\lambda : \mathfrak{CMan} \to \mathfrak{Test}^\lambda$ associating to every manifold the corresponding test function space and to every conformal embedding the corresponding λ-weighted push-forward.

Definition 2.1.12.

- A covariant functor $C : \mathfrak{CMan} \to \mathfrak{Alg}$ is called a **locally covariant conformal quantum field theory**. Note that every locally covariant conformal quantum field theory C contains canonically a locally covariant quantum field theory $Q_C := C|_{\mathfrak{Man}}$.

- A natural transformation $\Phi^\lambda : T^{4-\lambda} \to C$ is called a **locally covariant conformal quantum field** with weight λ.

- A covariant functor $Z : \mathfrak{CMan} \to \mathfrak{Sts}$ is called a **locally contravariant conformal state space**. Note that every locally contravariant conformal state space Z contains canonically a locally contravariant state space $S_Z := Z|_{\mathfrak{Man}}$.

In the following it will be useful to define the notion of the representative of a locally covariant (conformal) quantum field (theory) or a locally contravariant state space for a certain spacetime $(\mathcal{M}, g)$. Let us for this purpose define the subcategories

$\mathfrak{Man}_\mathfrak{g}$:
$Obj(\mathfrak{Man}_\mathfrak{g})$: 4-dimensional, oriented, globally hyperbolic embedded Lorentz submanifolds of $(\mathcal{M}, g)$, embedded orientation- and time-orientation-preservingly, causally convex and isometrically.
$Hom_{\mathfrak{Man}_\mathfrak{g}}$: orientation- and time-orientation-preserving isometric embeddings with causally convex image.

Definition 2.1.13.

- Let Q (C) a locally covariant (conformal) quantum field theory then $Q_g = Q|_{\mathfrak{Man}_\mathfrak{g}}$ $(C_g = C|_{\mathfrak{Man}_\mathfrak{g}})$ is called its representative on the spacetime $(\mathcal{M}, g)$. Let Φ a locally covariant quantum field and $T_g = T|_{\mathfrak{Man}_\mathfrak{g}}$ then $\Phi_g = \Phi|_{T_g} : T_g \to Q_g$ is called the **representative** of Φ on $(\mathcal{M}, g)$.

- Let S (Z) a locally contravariant (conformal) state space then $S_g = S|_{\mathfrak{Man}_\mathfrak{g}}$ $(Z_g = Z|_{\mathfrak{Man}_\mathfrak{g}})$ is called its representative on the spacetime $(\mathcal{M}, g)$.

The restriction to the diagonal of locally covariant Wick products in the sense defined above are now required to be locally covariant quantum fields that only differ from the restriction to the diagonal of ω-Wick products by a smooth function. This can be achieved by renormalising by subtraction of $\frac{1}{4\pi^2}\mathfrak{H}_{k,\varepsilon}(f,g)$ for a large enough k to account for the possible derivatives instead of $\mathscr{W}_2^\omega(f,g)$ in (2.1.4). We are dealing with Gaussian states and their mixtures and are therefore only interested in the Wick squares in the following. We thus remark more precisely that k must at least be half the total number of derivatives involved in the Wick square in question.

It should be noted that the definitions of derivatives of covariant Wick squares still contain ambiguities. These can be understood as renormalisation ambiguities and have the form of local curvature terms, as shown in [21].

As explained above there are no locally contravariant states, as states depend non-locally on the whole spacetime. It was shown that the sets of Hadamard states on all spacetimes $(\mathcal{M}, g) \in Obj(\mathfrak{Man})$ form a locally contravariant state space. This follows from the formulation of the Hadamard condition in terms of wavefront sets [22]. For the discussion of certain types of physical phenomena, e.g. thermodynamics, one should define appropriate subsets of the sets of Hadamard states for an appropriate subcategory of $\mathfrak{Man}$ that form again a contravariant state space. One may keep this principle goal in mind, although the concept of states of local thermal equilibrium is still far from achieving it.

2.2. Local Thermal Equilibirum

States of thermal equilibrium are rather limited in their capacity to describe thermodynamical situations. The description of situations where the thermodynamic functions of state are not constant and homogeneous but change throughout spacetime, is a first step to the description of non-equilibrium systems. The concept of local thermal equilibrium (LTE) states introduced in [11] takes exactly this step, still neglecting the effects of matter flows but describing non-constant functions of state. The principal strategy to describe suitable states of local thermal equilibrium rests on two pillars: A set of thermal reference states and a set of thermal observables. The thermal observables are then used to compare a state locally to a reference state.

2.2.1. Global Thermodynamic Equilibrium - KMS States

As a first step we will introduce the set of thermal reference states. It was shown in [19] that thermodynamic equilibrium states can be characterised by the KMS condition for the time translation. The KMS condition was then refined in [8] to encompass a description of thermal equilibrium in Minkowski spacetime by observers who are not in the rest frame with respect to which equilibrium is defined. We will call this condition the relativistic KMS condition. In the following we will however refer to both KMS states and relativistic KMS states in different contexts, therefore we will define both types of states.

As a preliminary step we will define what a static spacetime is, as the KMS states we are interested in can only be defined on such spacetimes.

Definition 2.2.1.
A spacetime $(\mathcal{M}, g)$ is called **static** if it admits a globally non-vanishing, irrotational[1], time-like Killing field.

To fix notation for the definition of the KMS conditions let $(\mathcal{M}, g)$ be a globally hyperbolic static spacetime and t a time coordinate such that t-translations $\chi_t(x) = \exp_x(ut)$ with $g(u,u) = 1$ are isometries of the metric. For $\phi(f) \in \mathcal{A}(\mathcal{M}, g)$ a generator of the algebra let $\alpha_t(\phi(f)) = \phi(f_t)$ with $f_t(x) = f(\chi_t^{-1}(x))$; α_t is then a one-parameter group of $\mathcal{A}(\mathcal{M}, g)$-isomorphisms. For Minkowski spacetime all translations are isometries of the metric and we can thus analogously define $\alpha_{\underline{a}}$ for any $\underline{a} \in \mathbb{R}^4$ as a group of $\mathcal{A}(\mathbb{R}^4, \eta)$-isomorphisms. We will define (r)KMS states as Gaussian for simplicity.

[1] A vector field is irrotational, if it is orthogonal to a foliation of spacetime by Cauchy surfaces.

Definition 2.2.2.

- A Gaussian state ω_β is called a **KMS state** with inverse temperature $\beta > 0$ with respect to t if for all $A, B \in \mathcal{A}(\mathcal{M}, g)$ there exists a function F_{AB} analytic in the strip $\{z \in \mathbb{C} \,|\, 0 < \mathrm{Im}(z) < \beta\}$ and continuous on the boundaries such that

$$\omega_\beta(B\alpha_t(A)) = F_{AB}(t) \qquad \omega_\beta(\alpha_t(A)B) = F_{AB}(t + i\beta)$$

- For $(\mathcal{M}, g)$ being Minkowski spacetime a Gaussian state ω_β is called a **rKMS state** with inverse temperature $\beta > 0$ in the rest frame given by the future pointing time-like unit vector $\underline{e}$ if for all $A, B \in \mathcal{A}(\mathcal{M}, g)$ there exists a function F_{AB} analytic in $\mathbb{R}^4 + i\,(V^+(\underline{0}) \cap V^-(\beta\underline{e}))$ and continuous on the boundaries such that

$$\omega_\beta(B\alpha_{\underline{a}}(A)) = F_{AB}(\underline{a}) \qquad \omega_\beta(\alpha_{\underline{a}}(A)B) = F_{AB}(\underline{a} + i\beta\underline{e})$$

  We will often use shorthand notation $\underline{\beta} := \beta\underline{e}$. We will not use the underlined notation whenever the context is clear.

Note. In general, a KMS condition can be defined for any one-parameter group of symmetries. As the thermal interpretation of states is however linked to the time translation the general notion of a KMS condition is never relevant in the present work. Therefore the term “KMS condition” will always refer to the KMS condition with respect to the time translation.

It should be noted that the rKMS condition is more restrictive than the KMS condition, as it can only be applied to Lorentz invariant systems and requires stronger analyticity of the two-point function. As Lorentz invariance is a specific characteristic of Minkowski spacetime, rKMS states do not in general exist in generic globally hyperbolic, static spacetimes.

As we are dealing with Gaussian states here and thus each state is uniquely characterised by its two-point function, it suffices for our means to express the KMS and rKMS conditions in terms of the two-point function. For simplicity we will assume states that are invariant under spatial rotations in the rest frame of equilibrium and translations. We will furthermore assume the existence of exactly one (r)KMS state per β or $\underline{\beta}$ respectively. This means we will not deal with phenomena like phase transitions and moreover we will ignore the chemical potential for massive fields. The latter is of course a severe restriction on the set of KMS states we consider.

The requirement of uniqueness implies extremality, meaning that a (r)KMS state cannot be decomposed into other (r)KMS states. This yields the symbolic form of the two-point function, suppressing the smearing functions, for a KMS state in Minkowski spacetime

$$\mathscr{W}_2^{\beta}(x,y) = \int \frac{e^{-i(x^\mu - y^\mu)p_\mu}}{(2\pi)^3(1-e^{-\beta p^0})}\varepsilon(p^0)\delta(p_\mu p^\mu - m^2)d^4p$$

where $\varepsilon(x) = \begin{cases} -1 & \text{for} \quad x<0 \\ 0 & \text{for} \quad x=0 \\ 1 & \text{for} \quad x>0 \end{cases}$ is the sign function.

The symbolic form of the two-point function for a rKMS state is correspondingly

$$\mathscr{W}_2^{\beta}(x,y) = \int \frac{e^{-i(x^\mu - y^\mu)p_\mu}}{(2\pi)^3(1-e^{-\beta_\mu p^\mu})}\varepsilon(p^0)\delta(p_\mu p^\mu - m^2)d^4p$$

On a general static spacetime the two-point function of a KMS state can be constructed by a procedure detailed and applied for a special spacetime below.

Next we want to define mixtures of KMS and rKMS states, as these are the reference states we will use in the following. It should be noted that a mixture of Gaussian states need not be Gaussian. In fact the non-Gaussianities of mixtures of KMS states are the only ones that occur in the present work. Therefore, the fact the mixtures of KMS states are not Gaussian will be mostly ignored.

Definition 2.2.3.
Let $d\mu(\beta)$ be a probability measure on $\mathbb{R}^+ \cup \{0\}$ for KMS states, on $V^+(0) \cup \{0\}$ for rKMS states, with the respective Borel σ-algebras. Then $\mathscr{W}_n^{\mu} = \int \mathscr{W}_n^{\beta}\, d\mu(\beta)$ are well defined distributions. The state ω_μ with n-point functions $\mathscr{W}_n^{\mu}$ is called a mixture of (r)KMS states. One usually writes $\omega_\mu = \int \omega_\beta d\mu(\beta)$ which is a well defined integral on state space. If the support of $d\mu(\beta)$ is compact we call the mixture compact.

We would like to extend mixtures of KMS and rKMS states to the algebra $\mathcal{W}^{\mathrm{d}}(\mathcal{M}, g)$ which can be achieved for all Hadamard states as we have seen above. From the result of [38] it follows that mixtures of KMS states are Hadamard for a free scalar field on any stationary globally hyperbolic spacetime, which allows extending mixtures of KMS states to the algebra $\mathcal{W}^{\mathrm{d}}(\mathcal{M}, g)$. We will use the set of all mixtures of rKMS states as the set of reference states for Minkowski spacetime. For other static spacetimes we will use the set of all mixtures of KMS states with respect to some time coordinate which must be specified separately.

For KMS and rKMS states we shall assume in the following that

$$\forall\, A \in \mathcal{W}^{\mathrm{d}}(\mathcal{M}, g): \quad \beta \mapsto \omega_\beta(A) \text{ continuous.}$$

As we have already excluded phase transitions by our uniqueness assumption, this requirement is in general not expected to impose additional restrictions on the set of states we consider. We also note that translation invariance of the KMS and rKMS states in Minkowski spacetime implies for any local observable $A(f) \in \mathcal{W}^{\mathrm{d}}(\mathbb{R}^4, \eta)$ and for any mixture of (r)KMS states ω_μ that if $\omega_\mu(A)$ is regular, $\omega_\mu(A(x))$ is independent of $x \in \mathbb{R}^4$. The case of regular $\omega_\mu(A)$ is the only relevant one for the observables and states considered in the present work.

2.2.2. Local Thermal Observables

The local thermal observables are used to compare states to the reference states. As we want to compare states in terms of their thermal behaviour, the thermal observables should have a thermodynamic significance. To have a "gradual" concept one may also want the thermal observables to be endowed with some sort of hierarchy. The set of thermal observables that was considered in [11] is indeed hierarchical in that a natural hierarchy of subsets can be considered. Thereby a "degree of local thermality" can be measured. However in [12] and [23] extended sets of observables were considered which still include the hierarchy of sets considered in [11], but focus on the description of states with a maximal degree of local thermality.

We will first define the basic set of thermal observables on Minkowski spacetime. Then we will discuss the extended set of observables for the massless field. In the last part we will discuss the topic of thermal observables in curved spacetimes. The last point will need careful attention as these observables are not uniquely fixed by the requirement of covariance and the known thermal observables in flat spacetime. Also we lack a general physical principle on a generic spacetime to identify thermal observables. This leaves considerable freedom in the definition of thermal observables.

One would want the local thermal observables to have good localisation properties and one would want their expectation values to be bounded by the energy in some suitable sense. The latter requirement led [11] to base the selection of the basic thermal observables for Minkowski spacetime on the work on H-bounds, especially in the context of the operator product expansion as investigated in [6]. From this approach one can conclude that the normal products of the fields can be approximated by pointwise definition of observables in the form sense, which makes them tractable candidates for local thermal observables. In our case of a free scalar field and Gaussian states the normal products simply reduce to the Wick square and its balanced derivatives (for consistency with later chapters we use the index η to denote the Minkowski metric), defined in the form sense as

$$\theta_{\eta,\boldsymbol{\mu}}(x+\zeta,x-\zeta) = \eth_{\boldsymbol{\mu}} : \phi_\eta^2 : (x+\zeta,x-\zeta)$$
$$:= \partial^\zeta_{\boldsymbol{\mu}} \left(\phi_\eta(x+\zeta)\phi_\eta(x-\zeta) - \omega_\infty\left(\phi_\eta(x+\zeta)\phi_\eta(x-\zeta)\right)\mathbb{1}\right) \quad (2.2.1)$$

$$\theta_{\eta,\boldsymbol{\mu}}(x) := \lim_{\zeta\to 0} \theta_{\eta,\boldsymbol{\mu}}(x+\zeta,x-\zeta) \quad (2.2.2)$$

Here and sometimes in the following the balanced derivatives are not written as evaluated in a state, for readability. This expression is purely formal and always has to be understood in the form sense, which means that the expression only makes sense evaluated in a state.

In the following it will be helpful to introduce the notion of thermal macroobservables. The basic idea is to define

$$\Psi(\underline{\beta}) := \omega_{\underline{\beta}}(\psi(x)) \quad (2.2.3)$$

for any local thermal observable $\psi(x)$ and then by a slight overload of notation define $\omega_\mu(\Psi(\underline{\beta})) := \int \Psi(\underline{\beta})\, d\mu(\underline{\beta})$. The formal foundation for this is that the macroobservables can be defined as limits of certain central sequences of local observables, as detailed in [12]. Let $f \in C_0^\infty(\mathbb{R}^4)$ with $\int f(x)\, d^4x = 1$, $(x_n \in \mathbb{R}^4)_{n\in\mathbb{N}}$ a sequence tending rapidly to spacelike infinity and define the series $f_n(x) = n^{-4} f\left(\frac{x}{n} - x_n\right)$. Then any $A \in \mathcal{A}(\mathcal{M},g)$ commutes with $\psi(f_n)$ for almost all n, thus $(\psi(f_n))_{n\in\mathbb{N}}$ is a central sequence. Then one can define $\Psi = \lim_{n\to\infty} \psi(f_n)$ where the limit exists in all mixtures of (r)KMS states and defines a central observable. Due to the mean ergodic theorem we have

$$\omega_\mu(A^*\Psi A) = \int \omega_{\underline{\beta}}(A^*A)\, \omega_{\underline{\beta}}(\psi(x))\, d\mu(\underline{\beta})$$

which makes the connection to the expression $\Phi(\underline{\beta}) = \omega_{\underline{\beta}}(\phi(x))$ given above, now seen to be the central decomposition of Ψ.

The linear space $\mathcal{T}_\eta$ spanned by the identity and the balanced derivatives $\theta_{\eta,\boldsymbol{\mu}}(x)$ is the basic set of local thermal observables which we consider in the following. The space of balanced derivatives evaluated at some point x will be denoted by $\mathcal{T}_{\eta,x}$. We note that the balanced derivatives vanish for $n = |\boldsymbol{\mu}|$ odd, since the part antisymmetric in ζ is subtracted in the definition of the normal product. Alternatively we could use a symmetrised Wick square to begin with and then correspondingly subtract the symmetrised vacuum expectation value. There is a canonical hierarchy given by the maximal degree of derivative n. We denote the spaces that are spanned by all balanced derivatives up to a maximal degree n by $\mathcal{S}_{n,\eta}$.

It is clear that the spaces of thermal microobservables defined above have a straight forward interpretation as spaces of macroobservables. However, the space $\mathcal{T}_{\eta,x}$ does not include observables like the entropy current $S^\mu(x)$ and the phase space density $N_p(x)$. One might want to include such observables into the set of thermal observables as they are of considerable physical relevance. It turns out that these observables can be approximated arbitrarily well by elements of $\mathcal{T}_\eta$ in a suitable sense. This was sketched in [11] and further elaborated in [12] for the massless field. The case of massive fields was investigated in [23].

In the case of massless scalar fields it suffices to consider compact mixtures of (r)KMS states to get a suitable topology in which to take the closure of $\mathcal{T}_{\eta,x}$. It is also illustrative to consider the macroobservable point of view in this case. Let $B \subset V^+(0)$ be the compact support of the measure describing some compact mixture of KMS states. We can then define a seminorm

$$\tau_B(\Psi(\underline{\beta})) = \sup_{\underline{\beta}\in B} \Psi(\underline{\beta})$$

for all mixtures whose measures are supported in B and all $\Psi(\underline{\beta}) \in \mathcal{T}_\eta$. As the functions $\underline{\beta} \mapsto \Psi(\underline{\beta})$ are by assumption continuous, the supremum is well defined. Calling the closure of $\mathcal{T}_\eta$ with respect to this family of seminorms $\overline{\mathcal{T}}^\tau_\eta$ and the evaluation of these for at a point $\overline{\mathcal{T}}^\tau_{\eta,x}$ we can formulate the following lemma that follows directly from Lemma 3.1 in [12].

Lemma 2.2.4.
Let $\Psi(\underline{\beta})$ be a smooth solution of $\Box_{\underline{\beta}}\Psi(\underline{\beta}) = 0$ in the compact $B \subset V^+$. Then

$$\forall \underline{\beta} \in B : \quad \Psi(\underline{\beta}), \partial^{\beta}_{\nu}\Psi(\underline{\beta}) \in \overline{\mathcal{T}}^\tau_\eta$$

Using this lemma it was shown in [12] that the entropy current S^μ and the phase space density N_p are indeed included in $\overline{\mathcal{T}}^\tau_\eta$.

For massive fields however the situation is more complicated as some interesting examples discussed in [23] cannot be described using only compact mixtures of KMS states. For the situation of non-compact mixtures of KMS states a more general class of topologies is defined of which the seminorm topology defined above is a special case. This general class of topologies includes also topologies which allow the approximation of important thermal observables like the entropy current and the phase space density in the case of the massive scalar field. As we will not use these observables for the case of a massive field we will not introduce the topologies needed for this case, but simply refer the interested reader to [23].

Last in this section we will discuss the topic of thermal observables on a generic globally hyperbolic spacetime. We have introduced the balanced derivatives of the

Wick square as local thermal observables but as discussed before the derivatives of Wick squares have been constructed on general globally hyperbolic spacetimes as locally covariant quantum fields. This means we have natural candidates for the local thermal observables on general globally hyperbolic spacetimes. On the downside Wick products as locally covariant quantum fields are only unique up to renormalisation ambiguities, which on the upside are restricted to locally constructed geometric quantities.

The renormalisation ambiguities are however not the only ambiguities involved in the identification of thermal observables, because the correct thermal observables on curved spacetimes might not actually be the covariant Wick products corresponding to the balanced derivatives, but could be modified by adding any term which has the correct tensor covariance properties and vanishes on Minkowski spacetime. This ambiguity is considerably larger than the renormalisation ambiguity and could only be reduced by introducing an independent physical criterion of local thermality on a generic globally hyperbolic spacetime. A step towards such a physical criterion has been made by the investigation of an Unruh detector model in [41] and [42], but the extension of the detector model to curved spacetimes was only sketched roughly and the fixing of ambiguities has not been discussed in this context. The work on local thermal equilibrium for the free dirac field in [25] indicates that one should indeed not use simply the covariant balanced derivatives of Wick squares but modified observables in generic curved spacetimes.

We will thus propose a definition for the local thermal observables that implies considerable ambiguity. First we fix the definition of the Hadamard-Wick square. As pointed out above the Wick products can be interpreted as $C^k(\mathcal{M})$ functions in two variables. By restriction to the diagonal one is left even with $C^\infty(\mathcal{M})$ functions of one variable.

$$:\phi_g^2:_k (x,y) = \lim_{\varepsilon\to 0^+} \left(\phi_g(x)\phi_g(y) + \phi_g(y)\phi_g(x) - \mathfrak{H}_{g,k,\varepsilon}(x,y)\mathbb{1} - \mathfrak{H}_{g,k,\varepsilon}(y,x)\mathbb{1}\right)$$

$$:\phi_g^2:(x) = \lim_{y\to x} :\phi_g^2:_k (x,y)$$

where $k \geq 0$ is needed and the index g denotes the metric. For the definition of a balanced derivative with $|\boldsymbol{\nu}| = n$ we need $k \geq \frac{n}{2}$. We denote a partition of a multiindex as $\boldsymbol{\alpha} \cup \boldsymbol{\lambda} = \boldsymbol{\nu}$, so the sum below should be understood as the sum of all partitions.

$$\theta_{g,\boldsymbol{\nu}} = \eth_{\boldsymbol{\nu}} :\phi_g^2:(x) := \lim_{y\to x} \sum_{\boldsymbol{\alpha}\cup\boldsymbol{\lambda}=\boldsymbol{\nu}} C_{g,\boldsymbol{\alpha}\subset\boldsymbol{\nu},\boldsymbol{\alpha}} \left(\nabla^x - \nabla^y\right)_{\boldsymbol{\lambda}} :\phi_g^2:_k (x,y) + D_{g,\boldsymbol{\nu}}\mathbb{1} \quad (2.2.4)$$

where the index $\boldsymbol{\alpha} \subset \boldsymbol{\nu}$ is simply meant to distinguish on the basis of what $\boldsymbol{\nu}$ is, and how $\boldsymbol{\alpha}$ is embedded in it. We assume that all $C_{g,\boldsymbol{\alpha}\subset\boldsymbol{\nu},\boldsymbol{\alpha}}$ be purely geometric quantities that vanish in Minkowski spacetime except for the coefficient of the term for $\boldsymbol{\lambda} = \boldsymbol{\nu}$, which has to fulfil $C_{\eta,\boldsymbol{\nu},\emptyset} = 1$ on Minkowski spacetime. From the symmetry of $:\phi_g^2:_k(x,y)$ it follows that the balanced derivatives vanish for n odd. Therefore we imply $C_{g,\boldsymbol{\alpha}\subset\boldsymbol{\nu},\boldsymbol{\alpha}} = 0$ whenever $|\boldsymbol{\alpha}|$ is odd and $D_{g,\boldsymbol{\nu}} = 0$ whenever $|\boldsymbol{\nu}|$ is odd.

Despite our very general definition we will for the most part of this work ignore the ambiguity in the definition of the local thermal observables and will work with the simple form

$$\theta_{g,\boldsymbol{\nu}} = \eth_{\boldsymbol{\nu}} :\phi_g^2:(x) := \lim_{y\to x}(\nabla^x - \nabla^y)_{\boldsymbol{\nu}} :\phi_g^2:_k(x,y). \tag{2.2.5}$$

We will however refer several times to the principal ambiguity that is possible in the definition of local thermal observables.

The linear span of the identity and all balanced derivatives interpreted as locally covariant quantum fields is denoted by $\mathcal{T}$, the span of all balanced derivatives up to a maximal degree n interpreted as locally covariant quantum fields is denoted by $\mathcal{S}_n$. The linear span of the identity and all balanced derivatives on the spacetime $(\mathcal{M}, g)$ interpreted as functions in x is called $\mathcal{T}_g$, the span of all balanced derivatives on the spacetime $(\mathcal{M}, g)$ up to a maximal degree n is called $\mathcal{S}_{n,g}$. We will also call the $\mathcal{S}_{n,g}$ and $\mathcal{T}_g$ the representatives of the $\mathcal{S}_n$ and $\mathcal{T}$ on the spacetime $(\mathcal{M}, g)$.

It should further be noted that $\mathcal{T}$ as well as the $\mathcal{S}_n$ do not depend on the ambiguities in the definition of balanced derivatives. The exact definition of balanced derivatives is then only a matter of physical interpretation of the observables, i.e. a question of which observables on two different spacetimes are assumed to describe the same physical entity. In this sense, altering the tone compared to an argument that was made by [44], the point of view taken in the present work is: The balanced derivatives on different spacetimes are assumed to correspond to each other, whereas the physical correspondence of all other observables in the respective linear spaces is dictated by these.

If certain observables, which one wants to physically correspond on different spacetimes, can be constructed as "linear combinations" of thermal observables with possibly tensorial coefficients, one might expect this to have an impact on the definitions of the local thermal observables. As an example, one may want the trace of the energy-momentum tensor on different spacetimes to be seen as representative of the same physical entity. As this observable can be constructed as linear combination of the Wick square and the identity one may feel compelled to define the first thermal observable in such a way that the linear relation between the three observables becomes identical on all spacetimes. However, one would thereby imply that the physical relation between these observables was geometry independent, thereby potentially enforcing the loss of physical meaning. It is not very remote to expect that linear relations between observables on Minkowski spacetime do not carry over to general spacetimes as such a situation occurs for numerous classical relations. Therefore we will abstain from any such arguments.

2.2.3. LTE on Flat Spacetime

For Minkowski spacetime we have now specified all we need to give a definition of LTE states. In fact this definition can even be straight forwardly generalised to generic static spacetimes. For non-static globally hyperbolic spacetimes we face an additional problem, which will be considered in the next subsection.

Definition 2.2.5.
Let $\mathfrak{t}_\eta$ be a linear space of thermal observables. A state ω is a local thermal equilibrium or **LTE state** at some point x if there is a mixture of (r)KMS states represented by a probability measure $d\mu_x(\beta)$ such that

$$\forall A(x) \in \mathfrak{t}_{\eta,x} : \quad \omega(A(x)) = \int \omega_\beta(A(x)) d\mu_x(\beta)$$

A state is said to be an LTE state in an open region $\mathcal{O}$ if it is LTE $\forall x \in \mathcal{O}$. We will denote LTE states for $\mathfrak{t}_\eta = \mathcal{S}_{n,\eta}, \mathcal{T}_\eta, \overline{\mathcal{T}}^\tau_\eta$ as n, ∞, τ-LTE states, respectively.

An important consequence of the LTE condition is the fulfilment of certain dynamical equations by the thermal macroobservables, as pointed out in [12]. These equations follow from the Klein-Gordon equation and the application of the LTE condition for the micro-observables

$$\eta^{\nu\lambda}\partial^x_\nu \partial^\zeta_\lambda \theta_{\eta,\boldsymbol{\mu}}(x+\zeta, x-\zeta) = 0 \tag{2.2.6}$$

$$\Rightarrow \partial_\nu \omega\left(\theta_{\eta,}{}^{\nu}{}_{\boldsymbol{\mu}}\right)(x) = 0 \tag{2.2.7}$$

$$\Box^x \theta_{\eta,\boldsymbol{\mu}}(x+\zeta, x-\zeta) = -\Box^\zeta \theta_{\eta,\boldsymbol{\mu}}(x+\zeta, x-\zeta) - 4m^2 \theta_{\eta,\boldsymbol{\mu}}(x+\zeta, x-\zeta) \tag{2.2.8}$$

$$\Rightarrow \Box\omega\left(\theta_{\eta,\boldsymbol{\mu}}\right)(x) = -\,\omega\left(\theta_{\eta,}{}^{\nu}{}_{\nu\boldsymbol{\mu}}\right)(x) - 4m^2\omega\left(\theta_{\eta,\boldsymbol{\mu}}\right)(x) = 0 \tag{2.2.9}$$

where the last equality is the only one that uses the LTE condition as input. Therefore equation (2.2.7) holds for any state as it holds on the operator level, while the second equality of (2.2.9) is specific to ∞-LTE states. For n-LTE states the equation for the balanced derivative of highest order has the general form of (2.2.9) without the last equality. These equations are also fulfilled for observables in the extended set of thermal observables $\overline{\mathcal{T}}^\tau_\eta$.

Some insight about mixtures of (r)KMS states can be gained by an investigation of the two lowest order balanced derivatives. Consider a set of thermal observables containing at least the space $\mathcal{S}_{2,\eta}$. The expectation values of the two balanced derivatives of lowest order in an rKMS state for a massless field were given in [11]

$$\Theta = \omega_\beta\left(\theta_\eta\right) = \frac{1}{12\underline{\beta}^2} \tag{2.2.10}$$

$$\varepsilon_{\mu\nu} = -\frac{1}{4}\omega_\beta\left(\theta_{\eta,\mu\nu}\right) = \frac{\pi^2}{90(\underline{\beta}^2)^3}\left(4\beta_\mu\beta_\nu - \eta_{\mu\nu}\underline{\beta}^2\right) \tag{2.2.11}$$

For a KMS state we get

$$\Theta = \omega_\beta\left(\theta_\eta\right) = \frac{1}{12\beta^2} \tag{2.2.12}$$

$$\varepsilon_{\mu\nu} = -\frac{1}{4}\omega_\beta\left(\theta_{\eta,\mu\nu}\right) = \frac{\pi^2}{90\beta^4}\left(3\delta^0_\mu\delta^0_\nu - \delta^i_\mu\delta^j_\nu\delta_{ij}\right) \tag{2.2.13}$$

This allows us to derive "temperature candidates" with $T = \frac{1}{\beta}$

$$T_0 = \sqrt{12\Theta} \tag{2.2.14}$$

$$T_{20} = \sqrt[4]{\frac{30}{\pi^2}\varepsilon_{00}} \tag{2.2.15}$$

$$T_{2i} = \sqrt[4]{\frac{30}{\pi^2}\delta^{ij}\varepsilon_{ij}} \tag{2.2.16}$$

which are by definition identical for a KMS state. However, for a general rKMS state and mixed temperature states these temperature candidates will not in general coincide. While ε is still traceless, giving $T_{20} = T_{2i} =: T_2$, we will in general observe $T_0 \neq T_2$. We can show for a general measure $d\mu(\beta)$ on $\mathbb{R}^4$ that $T_0 \leq T_2$

$$\begin{aligned} T_0^4 = \left(\int \frac{1}{\beta_0^2 - \vec{\beta}^2} d\mu(\underline{\beta})\right)^2 &\leq \int \frac{1}{\left(\beta_0^2 - \vec{\beta}^2\right)^2} d\mu(\underline{\beta}) \\ &\leq \int \left[\frac{1}{\left(\beta_0^2 - \vec{\beta}^2\right)^2} + \frac{4\vec{\beta}^2}{3\left(\beta_0^2 - \vec{\beta}^2\right)^3}\right] d\mu(\underline{\beta}) = T_2^4 \end{aligned} \tag{2.2.17}$$

where the first inequality follows from Jensen's inequality.

For the case that all temperatures are taken to have the same rest frame this relation can be understood in terms of moments of a temperature distribution, if we assume the temperature to be a random field and $\tilde{\mu}(T)$ its probability distribution corresponding to the measure $\mu(\beta)$. Let M_i be the i-th moment and K_i the i-th cumulant of the distribution $\tilde{\mu}(T)$. Then by definition of moments and cumulants

$$
\begin{aligned}
T_0^2 =& M_2 = K_1^2 + K_2 \\
T_2^4 =& M_4 = K_1^4 + 6K_1^2 K_2 + 3K_2^2 + 4K_1 K_3 + K_4
\end{aligned}
$$

If we assume the cumulants to fulfil $K_n \propto \epsilon^n$ for some small ϵ we can recover approximations for the first cumulants from the even moments we get from the thermal observables. The assumption $K_n \propto \epsilon^n$ holds for random variables that are composed of a large number of stochastically independent random variables with the same distribution by the central limit theorem. For an ensemble of classical identical non-interacting particles this assumption seems reasonable so it should have some validity for our model. In our example of only two thermal observables we get

$$K_1 \approx \sqrt[4]{\frac{6M_2^2 - M_4}{5}} \tag{2.2.18}$$

$$K_2 \approx \frac{M_4 - M_2^2}{\sqrt{30M_2^2 - 5M_4}} \tag{2.2.19}$$

In the massive case the expectation values of the thermal observables no longer have such a simple interpretation. Also ε, which corresponds to the thermal part of the energy-momentum tensor, is not trace free as the model is no longer conformally invariant.

$$\Theta = \frac{1}{12\beta^2} \frac{6}{\pi^2} \int_0^\infty \frac{\rho^2}{(\exp(\sqrt{\rho^2 + m^2\beta^2}) - 1)\sqrt{\rho^2 + m^2\beta^2}} d\rho \tag{2.2.20}$$

$$\delta^{ij}\varepsilon_{ij} = \frac{\pi^2}{90\beta^4} \frac{90}{\pi^4} \int_0^\infty \frac{\rho^4}{(\exp(\sqrt{\rho^2 + m^2\beta^2}) - 1)\sqrt{\rho^2 + m^2\beta^2}} d\rho \tag{2.2.21}$$

$$\varepsilon_\mu^\mu = m^2\Theta \tag{2.2.22}$$

Lemma 2.2.6.
Θ and $\delta^{ij}\varepsilon_{ij}$ increase monotonously as functions of T, decrease monotonously as functions of m and are always non-negative.

Proof. The integrands are positive everywhere and the integration range is positive, thus the positivity is trivial. For monotonicity, we first note that both functions are continuous for all m and T as the integrals are majorised by the respective $m = 0$ special cases. The derivative with respect to m or T of the integrand is also continuous except for $m = 0$ thus we can interchange derivation and integration. This yields

$$\partial_m \Theta = -\frac{m}{2\pi^2} \int_0^\infty \frac{\rho^2 \left(\left(\sqrt{\rho^2 + \frac{m^2}{T^2}} + 1 \right) \exp\left(\sqrt{\rho^2 + \frac{m^2}{T^2}} \right) - 1 \right)}{\left(\exp\left(\sqrt{\rho^2 + \frac{m^2}{T^2}} \right) - 1 \right)^2 \left(\rho^2 + \frac{m^2}{T^2} \right)^{\frac{3}{2}}} d\rho < 0$$

$$\partial_m (\delta^{ij} \varepsilon_{ij}) = -\frac{mT^2}{\pi^2} \int_0^\infty \frac{\rho^4 \left(\left(\sqrt{\rho^2 + \frac{m^2}{T^2}} + 1 \right) \exp\left(\sqrt{\rho^2 + \frac{m^2}{T^2}} \right) - 1 \right)}{\left(\exp\left(\sqrt{\rho^2 + \frac{m^2}{T^2}} \right) - 1 \right)^2 \left(\rho^2 + \frac{m^2}{T^2} \right)^{\frac{3}{2}}} d\rho < 0$$

$$\partial_T \Theta = \frac{2}{T}\Theta - \frac{m}{T}\partial_m \Theta > 0$$

$$\partial_T (\delta^{ij} \varepsilon_{ij}) = \frac{4}{T}(\delta^{ij} \varepsilon_{ij}) - \frac{m}{T}\partial_m (\delta^{ij} \varepsilon_{ij}) > 0$$

This implies monotonicity for all $T \geq 0$ and $m > 0$. This can be extended to the point $m = 0$ due to continuity. □

Thus from a physical point of view the corresponding observables are still reasonable "temperature measurement devices". However the dependence on temperature is no longer given by a simple power law as in the massless case. This suggests that numerical methods are needed to establish a relation between the expectation values of the thermal observables and cumulants of the temperature distribution. Conversely, one might opt for choosing more complicated microobservables in order to have more tractable macroobservables.

2.2.4. LTE in Cosmological Spacetimes

As explained above there is a serious problem defining LTE states for non-static globally hyperbolic spacetimes. On such spacetimes no globally isometric time evolution exists, which precludes the definition of KMS states. Thus it is not clear which states should be chosen as thermal reference states or on a heuristic level how to gauge the thermal measurement apparatus. A heuristic concept which seems straight forward is to gauge the measurement apparatus in a "Minkowskian region" of spacetime and then use the Minkowski scale for measurements of thermal observables. If one decides to adopt this strategy, one is lead to the so-called "extrinsic LTE states" put forth first in [40][13]. A state is in this context called an extrinsic LTE state, if the expectation values of the thermal microobservables in this state are identical to the expectation values of the corresponding observables on Minkowski spacetime in a mixture of (r)KMS states. This means that the macroobservable interpretation of corresponding microobservables are assumed to be identical. The correspondence of microobservables on different spacetimes is given by the concept of locally covariant quantum fields as explained above.

Let the components of some tensor T with respect to some tetrad e be denoted as $T|_e$. For two tensors S and T of the same rank, possibly defined on different spacetimes, two tetrads e and f and points x and y defined on the appropriate spacetimes, let $S|_{e(x)} = T|_{f(y)}$ denote componentwise identity. This identity is in general without mathematical context and is to be simply understood as an identity of numbers.

Definition 2.2.7.
Let $\mathfrak{t}$ be a linear space of locally covariant thermal observables. Let e_g be a tetrad defined in a neighbourhood of $x \in \mathcal{M}$ and let $e_\eta(0)$ be that canonical Minkowski coordinate tetrad. A state ω is an extrinsic local thermal equilibrium or **extrinsic LTE state** at some point $x \in \mathcal{M}$ if there is a mixture of rKMS states represented by a probability measure $d\mu_x(\beta)$ such that

$$\forall A \in \mathfrak{t}: \quad \omega(A_g(x))\Big|_{e_g(x)} = \int \omega_\beta(A_\eta(0))\Big|_{e_\eta(0)} d\mu_x(\beta)$$

A state is said to be an LTE state in an open region $\mathcal{O} \subset \mathcal{M}$ if it is LTE $\forall x \in \mathcal{O}$. We will denote extrinsic LTE states for $\mathfrak{t} = \mathcal{S}_n, \mathcal{T}$ as (extrinsic) n, ∞-LTE states, respectively.

The choice of the origin in Minkowski spacetime is arbitrary and implies no loss of generality due to the translation invariance of Minkowski KMS states. Also the choice of tetrad is arbitrary and as shown in [44] choosing another tetrad will simply lead to a Lorentz transformation of the temperatures of the mixture of Minkowski rKMS states that is used for comparison.

This concept of thermality on curved spacetimes has had some success. It was used to investigate the KMS states in the static portion of de Sitter spacetime in [40][13] and to derive energy inequalities in quantum field theory on curved spacetimes for non-minimally coupled fields in [43]. The existence of extrinsic LTE states for definite temperature on a Cauchy surface in Friedmann-Robertson-Walker spacetime was proved in [42].

The principle of local covariance fixes the space of thermal observables unambiguously, thus providing an important ingredient to a concept of local thermality on curved spacetimes. However the physical, macroobservable, meaning of the microobservables is not fixed by the local covariance principle, which has profound implications for the extrinsic LTE condition. It is not clear which microobservables should really physically correspond to the thermal microobservables on Minkowski spacetime, but the extrinsic LTE condition depends on this correspondence. It should more generally be noted that the principle of local covariance gives no justification for the direct comparison of macroobservables given as expectation values for quantum field theories and their states on different spacetimes. From a heuristic point of view this amounts to gauging a set of measurement devices in Minkowski spacetime and then transferring the measurement devices and the scales into another spacetime. It is by no means ensured that the readings of the scales are sensibly connected to the physical processes in this spacetime, even more so as the curvature sensitivities of the measurement devices are unknown.

In this work we will highlight some problems that arise in the context of the extrinsic LTE condition. In light of the principal problem outlined here, we will take the point of view that the problems can be traced back, not to choosing the local covariance principle to acquire a space of thermal observables, but to the ambiguity in the choice of thermal observables i.e. of physical interpretation, and to the direct comparison of expectation values on different spacetimes.

2.3. Linear Scalar Cosmological Perturbations

Cosmological perturbation theory is a special case of perturbation theory in general relativity. The present work will only be concerned with linear perturbation theory, which means that only the tree level and the first order in the perturbations are considered and higher orders are neglected. The basic idea is to split all quantities up into a background part and a perturbation. In the case of geometric quantities, most prominently the metric, this is nontrivial due to the role of diffeomorphism covariance in general relativity. It turns out that only part of this covariance survives in the setting of linear perturbation theory, which is interpreted as covariance under infinitesimal diffeomorphisms and labelled gauge freedom. For physically unambiguous results it is reasonable to define gauge invariant quantities.

Using a $3+1$ decomposition of the background metric, it is possible to classify perturbations by their transformation behaviour under symmetries of the spatial section. This will lead to the definition of scalar, vector and tensor perturbations. In the present work we will only be concerned with scalar perturbations, thus vector and tensor perturbations will be dropped, after they have been identified.

The treatment in this section mostly follows [47] where no other sources are cited.

2.3.1. Robertson-Walker Cosmology

First we describe the basic properties of the background spacetime. As we are aiming for the description of a cosmological situation, the background spacetime is taken to be the simplest model which is thought to describe the universe on very large scales. Following the cosmological principle that no place in the universe is special if one considers only large scales, one is lead to the conclusion that spatial homogeneity and isotropy are appropriate simplifying assumptions for a simple approximate cosmological model. From these assumptions it follows that the spacetime is globally hyperbolic and the spatial section Σ must be a maximally symmetric space, which implies an at least 6-dimensional symmetry group of the spacetime. As in general singularities are possible, the spacetime is in general homeomorphic to $I \times \Sigma$ where $I \subset \mathbb{R}$ is some open, possibly unbounded, set. These spacetimes are called Robertson-Walker spacetimes.

Remarkably, a global comoving time t can be defined in Robertson-Walker spacetimes and, using t as a time coordinate and canonical coordinates for the spatial section, the line element takes the form

$$ds^2 = dt^2 - a^2(t) ds_\Sigma^2$$

where ds_Σ^2 symbolises the line element of the spatial hypersurface. The spatial hypersurfaces defined by a fixed value of the time coordinate are Cauchy surfaces of the spacetime, thus this choice of coordinates obviates the foliation of the spacetime by Cauchy surfaces. It is furthermore clear that Robertson-Walker spacetimes are static if and only if $a(t) = \text{const.}$, which makes them one of the simplest examples of non-static spacetimes. As the most accurate available measurements by WMAP [51] indicate that the spatial section of the universe is indeed flat with only an uncertainty of about 0.01 the critical density, we will assume $ds_\Sigma^2 = d\vec{x}^2$ in the following.

An important alternative set of coordinates can be acquired using the time coordinate $\eta(t) = \int\limits_{t_0}^{t} \frac{dt'}{a(t')}$ with some fixed time t_0. This obviously implies $a d\eta = dt$ and leads to the line element

$$ds^2 = a^2(\eta) \left(d\eta^2 - d\vec{x}^2 \right)$$

Using these coordinates one can immediately see that the spacetime is conformally equivalent to Minkowski spacetime, thus η is called conformal time. In the following we will mostly work with conformal time.

For some given quantity X we will denote the derivative with respect to comoving time as $\dot{X}$ and the derivative with respect to conformal time as X'. We also denote $H = \frac{\dot{a}}{a}$ and $\mathcal{H} = \frac{a'}{a}$.

The time dependence of the scale factor a depends crucially on the matter model coupled to the spacetime via the Einstein equations which do in this case reduce to the Friedmann equations

$$3H^2 = 8\pi G\rho$$

$$\dot{H} = -4\pi G(\rho + p)$$

In these equations ρ and p are the energy density and the pressure respectively, the only two free parameters of a matter model that is compatible with a Robertson-Walker spacetime. Assuming a linear equation of state $\rho = wp$ with constant w to hold, we can derive the dynamics of the matter

$$\dot{\rho} + 3H(1+w)\rho = 0 \quad \Rightarrow \quad \rho \propto a^{-3(1+w)}$$

If we assume the matter content to consist of components with different equations of state it is clear that the component with the lowest w will dominate for a very large a, while the component with the highest w will dominate for very small a. As the universe expands, i.e. $H > 0$, we can expect the component with largest w to dominate at early times, while the component with the lowest w should dominate at late times. Plugging the matter dynamics into the first Friedmann equation we get

$$\dot{a} = \sqrt{\frac{8\pi G\rho_0}{3}} a^{-\frac{1+3w}{2}} \quad \Rightarrow \quad a \propto \begin{cases} e^{Ht} & \text{for} \quad w = -1 \\ t^{\frac{2}{3(1+w)}} & \text{else} \end{cases}$$

where the special case $w = -1$ amounts to a matter model that is equivalent to an effective cosmological constant.

A naive extrapolation backwards in time leads to a singularity $a = 0$ with infinite energy density, as long as there are other matter components except a cosmological constant. The singularity theorems by Hawking and Penrose suggest that the singularity is not a defect of this simple model but a generic feature of expanding universe models. As the laws of physics that hold at very high energy density are unknown, it is customary to exclude at least the region where the energy density is of the order of the Planck scale from the cosmological standard model.

To add some context to the following explanation of the formalism, we will give a short overview of the main stages of development of the universe according to the cosmological standard model. The background model is assumed to be purely classical, such that quantum effects only play a significant role for the evolution of perturbations. The first phase of cosmological evolution is the phase of inflation. It is thought to have lasted from $t \leq 10^{-35}s$ to $t \approx 10^{-33}s \sim 10^{-30}s$. Within this time span the scale factor is supposed to have increased by a factor of $\sim 10^{30}$ in an approximately exponential fashion $a(t) \sim e^{Ht}$ which implies $w \approx -1$. Such an exponential expansion can be modelled by a homogeneous classical scalar field with large potential energy, as will be detailed below.

The phase of inflation was originally introduced to solve two problems, the horizon problem and the flatness problem. First we turn to an explanation of the horizon problem. Assuming the matter content of the universe to fulfil $w \geq 0$ even to very early times, we can draw the conclusion that at the time of hydrogen recombination, when the cosmic microwave background emerged, only the matter in rather small regions had ever been in causal contact and only there had the possibility to equilibrate. There is thus no explanation for the isotropy of the cosmic microwave background over large angles. A suitably rapid and large increase in size of the universe at an early stage can enlarge the regions of causal contact such that one region of causal contact fills all of the sky. The flatness problem consists simply of the question why the universe is to such a good degree spatially flat. A phase of inflation would decrease the magnitude of scalar curvature greatly, thus increasing the range of initial data compatible with the observed flatness.

A number of authors have formulated criticism of the inflationary scenario on different grounds. We will not consider these objections here but simply take the inflationary scenario for granted as a part of the cosmological standard model.

After the inflationary phase, the general matter model is assumed to consist of three components, namely radiation with $w = \frac{1}{3}$, which dominates the evolution for roughly the first $80,000$ years of the universe, matter with $w = 0$ which dominates in the time span from $80,000$ years to about 5 billion years and finally a cosmological constant or “dark energy” with $w \approx -1$ which dominates since an age of the universe of 5 billion years. However these transition times have no immediate physical importance.

A time which is physically very significant, especially for our purposes, is the time of hydrogen recombination. As the spacetime expands, the temperature of the classical matter decreases and at some point temperature will be so low that the energy of photons will not suffice to ionise hydrogen atoms. The period of time within which this transition occurs all over the universe is called the time of recombination, although strictly speaking the prefix “re” is misplaced, as no neutral atoms have stably existed before. During the time of recombination the mean free path of photons increased to infinity, such that photons after recombination can be assumed to be free particles for cosmological purposes. The epoch before recombination is called the tight coupling regime, while the epoch after recombination is called the regime of free streaming.

As the photon energy distribution follows a thermal spectrum and there are small temperature inhomogeneities, the time of recombination is really a time span in the order of magnitude of $100,000$ years. The phase of recombination occurred around $400,000$ years after the initial singularity.

2.3.2. Mathematical Background

This section will be dedicated to the explanation of the mathematical background of linear perturbation theory and gauge invariance. The approach taken here differs slightly from the usual treatment in the literature. We are following the presentation of [36] because it leads to a quite appealing formulation of the foundations of linear perturbation theory and gauge transformations. The key element for our description of linear perturbations and gauge freedom is the interpretation of perturbed quantities as one-parameter families of tensor fields.

Definition 2.3.1.

- Let $\mathcal{O} \subset \mathbb{R}$ an open neighbourhood of 0 and let $T : \mathcal{O} \to \Gamma(T^r_s\mathcal{M})$ a smooth one-parameter family of smooth r-s-tensor fields. Then $T_0 := T(0)$ is called the background quantity and $\delta T := \frac{d}{d\lambda}T(\lambda)|_{\lambda=0}\lambda$ is called the linear perturbation.
- Let $\Phi : \mathcal{O} \to \mathrm{Diff}\mathcal{M}$ a smooth one-parameter family of diffeomorphisms generated by the vector field X, i.e. $\Phi(0) = \mathrm{id}_{\mathcal{M}}$, $X = \frac{d}{d\lambda}\Phi(\lambda)|_{\lambda=0}$ and for the pull-back $(T^r_s\Phi)(0) = \mathrm{id}_{\Gamma(T^r_s\mathcal{M})}$. Then we define $\widetilde{\delta T} := \frac{d}{d\lambda}\Big((T^r_s\Phi)(\lambda)T(\lambda)\Big)|_{\lambda=0}\lambda$ as the transformed perturbation while the background quantity is unchanged $\tilde{T}_0 := (T^r_s\Phi)(0)T_0 = T_0$.

The above definition has the benefit that it is mathematically concise and yields the transformation law of the perturbations under gauge transformations in a very transparent way.

$$
\begin{aligned}
\widetilde{\delta T} =& \frac{d}{d\lambda}\Big((T^r_s\Phi)(\lambda)T(\lambda)\Big)\Big|_{\lambda=0}\lambda \\
=& \frac{d}{d\lambda}\Big((T^r_s\Phi)(0)T(\lambda)\Big)\Big|_{\lambda=0}\lambda + \frac{d}{d\lambda}\Big((T^r_s\Phi)(\lambda)T(0)\Big)\Big|_{\lambda=0}\lambda \\
=& \delta T + \lambda\mathscr{L}_X T_0 =: \delta T + \mathscr{L}_\xi T_0
\end{aligned}
$$

In this equation $\xi = \lambda X$ is often interpreted as an “infinitesimal vector field” to justify the linearisation. In any case the linearisation is seen to be essentially a linearisation of the Taylor expansion in λ of one-parameter families of tensor fields. Using the

Levi-Civita connection and local coordinates with respect to the background metric g_0 to express the Lie derivative we get

$$\widetilde{\delta T}^{\boldsymbol{\rho}}{}_{\boldsymbol{\sigma}} = \delta T^{\boldsymbol{\rho}}{}_{\boldsymbol{\sigma}} + \xi^\alpha \nabla_\alpha T_0{}^{\boldsymbol{\rho}}{}_{\boldsymbol{\sigma}} - \sum_{n=1}^{r} (\nabla_\alpha \xi^{\rho_n}) T^{\hat{\boldsymbol{\rho}}_n}{}_{\boldsymbol{\sigma}} + \sum_{n=1}^{s} (\nabla_{\sigma_n} \xi^\alpha) T^{\boldsymbol{\rho}}{}_{\hat{\boldsymbol{\sigma}}_n}$$

where the multiindices $\hat{\boldsymbol{\sigma}}_n$ and $\hat{\boldsymbol{\rho}}_n$ are equal to the multiindices $\boldsymbol{\sigma}$ and $\boldsymbol{\rho}$ respectively, except that the index at the n-th position, i.e. σ_n or ρ_n respectively, is replaced by α. Due to the metric compatibility of the Levi-Civita connection this yields an especially simple transformation law for the metric perturbation δg given by

$$\widetilde{\delta g}_{\mu\nu} = \delta g_{\mu\nu} + \nabla_\mu \xi_\nu + \nabla_\nu \xi_\mu$$

It is customary to classify metric perturbations using a $3+1$ decomposition of the background spacetime into spatial section and time direction if the background metric is sufficiently symmetric. In our case the background metric is a Robertson-Walker metric with flat spatial sections therefore such a decomposition is indeed beneficial. The perturbations are decomposed into scalar, vector and tensor part, dependent on their transformation behaviour under the symmetry group of the spatial section.

Let γ denote the metric of the spatial section Σ and let $X_{|i}$ denote the application of the Levi-Civita connection of (Σ, γ) on X expressed in the coordinates of the $3+1$ decomposition. In this context, $\delta g_{00} =: s_1$ is considered scalar; $\delta g_{0i} =: s_{2|i} + v_{1i}$ is decomposed into a pure gradient scalar part s_2 and a divergence free vector part v_1 with ${v_1}^i{}_{|i} = 0$; $\delta g_{ij} =: s_{3|ij} + s_4 \gamma_{ij} + v_{2i|j} + v_{2j|i} + t_{ij}$ is decomposed into two scalar parts, one pure gradient s_3 and the trace s_4, the gradient of a divergence free vector part v_2 with ${v_2}^i{}_{|i} = 0$ and a trace and divergence free tensor part t_{ij} with $t^i{}_i = t^i{}_{j|i} = 0$.

Counting the degrees of freedom, one naively gets 4 scalar, 4 vector and 2 tensor degrees of freedom. However, vector fields ξ used for gauge transformations, can be decomposed into a scalar part $\xi_s = \xi^0 \partial_0 + \xi^{|i} \partial_i$ and a vector part $\xi_v = x^i \partial_i$ with $x^i_{|i} = 0$, with two components each. This means that the gauge freedom reduces the degrees of freedom such that 2 gauge invariant degrees of freedom of every type remain. The total number of degrees of freedom is 10 without considering symmetries and 6 if the freedom to choose coordinates is considered. These degrees of freedom are simply the linearised version of the 10 degrees of freedom of the metric, which reduce to only 6 degrees of freedom if coordinate ambiguity in the guise of the Bianchi identity is considered.

An important point of this decomposition is that the different types of perturbations do not mix under gauge transformations. As implicitly claimed above, this can be traced back to an analogous decomposition of the gauge vector fields. We will state this fact in the following lemma.

Lemma 2.3.2.
Let $\underline{\xi} = \xi^0\partial_0 + (\xi^{|i} + x^i)\partial_i$ *be a vector field where* ${x^i}_{|i} = 0$*, and let* δg *be decomposed into scalar, vector and tensor part as explained above. Then, decomposing* $\widetilde{\delta g} = \delta g + \mathscr{L}_\xi g_0$ *in the same way, one sees comparing the scalar perturbations* $\tilde{s}_n = f_n(\xi^0, \xi, \boldsymbol{s})$*, for vector perturbations* $\tilde{v}_n = g_n(\vec{x}, \boldsymbol{v})$ *and for the tensor perturbation* $\tilde{t} = t$*, where the functions* f_n*,* g_n *may include time derivatives of the arguments. This means, the different types of perturbations are not mixed by gauge transformations.*

Proof. The proof can be done by direct calculation.

$$\widetilde{\delta g}_{00} = \delta g_{00} + 2(\xi^0)' + 2\Gamma^0_{00}\xi^0 + \Gamma^i_{00}(\xi_{|i} + x_i)$$

$$\widetilde{\delta g}_{0i} = \delta g_{0i} + {\xi'}_{|i} + x'_i + \Gamma^0_{0i}\xi^0 + \Gamma^j_{0i}(\xi_{|j} + x_j) + {\xi^0}_{|i}$$

$$\widetilde{\delta g}_{ij} = \delta g_{ij} + \xi_{|ij} + x_{i|j} + \xi_{|ji} + x_{j|i}$$

One immediately sees that the gauge transformation terms can be linked to the perturbations such as to fulfil the claim, if $\Gamma^i_{00} = \Gamma^0_{0i} = 0$ holds. This does indeed follow from the fact that the $3+1$ decomposition implies that $(g_0)_{0i} = 0$ and $(g_0)_{00}$ depends only on time. This proves the claim. □

2.3.3. Technical Framework and Formulae

In the following the necessary formulae for a basic treatment of cosmological questions in the context of linear perturbation theory are derived. As the perturbations of the cosmic microwave background are explained as an effect of quantum fluctuations in the early universe, the perturbations will be quantised at some point. This gives rise to questions in the context of more rigorous quantum field theory some of which are discussed in this work.

As explained above, the background metric used for cosmological perturbation theory is a Robertson-Walker metric with flat spatial section. As we restrict now to scalar perturbations, the perturbed metric can be expressed using conformal time as

$$ds^2 = a^2(\eta)\Big((1+2A)d\eta^2 + 2B_{|i}d\eta dx^i - \Big((1+2D)\delta_{ij} + 2E_{|ij}\Big)dx^i dx^j\Big)$$

where A, B, D and E are functions of all coordinates. It should be noted that A, B, D and E are not exactly the same as the s_n used above, but differ by a factor of $2a^2(\eta)$. This yields slightly different behaviour under gauge transformations.

As we restrict to scalar perturbations we also restrict to scalar gauge vector fields $\underline{\xi} = \xi^0 \partial_0 + \xi^{|i} \partial_i$. This yields transformation laws

$$\tilde{A} = A + \mathcal{H}\xi^0 + (\xi^0)' \qquad \tilde{B} = B + \xi^0 - \xi'$$

$$\tilde{D} = D + \mathcal{H}\xi^0 \qquad \tilde{E} = E + \xi$$

Obviously any two of the perturbations can be brought to vanish except A and D, as they are both only changed due to ξ^0. This means if A and D can both be brought to vanish in some gauge, this has a physical implication. An often used gauge is the conformal gauge, where $B_c = E_c = 0$. To separate physical contents from gauge effects, it is useful to work with gauge invariant variables. As we have four scalar perturbations and two gauge parameters we can derive two gauge invariant scalar perturbations. The ones usually defined in the literature are the Bardeen potentials

$$\Psi = A - \frac{1}{a}\Big((B - E')\Big)' \qquad \phi = D - \mathcal{H}(B - E')$$

For the Einstein equation it is necessary to calculate the Einstein tensor, which is not gauge invariant. However $G^\mu_\nu - 8\pi G T^\mu_\nu$ can be cast into a gauge invariant form, as it vanishes in any gauge. This implies that the Einstein equations can be formulated using only gauge invariant variables. This means we can calculate the Einstein tensor and the energy momentum tensor in some arbitrary gauge, and the resulting Einstein equations will be true for any gauge. This means we can replace the perturbation variables in the Einstein equations by gauge invariant variables that are equal to them in the chosen gauge. The resulting equation, containing only gauge invariant variables, still holds in any gauge.

The calculation of the perturbation of the Einstein tensor in conformal gauge is tedious and has been done in [47], therefore we will not redo it here but simply give the result. We remark that in conformal gauge $A_c = \Psi$, $D_c = \Phi$ and $B_c = E_c = 0$. This means that the Einstein tensor will only contain A_c and D_c which can be straight forwardly replaced by the Bardeen potentials in the full Einstein equation. In the following, the indices denoting conformal gauge will be suppressed for readability and all expressions containing only the perturbations A and D are to be understood in conformal gauge.

$$\delta G^0_0 = -\frac{2}{a^2}\Big(3\mathcal{H}(\mathcal{H}A - D') + \triangle D\Big)$$

$$\delta G^0_i = \frac{2}{a^2}(\mathcal{H}A - D')_{,i}$$

$$\delta G^i_j = -\frac{2}{a^2}\Big((2\mathcal{H}' + \mathcal{H}^2)A + \mathcal{H}A' - D'' - 2\mathcal{H}D' + \frac{1}{2}\triangle(A + D)\Big)\delta^i_j + \frac{1}{a^2}(A + D)^{|i}{}_{|j}$$

The last expression can be considerably simplified by subtracting the trace

$$\delta G^i_j - \frac{1}{3}\delta G^k_k \delta^i_j = \frac{1}{a^2}\Big((A+D)^{|i}{}_{|j} - \frac{1}{3}(A+D)^{|k}{}_{|k}\delta^i_j\Big)$$

For the matter model we will only discuss the case of a scalar field. In [47] more general fluid matter models are discussed and some interesting applications are briefly shown. For the present work however the application to the scalar field model suffices, as this is the only model where a quantum treatment of the perturbations occurs. We will also be concerned with part of the perturbation theory which is usually treated classically and we will investigate this topic from the point of view of quantum field theory on curved spacetimes. However in said case it is customary to use the Boltzmann equation and not the Einstein equation as one is interested in a photon spectrum. Thus our restriction to the scalar field case still suffices to keep the treatment self-contained.

We use the general field equation

$$\Box\phi = -\frac{\partial V}{\partial\phi}(\phi) =: -V_{,\phi}$$

where $V(\phi)$ is some potential. Strictly speaking the potential must not be dependent on the metric, otherwise the suggested form of the energy momentum tensor

$$T^\mu_\nu = \partial^\mu\phi\partial_\nu\phi - \delta^\mu_\nu\Big(\frac{1}{2}\partial^\lambda\phi\partial_\lambda\phi - V(\phi)\Big)$$

would be wrong. If, for instance $V(\phi, g_{\mu\nu}) = \widetilde{V}(\phi) - \frac{\xi}{2}R\phi^2$, which is only the simplest form of coupling the field to gravity, the energy momentum tensor would include an additional term

$$\begin{aligned}T^\mu_\nu =&\partial^\mu\phi\partial_\nu\phi - \delta^\mu_\nu\Big(\frac{1}{2}\partial^\lambda\phi\partial_\lambda\phi - \widetilde{V}(\phi)\Big)\\ &+\xi\Big[G^\mu_\nu\phi^2 + 2\delta^\mu_\nu\Big(\phi\Box\phi + \partial^\lambda\phi\partial_\lambda\phi\Big) - 2\Big(\phi\nabla^\mu\partial_\nu\phi + \partial^\mu\phi\partial_\nu\phi\Big)\Big]\end{aligned}$$

It is clear that such a modification could have a significant impact.

For now we will follow the standard treatment and assume the potential to be independent of the metric. In keeping with the idea of linear perturbation theory also the scalar field is decomposed into a background part and a perturbation $\phi = \phi_0 + \delta\phi$. The background field is assumed to be spatially homogeneous such that one gets

$$\begin{aligned}T^0_0 =&\frac{1}{2a^2}(\phi_0')^2 + V(\phi_0)\\ T^i_j =&\Big(-\frac{1}{2a^2}(\phi_0')^2 + V(\phi_0)\Big)\delta^i_j\end{aligned}$$

The gauge transformation behaviour of the field perturbation is

$$\widetilde{\delta\phi} = \delta\phi + \xi^0\phi_0'$$

which implies the following gauge invariant perturbation

$$\chi = \delta\phi - \phi_0'(B + E')$$

Again in conformal gauge $\delta\phi_c = \chi$; in the following the subscript indicating conformal gauge will be suppressed and whenever expressions contain $\delta\phi$ they are to be understood in conformal gauge. Inserting $\phi = \phi_0 + \delta\phi$ in the formula for the energy-momentum tensor we get the linear perturbation

$$\begin{aligned}
\delta T^0_0 =& \frac{1}{a^2}\Big(- (\phi_0')^2 A + \phi_0'\delta\phi' + V_{,\phi}a^2\delta\phi\Big) \\
\delta T^0_i =& \frac{1}{a^2}\phi_0'\delta\phi_{,i} \\
\delta T^i_j =& \frac{1}{a^2}\Big((\phi_0')^2 A - \phi_0'\delta\phi' + V_{,\phi}a^2\delta\phi\Big)\delta^i_j
\end{aligned}$$

The idea of perturbation theory is to assume the equations to hold order by order. This means we will have a background Einstein equation and a perturbation to the Einstein equation which will be assumed to hold separately. The background Einstein equations are

$$\begin{aligned}
-3\mathcal{H}' =& 4\pi G(\phi_0')^2 + 8\pi G V(\phi_0)a^2 \\
-\mathcal{H}' - 2\mathcal{H}^2 =& - 4\pi G(\phi_0')^2 + 8\pi G V(\phi_0)a^2 \\
-\mathcal{H}' + \mathcal{H}^2 =& 4\pi G(\phi_0')^2
\end{aligned}$$

and the background Klein-Gordon equation reduces to

$$\phi_0'' + 2\mathcal{H}\phi_0' + V_{,\phi}(\phi_0)a^2 = 0 \tag{2.3.1}$$

The perturbation Klein-Gordon and Einstein equations will lead to a set of three independent equations. We start with the equation

$$\delta G^i_j - \frac{1}{3}\delta G^k_k\delta^i_j = \frac{1}{a^2}\left((A + D)^{|i}{}_{|j} - \frac{1}{3}(A + D)^{|k}{}_{|k}\delta^i_j\right) = 0$$

which implies $A + D = 0$ up to an irrelevant homogeneous term. In gauge invariant notion this becomes $\Phi = -\Psi$. The 0-i-equation of the Einstein equations becomes

$$\mathcal{H}A + A' = 4\pi G\phi_0'\delta\phi \quad \Leftrightarrow \quad \Psi' + \mathcal{H}\Psi = 4\pi G\phi_0'\chi \tag{2.3.2}$$

again up to a homogeneous term. For the last Einstein equations we take

$$
\begin{aligned}
-\delta G^0_0 - \frac{1}{3}\delta G^k_k =& \frac{2}{a^2}\Big(3\mathcal{H}(\mathcal{H}A + A') - \triangle A\Big) + \frac{2}{a^2}\Big((2\mathcal{H}' + \mathcal{H}^2)A + 3\mathcal{H}A' + A''\Big) \\
=& \frac{2}{a^2}\Big(A'' + 6\mathcal{H}A' + (2\mathcal{H}' + 4\mathcal{H}^2)A - \triangle A\Big) \\
=& -8\pi G\delta T^0_0 - \frac{8\pi G}{3}\delta T^k_k = -8\pi G\frac{2}{a^2}V_{,\phi}a^2\delta\phi
\end{aligned}
$$

Then we can use the Klein-Gordon equation and the 0-i-equation to recast this in the form

$$
A'' - \triangle A + 6\mathcal{H}A' + (2\mathcal{H}' + 4\mathcal{H}^2)A = \frac{2}{\phi_0'}(A' + \mathcal{H}A)(\phi_0'' + 2\mathcal{H}\phi_0')
$$

$$
\Rightarrow \quad \Psi'' - \triangle\Psi + 2\left(\mathcal{H} - \frac{\phi_0''}{\phi_0'}\right)\Psi' + 2\left(\mathcal{H}' - \frac{\phi_0''}{\phi_0'}\mathcal{H}\right)\Psi = 0 \tag{2.3.3}
$$

The perturbation of the Klein-Gordon equation is

$$
\chi'' - \triangle\chi + 2\mathcal{H}\chi' + V_{,\phi\phi}(\phi_0)a^2\chi = 4\phi_0'\Psi' - 2V_{,\phi}(\phi_0)a^2\Psi \tag{2.3.4}
$$

The coupled differential equations (2.3.2), (2.3.3) and (2.3.4) govern the dynamics of the gauge invariant perturbations Ψ and χ. We will investigate in this work the quantisation of perturbations using these equations. Especially the constraint equation (2.3.2) will play a major role.

In the standard treatment one usually defines a field

$$
u = a\chi + z\Psi \qquad \text{where} \qquad z = \frac{a\phi_0'}{\mathcal{H}} \tag{2.3.5}
$$

which fulfils the equation of motion

$$
u'' - \triangle u - \frac{z''}{z}u = 0. \tag{2.3.6}
$$

This field is then usually quantised and the Fourier transform of its associated two-point function, the so-called power spectrum, is derived. The power spectrum is later used to derive the spectrum of temperature perturbations of the cosmological background radiation. To achieve a reasonably well defined model, some assumptions have to be made about the inflationary period. In the context of this work it suffices to elaborate the "slow-roll" model. We define the so-called slow-roll parameters

$$\varepsilon = 1 - \frac{\mathcal{H}'}{\mathcal{H}^2} = 4\pi G \frac{z^2}{a^2} \tag{2.3.7}$$

$$\delta = 1 + \varepsilon - \frac{z'}{z\mathcal{H}} \tag{2.3.8}$$

where ε also implement the background Friedmann equation, and assume them to be small. Noting

$$\frac{z''}{z} = \left(2 + 2\varepsilon - 3\delta + 2\varepsilon^2 - 3\varepsilon\delta + \delta^2 - \frac{\delta'}{\mathcal{H}}\right)\mathcal{H}^2$$

and remembering that the inflationary model implies an approximate de Sitter phase with $\mathcal{H} \approx -\frac{1+\varepsilon}{\eta}$ this implies the approximate equation of motion

$$u'' - \triangle u - \frac{2 + 4\varepsilon - 3\delta}{\eta^2} u = 0.$$

For simplicity, ε and δ are usually treated as constants, which means that the equation of motion is that of an almost minimally coupled scalar field in de Sitter spacetime.

Next it is assumed that the ultraviolett asymptotics of the two-point function are fixed in such a way that the state is compatible with the Hadamard condition. It is then argued heuristically that the power spectrum tends to that of the Bunch-Davies state during the inflationary period. The property in question here is in fact the infrared stability of de Sitter spacetime which has been studied to some degree. While there is no final consent about this, this assumption can be taken for granted for a free field as long as it is not massless. This finally yields the so-called "scale-free power spectrum", which is simply the infrared limit power spectrum of the Bunch-Davies state.

$$\omega\Big(\tilde{u}(\vec{k})\tilde{u}(\vec{k}')\Big) = \frac{2\pi^2}{k^3} P_{\text{prim}}(k)\delta(\vec{k} - \vec{k}') \quad \Rightarrow \quad P_{\text{prim}}(k) \propto k^{3\delta - 4\varepsilon}$$

Quite oddly, one writes $P_{\text{prim}}(k) = k^{n-1}$, where the spectrum calculated here is approximately the so-called Harrison-Zel'dovich spectrum for which $n = 1$.

In the present work the quantisation procedure will be investigated in some detail, showing that the choice of field to quantise is ambiguous. However, the field u which is usually chosen for quantisation will be seen to be among the preferred options for fields to quantise. It would be preferable to formulate a sound quantum theory for the linear perturbations that takes into account gauge issues and provides a well founded quantisation mechanism. However, such an endeavour is beyond the scope of this work. In [17] an algebraic quantum theory for linear perturbations of the metric has been formulated for vacuum spacetimes. However, the very procedure applied in that article prevents a coupling to matter and thus a treatment of cosmological problems.

2.3.4. The Boltzmann Equation

In this subsection we will introduce the necessary formalism to derive the temperature perturbations of the cosmic microwave background from the primordial power spectrum. This means that the evolution of the perturbations after the end of inflation is to be described. To describe the photon fluid after the era of inflation one uses the Boltzmann equation. The Boltzmann equation in the form derived in the present subsection will be used in the following derivation of the Sachs-Wolfe effect and in section 4.2.

There are two main procedures to motivate the Boltzmann equation in the literature. The treatment that is pursued for example in [15] is rather heuristic and uses a classical mechanics analogy. The treatment in [47] is in contrast rather technical but sheds more light on the geometrical background. We will therefore follow the latter approach. The description is purely classical and light is not modelled as waves but as classical particles traveling on null geodesics. Thus one essentially looks for the Liouville operator corresponding to geodesic motion.

First of all we note that the cotangent bundle $T^*\mathcal{M}$ of spacetime can be interpreted as a symplectic manifold with a symplectic form ω_g expressed in natural bundle coordinates (x^μ, p_ν), which are Darboux coordinates in the symplectic setting, as

$$\omega = dx^\mu \wedge dp_\mu \quad \longrightarrow \quad \omega_g = dx^\mu \wedge d(g_{\mu\nu}p^\nu)$$

The second equality uses the metric isomorphism to define a corresponding symplectic form ω_g on the tangent bundle $T\mathcal{M}$. On the tangent bundle the Hamiltonian function for geodesic motion can be expressed as

$$L = \frac{1}{2} g_{\mu\nu} p^\mu p^\nu$$

which yields the Hamiltonian vector field as solution to $i_{X_g}\omega_g = dL$. The Hamiltonian vector field in this case is the geodesic spray

$$X_g = p^\mu \frac{\partial}{\partial x^\mu} - \Gamma^\mu_{\nu\lambda} p^\nu p^\lambda \frac{\partial}{\partial p^\mu}$$

With some additional geometric apparatus one can show that the collisionless Boltzmann equation is $\mathcal{L}_{X_{m,g}} f = 0$ where $X_{m,g} = X_g|_{\Phi_m}$ and

$$\Phi_m = \{v \in T\mathcal{M} | v \text{ future directed, } g(v,v) = m^2\}$$

can be interpreted as the mass shell. As this is done in some detail in [47] we will not repeat the argument here. Note that X_g can be cast in the form

$$X_g = p^{\overline{\mu}} e_{\overline{\mu}} - \omega^{\overline{\mu}}{}_{\overline{\nu}}(p) p^{\overline{\nu}} \frac{\partial}{\partial p^{\overline{\mu}}}$$

where overlines denote tetrad indices. The tetrad used in this setting is the canonical lift of the tetrad given by

$$e_{\overline{0}} = \frac{1-A}{a}\partial_\eta \qquad e_{\overline{i}} = \frac{1-D}{a}\partial_i$$

in conformal gauge to a tetrad on $T(T\mathcal{M})$. This canonical lift is defined via the identification of $T_x\mathcal{M}$ and its basis with its tangent space. The restriction to Φ_m in terms of this tetrad is given as

$$X_{m,g} = p^{\overline{\mu}} e_{\overline{\mu}} - \omega^{\overline{i}}{}_{\overline{\nu}} p) p^{\overline{\nu}} \frac{\partial}{\partial p^{\overline{i}}}$$

where $\omega^{\overline{i}}_{\overline{\nu}}(p)$ are the connection forms. In keeping with the idea of perturbation theory we assume the phase space density $f(x,\vec{p}) = f_0(\eta, p) + \delta f(\eta, \vec{x}, p, \hat{p})$. Now we can separate the background terms from the perturbation in $\mathcal{L}_{X_{m,g}} f$. In the linear term we use the "comoving momentum" $q = ap$ instead of the "conformal momentum", given by the tetrad components of p. Additionally we Fourier transform from $\vec{x}$ to $\vec{k}$ and use $\mu = \hat{k}\cdot\hat{p}$. Denoting the background part and the perturbation by $\widetilde{X_g(f)} =: \left(\widetilde{X_g(f)}\right)_0 + \left(\widetilde{X_g(f)}\right)_1$, we get

$$\frac{a}{p^0}\left(\widetilde{X_g(f)}\right)_0 = f_0' - \mathcal{H}p\frac{\partial f_0}{\partial p} \tag{2.3.9}$$

$$\frac{a}{p^0}\left(\widetilde{X_g(f)}\right)_1 = \left(\widetilde{\delta f}' - \tilde{A}' q \frac{\partial f_0}{\partial q}\right) + ik\mu\left(\widetilde{\delta f} - \tilde{A} q\frac{\partial f_0}{\partial q}\right) + (\tilde{A} - \tilde{D})' q \frac{\partial f_0}{\partial q} \tag{2.3.10}$$

This can be recast in a gauge invariant form, which is however more complicated than with the quantities treated so far, as δf is a function on a subspace of the tangent bundle. The details are explained in [47] and we just give the gauge invariant form here.

$$\mathcal{F} = \delta f - q\frac{\partial f_0}{\partial q}\Big(\mathcal{H}(B + E') + \hat{p}^i (B + E')_{,i}\Big)$$

In the following we drop the tildes from the Fourier transform; as we use only the Fourier transformed quantities in the following, no confusion should arise.

It is then customary to define the background rescaled bolometric phase space density

$$\Lambda = \frac{\int\limits_0^\infty \mathcal{F} q^3 dq}{4 \int\limits_0^\infty f_0 q^3 dq} \tag{2.3.11}$$

where the factor $\frac{1}{4}$ is multiplied to allow an interpretation as a background rescaled temperature perturbation due to the Stefan-Boltzmann law. Observing

$$\int\limits_0^\infty \frac{\partial f_0}{\partial q} q^4 dq = -4 \int\limits_0^\infty f_0 q^3 dq$$

one gets, integrating equation (2.3.10) and using (2.3.11)

$$\frac{a \int\limits_0^\infty \frac{1}{p^0} \left(\widetilde{X_g(f)}\right)_1 q^3 dq}{4 \int\limits_0^\infty f_0 q^3 dq} = (\Lambda + \Psi)' + (ik\mu)(\Lambda + \Psi) - (\Psi - \Phi)'$$

The second ingredient to the Boltzmann equation is a description of non-gravitational interaction. In the case of the photon fluid we expect strong interaction with charged particles as long as the photon energy is high enough. The process that is most important for photon energies close to the ionisation energy is Thomson scattering with electrons. As the last interaction before decoupling is overwhelmingly likely to be a Thomson scattering, it suffices to consider this process for an adequate description of decoupling and free streaming. We will not derive the scattering amplitude in the usual form here. A quite accessible derivation is given in [47]. We will assume Λ to be scalar, which means that it only depends on η, k and μ. Furthermore we will use cylindrical moments defined by $\Lambda(\eta, k, \mu) = \sum\limits_{l=0}^{\infty} (-i)^l \lambda_l(\eta, k) P_l(\mu)$.

The full Boltzmann equation with Thomson scattering is

$$(\Lambda + \Psi)' + (ik\mu + \dot{\tau})(\Lambda + \Psi) = (\Psi - \Phi)' + \dot{\tau} \left(\lambda_0 + \Psi - i\mu\lambda_1 - \tfrac{1}{10} P_2(\mu)\lambda_2\right) \tag{2.3.12}$$

where $\dot{\tau} = n_{\text{fe}} \sigma_T a$ with n_{fe} being the density of free electrons and σ_T the Thomson cross section. As the cross section is strongly dependent on photon energy and thereby temperature, it is evident that $\dot{\tau}$ is strongly time dependent in the temperature range where the average photon energy drops below the ionisation energy of hydrogen. (To be more precise one should note that the extreme excess of photons over electrons actually lowers the temperature of decoupling by almost two orders of magnitude below the ionisation energy of hydrogen.)

2.3.5. The Sachs-Wolfe Effect for Adiabatic Perturbations

The Sachs-Wolfe effect, first described in [37], provides an explanation for the large angle part of the angular spectrum of temperature fluctuations of the cosmic microwave background. In the previous subsections almost all necessary tools for the derivation of the Sachs-Wolfe angular spectrum of perturbations have been collected. In this subsection the angular spectrum will be derived for completeness. The Sachs-Wolfe angular spectrum will only briefly be referenced in the remainder of this work but its derivation highlights an interesting point which plays a role in all semiclassical treatments of gravity. The treatment in this section largely follows [47] and [15].

The temperature fluctuations of the cosmic microwave background are fundamentally random, so the theory of cosmological perturbations cannot predict a certain map of the sky with hot and cool spots. However, the randomness of the fluctuations can be quantified in the sense that the angular correlation of temperature fluctuations can be investigated. So the questions that can be answered by cosmological perturbation theory are of the type: "Randomly taking $1,000$ pairs of points in the sky where each pair are an angle of one degree apart, how strongly are the measured pairs of temperatures of the cosmic microwave background at the two points correlated?" Therefore the principal object of investigation is the statistical autocorrelation of temperature fluctuations at different angles of measurement

$$C(\eta, \vec{x}, \hat{p}\cdot\hat{p}') := \left\langle \frac{\Delta T(\hat{p})}{T}\frac{\Delta T(\hat{p}')}{T} \right\rangle$$

$$:= \int \frac{d^3k d^3k'}{(2\pi)^6} e^{i\vec{x}(\vec{k}-\vec{k}')} \left\langle (\Lambda+\Psi)(\eta,\vec{k},\hat{p})(\Lambda+\Psi)^*(\eta,\vec{k}',\hat{p}')\right\rangle$$

where $\hat{p}$ and $\hat{p}'$ are directions of measurement, i.e., telescope alignments, $(\vec{x},\eta)$ marks the spacetime location of the telescope and $\Lambda+\Psi = \frac{\Delta T}{T}$ by definition. In this expression Λ is interpreted as a random variable with vanishing expectation value, because the background temperature is chosen such that the mean of the fluctuation vanishes.

As the object of interest is an angular correlation, considering an angular expansion is rather natural. An expansion in spherical harmonics is given by

$$\int \frac{d^3k}{(2\pi)^3} e^{i\vec{x}\vec{k}}(\Lambda+\Psi)(\eta,\vec{k},\hat{p}) = \sum_{l,m} a_{lm}(\eta,\vec{x})Y_{lm}(\hat{p})$$

where the a_{lm} are again understood as random variables. Due to spatial homogeneity and isotropy these random variables satisfy

$$\langle a_{lm}(\eta,\vec{x})a^*_{l'm'}(\eta,\vec{x})\rangle = \delta_{ll'}\delta_{mm'}C_l(\eta)$$

which bears two important implications. Firstly, it suffices to consider an expansion of $C(\eta, \vec{x}, \hat{p} \cdot \hat{p}')$ in cylindrical moments and secondly the variance of the cylindrical moments is constrained by their relation to the correlation of the a_{lm}. The expansion in cylindrical moments is

$$C(\eta, \hat{p} \cdot \hat{p}') = \sum_{l=2}^{\infty} \frac{2l+1}{4\pi} C_l(\eta) P_l(\hat{p} \cdot \hat{p}')$$

In the following, the Ψ added to Λ at measurement time is ignored, as it only affects the moment C_0, because of the independence of Ψ on μ.

The correlations of the temperature fluctuations are assumed to stem from primordial fluctuations, which means that the correlation function is decomposed as

$$\left\langle \Lambda(\eta, \vec{k}, \hat{p}) \Lambda^*(\eta, \vec{k}', \hat{p}') \right\rangle = \left\langle u(\eta, \vec{k}) u^*(\eta, \vec{k}') \right\rangle \frac{\Lambda(\eta, \vec{k}, \hat{p})}{u(\eta, \vec{k})} \frac{\Lambda^*(\eta, \vec{k}', \hat{p}')}{u^*(\eta, \vec{k}')} \tag{2.3.13}$$

where the quotients $\frac{\Lambda}{u}$ are assumed to evolve deterministically. The autocorrelation of u is then identified with the Fourier transform of its two-point function. So essentially the quantum expectation value at the end of inflation is interpreted as the autocorrelation of a classical random field. This is a generic way of doing a quantum-classical transition in a semiclassical setting, where the present case is still peculiar when compared to semiclassical electrodynamics or the semiclassical Einstein equation, as pointed out by [33]. In the latter cases, a quantum expectation value is interpreted as a classical quantity, or to make an analogy to the present case, as a classical expectation value. In the present case however, the quantum two-point function is interpreted as a classical autocorrelation, i.e. statistical information on pairs of points. In [33] the troublesome features of the quantum-classical transition are discussed in some detail. In the present work the usual procedure is not questioned.

To get an expression for $\frac{\Lambda}{u}$ at present time, it is necessary to solve the Boltzmann equation formulated above. However, to achieve this a model for the time dependence of the Thomson cross section, i.e., some information about $\dot{\tau}$ is needed. Before addressing this problem, consider the general solution of equation (2.3.12)

$$\Lambda + \Psi = \int_0^\eta \left[\dot{\tau} \left(\lambda_0 + \Psi - i\mu\lambda_1 - \frac{P_2(\mu)}{10} \lambda_2 \right) + (\Psi - \Phi)' \right] e^{-ik\mu(\eta - \eta') - \tau(\eta', \eta)} d\eta' \tag{2.3.14}$$

where $\tau(\eta', \eta) = \int_{\eta'}^{\eta} \dot{\tau} d\eta''$ and $\dot{\tau} e^{-\tau(\eta', \eta)}$ is called the visibility function. The visibility function is a probability density for the time of last scattering of photons in such a fashion that the model of all photons being last scattered at a fixed time η_*

implies $\dot{\tau}e^{-\tau(\eta',\eta)} = \delta(\eta' - \eta_*)$. This approximation is called the sudden decoupling approximation and leads to an explicitly calculable spectrum. In this approximation

$$(\Lambda + \Psi)(\eta, \mu, k) = \Big(\lambda_0(\eta_*) + \Psi(\eta_*) - i\mu\lambda_1(\eta_*) - \frac{1}{10}P_2(\mu)\lambda_2(\eta^*)\Big)e^{-ik\mu(\eta-\eta_*)} + \text{ISW}$$

where $\text{ISW} := \int_0^\eta (\Psi - \Phi)' e^{-ik\mu(\eta-\eta')-\tau(\eta',\eta)} d\eta'$ is responsible for the so-called integrated Sachs-Wolfe effect. If decoupling is modelled not as instantaneous but the time of decoupling is instead smeared out, the results change slightly but qualitatively remain largely the same, as indicated in [15].

To extract the cylindrical moments at late times from the solution, it is necessary to expand $e^{-ik\mu(\eta-\eta_*)}$ into Legendre polynomials. This yields

$$e^{-ik\mu(\eta-\eta_*)} = \sum_l (-i)^l (2l+1) j_l(k(\eta - \eta_*)) P_l(\mu)$$

$$-i\mu e^{-ik\mu(\eta-\eta_*)} = \sum_l (-i)^l (2l+1) j_l'(k(\eta - \eta_*)) P_l(\mu)$$

$$(-i)^2 P_2(\mu) e^{-ik\mu(\eta-\eta_*)} = \sum_l (-i)^l (2l+1) \frac{1}{2}\Big(3j_l'' + j_l\Big)(k(\eta - \eta_*)) P_l(\mu)$$

which leads to the moments

$$\frac{\lambda_l(\eta, k)}{2l+1} = (\lambda_0(\eta_*, k) + \Psi(\eta_*, k)) j_l(k(\eta - \eta_*)) + \lambda_1(\eta_*, k) j_l'(k(\eta - \eta_*))$$

$$+ \frac{1}{20}\Big(3j_l''(k(\eta - \eta_*)) + j_l(k(\eta - \eta_*))\Big)\lambda_2(\eta^*, k) + \text{ISW}_l \qquad (2.3.15)$$

for $l \geq 2$.

To calculate the cylindrical modes of the variance of the temperature fluctuations from (2.3.15), a mode form of equation (2.3.13) is needed. This can be achieved using the relation between Legendre polynomials and spherical harmonics. Inserting (2.3.9) we get

$$\Big\langle \Lambda(\eta, \vec{k}, \hat{p}) \Lambda^*(\eta, \vec{k}', \hat{p}') \Big\rangle = 2\pi^2 \delta(\vec{k} - \vec{k}') \frac{P_{\text{prim}}(k)}{k^3} \frac{\Lambda(\eta, \vec{k}, \hat{p})}{u(\eta, k)} \frac{\Lambda^*(\eta, \vec{k}', \hat{p}')}{u^*(\eta, k')}$$

$$\int e^{i\vec{x}(\vec{k}-\vec{k}')} \Big\langle \Lambda(\eta, \vec{k}, \hat{p}) \Lambda^*(\eta, \vec{k}', \hat{p}') \Big\rangle d^3k d^3k'$$

$$= 2\pi^2 \int \frac{P_{\text{prim}}(k)}{k^3} \frac{\Lambda(\eta, \vec{k}, \hat{p})}{u(\eta, k)} \frac{\Lambda^*(\eta, \vec{k}, \hat{p}')}{u^*(\eta, k)} d^3k$$

$$= 2\pi^2 \int \sum_{l=0}^{\infty} \sum_{l'=0}^{\infty} (-i)^{l-l'} \frac{P_{\text{prim}}(k)}{k^3} \frac{\lambda_l(\eta,k) P_l(\hat{k}\cdot\hat{p})}{u(\eta,k)} \frac{\lambda_l^*(\eta,k) P_l(\hat{k}\cdot\hat{p}')}{u^*(\eta,k)} d^3k$$

$$= (2\pi)^3 \int \sum_{l,l'} i^{l'-l} 4\pi \frac{P_{\text{prim}}(k)}{k^3} \sum_{m,m'} \frac{|\lambda_l(\eta,k)|^2 Y_{lm}(\hat{k}) Y_{lm}^*(\hat{p}) Y_{l'm'}(\hat{k}) Y_{l'm'}^*(\hat{p}')}{|u(\eta,k)|^2 (2l+1)(2l'+1)} d^3k$$

$$= (2\pi)^3 \int_0^{\infty} \sum_{l=0}^{\infty} \frac{4\pi}{2l-1} \frac{P_{\text{prim}}(k)}{k} \sum_{m=-l}^{l} \frac{|\lambda_l(\eta,k)|^2 Y_{lm}^*(\hat{p}) Y_{lm}^*(\hat{p}')}{|u(\eta,k)|^2} dk$$

$$= (2\pi)^3 \int_0^{\infty} \sum_{l=0}^{\infty} \frac{P_{\text{prim}}(k)}{k} \left| \frac{\lambda_l(\eta,k)}{u(\eta,k)} \right|^2 P_l(\hat{p}\cdot\hat{p}') dk$$

This finally leads to

$$\frac{(2l+1)^2}{4\pi} C_l = \int_0^{\infty} \frac{P_{\text{prim}}(k)}{k} \left| \frac{\lambda_l(\eta,k)}{u(\eta,k)} \right|^2 P_l(\hat{p}\cdot\hat{p}') dk$$

for $l \geq 2$

To calculate $\frac{\lambda_l}{u}$ it is necessary to relate the Bardeen potentials and cylindrical modes of the temperature fluctuations at decoupling to the field u. To do this requires an investigation of the evolution during the phase of tight coupling, which is done in some detail in [47] and [15]. As this investigation takes up a lot of space and is unrelated to the present work it will not be reproduced here. For the Sachs-Wolfe effect one restricts to the first term in equation (2.3.15) and gets the expression

$$\frac{\lambda_l(\eta,k)}{u(2l+1)} = K_0(\eta) j_l(k(\eta-\eta_*))$$

where $K_0(\eta)$ is some function of cosmological parameters at the time of measurement, whose form is relevant for quantitative but not qualitative understanding of the result. This leads to

$$C_l(\eta) = K_1'\eta) \int_0^{\infty} \frac{1}{k} e^{i\vec{x}(\vec{k}-\vec{k}')} \delta(\vec{k}-\vec{k}') P_{\text{prim}}(k) j_l(k(\eta-\eta_*)) j_l^*(k'(\eta-\eta_*)) dk$$

$$= K_1(\eta) \int_0^{\infty} k^{n-2} |j_l(k(\eta-\eta_*))|^2 dk$$

$$= K_2(\eta) \frac{\Gamma(3-n)\Gamma(\frac{2l+n-1}{2})}{[\Gamma(\frac{4-n}{2})]^2 \Gamma(\frac{2l-n+5}{2})}$$

where $K_1(\eta)$ and $K_2(\eta)$ are again functions of time whose exact forms are irrelevant for the present qualitative treatment. (Indeed, in a quantitative treatment, this prefactor contains a free parameter that is fixed by measurement.) For $n = 1$ the result ist thus $l(l+1)C_l = K_3(\eta)$, which accounts for the so-called Sachs-Wolfe plateau for low l, i.e., large angles, in a plot of $l(l+1)C_l$ versus l.

3. Towards a Refinement of the LTE Condition on Curved Spacetimes

This chapter is devoted to pointing out some open questions connected to the extrinsic LTE condition. We will especially remark inconsistencies of the extrinsic LTE condition with native thermality conditions, i.e. the native (conformal) KMS condition, in two simple models. We will furthermore show that extrinsic $\mathcal{S}_4$ states for a massless field show a temperature behaviour which is very different from the temperature behaviour of an analogous classical ensemble. We will also illustrate, referring to a specific model, that the LTE condition is very difficult to check when a two-point function is explicitly given.

In the light of the described problems and open questions we will review the extrinsic LTE concept. Aiming to modify the LTE condition as little as possible, we argue that certain minimum requirements should be met in order to address the problems. An explicit modification of the LTE concept on curved spacetimes is put forward and discussed in the context of the problems. We will point out that the suggested modification still leaves open some problems and questions which seem to be solvable only with additional physical input. We will however illustrate the modified condition with a simple example to show how it can be applied to address at least some of the problems.

3.1. Non-Minimal Coupling

This section is devoted to the study of the simple model of scalar field in Einstein static spacetime $\mathbb{R} \times S^3$. Our investigation shows that the properties of KMS states on the Einstein static spacetime are fundamentally incompatible with the extrinsic LTE condition. Furthermore we argue that the coupling to curvature needs to be considered in the context of local thermal equilibrium on curved spacetimes, if the KMS states are interpreted as reasonable thermodynamic equilibrium states.

For our investigation we must derive the two-point function for maximally symmetric KMS states on the Einstein static spacetime. To achieve this we follow a generic recipe to derive KMS two-point functions. First we establish the commutator distribution on the Einstein static spacetime then we derive the KMS two-point function using Fourier transform in time direction and some functional analytic argument. Having determined the KMS two-point function we calculate balanced derivatives, where we regularise using the zero temperature KMS state. This means we determine the balanced derivatives up to a state independent, purely geometric term.

The special case $m = 0$ and $\xi = \frac{1}{6}$ of this model has been investigated in [46]. Only the first thermal observable was considered there. Our treatment will be somewhat different and more general than the one in [46]. We will also focus on different aspects of the model than said work.

3.1.1. Commutator Distribution

According to theorem 3.3.1 in [1] the advanced/retarded fundamental solutions to a wave equation on a globally hyperbolic manifold are the unique fundamental solutions with past/future compact support. This means that it suffices to check that a fundamental solution is supported only for $t > t'$ or $t < t'$ to show that it is the advanced/retarded solution. Due to [40] we know that advanced and retarded solutions can be constructed from a bidistribution E that weakly fulfils the following initial value problem

$$\begin{aligned}(\Box^x + m^2 - \xi R)E(t,x;t'x') &= 0 \qquad (3.1.1)\\ \delta(t,t')E(t,x;t'x') &= 0\\ \delta(t,t')\partial_t E(t,x;t'x') &= -i\delta(t,t')\delta(x,x')\end{aligned}$$

The solution to this initial value problem is thus the commutator distribution we are looking for.

Lemma 3.1.1.
Denoting $\omega_n = \sqrt{m^2 + n(n+2) + 6\xi}$ and $\Delta t = t - t'$ the bidistribution

$$\begin{aligned}E(t,\chi,\theta,\phi;t',\chi',\theta',\phi') = \sum_{n=0}^{\infty} \frac{1}{2\omega_n}\left(e^{-i\omega_n\Delta t} - e^{i\omega_n\Delta t}\right)\\ \sum_{l=0}^{n}\sum_{m=-l}^{l} Y_{nlm}(\chi,\theta,\phi)Y^*_{nlm}(\chi',\theta',\phi') \qquad (3.1.2)\end{aligned}$$

weakly fulfils the initial value problem (3.1.1).

Proof. The result from [24] ensures that we can interchange integration and infinite summation in this case, such that the smearing integrals of the test function can be moved into each summand which allows for partial integration.

To see that the E given above fulfils the Klein-Gordon equation, we use that

$$(-\triangle_{S^3} + m^2 + 6\xi)Y_{nlm}(\chi, \theta, \phi) = \omega_n^2 Y_{nlm}(\chi, \theta, \phi)$$

We then smear $\int E(t, \chi, \theta, \phi; t', \chi', \theta', \phi')(\Box^x + m^2 + 6\xi)f(t, \chi, \theta, \phi)dtd\Omega$, interchange integration and the summation over n and use partial integration to apply the derivatives on the summands. The boundary terms vanish for all summands, as f is compactly supported. It is obvious that the result vanishes.

For the initial conditions first note that

$$E_f(t, t', \chi, \theta, \phi) := \int E(t, \chi, \theta, \phi; t', \chi', \theta', \phi')f(t', \chi', \theta', \phi')d\Omega'$$

is a convergent series, as well as its termwise time derivative. This follows from the fact that for $n > 0$ and any Δt we have

$$\left|\frac{1}{2\omega_n}\left(e^{-i\omega_n\Delta t} - e^{i\omega_n\Delta t}\right)\right| \leq 1 \qquad \left|\frac{-i}{2}\left(e^{-i\omega_n\Delta t} + e^{i\omega_n\Delta t}\right)\right| \leq 1$$

and the completeness relation for the hyperspherical harmonics

$$\sum_{n=0}^{\infty}\sum_{l=0}^{n}\sum_{m=-l}^{l} Y^*_{nlm}(\chi, \theta, \phi)Y_{nlm}(\chi', \theta', \phi') = \delta_{S^3}(\chi, \theta, \phi; \chi', \theta', \phi')$$

This implies that by interchangeability of integration and summation E_f and its termwise time derivative are majorised by f. (To be precise, for some values of m and ξ the $n = 0$-Term has to be subtracted for this claim to be true. However as one is a finite number of terms, this poses no problem in the following argument.) This implies that the derivative of E_f is given by its termwise derivative. Given this, it is clear that E fulfils the first initial condition $\delta(t, t')E(t, x; t'x') = 0$ as this can easily be seen to hold termwise for E_f. For the second initial condition $\delta(t, t')\partial_t E(t, x; t'x') = -i\delta(t, t')\delta(x, x')$, calculation of termwise derivative of E_f and then termwise application of the delta distribution yields the desired equality $\int \delta(t, t')\partial_t E_f(t, t', \chi, \theta, \phi) = -if(t, \chi, \theta, \phi)$. □

Comparing the commutator distribution (3.1.2) to the Fourier transformed Minkowski commutator distribution, one sees that it is a straight forward adaption of the latter, where the expansion in plane waves has been substituted for an expansion in hyperspherical harmonics.

3.1.2. KMS Two-Point Function

To acquire the KMS two-point function from the commutation distribution we use a generic recipe which is generally applicable. The idea is to use the Fourier transform of the KMS condition for the two-point function. This leads to a distributional relation, which has to be treated with some care, but finally leads to an expression of the KMS two-point function in terms of the commutator distribution. We will briefly review the origin of the recipe before applying it to our case.

We begin by fixing our notation

$$g_\tau(t',\chi',\theta',\phi') :=g(t'-\tau,\chi',\theta',\phi')$$

$$F^\beta_{f,g}(\tau) :=\mathscr{W}^\beta_2(f,g_\tau)$$

$$G^\beta_{f,g}(\tau) :=\mathscr{W}^\beta_2(g_\tau,f)$$

$$E_{f,g}(\tau) :=E_{f,g_\tau}$$

which obviously implies $F^\beta_{f,g}(\tau)-G^\beta_{f,g}(\tau)=E_{f,g}(\tau)$. Fourier transforming this relation with respect to τ and using the KMS condition we get

$$\tilde{E}_{f,g}(\epsilon)=\tilde{F}^\beta_{f,g}(\epsilon)-(2\pi)^{-\frac{1}{2}}\int G^\beta_{f,g}(\tau)e^{-i\epsilon\tau}d\tau \tag{3.1.3}$$

$$=\tilde{F}^\beta_{f,g}(\epsilon)-(2\pi)^{-\frac{1}{2}}\int F^\beta_{f,g}(\tau+i\beta)e^{-i\epsilon\tau}d\tau$$

$$=\tilde{F}^\beta_{f,g}(\epsilon)-(2\pi)^{-\frac{1}{2}}\int F^\beta_{f,g}(\tau)e^{-i\epsilon\tau}e^{-\beta\epsilon}d\tau=(1-e^{-\beta\epsilon})\tilde{F}^\beta_{f,g}(\epsilon) \tag{3.1.4}$$

It should be noted that these Fourier transforms are in general distributions, even if the original expressions are smooth functions. The resulting relation (3.1.4) is thus to be understood in the sense of distributions and not straight forward to solve for $\tilde{F}^\beta_{f,g}(\epsilon)$. If however $\tilde{E}_{f,g}(\epsilon)$ is regular for a neighbourhood of $\epsilon=0$ one can explicitly give a solution using the principal value

$$\tilde{F}_{f,g}(h)=\left(\tilde{E}_{f,g}\mathrm{P}\frac{1}{1-e^{-\beta\cdot}}\right)(h)+(2\pi)^{\frac{1}{2}}c_{f,g}\delta(h)$$

where h is a test function and the ambiguity stems from the fact that $(1-e^{-\beta\epsilon})$ is of order ϵ^1 which annihilates the delta distribution. The full argument that the ambiguity is given only by this delta distribution is given in [5]. To see that the above expression is indeed a solution to (3.1.4), it remains to show that $(1-e^{-\beta\epsilon})$

is a multiplicator for it, which it is obviously by definition. Then we can apply the inverse Fourier transform to get the distribution

$$F_{f,g}(h') = \left((2\pi)^{-\frac{1}{2}} \int e^{i\epsilon\cdot} \tilde{E}_{f,g} \mathrm{P}\frac{1}{1-e^{-\beta\epsilon}} d\epsilon\right)(h') + c_{f,g}$$

where we assume the test function h' normalised for simplicity, such that $c_{f,g}$ does not get a prefactor. Next we need regularity of this distribution at $\tau = 0$, such that the limit

$$\mathscr{W}_2^\beta(f,g) = F_{f,g}(0)$$

is well defined. We will see that the two requirements are fulfilled in the case considered here.

Lemma 3.1.2.

- *$\tilde{E}_{f,g}(\epsilon)$ vanishes in a neighbourhood of $\epsilon = 0$, except for $m = \xi = 0$.*
- *$F_{f,g}(\tau)$ is regular at $\tau = 0$.*

The two-point function is

$$\mathscr{W}_2^\beta(f,g) = \int \sum_{n=0}^{\infty} \frac{1}{2\omega_n} \left(\frac{e^{-i\omega_n \Delta t}}{1-e^{-\beta\omega_n}} - \frac{e^{i\omega_n \Delta t}}{1-e^{\beta\omega_n}}\right) \sum_{l,m} f^*_{nlm}(t) g_{nlm}(t') dt dt' \\ (1-\delta_{\omega_n,0}) \tag{3.1.5}$$

Proof. Shifting the integration $t' \to t'' = t' - \tau$, we essentially get $\Delta t \to \Delta t - \tau$ in E. This yields

$$\tilde{E}_{f,g}(\epsilon) = \int e^{-i\epsilon\tau} \sum_{n=0}^{\infty} \frac{1}{2\omega_n (2\pi)^{\frac{1}{2}}} \left(e^{-i\omega_n(\Delta t - \tau)} - e^{i\omega_n(\Delta t-\tau)}\right) \sum_{l,m} f^*_{nlm}(t) g_{nlm}(t') d\tau dt dt'$$

$$= \int \sum_{n=0}^{\infty} \frac{(2\pi)^{\frac{1}{2}}}{2\omega_n} \left(e^{-i\omega_n\Delta t}\delta(\epsilon-\omega_n) - e^{i\omega_n \Delta t}\delta(\epsilon+\omega_n)\right) \sum_{l,m} f^*_{nlm}(t) g_{nlm}(t') dt dt'$$

which is obviously regular in a neighbourhood of $\epsilon = 0$ because $\forall n : \omega_n > 0$ as required for the explicit construction of the solution to (3.1.4). As it even vanishes for $\epsilon = 0$ the principal value can be ignored here and does not add complication.

We get

$$F_{f,g}(\tau) = \int \sum_{n=0}^{\infty} \frac{1}{2\omega_n} \left(\frac{e^{-i\omega_n(\Delta t-\tau)}}{1-e^{-\beta\omega_n}} - \frac{e^{i\omega_n(\Delta t-\tau)}}{1-e^{\beta\omega_n}}\right) \sum_{l,m} f^*_{nlm}(t) g_{nlm}(t') dt dt' + c_{f,g}$$

which inherits the property of regularity at $\tau = 0$ from the same property of $E_{f,g}(\tau)$, which can be seen by a straight forward majorant property.

This finally leads to the well defined two-point distribution

$$\mathscr{W}_2^\beta(f,g) = \int \sum_{n=0}^{\infty} \frac{1}{2\omega_n} \left(\frac{e^{-i\omega_n \Delta t}}{1 - e^{-\beta\omega_n}} - \frac{e^{i\omega_n \Delta t}}{1 - e^{\beta\omega_n}} \right) \sum_{l,m} f^*_{nlm}(t) g_{nlm}(t') dt dt' + c_{f,g}$$

However there is one special case which has to be considered, namely the case of $m = \xi = 0$. In this case the summand for $n = 0$ in the commutator distribution takes the form

$$E^0(x,x') = \lim_{n\to 0} \frac{1}{4\pi^2\omega_n} \left(e^{-i\omega_n \Delta t} - e^{i\omega_n \Delta t} \right) = \frac{-i\Delta t}{2\pi^2}$$

where $Y^2_{000} = \frac{1}{2\pi^2}$ was used. Now we use $\underline{f}(t) = \int d\mu_{S^3} f(t,\chi,\theta,\phi)$ and $\underline{h}(t) = \underline{f}(t) - \underline{g}(t)$, and without loss of generality we demand for simplicity $\int \underline{f}(t)dt = \int \underline{g}(t)dt = 1$. Then we get the smeared form

$$E^0_{f,g} = \frac{-i}{2\pi^2} \int \underline{h}(t) t dt$$

We also get $\int \underline{g}_\tau(t) t dt = \int \underline{g}(t) t dt + \tau$ which leads to

$$E^0_{f,g}(\tau) = \frac{-i}{2\pi^2} \left(\int \underline{h}(t) t dt - \tau \right)$$

$$\tilde{E}^0_{f,g}(\epsilon) = \frac{-i}{2\pi^2} \left(\delta(\epsilon) \int \underline{h}(t) t dt - i\delta'(\epsilon) \right)$$

which is obviously irregular at $\epsilon = 0$. We can however still solve (3.1.4) using a trick. We make the ansatz that $\tilde{F}^\beta_{f,g}(\epsilon)$ is a series, then we separate the summand $n = 0$ from the rest of the series on both sides of the relation and assume the relation to hold separately. The rest of the sum can then be treated as before and only the $n = 0$ term remains to be dealt with. The simple form of $\tilde{E}^0_{f,g}(\epsilon)$ allows for a straight forward ansatz for $\tilde{F}^{\beta,0}_{f,g}(\epsilon)$. The equation we have to fulfil in the distributional sense is

$$\tilde{F}^{\beta,0}_{f,g}[(1 - e^{-\beta\cdot})u] = \tilde{E}^0_{f,g}[u] = \frac{-i}{2\pi^2} \left(u(0) \int \underline{h}(t) t dt - iu'(0) \right)$$

which motivates the ansatz

$$\tilde{F}^{\beta,0}_{f,g}(\epsilon) = \sum_{k=0}^{\infty} a_k \delta^{(k)}(\epsilon)$$

A straight forward calculation yields

$$\tilde{F}^{\beta,0}_{f,g}(\epsilon) = c_{f,g}\delta(\epsilon) + \left(\frac{-i}{2\pi^2\beta}\int \underline{h}(t)tdt - \frac{1}{4\pi^2}\right)\delta'(\epsilon) - \frac{1}{4\pi^2\beta}\delta''(\epsilon)$$

$$F^{\beta,0}_{f,g}(\tau) = c_{f,g} + \left(\frac{1}{2\pi^2\beta}\int \underline{h}(t)tdt - i\frac{1}{4\pi^2}\right)\tau + \frac{1}{4\pi^2\beta}\tau^2$$

This term is regular for $\tau = 0$, such that we get a well defined two-point function. Thus, in the special case $m = \xi = 0$ we simply eliminate the summand for $n = 0$ from the two-point function.

Last we turn to the task of determining $c_{f,g}$. We follow the procedure described in [23]. This means we want our states to be extremal, meaning they shall not be expandable in other time translation invariant states. Thus they are primary and fulfil the weak cluster property (see [20]). As we also want the one point functions to vanish for simplicity, we are led to the following expression for the weak cluster property

$$\lim_{T\to\infty}\frac{1}{2T}\int\limits_{-T}^{T} F^{\beta}_{f,g}(\tau)d\tau = 0$$

Again these limits can be interchanged with the sum to get

$$\lim_{T\to\infty}\frac{1}{2T}\int\limits_{-T}^{T}\frac{1}{2\omega_n}\frac{e^{i\omega_n\tau}}{1-e^{-\beta\omega_n}}\sum_{l,m}\tilde{f}_{nlm}(\omega_n)\tilde{g}_{nlm}(-\omega_n)d\tau - (\omega_n \to -\omega_n) + c_{f,g}$$

$$= \lim_{T\to\infty}\frac{\sin(\omega_n T)}{2\omega_n^2 T}\frac{1}{1-e^{-\beta\omega_n}}\sum_{l,m}\tilde{f}_{nlm}(\omega_n)\tilde{g}_{nlm}(-\omega_n)d\tau - (\omega_n \to -\omega_n) + c_{f,g} = 0$$

which means that the condition is fulfilled if $c_{f,g} = 0$. This finally proves the claim. □

We want to give a simpler symbolic form of the two-point function, which will be of use when calculating the balanced derivatives. Consider $s = \arccos\left(\frac{XY}{\sqrt{X^2Y^2}}\right)$ for vectors in $\mathbb{R}^4$. The restriction of this function to S^3 will be denoted with s too and is the geodesic distance on the hypersphere. Using this, we get

$$\sum_{l=0}^{n}\sum_{m=-l}^{l} Y^*_{nlm}(\chi,\theta,\phi)Y_{nlm}(\chi',\theta',\phi') = \frac{n+1}{2\pi^2}U_n(\cos s) = \frac{n+1}{2\pi^2}\frac{\sin((n+1)s)}{\sin s}$$

where U_n are the Chebyshev polynomials of second kind. This yields the symbolic form

$$\mathscr{W}_2^\beta(x,x') = \sum_{n=0}^{\infty} \frac{n+1}{4\pi^2\omega_n}\left(\frac{2\cos(\omega_n\Delta t)}{e^{\beta\omega_n}-1} + e^{-i\omega_n\Delta t}\right)\frac{\sin((n+1)s)}{\sin s}(1-\delta_{\omega_n,0}) \quad (3.1.6)$$

3.1.3. Balanced Derivatives

Note that

$$\langle :\phi(x)\phi(x'):\rangle_\beta = \langle\phi(x)\phi(x')\rangle_\beta - \langle\phi(x)\phi(x')\rangle_\infty + \langle :\phi(x)\phi(x'):\rangle_\infty$$

We ignore the last term for now and only calculate $\theta_\beta(x,x') := \langle\phi(x)\phi(x')\rangle_\beta - \langle\phi(x)\phi(x')\rangle_\infty$. The last term is obviously independent on temperature and only yields a purely geometric contribution.

$$\theta_\beta(x,x') = \sum_{n=0}^{\infty}\frac{n+1}{2\pi^2\omega_n}\frac{\cos(\omega_n\Delta t)}{e^{\beta\omega_n}-1}\frac{\sin((n+1)s)}{\sin s}(1-\delta_{\omega_n,0})$$

This easily yields

$$\Theta = \theta_\beta(x,x) = \sum_{n=1}^{\infty}\frac{n^2}{2\pi^2\omega_{n-1}(e^{\beta\omega_{n-1}}-1)}(1-\delta_{\omega_{n-1},0}) \quad (3.1.7)$$

To get an understanding of Θ we will prove the following estimate.

Lemma 3.1.3.
Θ fulfils the following estimate

$$\Theta \le \frac{1}{2\pi^2(e^{\beta\omega_0}-1)}(1-\delta_{\omega_0,0}) - \frac{1}{\sqrt{3}\pi^2}e^{-\frac{\beta}{2}}$$
$$+\frac{1}{\sqrt{3}\pi^2}\left(\frac{2}{\beta^2}-\frac{1}{\beta}\right)e^{-\beta} + \frac{1}{\sqrt{3}\pi^2}\frac{1}{\cosh\left(\frac{\beta}{2}\right)-1} \quad (3.1.8)$$

Proof.
For $n > \frac{1}{\beta}+1$ and $\left[n \ge \frac{5}{4} \Rightarrow 2\sqrt{\frac{n+1}{n-1}} - \frac{n}{n-1} \ge 1\right]$ we have

$$e^{-\frac{\beta n}{2}}(e^{\beta\omega_{n-1}}-1) \ge e^{\frac{\beta}{2}\left(2\sqrt{n^2-1}-n\right)} - e^{-\frac{\beta n}{2}} \ge e^{\frac{\beta}{2}\left(2\sqrt{n^2-1}-n\right)} - e^{-\frac{\beta}{2}\left(2\sqrt{n^2-1}-n\right)}$$
$$= 2\sinh\left(\frac{\beta}{2}\left(2\sqrt{n^2-1}-n\right)\right) \ge \beta\left(2\sqrt{n^2-1}-n\right)$$
$$\ge 2\sqrt{\frac{n+1}{n-1}} - \frac{n}{n-1} \ge 1$$

and for $n \geq 2$ we have $\frac{n}{\omega_{n-1}} < \frac{2}{\sqrt{3}}$. This yields

$$\Theta = \sum_{n=1}^{\infty} \frac{n^2}{2\pi^2\omega_{n-1}(e^{\beta\omega_{n-1}} - 1)}(1 - \delta_{\omega_{n-1},0})$$

$$\leq \frac{1}{2\pi^2(e^{\beta\omega_0} - 1)}(1 - \delta_{\omega_0,0}) + \frac{1}{\sqrt{3}\pi^2} \sum_{n=2}^{\lfloor \frac{1}{\beta}+1 \rfloor} \frac{n}{(e^{\beta\omega_{n-1}} - 1)} + \frac{1}{\sqrt{3}\pi^2} \sum_{n=\lceil \frac{1}{\beta}+1 \rceil}^{\infty} \frac{n}{e^{\frac{\beta n}{2}}}$$

$$= \frac{1}{2\pi^2(e^{\beta\omega_0} - 1)}(1 - \delta_{\omega_0,0}) - \frac{1}{\sqrt{3}\pi^2} e^{-\frac{\beta}{2}}$$

$$+ \frac{1}{\sqrt{3}\pi^2} \sum_{n=2}^{\lfloor \frac{1}{\beta}+1 \rfloor} n \left(\frac{1}{e^{\beta\omega_{n-1}} - 1} - e^{-\frac{\beta n}{2}} \right) + \frac{1}{\sqrt{3}\pi^2} \frac{e^{-\frac{\beta}{2}}}{\left(1 - e^{-\frac{\beta}{2}}\right)^2}$$

where the last equality is due to the geometric series. To further simplify the remaining sum we note for $\frac{5}{4} \leq n \leq \frac{1}{\beta} + 1$

$$\frac{1}{e^{\beta\omega_{n-1}} - 1} \leq \frac{e^{-\frac{\beta n}{2}}}{\beta(n-1)}$$

$$n \left(\frac{1}{\beta(n-1)} - 1 \right) e^{-\frac{\beta n}{2}} \geq (n+1) \left(\frac{1}{\beta n} - 1 \right) e^{-\frac{\beta(n+1)}{2}}$$

To see that the latter inequality holds, note that

$$n \left(\frac{1}{\beta(n-1)} - 1 \right) e^{-\frac{\beta n}{2}} \geq (n+1) \left(\frac{1}{\beta(n)} - 1 \right) e^{-\frac{\beta(n+1)}{2}}$$

$$\Leftrightarrow \quad n^2 - \beta n^2(n-1) \geq \Big(n^2 - 1 - \beta n(n^2 - 1)\Big) e^{-\frac{\beta}{2}}$$

$$\Leftrightarrow \quad \beta n^2 - (\beta n - 1)n^2 \geq -(\beta n - 1)n^2 e^{-\frac{\beta}{2}} + (\beta n - 1)e^{-\frac{\beta}{2}}$$

$$\Leftrightarrow \quad \beta n^2 - (\beta n - 1)n^2(1 - e^{-\frac{\beta}{2}}) \geq (\beta n - 1)e^{-\frac{\beta}{2}}$$

$$\Leftarrow \quad \beta n^2 - \beta n^2(1 - e^{-\frac{\beta}{2}}) \geq \beta e^{-\frac{\beta}{2}}$$

$$\Leftrightarrow \quad n^2 \geq 1$$

This allows the estimate

$$\Theta \leq \frac{1}{2\pi^2(e^{\beta\omega_0}-1)}(1-\delta_{\omega_0,0}) - \frac{1}{\sqrt{3}\pi^2}e^{-\frac{\beta}{2}}$$

$$+\frac{1}{\sqrt{3}\pi^2}\left(\frac{2}{\beta^2}-\frac{1}{\beta}\right)e^{-\beta} + \frac{1}{\sqrt{3}\pi^2}\frac{1}{\cosh\left(\frac{\beta}{2}\right)-1}$$

□

Although this estimate is not straight forward to interpret it is obvious that the decay property for $\beta \to \infty$ is exponential, as all terms include exponentials of $-\beta$, in the last term disguised as cosh. One might have guessed this from formula (3.1.7) however it should be noted that our estimate does away with the infinite sum, leaving no doubt about the expressiveness of the result. This decay property is incompatible with the quadratic decay in the temperature observed for the Wick square in Minkowski spacetime. This illustrates that the extrinsic LTE temperature is incompatible with the KMS temperature on Einstein static spacetime.

Furthermore, we can investigate the $\beta \to 0$ asymptotics in the special case $m = 0$ and $\xi = \frac{1}{6}$. We calculate

$$\Theta = \sum_{n=1}^{\infty} \frac{n}{2\pi^2(e^{\beta n}-1)} = \frac{1}{2\pi^2}\sum_{n=1}^{\infty}\sum_{k=1}^{\infty} n e^{-\beta k n} = \frac{1}{4\pi^2}\sum_{k=1}^{\infty}\frac{1}{\cosh(\beta k)-1}$$

$$\to \frac{1}{2\pi^2}\sum_{k=1}^{\infty}\frac{1}{\beta^2 k^2} = \frac{1}{12\beta^2}$$

which shows that the high temperature asymptotics matches the behaviour for the massless field in Minkowski spacetime. Heuristically this can be understood in the sense that high temperatures correspond to short wavelengths and the geometry mainly influences long wavelengths as these probe larger patches of space.

In the general case one can see that the $\beta \to 0$ asymptotics are the same, by looking at the difference

$$\Theta_{\xi=\frac{1}{6}} - \Theta = \frac{1}{2\pi^2}\sum_{n=1}^{\infty}\left(\frac{n}{(e^{\beta n}-1)} - \frac{n^2}{\sqrt{n^2+a}(e^{\beta\sqrt{n^2+a}}-1)}\right)$$

$$\to \frac{1}{2\pi^2}\sum_{n=1}^{\infty}\left(\frac{1}{\beta} - \frac{n^2}{\beta(n^2+a)}\right) = \frac{1}{2\pi^2\beta}\sum_{n=2}^{\infty}\frac{a}{n^2+a}$$

where the sum converges for any $a = m^2 + 6\xi - 1$. Thus the difference is of lower order in β than the asymptotics of $\Theta_{\xi=\frac{1}{6}}$ which means that the asymptotics of the two quantities are the same.

Next we calculate the components of the thermal energy-momentum tensor for the KMS states on Einstein static spacetime. The 00-component is straight forward to calculate

$$\varepsilon_{00} = \sum_{n=1}^{\infty} \frac{n^2 \omega_{n-1}}{2\pi^2 (e^{\beta \omega_{n-1}} - 1)} (1 - \delta_{\omega_{n-1},0}) \tag{3.1.9}$$

To calculate ε_{ii} we can take different routes. The simplest is to set $\theta = \theta'$ and $\phi = \phi'$ such that $s = \Delta\chi$. We get

$$\varepsilon_{\chi\chi} = \sum_{n=1}^{\infty} \frac{n^2 (n^2 - 1)}{6\pi^2 \omega_{n-1} (e^{\beta \omega_{n-1}} - 1)} (1 - \delta_{\omega_{n-1},0}) \tag{3.1.10}$$

We will show by a calculation in normal coordinates that one can take $\varepsilon_{\chi\chi} = \varepsilon_{ii}$, i.e. the other components are given straight forwardly by multiplying $\varepsilon_{\chi\chi}$ with the appropriate angular functions to yield $-g_{ij}\varepsilon_{ij} = 3\varepsilon_{\chi\chi}$.

The angular dependence stems only from the terms $U_n(\hat{X}\hat{Y})$ where X and Y are vectors in an ambient $\mathbb{R}^4$. We will pick our coordinates such that the vector $\widehat{X+Y}$ is identified with the coordinates $\phi = 0$, $\theta = \chi = \frac{\pi}{2}$. Defining the auxiliary coordinates $\alpha_1 = \phi$, $\alpha_2 = \theta - \frac{\pi}{2}$ and $\alpha_3 = \chi - \frac{\pi}{2}$ we then get

$$\hat{X} = \begin{pmatrix} \cos\alpha_3 \cos\alpha_2 \cos\alpha_1 \\ \cos\alpha_3 \cos\alpha_2 \sin\alpha_1 \\ \cos\alpha_3 \sin\alpha_2 \\ \sin\alpha_3 \end{pmatrix} \qquad \hat{Y} = \begin{pmatrix} \cos\alpha_3 \cos\alpha_2 \cos\alpha_1 \\ -\cos\alpha_3 \cos\alpha_2 \sin\alpha_1 \\ -\cos\alpha_3 \sin\alpha_2 \\ -\sin\alpha_3 \end{pmatrix}$$

Denoting the normal coordinates by x we have

$$\begin{aligned} \alpha_1 &= x_1 + \mathcal{O}(x^4) \\ \alpha_2 &= x_2 - \frac{1}{6} x_1^2 x_2 + \mathcal{O}(x^4) \\ \alpha_3 &= x_3 - \frac{1}{6} x_1^2 x_3 - \frac{1}{6} x_2^2 x_3 + \mathcal{O}(x^4) \end{aligned}$$

and using the Taylor series of sin and cos we get

$$\hat{X}\hat{Y} = 1 - 2\vec{x}^2 + \frac{2}{3}(\vec{x}^2)^2 + \frac{4}{3}\Big(x_1^2 x_2^2 + x_1^2 x_3^2 + x_2^2 x_3^2\Big) + \mathcal{O}(x^5)$$

Now we use the series expansion of the Chebyshev polynomials

$$U_n(z) = \sum_{r=0}^{\lfloor \frac{n}{2} \rfloor} \begin{pmatrix} n+1 \\ 2r+1 \end{pmatrix} z^{n-2r} (z^2 - 1)^r$$

where we first note that $(\hat{X}\hat{Y})^2 - 1 = -4\vec{x}^2 + \mathcal{O}(x^3) = \mathcal{O}(x^2)$. This means that the index r provides an ordering by orders in x in our case. Thus it suffices to look at the first two terms

$$U_n(\hat{X}\hat{Y}) = (n+1)(1-2\vec{x}^2) + \frac{(n-1)n(n+1)}{6}(-4\vec{x}^2) + \mathcal{O}(x^3)$$

$$= n+1-\frac{2}{3}n(n+1)(n+2)\vec{x} + \mathcal{O}(x^3)$$

Now we get $\partial^2_{x_i} U_n(\hat{X}\hat{Y})\Big|_{x=0} = -4\frac{1}{3}n(n+1)(n+2)$ which leads to the same result as we calculated for $\varepsilon_{\chi\chi}$.

This finally yields

$$\mathrm{Tr}(\varepsilon) = \sum_{n=1}^{\infty} \frac{n^2(\omega_{n-1}^2 - (n^2-1))}{2\pi^2\omega_{n-1}(e^{\beta\omega_{n-1}}-1)}(1-\delta_{\omega_{n-1},0})$$

$$= \sum_{n=1}^{\infty} \frac{n^2(m^2+6\xi)}{2\pi^2\omega_{n-1}(e^{\beta\omega_{n-1}}-1)}(1-\delta_{\omega_{n-1},0})$$

$$= (m^2+6\xi)\Theta = (m^2-\xi R)\Theta \tag{3.1.11}$$

where the last sign is due to our sign convention of the curvature. This shows another incompatibility of the extrinsic LTE condition with the KMS condition on Einstein static spacetime. The extrinsic LTE condition would demand that the trace of the thermal energy-momentum tensor be independent on ξ, as is the case in Minkowski spacetime. Especially for $m = 0$ the trace would have to vanish for all ξ, which is not the case. This deviation goes beyond a mere difference in temperature definition and may be seen as indicative of a need for a modified definition of thermal observables. A modified thermal energy-momentum tensor has been proposed in [45], whose trace for KMS states on Einstein static spacetime has the same form as for KMS states on Minkowski spacetime for conformal coupling. Although this feature is not general, the modified thermal reference observables proposed in [45] are well motivated and yield interesting results for static spacetimes.

3.2. Conformally Static Spacetimes

In this section we will discuss the question, whether conformal KMS states of a conformally invariant free field on a conformally static spacetime should be considered thermal states and which implication this bears for the expectation values of thermal observables. We will introduce a model already discussed by [4] and specialise to the conformally invariant field to argue that conformally KMS states might indeed be interpreted as thermal with some caution. We will then calculate the expectation values of thermal observables on a general conformally flat spacetime and discuss some problems arising in this context.

We will also investigate the consequence of the extrinsic LTE condition on the dynamical equations of the thermal observables. The resulting equations lead to questionable results which are qualitatively radically different from the classical temperature behaviour. This problem can be remedied by adjusting the definition of thermal observables, as we will show. However, such an adjustment of thermal observables leads to a physical interpretation which is still very different from the classical case. We will therefore argue that from the point of view of the correspondence principle a modification of the extrinsic LTE concept is more desirable than a simple redefinition of thermal observables.

3.2.1. Conformal KMS States

In this chapter we will use the tools for conformal quantum field theories introduced earlier. To fix terminology we define

Definition 3.2.1.
Let ds^2 the line element of a static spacetime $(\mathcal{M}, g)$ and $\Omega : \mathcal{M} \to \mathbb{R}^+$ a smooth function called the conformal factor, then the spacetime $(\mathcal{M}, \tilde{g})$ with line element

$$\widetilde{ds}^2 = \Omega^2(x) ds^2$$

is called **conformally static**. If the spacetime $(\mathcal{M}, g)$ is Minkowski spacetime, the spacetime $(\mathcal{M}, \tilde{g})$ is called conformally flat.

Summarising lemmas 2.2. and 2.4. of [35] one can use

Lemma 3.2.2.
Let $(\mathcal{M}, g)$ and $(\mathcal{M}, \tilde{g})$ two spacetimes which are conformally related, i.e. $\widetilde{ds}^2 = \Omega^2(x) ds^2$ with $\Omega : \mathcal{M} \to \mathbb{R}^+$ a smooth function. This implies that the spacetimes are diffeomorphic to each other. Let C a locally covariant conformal quantum field theory, Q_C the corresponding locally covariant quantum field theory, S the locally contravariant state space of Gaussian Hadamard states corresponding to Q_C. Then the representatives S_g and $S_{\tilde{g}}$ are canonically isomorphic with

$$\widetilde{\mathscr{W}^{\omega}}(f, g) = \mathscr{W}^{\omega}(\Omega^3 f, \Omega^3 g) \quad \Leftrightarrow \quad \widetilde{\mathscr{W}^{\omega}}(x, x') = \Omega^{-1}(x)\Omega^{-1}(x')\mathscr{W}^{\omega}(x, x')$$

where the identification of f and g on the different spacetimes is done via conformal coordinates $\widetilde{ds}^2 = \Omega^2(x) ds^2$.

This lemma essentially implies that for any locally covariant conformal quantum field theory C the locally contravariant state space S of Gaussian Hadamard states corresponding to the locally covariant quantum field theory Q_C contained in C can be canonically extended to a locally contravariant conformal state space Z which contains S. Note that the relation between two-point functions also holds for non-Gaussian states, but additionally analogous relations have to hold for the other n-point functions. On the practical side the lemma provides a simple prescription to explicitly construct two-point functions for states of a conformal field theory on a conformally static spacetime. We will use this prescription in the following definition.

Definition 3.2.3. Let $(\mathcal{M}, g)$ be a static spacetime and $(\mathcal{M}, \widetilde{g})$ a conformally static spacetime with $\widetilde{ds}^2 = \Omega^2(x)ds^2$. Let C be a locally covariant conformal quantum field theory, Z its corresponding locally contravariant conformal state space of Gaussian Hadamard states. For the KMS state $\omega_\beta \in Z_g$ with two-point function $\mathscr{W}^\beta(f, g)$ we call $\widetilde{\omega}_\beta \in Z_{\widetilde{g}}$ defined by the two-point function

$$\widetilde{\mathscr{W}}^\beta(f, g) := \mathscr{W}^\beta(\Omega^3 f, \Omega^3 g) \quad \Leftrightarrow \quad \widetilde{\mathscr{W}}^\beta(x, x') := \Omega^{-1}(x)\Omega^{-1}(x')\mathscr{W}^\beta(x, x')$$

a **conformal KMS state**. In this case β will not be straight forwardly interpreted as the inverse temperature.

This definition can be straight forwardly extended to mixtures of conformal KMS states, where the conformal relation of n-point functions commutes with taking the mixture. This means that the mixture of conformal KMS states is related by conformal transformation to the corresponding mixture of the corresponding KMS states.

The model which serves us as motivation is a conformally flat Robertson-Walker spacetime that is flat in the asymptotic time-like future and past.

$$ds^2 = \left(\frac{1+\epsilon^2}{2} + \frac{1-\epsilon^2}{2}\tanh(\rho\eta)\right)\left(d\eta^2 - d\vec{x}^2\right)$$

This line element implies $a(\eta) \to \epsilon$ for $\eta \to -\infty$ and $a(\eta) \to 1$ for $\eta \to \infty$. On this spacetime we consider a conformally coupled scalar quantum field

$$\left(\Box + m^2 - \frac{1}{6}R\right)\phi = 0$$

where we can make a mode decomposition in spatial direction and rescale the field modes $\chi_p(\eta) = a(\eta)\phi_p(\eta)$ to get the equation

$$\chi_p'' + (p^2 + m^2a^2)\chi_p = 0$$

Thus in the massless case which will concern us here, we get a generic harmonic oscillator equation for the modes χ_p. This means that the modes of the field ϕ are simply scaled with a^{-1}.

As the asymptotic initial state we choose a KMS state with the two-point function

$$\mathscr{W}_2^\beta(x,y) = \frac{1}{\epsilon^2}\int \frac{1}{(2\pi)^3 2p}\left(\frac{e^{-i(x^0-y^0)p}}{1-e^{-\beta p}} - \frac{e^{i(x^0-y^0)p}}{1-e^{\beta p}}\right) e^{i(\vec{x}-\vec{y})\vec{p}} d^3p$$

The KMS inverse temperature is $\epsilon\beta$, as can be seen by rescaling $p = \epsilon q$ and $x = \frac{x'}{\epsilon}$. The inverse temperature $\epsilon\beta$ is also what is measured by the LTE observables as is best seen in rescaled coordinates. As the field is conformally invariant, the two-point function of the state corresponding to the above given KMS initial state is

$$\mathscr{W}_2^\beta(x,y) = \frac{1}{a(x^0)a(y^0)}\int \frac{1}{(2\pi)^3 2p}\left(\frac{e^{-i(x^0-y^0)p}}{1-e^{-\beta p}} - \frac{e^{i(x^0-y^0)p}}{1-e^{\beta p}}\right) e^{i(\vec{x}-\vec{y})\vec{p}} d^3p$$

which is the two-point function of a conformal KMS state. This means that the asymptotic final state is also a KMS state with two-point function

$$\mathscr{W}_2^\beta(x,y) = \int \frac{1}{(2\pi)^3 2p}\left(\frac{e^{-i(x^0-y^0)p}}{1-e^{-\beta p}} - \frac{e^{i(x^0-y^0)p}}{1-e^{\beta p}}\right) e^{i(\vec{x}-\vec{y})\vec{p}} d^3p$$

corresponding to the KMS inverse temperature β. This means the temperature is redshifted with a as is the case for a classical fluid of massless particles. Ignoring the intermediate state, the initial and final states of this model reproduce exactly the behaviour that would classically be expected for a fluid in thermodynamic equilibrium. The temperature evolution in the intermediary region is identical to the behaviour of a classical ideal gas of massless particles in an initial state of equilibrium in an expanding spacetime. One could therefore expect that the state should be interpreted as thermal all along.

If one deforms the spacetime to be some general Robertson-Walker spacetime in the future, propagates the state to this region and then also deform the past arbitrarily, one gets a conformal KMS state on a general Robertson-Walker spacetime. This procedure could even be extended to arbitrary conformally flat spacetimes and the resulting state will always correspond to a conformal KMS state. One could therefore argue that in general conformal KMS states for the conformally invariant field on conformally flat (or more generally, conformally static) spacetime may be considered thermal states.

Indeed the temperature measured by the local thermal observables in conformal KMS states conforms with the correspondence principle, as for large temperature, i.e. small $a(t)\beta$, the curvature terms can be neglected. Thus a simple redshift, the temperature behaviour for a classical fluid, is recovered in the semiclassical limit, as long as it is justified.

We will now calculate a trace relation for the first two thermal observables as we have done in the case of the Einstein static spacetime. In the following we will denote quantities for the static spacetime as usual and respective quantities for the corresponding conformally flat spacetimes with tildes. For the Ricci tensor and scalar the following relations hold

$$\widetilde{R}_{\mu\nu} = R_{\mu\nu} + \frac{1}{\Omega}\Big(- 2\nabla_\mu\partial_\nu\Omega - g_{\mu\nu}g^{\alpha\beta}\nabla_\alpha\partial_\beta\Omega\Big) + \frac{1}{\Omega^2}\Big(4\partial_\mu\Omega\partial_\nu\Omega - g_{\mu\nu}g^{\alpha\beta}\partial_\alpha\Omega\partial_\beta\Omega\Big)$$

$$\widetilde{R} = \frac{1}{\Omega^2}\Big(R - 6\frac{\Box\Omega}{\Omega}\Big)$$

Considering the case of conformally coupled massless field, the two-point functions of conformal KMS states are related to two-point functions of KMS states on the static spacetime by

$$\widetilde{\mathscr{W}}_2^\beta(x,y) = \frac{1}{\Omega(x)\Omega(y)}\mathscr{W}_2^\beta(x,y)$$

using conformal coordinates. However the label β should in the case of the conformally static spacetime not be interpreted as the physical inverse temperature. Inserting a constant conformal factor or calculating Θ rather suggests $\Omega(x)\beta$, possibly modified by a geometric term, to be the physical inverse temperature. We define Θ and ε via the difference $\widetilde{\theta}(x,y) := \widetilde{\mathscr{W}}_2^\beta(x,y) - \widetilde{\mathscr{W}}_2^\infty(x,y)$ as in the Einstein static case, so we again ignore the curvature term for the time being as its explicit form has little relevance for now.

Lemma 3.2.4.
The trace of the thermal energy-momentum tensor for a conformal KMS state on a conformally static spacetime is

$$\tilde{\varepsilon}^\mu_\mu = \frac{1}{\Omega^4}\left(\varepsilon^\mu_\mu + \frac{1}{2}\Big(\frac{\Box\Omega}{\Omega} + g^{\mu\nu}\frac{\partial_\mu\Omega\partial_\nu\Omega}{\Omega^2}\Big)\Theta\right) \tag{3.2.1}$$

Proof.
We start with the definition of the trace of the thermal energy momentum tensor

$$\begin{aligned}\tilde{\varepsilon}^\mu_\mu(x,y) &:= -\frac{1}{4}(\widetilde{\nabla}^x - \widetilde{\nabla}^y)_\mu(\widetilde{\nabla}^x - \widetilde{\nabla}^y)^\mu\widetilde{\theta}(x,y)\\ &= \frac{1}{2}\Big(- \widetilde{\Box}^x + \tilde{g}^{\mu\nu}\partial^x_\mu\partial^y_\nu\Big)\Big(\frac{1}{\Omega(x)\Omega(y)}\theta(x,y)\Big)\end{aligned}$$

then we calculate

$$\widetilde{\Box}^x\Big(\frac{1}{\Omega(x)}\theta(x,y)\Big) = \frac{1}{\Omega^4(x)\sqrt{|g|}}\partial^x_\mu\Big(\Omega^2(x)g^{\mu\nu}\sqrt{|g|}\partial^x_\nu\Big(\frac{1}{\Omega(x)}\theta(x,y)\Big)\Big)$$

$$= \frac{1}{\Omega^4(x)\sqrt{|g|}}\partial^x_\mu\Big(g^{\mu\nu}\sqrt{|g|}\big(\Omega(x)\partial^x_\nu\theta(x,y) - (\partial^x_\nu\Omega(x))\theta(x,y)\big)\Big)$$

$$= \frac{1}{\Omega^4(x)}\big(\Omega(x)\Box^x\theta(x,y) - (\Box^x\Omega(x))\theta(x,y)\big)$$

This leads to

$$\tilde{\varepsilon}^\mu_\mu(x,y) = \frac{1}{2\Omega^4(x)\Omega^2(y)}\Big(\Omega(y)\Big(- \Omega(x)\Box^x\theta(x,y) + (\Box^x\Omega(x))\theta(x,y)$$

$$+ g^{\mu\nu}\Big(\Omega(x)\partial^x_\mu\partial^y_\nu\theta(x,y) - (\partial^x_\mu\Omega(x))\partial^y_\nu\theta(x,y)\Big)\Big)$$

$$+ g^{\mu\nu}\Big(- \Omega(x)(\partial^y_\mu\Omega(y))\partial^x_\nu\theta(x,y) + (\partial^x_\mu\Omega(x))(\partial^y_\nu\Omega(y))\theta(x,y)\Big)\Big)$$

and thus we get in the limit $x = y$

$$\tilde{\varepsilon}^\mu_\mu = \frac{1}{2\Omega^4}\Big(- \Box^x + g^{\mu\nu}\partial^x_\mu\partial^y_\nu + \frac{\Box\Omega}{\Omega} + g^{\mu\nu}\frac{\partial_\mu\Omega\partial_\nu\Omega}{\Omega^2} - g^{\mu\nu}\frac{\partial_\mu\Omega}{\Omega}(\partial^x_\nu + \partial^y_\nu)\Big)\theta(x,y)\Big|_{x=y}$$

Now we can use $\varepsilon^\mu_\mu = \frac{1}{2}(-\Box^x + g^{\mu\nu}\partial^x_\mu\partial^y_\nu)\theta(x,y)\Big|_{x=y}$ and $(\partial^x_\nu + \partial^y_\nu)\theta(x,y)\Big|_{x=y} = 0$ where the latter follows from the canonical commutation relations at equal times. This finally yields the result

$$\tilde{\varepsilon}^\mu_\mu = \frac{1}{\Omega^4}\Big(\varepsilon^\mu_\mu + \frac{1}{2}\Big(\frac{\Box\Omega}{\Omega} + g^{\mu\nu}\frac{\partial_\mu\Omega\partial_\nu\Omega}{\Omega^2}\Big)\Theta\Big)$$

□

In the case of conformally flat spacetimes we get the simple expression

$$\tilde{\varepsilon}^\mu_\mu = \frac{1}{2\Omega^2}\Big(- \frac{1}{6}\tilde{R} + g^{\mu\nu}\frac{\partial_\mu\Omega\partial_\nu\Omega}{\Omega^4}\Big)\Theta \qquad (3.2.2)$$

which is obviously incompatible with the requirements of the external LTE condition. This means, analogously to the Einstein static case, that the LTE condition is in general incompatible with the conformal KMS condition. In this case the incompatibility persists, if we choose the modified reference observables proposed by [45]. As before, the question which concept of thermality is physically more viable has to be addressed. This will be done in the rest of the section.

The trace relation is also in general different from the result acquired for KMS states in the Einstein static spacetime. If we interpret conformal KMS states as reasonable thermal states for conformal quantum field theories on conformally flat spacetimes, this leads to the conclusion that, even ignoring the geometric terms, a general expression for the trace of ε in terms of Θ is not straight forward for thermal states. This will be of importance later, when we discuss a modified approach to local thermal equilibrium states on curved spacetimes.

3.2.2. Extrinsic LTE in de Sitter Spacetime

Considering the special case of a massless field with arbitrary coupling to curvature on de Sitter spacetime we can highlight another difficulty of the extrinsic LTE concept. In the following we will not consider conformal KMS states, but take the extrinsic LTE condition for granted and consider a space of thermal observables containing $\mathcal{S}_4$. In this case the de Sitter equivalent of equation (2.2.9) simplifies for the two balanced derivatives of lowest order.

As we are dealing in the following with balanced derivatives of order 4, it is important to point out that the extrinsic LTE concept is not straight forwardly applicable in the case of higher orders of derivative than 2. This is due to the fact that on a curved spacetime the resulting tensor fields are not symmetric in the tensor indices, as they are on Minkowski spacetime. Therefore the expectation values cannot be equated without additional input. We will for simplicity assume the balanced derivatives straight forwardly symmetrised for the following consideration.

To derive the generalised forms of the equations (2.2.6)-(2.2.9) we have to find a suitable definition for the point split quantities $\theta_{g,\boldsymbol{\mu}}(x+\zeta, x-\zeta)$. However, it is not a priori clear what $x+\zeta$ should mean, as it was in flat spacetime. To avoid referring to normal coordinates we will thus slightly modify the treatment that was done for flat spacetimes. We therefore note

$$\partial^z_\nu f(z+\zeta, z-\zeta) = \Big((\partial^x_\nu + \partial^y_\nu) f(x,y)\Big)|_{x=z+\zeta, y=z-\zeta}$$

$$\partial^\zeta_\nu f(z+\zeta, z-\zeta) = \Big((\partial^x_\nu - \partial^y_\nu) f(x,y)\Big)|_{x=z+\zeta, y=z-\zeta}$$

in flat spacetimes. This reformulation allows a translation of equations (2.2.6)-(2.2.9) into a more general form. In the following we use abbreviations

$$\nabla^{\pm}_{\mu} := \nabla^{x}_{\mu} \pm \nabla^{y}_{\mu} \qquad \Box^{\pm} := g^{\mu\nu}\nabla^{\pm}_{\mu}\nabla^{\pm}_{\nu}$$

The curvature terms stemming from the Hadamard parametrix will be denoted by $C^{x}_{\boldsymbol{\mu}}(x,y) := P^{x}_{m,\xi}\nabla_{\boldsymbol{\mu}}\theta_g(x,y)$, $C_{\boldsymbol{\mu}}(x) := C^{x}_{\boldsymbol{\mu}}(x,y)|_{x=y} = C^{y}_{\boldsymbol{\mu}}(x,y)|_{x=y}$. In the de Sitter model we investigate, these curvature terms have no coordinate dependence which simplifies the calculations a lot. The equations for the Wick square are

$$g^{\mu\nu}\nabla^{+}_{\mu}\nabla^{-}_{\nu}\theta_g(x,y) = 0 \tag{3.2.3}$$

$$\Rightarrow g^{\mu\nu}\nabla_{\mu}\omega\left(\theta_{g,\nu}\right)(x) = 0 \tag{3.2.4}$$

$$(\Box^{+} + \Box^{-})\theta_g(x,y) = -4(m^2 - \xi R)\theta_g(x,y) + 4C \tag{3.2.5}$$

$$\Rightarrow \Box\,\omega\left(\theta_g\right)(x) = -\omega\left(\theta_{g,}{}^{\nu}{}_{\nu}\right)(x) - 4(m^2 - \xi R)\omega\left(\theta_g\right)(x) + 4C \tag{3.2.6}$$

Obviously a generalisation of these equations to higher order thermal observables is not straight forward, as the derivatives do not commute. Equations (3.2.3) and (3.2.4) can be generalised to non-symmetrised thermal observables, as they are symmetric in x and y and $g^{\mu\nu}\nabla^{+}_{\mu}\nabla^{-}_{\nu} = \Box^{x} - \Box^{y}$ such that the geometric terms that are produced by interchange of derivatives cancel out. However a version using only symmetrised thermal observables is less straight forward to give. Things are even worse for equations (3.2.5) and (3.2.6) in the general case, ever more so if symmetrisation is required. In the de Sitter model the fact that R and C are constant greatly simplifies the treatment.

Due to these difficulties, we will not give a general version of these equations for symmetrised thermal observables here but rather restrict to the scenario we are interested in, which requires only the calculation of the equations for the second order thermal observable, which however implies a trace of the fourth order thermal observable. This means we have to calculate the effect of symmetrisation. We define the symmetrised thermal observables as

$$\theta_{g,\boldsymbol{\nu}}(x,y) := \nabla^{-}_{(\boldsymbol{\nu})} :\phi^2_g:_k (x,y). \tag{3.2.7}$$

where the brackets indicate symmetrisation.

We collect some calculational tools that will be needed in the following

Lemma 3.2.5.
The following relations hold

(a) *Elementary relations*

$$[\nabla^-_\alpha, \nabla^+_\beta] = [\nabla^x_\alpha, \nabla^x_\beta] - [\nabla^y_\alpha, \nabla^y_\beta]$$

$$[\nabla^-_\alpha, \nabla^-_\beta] = [\nabla^x_\alpha, \nabla^x_\beta] + [\nabla^y_\alpha, \nabla^y_\beta]$$

(b) *Relations relevant for generalisation of equations (3.2.3) and (3.2.4)*

$$\nabla^+_\lambda [\nabla^-_\rho, \nabla^-_\mu] \nabla^-_\nu \theta(x,y)|_{x=y} = R^\alpha{}_{\nu\mu\rho} \nabla_\lambda \theta_\alpha$$

$$\nabla^-_\mu [\nabla^+_\lambda, \nabla^-_\nu] \nabla^-_\rho \theta(x,y)|_{x=y} = R^\alpha{}_{\rho\nu\lambda} \nabla_\alpha \theta_\mu$$

$$[\nabla^+_\lambda, \nabla^-_\mu] \nabla^-_\nu \nabla^-_\rho \theta(x,y)|_{x=y} = R^\alpha{}_{\nu\mu\lambda} \nabla_\alpha \theta_\rho + R^\alpha{}_{\rho\mu\lambda} \nabla_\alpha \theta_\nu$$

(c) *Relations relevant for generalisation of equations (3.2.5) and (3.2.6)*

$$\nabla^+_\lambda [\nabla^+_\rho, \nabla^-_\mu] \nabla^-_\nu \theta(x,y)|_{x=y} = R^\alpha{}_{\nu\mu\rho} \nabla_\lambda \nabla_\alpha \theta + (\nabla_\lambda R^\alpha{}_{\nu\mu\rho}) \nabla_\alpha \theta$$

$$\nabla^-_\mu [\nabla^+_\lambda, \nabla^-_\nu] \nabla^+_\rho \theta(x,y)|_{x=y} = R^\alpha{}_{\rho\nu\lambda} \theta_{\mu\alpha} + (\nabla_\mu R^\alpha{}_{\rho\nu\lambda}) \nabla_\alpha \theta$$

$$\nabla^-_\lambda [\nabla^-_\rho, \nabla^-_\mu] \nabla^-_\nu \theta(x,y)|_{x=y} = R^\alpha{}_{\nu\mu\rho} \theta_{\lambda\alpha} + (\nabla_\lambda R^\alpha{}_{\nu\mu\rho}) \nabla_\alpha \theta$$

$$[\nabla^+_\lambda, \nabla^-_\mu] \nabla^-_\nu \nabla^+_\rho \theta(x,y)|_{x=y} = R^\alpha{}_{\nu\mu\lambda} \nabla_\alpha \nabla_\rho \theta + R^\alpha{}_{\rho\mu\lambda} \theta_{\nu\alpha}$$

$$[\nabla^-_\lambda, \nabla^-_\mu] \nabla^-_\nu \nabla^-_\rho \theta(x,y)|_{x=y} = R^\alpha{}_{\nu\mu\lambda} \theta_{\alpha\rho} + R^\alpha{}_{\rho\mu\lambda} \theta_{\nu\alpha}$$

Proof.
All relations are shown by straight forward calculation in appendix A.1. □

Now we derive the dynamical equations, using the above formulae.

Lemma 3.2.6.
The dynamical equations for $\theta_{\mu\nu}$ and $\theta_{\mu\nu\lambda}$ are

$$\nabla_\lambda \theta^\lambda_{\mu\nu} = 0 \tag{3.2.8}$$

$$\Box\theta_{\mu\nu} + \Big(\frac{32}{3} + 48\xi\Big) H^2 \theta_{\mu\nu} = -\theta^\lambda_{\lambda\mu\nu} + \frac{2}{3} H^2 g_{\mu\nu} \theta^\lambda_\lambda + 2H^2 \Big(g_{\mu\nu}\Box - \nabla_\mu \nabla_\nu\Big)\theta + 4C_{\mu\nu} \tag{3.2.9}$$

Proof.
The proof is done by straight forward application of the relations from lemma 3.2.5. The calculations can be found in appendix A.2. □

The physical meaning of equations (3.2.3) and (3.2.8) is not straight forward in the de Sitter case. In the case of the free massless field in Minkowski spacetime the implication of this type of equation was demonstrated in [12] to be straight forward, as the balanced derivatives ∇^{-} can be understood in the sense of derivatives of the macroobservables with respect to the inverse temperature β.

Using an appropriate extended set of thermal observables a similar result was found by [23] for the massive field. In this case the argument was more indirect however, as the balanced derivatives do not directly translate into derivatives of macroobservables with respect to β, but these derivatives of macroobservables were themselves found to be macroobservables contained in the extended set of thermal observables. This in turn allowed to simply pick suitable allowed macroobservables to extract physical meaning, completely prescinding from the balanced derivatives used to construct the space of observables.

A treatment analogous to the massive case would be desirable in the case of LTE on curved spacetimes in general and on de Sitter spacetime especially. However, the extrinsic LTE concept can only offer carrying over the framework from Minkowski spacetime to general spacetimes. Still it is not reasonably clear, whether a straight forward simultaneous extension of the microobservable and macroobservable interpretations from Minkowski spacetime to curved spacetimes in the spirit of the extrinsic LTE condition is possible. This will be explored later in this subsection.

Next we investigate the implications of equations (3.2.5) and (3.2.9) in the extrinsic LTE framework. First we note that using the extrinsic LTE concept, the traces $\Theta^{\lambda}_{\lambda}$ and $\Theta^{\lambda}_{\lambda\mu\nu}$ vanish, as they do for the massless field in Minkowski spacetime. Furthermore we want to restrict to spatially homogeneous isotropic states, which implies that the thermal observables will only be dependent on time and not on space. The following consideration will be simplified by picking coordinates with comoving time, such that

$$ds^2 = dt^2 - e^{2Ht} d\vec{x}^2.$$

As we are interested in the 00-component of $\Theta_{\mu\nu}$, we are left with the equations

$$\ddot{\Theta} + 3H\dot{\Theta} + 48\xi H^2 \Theta = 4C \tag{3.2.10}$$

$$\ddot{\Theta}_{00} + 3H\dot{\Theta}_{00} + \left(\frac{32}{3} + 48\xi\right) H^2 \Theta_{00} = 6H^3\dot{\Theta} + 4C_{00} \tag{3.2.11}$$

Defining the numbers $\alpha_\pm = \frac{3}{2} \pm \sqrt{\frac{9}{4} - 48\xi}$ we get the solution to equation (3.2.10) as

$$\Theta = A_+ e^{-\alpha_+ Ht} + A_- e^{-\alpha_- Ht} + \frac{C}{3H} t\delta_{\xi,0} + \frac{C}{12\xi H^2}(1 - \delta_{\xi,0}) \tag{3.2.12}$$

This obviously leads to an oscillatory solution for $\xi > \frac{3}{64}$. Thus, depending on the relation between C and $A_\pm$, negative values for the squared temperature are possible, which is not physically sensible. In these unphysical cases, extrinsic local thermal equilibrium is unstable, as a state initially in extrinsic LTE will after a finite time exhibit physically unacceptable temperature behaviour. This "life time" of LTE is dependent on temperature, as the prefactors $A_\pm$ may be temperature dependent. If one fixes $A_\pm$ through an initial condition on the temperature and considers the comparison to $\Theta \propto T^2$, which holds for Minkowski spacetime, this suggests that $A_\pm$ will be larger for large temperatures, such that the life time of LTE is shorter.

It should be noted that finite life time of LTE can occur for conformal coupling $\xi = \frac{1}{6}$. In fact, $C = \frac{3}{4\pi^2}\left((1-6\xi)^2 - \frac{1}{30}\right)H^4$, which is negative for the conformally coupled field, such that the life time of LTE is limited for any temperature in this case.

Now we turn to the solution of equation (3.2.11). Defining $\gamma_\pm = \frac{3}{2} \pm i\sqrt{\frac{101}{12} + 48\xi}$ we get the general solution

$$\begin{aligned}\Theta_{00} = {} & A_{00,+}e^{-\gamma_+ Ht} + A_{00,-}e^{-\gamma_- Ht} - \frac{9}{16}H^2\alpha_+ A_+ e^{-\alpha_+ Ht} - \frac{9}{16}H^2\alpha_- A_- e^{-\alpha_- Ht} \\ & + \frac{3C}{H^3(16+72\xi)}\delta_{\xi,0} + \frac{3C_{00}}{(8+36\xi)H^2}\end{aligned} \tag{3.2.13}$$

Again there is a wide range of parameters within which this result is oscillatory and also a wide range where the life time of LTE is finite.

However, taking the two results together, an additional obstacle for the extrinsic LTE condition becomes apparent. As shown in equation (2.2.17) a necessary condition for Minkowski KMS states for the massless field and thus also for extrinsic LTE states is

$$(12\Theta)^2 \leq -\frac{120}{\pi^2}\Theta_{00}$$

Of the exponents $\alpha_\pm$ and $\gamma_\pm$ the one with the largest real part is α_+, such that the exponential $e^{-\alpha_+ Ht}$ dominates for small t, whereas the constant terms dominate for large t. Thus for small t

$$\Theta^2 \to A_+^2 e^{-2\alpha_+ Ht} \qquad\qquad -\Theta_{00} \to \frac{9}{16}H^2\alpha_+ A_+ e^{-\alpha_+ Ht}$$

This means, as long as A_+ is nonzero, the inequality will always be violated for some suitably small t.

If we define $\gamma = \sqrt{\frac{101}{12} + 48\xi}$, denote the constant and linear term of Θ by $B(t)$, the constant term of $-\frac{5}{6\pi^2}\Theta_{00}$ by $\hat{B}$ and $-\frac{5}{6\pi^2}A_{00,\pm} =: \hat{A}_\pm$ this inequality for the case $A_+ = 0$ is

$$A_-^2 e^{-2\alpha_- Ht} + 2A_- B(t) e^{-\alpha_- Ht} + B^2(t) \leq (\hat{A}_+ e^{-i\gamma Ht} + \hat{A}_- e^{i\gamma Ht}) e^{-\frac{3}{2}Ht} + \frac{15}{32\pi^2} H^2 \alpha_- A_- e^{-\alpha_- Ht} + \hat{B}$$

A necessary condition for this to hold true for all times is that $\alpha_- = \frac{3}{4}$ which is equivalent to $\xi = \frac{9}{256}$, a value for the coupling to curvature which has no precedent. Still the oscillatory prefactor on the right hand side, which will periodically be negative, even if it is chosen to be real cannot be accounted for on the left hand side by any real choice of A_-. Thus it is impossible to fulfil the inequality for all t.

This means that in general the inequality can at most be fulfilled in the future of a Cauchy surface, where equality holds on the Cauchy surface and the two sides of the inequality become ever more unequal later. As the geometric terms are negative for some choices of ξ, Θ will become negative at some time for these cases, which means that it will only be an extrinsic LTE state for a finite time span. This result is very remote from the classical picture, where essentially a redshift would be expected. Although particle production effects are to be expected, the behaviour seen here goes considerably beyond a small perturbation. One should also note that, while the finding of instability under time evolution remains, the quantitative result changes if Θ_0^0 or even Θ^{00} is considered instead of Θ_{00}. This calls into question the standard extrinsic LTE condition and suggests at least a careful choice of thermal observables to compare. One may for instance expect that only observables with as many upper as lower tensor indices should be compared as then the effect of the metric should cancel out.

Last it will be illustrated that a straight forward simultaneous extension of the microobservable and macroobservable interpretations from Minkowski spacetime to curved spacetimes in the spirit of the extrinsic LTE condition is not possible. To show this, equation (3.2.3) for de Sitter spacetime will be treated using a straight forward extension of the macroobservable interpretation from Minkowski spacetime. This point of view simply leads to the equation

$$\nabla_\mu \left(\partial_\beta^\mu \frac{1}{\underline{\beta}^2} \right)(x) = 0 \tag{3.2.14}$$

if we assume a "pure temperature" state for simplicity.

Using $\Gamma^{\mu}_{\mu\nu} = 3H\delta^{0}_{\nu}$, assuming homogeneity and isotropy, i.e. $\underline{\beta}(x) = \underline{\beta}(t)$ and restricting to the simple case $\vec{\beta} = \vec{0}$ we get the simple equation

$$\dot{\beta}_0 - H\beta_0 = 0 \quad \Rightarrow \quad \beta_0(t) = \beta_0(0)e^{Ht}$$

This equation implies $T \propto a^{-1}$, a simple redshift, compatible with the correspondence principle. However this result is in general not compatible with

$$\Theta = \frac{1}{\beta_0^2} = A_+e^{-\alpha_+Ht} + A_-e^{-\alpha_-Ht} + \frac{C}{3H}t\delta_{\xi,0} + \frac{C}{12\xi H^2}$$

which is the solution to equation (3.2.5). These equations were derived on the level of microobservables, i.e. local quantum observables, however their interpretation in the framework of extrinsic LTE amounts to straight forwardly extend the macroobservable interpretation from certain microobservables in Minkowski spacetime to corresponding locally covariant microobservables in curved spacetime. This extension of the macroobservable interpretation leads to inconsistencies even in the simple model of a massless scalar field in de Sitter spacetime.

One way to try and overcome these inconsistencies is to adjust the definition of the thermal observables in de Sitter spacetime, as indicated in (2.2.4). However, a comparison to the difference between the cases of massive and massless fields on Minkowski spacetime may lead one to the expectation that such simple adjustments are not sufficient, but instead one would have to turn to suitable extended spaces of thermal observables, which include macroobservables that are suitable functions of $\underline{\beta}$. As in the case of the massive field in Minkowski spacetime it is then not at all clear which series of balanced derivatives approximates the function one is interested in. Also identifying the meaningful physical quantities, like thermodynamic state variables, as functions of $\underline{\beta}$ and even more as series of balanced derivatives is not straight forward.

Under any circumstances the extrinsic LTE concept seems to be inconsistent, as equation (3.2.14) allows for a solution which exhibits exactly the temperature behaviour of a classical radiation fluid in an expanding universe, while equation (3.2.5) yields a solution, which is much less straight forward. However, in light of the above considerations about extended sets of observables, one could expect an equation like

$$\nabla_\mu \left(\partial^\mu_\beta \Theta\right)(x) = 0 \tag{3.2.15}$$

to hold on an extended set of macroobservables Θ, which includes the macroobservable $\frac{1}{\underline{\beta}^2}$, such that indeed a classical-like behaviour would be physically realised in quantum field theory.

An investigation of suitable extended sets of thermal observables and the implication of the macroobservable point of view in terms of metric dependence of thermal observables is beyond the scope of this work. We will instead propose a modification of the extrinsic LTE concept, which is as minimal as possible but addresses the problems discussed in this work. This is necessary from our point of view because a solid foundation on the level of microobservables is necessary for any considerations about macroobservables to be meaningful at all.

3.3. Massive Fields

In this section we will discuss the general massive case of the model of a scalar field in a spacetime which is asymptotically flat in the far future and past. The initial state is taken to be a pure temperature KMS state and it is checked whether the final state satisfies the KMS condition or whether it is at least a suitable mixture of KMS states. To this avail the two-point function of the state in the limit of future infinity is calculated using the Bogoliubov coefficients for the model at hand. This model has been investigated in [28], however that treatment contained mistakes which are corrected here.

3.3.1. Properties of the Model

The model discussed in this section is a conformally flat Robertson-Walker spacetime that is flat in the asymptotic future and past.

$$ds^2 = \left(\frac{1+\epsilon^2}{2} + \frac{1-\epsilon^2}{2}\tanh(\rho\eta)\right)\left(d\eta^2 - d\vec{x}^2\right)$$

Towards past infinity the scale factor converges to $a(-\infty) = \epsilon$ and for future infinity the limit is $a(\infty) = 1$. This model can be interpreted as a very simplistic inflationary scenario, where ϵ fixes the magnitude of inflation and ρ quantifies the speed of inflation. The implications of this metric as a model for inflation are best illustrated by calculating the Hubble parameter $H = \frac{a'}{a^2}$ as a function of the scale factor a.

We get

$$H = \frac{a'}{a^2} = \rho\frac{(1-a^2)(a^2-\epsilon^2)}{(1-\epsilon^2)a^3}$$

which can be interpreted particularly easily in a doubly logarithmic visualisation.

One can see in figure 3.1 that the Hubble parameter H quickly rises to a maximum, then decays as $H \sim a^{-1}$ until the "end of inflation", where H quickly drops again.

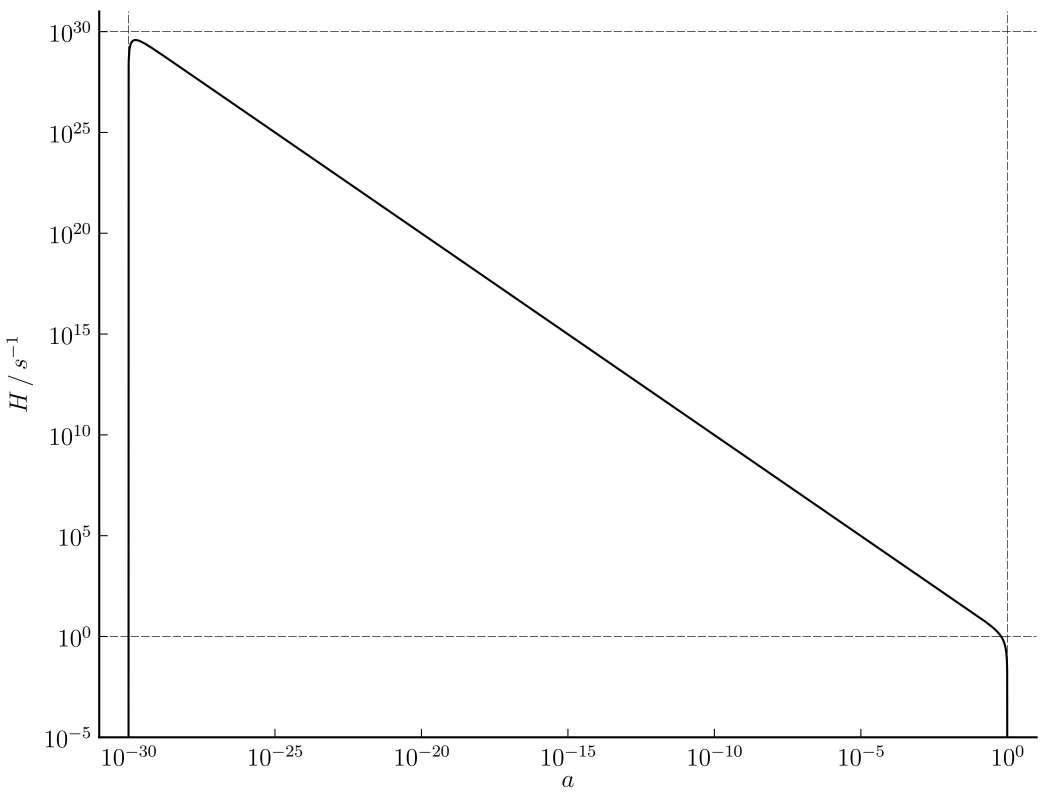

Figure 3.1.: Scale factor visualisation for $\epsilon = 10^{-30}$ and $\rho = 1s^{-1}$

On this spacetime we consider a conformally coupled scalar quantum field which is decomposed in modes in spatial direction and rescaled $\chi_p(\eta) = a(\eta)\phi_p(\eta)$ to get the equation

$$\chi_p'' + (p^2 + m^2a^2)\chi_p = 0$$

The metric becomes flat for time-like past and future infinity, but it is not asymptotically flat. For the sake of asymptotic considerations, we define asymptotic spacetimes $\mathcal{M}^{\mathrm{in/out}}$, which are isometric copies of Minkowski spacetime. However it is of significance that the volume elements of the asymptotic spacetimes are different, because the scale parameter asymptotes to different values. Essentially $\mathcal{M}^{\mathrm{out}}$ can be understood as the ordinary Minkowski spacetime, while the metric of $\mathcal{M}^{\mathrm{in}}$ is a Minkowski metric scaled by ϵ^2.

On the asymptotic spacetimes $\mathcal{M}^{\mathrm{in/out}}$ one can consider Minkowski equations of motion which emerge as limits of the equation of motion for past and future infinity.

Correspondingly, field algebras and state spaces can be defined on the asymptotic spacetimes. These state spaces contain unique Poincaré invariant vacuum states, whose associated GNS representation is the well known vacuum Fock space. These states can be interpreted as asymptotic vacuum states in this model, emerging as past and future time-like infinity limits of certain states in the bulk [4]. It should be noted that this is not identical to the usual notion of asymptotic vacuum states in asymptotically flat spacetimes, as the spacetime considered here is not asymptotically flat. Due to the well defined limits of n-point functions one can nevertheless attach meaning to the states on the asymptotic spacetimes $\mathcal{M}^{\text{in/out}}$ as asymptotic initial or final states.

3.3.2. Bogoliubov Transformation

To fix notation with respect to the asymptotic spacetimes and their corresponding vacuum states, let the limit of some quantity X for the asymptotic past and future be denoted as $X\Big|_{\text{in/out}}$. Such limits of mode functions or two-point functions can be interpreted as mode functions or two-point functions on the asymptotic spacetimes $\mathcal{M}^{\text{in/out}}$. The mode functions $\chi_p^{\text{in/out}}$ for asymptotic vacuum states are simply plane waves in the respective asymptotic limit. This means, by definition $\chi_p^{\text{in}}(x^0)\Big|_{\text{in}} = \chi_p^{\text{out}}(x^0)\Big|_{\text{out}} = e^{-i\omega_p x^0}$. In this subsection the slightly more general case of a free scalar field in a conformally flat, spatially homogeneous and isotropic spacetime that is flat in the far future and past will be discussed without reference to the specific spacetime. The general idea in treating this kind of problem is to calculate the Bogoliubov coefficients that relate the "in"-modes and "out"-modes.

The Bogoliubov transformation for a spatially homogeneous and isotropic spacetime can be expressed as

$$\chi_p^{\text{in}} = A_p \chi_p^{\text{out}} + B_p \chi_p^{\text{out}*}$$

where the consistency condition for the Bogoliubov coefficients

$$\forall p : \, |A_p|^2 - |B_p|^2 = 1$$

must be fulfilled. To calculate the Bogoliubov coefficients solutions for the "in"- and "out"-modes at the same time t_0 are needed. The model that is considered here has the advantage that solutions for all times have already been calculated in [4]. The general solution to the problem considered here will be given in terms of the Bogoliubov coefficients, which allows straight forward calculation of results as soon as the Bogoliubov coefficients are known.

As the initial state we choose a KMS state with the two-point function

$$\mathscr{W}_2^{\beta,\mathrm{in}}(x,y)\Big|_{\mathrm{in}} = \frac{1}{\epsilon^2}\int \frac{1}{(2\pi)^3 2\omega_p^{\mathrm{in}}}\left(\frac{e^{-i(x^0-y^0)\omega_p^{\mathrm{in}}}}{1-e^{-\beta\omega_p^{\mathrm{in}}}} - \frac{e^{i(x^0-y^0)\omega_p^{\mathrm{in}}}}{1-e^{\beta\omega_p^{\mathrm{in}}}}\right) e^{i(\vec{x}-\vec{y})\vec{p}} d^3p$$

where we define $\omega_p^{\mathrm{in}} = \sqrt{p^2+\epsilon^2 m^2}$. The KMS inverse temperature is $\epsilon\beta$, as can be seen by rescaling $p=\epsilon q$ and $x=\frac{x'}{\epsilon}$ analogous to the massless case. As this is only the asymptotic expression for the far past, the modes χ_k^{in} are used to express this two-point function in a form that holds for all times. Also the time dependence of the scale factor has to be taken into account, such that the resultant two-point function is

$$\mathscr{W}_2^{\beta,\mathrm{in}}(x,y) = \frac{1}{a(x^0)a(y^0)}\int \frac{1}{(2\pi)^3}\left(\frac{\chi_k^{\mathrm{in}}(x^0)\chi_k^{\mathrm{in}*}(y^0)}{1-e^{-\beta\omega_p^{\mathrm{in}}}} - \frac{\chi_k^{\mathrm{in}*}(x^0)\chi_k^{\mathrm{in}}(y^0)}{1-e^{\beta\omega_p^{\mathrm{in}}}}\right) e^{i(\vec{x}-\vec{y})\vec{p}} d^3p$$

It can be checked that this expression does indeed fulfil the Klein-Gordon equation in both arguments.

The next step is to find the form of this two-point function in the limit $t\to\infty$. This can be achieved by applying a Bogoliubov transformation. Using $x=z+\zeta$, $y=z-\zeta$ and $|A_p|^2=|B_p|^2+1$ the late time limit of the two-point function is

$$\begin{aligned}
\mathscr{W}_2^{\beta,\mathrm{in}}(x,y)\Big|_{\mathrm{out}} &= \int \frac{1}{(2\pi)^3}\left(\frac{\chi_k^{\mathrm{in}}(x^0)\chi_k^{\mathrm{in}*}(y^0)}{1-e^{-\beta\omega_p^{\mathrm{in}}}} - \frac{\chi_k^{\mathrm{in}*}(x^0)\chi_k^{\mathrm{in}}(y^0)}{1-e^{\beta\omega_p^{\mathrm{in}}}}\right)\Bigg|_{\mathrm{out}} e^{i(\vec{x}-\vec{y})\vec{p}} d^3p \\
&= \int \frac{1}{(2\pi)^3}\Bigg(\Big(|A_p|^2\chi_k^{\mathrm{out}}(x^0)\chi_k^{\mathrm{out}*}(y^0) + A_pB_p^*\chi_k^{\mathrm{out}}(x^0)\chi_k^{\mathrm{out}}(y^0) \\
&\quad + B_pA_p^*\chi_k^{\mathrm{out}*}(x^0)\chi_k^{\mathrm{out}*}(y^0) + |B_p|^2\chi_k^{\mathrm{out}*}(x^0)\chi_k^{\mathrm{out}}(y^0)\Big)\frac{1}{1-e^{-\beta\omega_p^{\mathrm{in}}}} \\
&\quad + \Big(|A_p|^2\chi_k^{\mathrm{out}*}(x^0)\chi_k^{\mathrm{out}}(y^0) + A_p^*B_p\chi_k^{\mathrm{out}*}(x^0)\chi_k^{\mathrm{out}*}(y^0) \\
&\quad + B_p^*A_p\chi_k^{\mathrm{out}}(x^0)\chi_k^{\mathrm{out}}(y^0) + |B_p|^2\chi_k^{\mathrm{out}}(x^0)\chi_k^{\mathrm{out}*}(y^0)\Big)\frac{1}{e^{\beta\omega_p^{\mathrm{in}}}-1}\Bigg)\Bigg|_{\mathrm{out}} \\
&\quad e^{i(\vec{x}-\vec{y})\vec{p}} d^3p
\end{aligned}$$

$$
\begin{aligned}
&= \int \frac{1}{(2\pi)^3 2\omega_p^{\mathrm{out}}} \Bigg(\bigg(|A_p|^2 e^{-i(x^0-y^0)\omega_p^{\mathrm{out}}} + A_p B_p^* e^{-i(x^0+y^0)\omega_p^{\mathrm{out}}} \\
&\quad + A_p^* B_p e^{i(x^0+y^0)\omega_p^{\mathrm{out}}} + |B_p|^2 e^{i(x^0-y^0)\omega_p^{\mathrm{out}}} \bigg) \left(\frac{1}{e^{\beta\omega_p^{\mathrm{in}}} - 1} + 1 \right) \\
&\quad + \bigg(|A_p|^2 e^{i(x^0-y^0)\omega_p^{\mathrm{out}}} + A_p B_p^* e^{-i(x^0+y^0)\omega_p^{\mathrm{out}}} \\
&\quad + A_p^* B_p e^{i(x^0+y^0)\omega_p^{\mathrm{out}}} + |B_p|^2 e^{-i(x^0-y^0)\omega_p^{\mathrm{out}}} \bigg) \frac{1}{e^{\beta\omega_p^{\mathrm{in}}} - 1} \Bigg) \Bigg|_{\mathrm{out}} e^{i(\vec{x}-\vec{y})\vec{p}} d^3p \\
&= \int \frac{1}{(2\pi)^3 2\omega_p^{\mathrm{out}}} \Bigg(\bigg(2\Big(2|B_p|^2 + 1\Big) \cos\Big(2\zeta^0 \omega_p^{\mathrm{out}} - 2\vec{\zeta}\vec{p}\Big) \\
&\quad + 2\Big(A_p B_p^* e^{-i2z^0\omega_p^{\mathrm{out}}} + A_p^* B_p e^{i2z^0\omega_p^{\mathrm{out}}} \Big) e^{i2\vec{\zeta}\vec{p}} \bigg) \frac{1}{e^{\beta\omega_p^{\mathrm{in}}} - 1} \\
&\quad + 2|B_p|^2 \cos\Big(2\zeta^0 \omega_p^{\mathrm{out}} - 2\vec{\zeta}\vec{p}\Big) + e^{-i2\left(\zeta^0\omega_p^{\mathrm{out}} - \vec{\zeta}\vec{p}\right)} \\
&\quad + \Big(A_p B_p^* e^{-i2z^0\omega_p^{\mathrm{out}}} + A_p^* B_p e^{i2z^0\omega_p^{\mathrm{out}}} \Big) e^{i2\vec{\zeta}\vec{p}} \Bigg) \Bigg|_{z^0\to\infty} d^3p
\end{aligned}
\tag{3.3.1}
$$

Obviously the oscillatory terms dependent on z^0 are problematic as they seem to prevent a reasonable limit for $z^0 \to \infty$. To permit a well defined limit and thus an unambiguous calculation of the thermal observables, it is necessary to show that these terms have a well defined limit for $z^0 \to \infty$. If ω_p^{out} were substituted by p in the terms $e^{\pm i2z^0\omega_p^{\mathrm{out}}}$ and $A_p^* B_p$ were a Schwartz function in p the desired convergence would follow as a property of the Fourier transformation. In the case at hand, the arguments from the proof of the Fourier transform's automorphism property on Schwartz space can be adapted to show a suitable decay property of the terms in question, as will be shown below.

3.3.3. Thermal Observables

In this subsection the thermal observables will be calculated. To achieve this goal, several limits have to be interchanged and especially the limit $z^0 \to \infty$ must be well defined for the thermal observables. All these problems are solved in the case that $|B_k|$ fulfils certain L^1-properties in k, which are slightly weaker than the requirement that $|B_k|$ be rapidly decaying. The needed property is given in the following definition.

Part of the present section is joint work with J. Zschoche, which will be indicated by [52]. Especially the proofs of lemmas 3.3.2 and 3.3.3 were found by J.Zschoche and are presented here in the interest of a self-contained treatment.

Definition 3.3.1. [52]
A function $f : \mathbb{R}^+ \to \mathbb{C}$ is of **essentially rapid decay** if

$$\forall n \in \mathbb{N} : \Big((1+\cdot)^n f \Big) \in L^1(\mathbb{R}^+)$$

A function $f : \mathbb{R}^k \to \mathbb{C}$ is of essentially rapid decay if

$$\forall n \in \mathbb{N} : \Big((1+|\cdot|)^n f \Big) \in L^1(\mathbb{R}^k)$$

To justify the chosen terminology note that rapidly decaying functions decay also essentially rapidly, while the converse is not true. Multiplying an essentially rapidly decaying function with a polynomially bounded function yields again an essentially rapidly decaying function.

As an example for a polynomially bounded function that is essentially rapidly decaying while not rapidly decaying one can consider a "comb function" where the teeth increase quadratically in height but shrink exponentially in width

$$f_{\text{erd}}(x) := \sum_{k=1}^{\infty} k^2 \chi(k - e^{-k}, k + e^{-k})(x)$$

where $\chi(k-e^{-k}, k+e^{-k})$ is the characteristic function of the interval $[k-e^{-k}, k+e^{-k}]$. One can see that f_{erd} is indeed essentially rapidly decaying by calculating

$$\begin{aligned} \int_{\mathbb{R}^+} (1+x)^n f_{\text{erd}}(x) dx &= \sum_{j=0}^{n} \binom{n}{j} \sum_{k=1}^{\infty} k^2 \int_{k-e^{-k}}^{k+e^{-k}} x^j dx \\ &= \sum_{j=0}^{n} \binom{n}{j} \sum_{k=1}^{\infty} \frac{k^2}{j+1} \Big((k+e^{-k})^{j+1} - (k-e^{-k})^{j+1} \Big) \end{aligned}$$

As every summand that does not cancel out has at least one factor e^{-k} the geometric series can be used to get a finite sum for this expression. This illustrates the convergence of the integrals and thus the essentially rapid decay. Adding any rapidly decaying function to the comb yields again an essentially decaying function, as does the multiplication with any polynomially bounded function.

The essentially rapid decay property is equivalent to a property that seems weaker at first glance, as is shown in the following lemma.

Lemma 3.3.2. [52]
If a function $f : \mathbb{R}^+ \to \mathbb{C}$ fulfils

$$\exists p \in \mathbb{N}\ \forall n \in \mathbb{N} : \Big((1+\cdot)^n f\Big) \in L^p(\mathbb{R}^+)$$

then it is of essentially rapid decay.

Proof.
The proof is done using the Hölder inequality.

$$||(1+\cdot)^n f||_1 = ||(1+\cdot)^{n+1} f (1+\cdot)^{-1}||_1 \leq ||(1+\cdot)^{n+1} f||_p ||(1+\cdot)^{-1}||_{\frac{p}{p-1}}$$

$$= ||(1+\cdot)^{n+1} f||_p \left(||(1+\cdot)^{-\frac{p}{p-1}}||_1\right)^{\frac{p-1}{p}} < \infty$$

As $\int\limits_{\mathbb{R}^+} |(1+x)^{-\frac{p}{p-1}}| dx$ is finite for any $p > 1$, the L^1-property for the monomial of order n follows from the L^p-property for the monomial of order $n+1$, independently of p, which proves the claim. □

The main mathematical result which will be used in the present treatment is given in the following lemma.

Lemma 3.3.3. [52]
Let $\phi : \mathbb{R}^n \to \mathbb{R}$ a non-negative polynomially bounded function and

$$\tilde{\phi}_r(x) = \lim_{\varepsilon \to 0} \int\limits_{\mathbb{R}^n} \phi(p) e^{ipx - \varepsilon|p|} d^n p$$

Then $\tilde{\phi}_r \in C^\infty(\mathbb{R}^n)$ if and only if ϕ is of essentially rapid decay.

Proof.
Let $t > 0$ and define operators for $f : \mathbb{R}^n \to \mathbb{C}$

$$(\Delta_1^i(t) f)(x) := f(x + te_i) - f(x - te_i)$$

$$(\Delta_n^i(t) f)(x) := [\Delta_1^i(t)(\Delta_{n-1}^i(t) f)](x) = \sum_{k=0}^{n} (-1)^k \binom{n}{k} f(x + (n-2k)te_i)$$

Application to $f(x) = e^{ipx}$ with $p \in \mathbb{R}^n$ yields

$$\Delta_n^i(t) e^{ipx} = e^{ipx} \sum_{k=0}^{n} (-1)^k \binom{n}{k} \left(e^{-itp^i}\right)^k \left(e^{itp^i}\right)^{n-k} = e^{ipx}(2i \sin(tp^i))^n$$

If $\tilde{\phi}_r \in C^\infty(\mathbb{R}^n)$ all derivatives exist and

$$\widetilde{M}_s := \left|\partial_i^{2s}\phi_r\Big|_{x=0}\right| = \lim_{t\to 0}\left|\frac{(\Delta_{2s}^i(t)\phi_r)(0)}{(2t)^{2s}}\right| < \infty$$

which allows the estimate

$$\widetilde{M}_s = \lim_{t\to 0}\lim_{\varepsilon\to 0}\int\limits_{\mathbb{R}^n}\left(\frac{\sin(tp^i)}{t}\right)^{2s}\phi(p)e^{-\varepsilon|p|}d^np \geq \lim_{t\to 0}\lim_{\varepsilon\to 0}\int\limits_{B_R(0)}\left(\frac{\sin(tp^i)}{t}\right)^{2s}\phi(p)e^{-\varepsilon|p|}d^np$$

$$= \lim_{t\to 0}\int\limits_{B_R(0)}\left(\frac{\sin(tp^i)}{t}\right)^{2s}\phi(p)d^np = \int\limits_{B_R(0)}\left(p^i\right)^{2s}\phi(p)d^np$$

for all $R > 0$. As the last Integral is monotonically growing in R but bounded by $\widetilde{M}_s$, the limit $R \to \infty$ is well defined and also bounded by $\widetilde{M}_s$. This proves the existence of all even p^i-moments, and thus all p^i-moments and by iteration all moments. This implies that ϕ is of essentially rapid decay. The backwards direction is trivial by the dominated convergence theorem. □

For the following treatment only a certain class of states is relevant, which is defined in the following.

Definition 3.3.4.
Let $(\mathcal{M}, g)$ a spatially flat FRW spacetime, Q_g the representative of a locally covariant scalar quantum field theory Q on $(\mathcal{M}, g)$. A state is called a Hadamard-Lüders-Roberts state or **HLR state** if it is a pure, Gaussian, homogeneous and isotropic Hadamard state on Q_g.

Note that the requirement that the states be pure refers to the states on $Q(\mathcal{M}, g)$, i.e. the algebra corresponding to all of the spacetime. Restrictions of pure states on $Q(\mathcal{M}, g)$ to subregions of the spacetime are not pure in general, which bears profound consequences like the Hawking and Unruh effects.

It was shown in [29] that HLR states can be specified by two functions. Let $\phi_p(t)$ the mode functions of the fields, where it follows from the homogeneity and isotropy of spacetime and state that these modes only depend on $p = |\vec{p}|$, and let $\pi_p(t) = \sqrt{|g|}g^{00}\partial_0\phi_p(t)$. These complex functions are polynomially bounded in p and have to fulfil

$$\forall t, p: \; \phi_p^*(t)\pi_p(t) - \phi_p(t)\pi_p^*(t) = i \tag{3.3.2}$$

which encodes the canonical commutation relations. The fact that the state is pure is encoded in the fact that the two-point function can be completely defined by giving $\phi_p(t)$ and $\pi_p(t)$ fulfilling (3.3.2) on a Cauchy surface. The implication of the Hadamard condition will be investigated in the following.

In the following construction some procedure is needed to identify states on different spacetimes in a way that allows carrying over Bogoliubov coefficients. To achieve this we will state a straight forward corollary of the work of [29].

Lemma 3.3.5. [52]
Let $(\mathcal{M}, g)$, $(\mathcal{M}', g')$ and $(\mathcal{M}'', g'')$ spatially flat FRW spacetimes, such that $(\mathcal{M}'', g'')$ is an isometrically, orientation and time orientation preservingly embedded submanifold of the other two manifolds, in both cases containing a Cauchy surface of the spacetime it is embedded into. Call these embeddings ψ and ψ'. Any HLR state defined on all of $(\mathcal{M}, g)$, $(\mathcal{M}', g')$ can be completely defined by suitable initial conditions in $\psi(\mathcal{M}'', g'')$, $\psi'(\mathcal{M}'', g'')$ (because it contains a Cauchy surface), and thus by an HLR state in $(\mathcal{M}'', g'')$. This yields a well defined method of identifying HLR state defined on all of $(\mathcal{M}, g)$ with HLR state defined on all of $(\mathcal{M}', g')$.

Let ω_1 and ω_1' HLR states identified via their initial conditions on the Cauchy surfaces within $\psi(\mathcal{M}'', g'')$, $\psi'(\mathcal{M}'', g'')$ as outlined above and ω_2 and ω_2' HLR states identified accordingly. Then the Bogoliubov coefficients relating ω_1 and ω_2 are the same as the Bogoliubov coefficients relating ω_1' and ω_2'.

Note that the identification of states given by this lemma is by no means general in any sense. If two spacetimes are isometric in two disjoint regions each containing Cauchy surfaces, states identified in one region will in general not be identified in the other region. This is an example for the fact that locally contravariant states do not exist in general, and is essentially the reason why the result of this section is not trivial. However, as the focus lies on Bogoliubov coefficients here, this caveat is no obstacle for the following treatment.

After these preparations it can now be shown that B_p is of essentially rapid decay in p for a certain class of models.

Theorem 3.3.6. [52]
Let $(\mathcal{M}, g)$ a spatially flat FRW spacetime, Q_g the representative of a locally covariant scalar quantum field theory Q on $(\mathcal{M}, g)$. Let ω_1 and ω_2 HLR states on Q_g. Then the Bogoliubov coefficient B_p corresponding to the Bogoliubov transformation from ω_1 to ω_2 is of essentially rapid decay in p.

Proof.
The idea for this proof stems largely from Nicola Pinamonti, [34].

As $(\mathcal{M}, g)$ is a spatially flat FRW spacetime its metric can be given as

$$ds^2 = a^2(\eta)\Big(d\eta^2 - d\vec{x}^2\Big)$$

in suitable coordinates, where η is defined on some open set $I \subseteq \mathbb{R}$. Let $\eta_1, \eta_2 \in I$ and $\eta_1 < \eta_2$ and define a spacetime $(\mathcal{M}', g')$ by the metric

$$ds^2 = \Big(1 - \sigma(\eta) + \sigma(\eta)a^2(\eta)\Big)\Big(d\eta^2 - d\vec{x}^2\Big)$$

where $\sigma(\eta)$ is a smooth function with $\forall \eta > \eta_2 : \sigma(\eta) = 1$ and $\forall \eta < \eta_1 : \sigma(\eta) = 0$ and η is defined in the open set $(-\infty, \sup I)$. The spacetimes $(\mathcal{M}, g)$ and $(\mathcal{M}', g')$ then conform with the assumptions of Lemma 3.3.5 for some neighbourhood of a Cauchy surface in the region $\eta > \eta_2$, such that HLR states on these spacetimes can be identified in the sense of this lemma, especially preserving their relation in terms of Bogoliubov coefficients. It thus suffices to show essentially rapid decay for B_p corresponding to the Bogoliubov transformation from ω_1' to ω_2'.

To prove the claim it is preferable to calculate in the Minkowski section of $(\mathcal{M}', g')$, i.e. at $\eta < \eta_1$. In this flat region there is a unique Poincaré invariant vacuum ω_∞' and as a first step we will treat the Bogoliubov transformation from ω_1' to the vacuum. In this case it is necessary to be cautious with the distribution character of the two-point function, therefore we take

$$\Big(\mathscr{W}_2^{\omega_1'} - \mathscr{W}_2^{\omega_\infty'}\Big)(f, g) = \iiint \frac{1}{(2\pi)^3 2\omega_p}\Big(|B_{1,p}|^2 e^{-i(x^0-y^0)\omega_p} + A_{1,p}B_{1,p}^* e^{-i(x^0+y^0)\omega_p}$$
$$+ A_{1,p}^* B_{1,p} e^{i(x^0+y^0)\omega_p} + |B_{1,p}|^2 e^{i(x^0-y^0)\omega_p}\Big) e^{i(\vec{x}-\vec{y})\vec{p}} f(x)g(y) d^4x\, d^4y\, d^3p$$

as can be derived from equation (3.3.1). This expression is a Schwartz distribution as $A_{1,p}$ and $B_{1,p}$ are polynomially bounded. This implies that derivatives in x and y can be defined in the weak sense.

Taking the expectation value of the point split energy density

$$\omega(T_{00})(x, y) := \frac{1}{2}\Big(\mathscr{W}_2^\omega(\partial_0 f, \partial_0 g) + \delta^{ij}\mathscr{W}_2^\omega(\partial_i f, \partial_j g) + m^2 \mathscr{W}_2^\omega(f, g)\Big)$$

the difference for the states at hand is

$$\Big(\omega_1'(T_{00}) - \omega_\infty'(T_{00})\Big)(f, g) = \iiint \frac{1}{(2\pi)^3 4\omega_p}\Big(\Big(\omega_p^2 + \vec{p}^2 + m^2\Big)|B_{1,p}|^2 e^{-i(x^0-y^0)\omega_p}$$
$$+ \Big(-\omega_p^2 + \vec{p}^2 + m^2\Big) A_{1,p}B_{1,p}^* e^{-i(x^0+y^0)\omega_p}$$
$$+ \Big(-\omega_p^2 + \vec{p}^2 + m^2\Big) A_{1,p}^* B_{1,p} e^{i(x^0+y^0)\omega_p}$$
$$+ \Big(\omega_p^2 + \vec{p}^2 + m^2\Big)|B_{1,p}|^2 e^{i(x^0-y^0)\omega_p}\Big) e^{i(\vec{x}-\vec{y})\vec{p}} f(x)g(y) d^4x\, d^4y\, d^3p$$
$$= \iiint \frac{\omega_p}{(2\pi)^3} |B_{1,p}|^2 \cos\Big((x^0 - y^0)\omega_p\Big) e^{i(\vec{x}-\vec{y})\vec{p}} f(x)g(y) d^4x\, d^4y\, d^3p$$

where the prefactors in the terms containing $A_{1,p}B^*_{1,p}$ vanish. To apply lemma 3.3.3 some further manipulations are necessary. First, $\lim_{\varepsilon\to 0} e^{-\varepsilon p}$ can be inserted in the p-integral, and because f and g have compact support and $|B_{1,p}|^2$ is polynomially bounded, the term

$$h(p) := \iint \frac{\omega_p}{(2\pi)^3}|B_{1,p}|^2 \cos\Big((x^0 - y^0)\omega_p\Big)e^{i(\vec{x}-\vec{y})\vec{p}}f(x)g(y)d^4x\, d^4y$$

is a Schwartz function, which allows interchanging the limit $\varepsilon \to 0$ with the p-integration. With the additional regularising term $e^{-\varepsilon p}$ the integrations can be interchanged such that the p integration is the innermost integration. As the difference of expectation values of the energy density is smooth, the smearing with test functions can be dropped to yield

$$\Big(\omega_1'(T_{00}) - \omega_\infty'(T_{00})\Big)(x,y) = \int \frac{\omega_p}{(2\pi)^3}|B_{1,p}|^2 \cos\Big((x^0 - y^0)\omega_p\Big)e^{i(\vec{x}-\vec{y})\vec{p}}d^3p$$

Setting $x^0 = y^0$ leads to an expression which fulfils the assumptions of lemma 3.3.3, which proves that $|B_{1,p}|^2$ and thus by lemma 3.3.2 finally $|B_{1,p}|$ is of essentially rapid decay.

The same holds for the corresponding coefficient $B_{2,p}$ for ω_2'. Recalling some relations for Bogoliubov coefficients one sees

$$\chi^1_p = A_{1,p}\chi^\infty_p + B_{1,p}\chi^{\infty *}_p \quad \chi^2_p = A_{2,p}\chi^\infty_p + B_{2,p}\chi^{\infty *}_p \quad \Rightarrow \quad \chi^\infty_p = A^*_{2,p}\chi^2_p - B_{2,p}\chi^{2*}_p$$

$$\chi^1_p = \Big(A_{1,p}A^*_{2,p} - B_{1,p}B^*_{2,p}\Big)\chi^2_p + \Big(B_{1,p}A_{2,p} - A_{1,p}B_{2,p}\Big)\chi^{2*}_p$$

The Bogoliubov coefficient $B_{12,p} := (B_{1,p}A_{2,p} - A_{1,p}B_{2,p})$ corresponding to the transformation from ω_1' to ω_2' is of essentially rapid decay, as the coefficients $A_{1/2,p}$ are polynomially bounded. This concludes the proof. □

The following lemma shows the connection of essentially rapid decay of B_k to the well-definedness of the limit $z^0 \to \infty$.

Lemma 3.3.7.
All functions in this lemma are understood to be complex valued. Let $f \in L^1(\mathbb{R}^+)$ and define

$$\forall x \in \mathbb{R} : \mathcal{F}_m[f](x) := \int_0^\infty f(p)e^{ix\sqrt{p^2+m^2}}dp$$

Then $\mathcal{F}_m[f](x) \in C_0(\mathbb{R})$.

Proof.
The idea of the proof is to adapt the proof of the corresponding theorem for the Fourier transform (see e.g. Satz V.2.2 in [50]).

First we show continuity of $\mathcal{F}_m[f]$ using the definition in terms of limits of sequences. Let $(x_n)_{n\in\mathbb{N}}$ a convergent series with $\lim\limits_{n\to\infty} x_n = x$, then

$$\forall p \in \mathbb{R}^+ : \lim_{n\to\infty} \left| e^{ix_n\sqrt{p^2+m^2}} - e^{ix\sqrt{p^2+m^2}} \right| = 0$$

By the convergence theorem of Lebesgue it then follows that

$$\lim_{n\to\infty} |\mathcal{F}_m[f](x_n) - \mathcal{F}_m[f](x)| \leq \int\limits_0^\infty |f(p)| \lim_{n\to\infty} \left| e^{ix_n\sqrt{p^2+m^2}} - e^{ix\sqrt{p^2+m^2}} \right| dp = 0$$

The limit can be interchanged with the integral, because the integrand is majorised by $2\,|f(p)| \in L^1(\mathbb{R}^+)$. This proves continuity of $\mathcal{F}_m[f]$.

Now we turn to the proof that $\mathcal{F}_m[f]$ vanishes for $x \to \infty$. Because $C_0^\infty(\mathbb{R}^+)$ is dense in $L^1(\mathbb{R}^+)$ and because of the inequality

$$\forall f \in L^1(\mathbb{R}^+) : \, ||\mathcal{F}_m[f]||_\infty \leq ||f||_1$$

it is sufficient to show

$$\forall g \in C_0^\infty(\mathbb{R}^+) : \, \lim_{x\to\infty} |\mathcal{F}_m[g](x)| = 0$$

Let $R \in \mathbb{R}^+$ and $g \in C_0^\infty(\mathbb{R}^+)$ then by partial integration

$$\begin{aligned}
|\mathcal{F}_m[g](x)| &= \left| \int\limits_0^\infty g(p) e^{ix\sqrt{p^2+m^2}} dp \right| \\
&= \left| \int\limits_0^\infty \frac{1}{ix} \sqrt{1 + \frac{m^2}{p^2}}\, g(p) \frac{d}{dp} e^{ix\sqrt{p^2+m^2}} dp \right| \\
&= \frac{1}{|x|} \left| \int\limits_0^\infty e^{ix\sqrt{p^2+m^2}} \frac{d}{dp} \left(\sqrt{1 + \frac{m^2}{p^2}}\, g(p) \right) dp \right| \\
&= \frac{1}{|x|} \left| \int\limits_0^\infty e^{ix\sqrt{p^2+m^2}} \left(-\frac{m^2}{p^2} \frac{1}{\sqrt{p^2+m^2}} g(p) + \frac{1}{p} \sqrt{p^2+m^2}\, g'(p) \right) dp \right| \\
&\leq \frac{1}{|x|} \int\limits_0^\infty \left(\left| \frac{m^2}{p^2} \frac{1}{\sqrt{p^2+m^2}} g(p) \right| + \left| \frac{1}{p} \sqrt{p^2+m^2}\, g'(p) \right| \right) dp
\end{aligned}$$

$$\leq \frac{1}{|x|}\left(\left|\left|\frac{m^2}{p^2}\frac{1}{\sqrt{p^2+m^2}}g(p)\right|\right|_1 + \left|\left|\frac{1}{p}\sqrt{p^2+m^2}g'(p)\right|\right|_1\right)$$

In the limits $x \to \pm\infty$ this expression decays like $|x|^{-1}$, which means that it converges to 0, if the remaining integrals exist. However the fact that $g \in C_0^\infty(\mathbb{R}^+)$ ensures the existence of the integrals, where the divergence of the prefactors at $p = 0$ are not problematic, as g has compact support on the open set $\mathbb{R}^+$.

To conclude the proof, note that for a series $(g_n)_{n\in\mathbb{N}} \subset C_0^\infty(\mathbb{R}^+)$ that converges to $f \in L^1(\mathbb{R}^+)$ we get

$$\begin{aligned}|\mathcal{F}_m[f](x)| &= |\mathcal{F}_m[g_n](x) + \mathcal{F}_m[f-g_n](x)| \\ &\leq |\mathcal{F}_m[g_n](x)| + |\mathcal{F}_m[f-g_n](x)| \\ &\leq |\mathcal{F}_m[g_n](x)| + ||\mathcal{F}_m[f-g_n]||_\infty \\ &\leq |\mathcal{F}_m[g_n](x)| + ||f-g_n||_1\end{aligned}$$

where the first term vanishes in the limit $x \to \pm\infty$ and the second term vanishes in the limit $n \to \infty$. This proves the claim. □

The thermal observables in the out-region are given by

$$\Theta_{\boldsymbol{\mu}}^{\text{out}} = \lim_{z^0\to\infty}\lim_{\zeta\to 0}\partial_{\boldsymbol{\mu}}^\zeta\left(\mathscr{W}_2^{\beta,\text{in}} - \mathscr{W}_2^{\infty,\text{out}}\right)\Big|_{\text{out}}(z^0,\zeta)$$

where the uniform convergence properties necessary for the interchange of the limits, differentials and integrals in this context hold if the L^1-properties used in Lemma 3.3.7 are fulfilled. Especially it suffices that B_p decays essentially rapidly because $\forall p \in \mathbb{R}^+ : |A_p| = \sqrt{|B_p|^2+1} \geq 1$.

For the terms containing $A_p^* B_p$ and its complex conjugate to not contribute to the expectation values of thermal observables up to order n in the limit $z^0 \to \infty$ the property

$$\forall k \leq n : \left(p \mapsto p^{2+k}A_p^*B_p\right) \in L^1(\mathbb{R}^+) \tag{3.3.3}$$

is needed. This property follows from the fact that B_p is of essentially rapid decay, so the expectation values of the balanced derivatives can be calculated as

$$\Theta_{\boldsymbol{\mu}}^{\text{out}} = \int \frac{1}{(2\pi)^3\omega_p^{\text{out}}}\left(\frac{2|B_p|^2+1}{e^{\beta\omega_p^{\text{in}}}-1} + |B_p|^2\right)\lim_{\zeta\to 0}\partial_{\boldsymbol{\mu}}^\zeta\cos\left(2\zeta^0\omega_p^{\text{out}} - 2\vec{\zeta}\vec{p}\right)d^3p \tag{3.3.4}$$

The spacetime model

$$ds^2 = \left(\frac{1+\epsilon^2}{2} + \frac{1-\epsilon^2}{2}\tanh(\rho\eta)\right)\left(d\eta^2 - d\vec{x}^2\right)$$

considered here has been treated in [4], where also the Bogoliubov coefficients were calculated. The term relevant to the present work is

$$|B_p|^2 = \frac{\sinh^2\left(\frac{\pi(\omega_p^{\text{out}}-\omega_p^{\text{in}})}{2\rho}\right)}{\sinh\left(\frac{\pi\omega_p^{\text{out}}}{\rho}\right)\sinh\left(\frac{\pi\omega_p^{\text{in}}}{\rho}\right)}$$

$$\Rightarrow \quad \lim_{p\to\infty}|B_p|^2 = \lim_{p\to\infty} e^{-\frac{\pi\omega_p^{\text{in}}}{\rho}} = \lim_{p\to\infty} e^{-\frac{\pi p}{\rho}} = 0$$

Thus, in this specific model, B_p is even of rapid decay in p.

Plugging the explicit form of $|B_p|^2$ into the definition of the thermal macroobservables (3.3.4), it is not at all obvious, whether the state is a KMS state, a mixture of KMS states or no KMS thermal state at all. By a numerical calculation it could be checked, whether the first thermal macroobservables are the same as for some KMS states, but a mixture of KMS states cannot be ruled out in the same way. The only intermediary result in equation (3.3.4) of the present section will be further investigated in a later section. For now the conclusion is that there is no apparent way except for numerical calculations to make headway on the interpretation of this result.

3.4. Towards an Alternative Concept

This section will be dedicated to a constructive critique of the LTE condition, especially the extrinsic LTE condition on curved spacetimes. First of all, the problems and open questions found in the previous sections will be discussed and it will be argued that such problems are unacceptable. This leads us to argue that a refinement of the LTE condition is necessary that should fulfil certain requirements to address the problems discussed above.

Next, a refinement of the LTE condition is proposed that enables one to address the problems pointed out before. Remaining weaknesses and problems of the refined condition will be discussed and two main problems will be identified. A solution to the first problem for a spacetime is necessary for the refined condition to be reasonable at all on that certain spacetime, and a partial solution will be given, which allows an application of the refined condition to conformally static spacetimes.

In the last part of this section it will be argued that the second problem can be solved gradually, where an optimal solution is desirable to minimise ambiguity of the refined condition. A partial solution in the special case of Minkowski spacetime will be demonstrated. The refined condition on Minkowski spacetime in the form presented here is thus not as exact as the original definition of LTE, meaning that some states which are not in LTE according to the LTE condition cannot be excluded as LTE states with the condition discussed here. An argument will be given why the refined condition is nevertheless useful as a tool to probe thermal states which are locally close to equilibrium.

3.4.1. Problems and Open Questions Concerning LTE

The previous sections have shown a number of problems of the LTE concept, especially the extrinsic LTE concept on curved spacetimes. In the following these problems will be reviewed and their perceived severety is commented upon.

The first problem discussed in section 3.1 is the inconsistency of the extrinsic LTE condition with the native KMS condition in static spacetimes. The same incompatibility was found in section 3.2 to the conformal KMS condition for a conformally invariant field in a conformally flat spacetime. In the Einstein static spacetime it was shown that the KMS condition is included in the extrinsic LTE condition in the limits of large temperature and small curvature. This is expected as large temperatures corresponds to mainly short wavelengths which probe little of the geometry. In the conformally flat case the inclusion of the conformal KMS condition in the extrinsic LTE condition is expected as the spacetime approaches Minkowski spacetime.

If the extrinsic LTE condition is to be upheld unchanged despite this problem, one has to draw the conclusion that the (conformal) KMS condition on other spacetimes than Minkowski spacetime has no thermodynamic relevance. Although an experimental examination of this question is not possible, one could try to establish an axiomatic concept of thermality from first principles, possibly extending the approach of [18][27] using adiabatic accessibility to gravitating systems. The point of view that an LTE concept with suitably modified observables should be preferred as a concept of thermality is taken in [45], where some interesting results for static spacetimes are presented. However, the modified observables do not solve the problems in conformally flat spacetime.

A subsidiary problem that emerges if one relies on the extrinsic LTE states is that the coupling to curvature ξ, which has no parallel on Minkowski spacetime, has to be dealt with. It is very doubtful in this context, whether the freedom in the definition of thermal observables as detailed in equation (2.2.4) is sufficient to restore the basic idea of the extrinsic LTE condition, namely the comparison of expectation values on different spacetimes. As explained before, a comparison to the difference between the cases of massive and massless fields on Minkowski spacetime may lead one to the expectation that such simple adjustments are insufficient to achieve a convincing macroobservable interpretation.

The second problem, discussed in section 3.2 of this work, is the blatant violation of the correspondence principle in the case of extrinsic LTE in de Sitter spacetime. Especially in the case of conformal coupling the results (3.2.12) and (3.2.13) for the time dependence of temperature are different from classical behaviour to an unacceptable degree. Also the instability of extrinsic LTE that was found, represents a huge departure from the classical behaviour. Even the limit of high temperature does no good in resolving this problem, which makes it particularly unacceptable. If one considers the modified observables proposed in [45], the correspondence principle is also violated.

However, it was also seen that the extrinsic LTE concept as applied in equation (3.2.14) reproduces the time dependence of temperature for the classical conformally coupled field. The latter finding could be investigated more closely and the expression for the trace from (3.2.2) could be substituted into equation (3.2.6) and geometric terms could be accounted for in the spirit of equation (2.2.4). This could be used to argue in favour of a modified extrinsic LTE condition. Such an effort would not address the other problems, however it may give a hint which direction a refined condition should take. It is therefore discussed in subsection 3.4.4.

The third problem is not a problem of principle but rather a technical inconvenience. The LTE condition is not straight forward to check, especially in the case of non-trivial temperature mixtures. This is especially true for massive fields, where the thermal integrals cannot be analytically solved in general. Although this is not a principal obstacle for the use of the LTE concept, it greatly infringes its usefulness. Therefore this problem should be taken seriously, not as calling the sensibility of the LTE concept into question but as strongly recommending an amendment. This holds true even for the simple case of mixtures of KMS states which are not straight forward to identify from the results of thermal measurements or even the full two-point function.

We contend that these problems point to the necessity for a refinement of the LTE condition. Such a refined LTE condition should have several properties to achieve the desired improvement without introducing too much ambiguity that threatens to render such a condition arbitrary. The properties we would like to achieve include

(a) In flat spacetime the refined LTE condition should be implied in the original LTE condition.

(b) The refined condition should be easier to check than the original one for a given state.

(c) The refined condition should be easier to generalise to curved spacetimes.

One might be interested in the stricter requirement that the refined condition be equivalent to the original condition for flat spacetimes. It is clear that such a requirement is rather difficult to fulfil. The draft for a refined condition presented here does not fulfil such a requirement of equivalence in general. We will point out, what type of further work could achieve such an equivalence. An example that illustrates which kind of unwanted effects are possible for our condition will be given to emphasise the need for further improvement of the condition. However, an equivalence is achieved if one restricts to mixtures of KMS states for a massless field with the same rest frame as reference states for the original LTE condition.

3.4.2. Dynamic Equations

The investigation of the correspondence principle in section 3.2 made heavy use of a generalisation of the dynamic equations (2.2.7) and (2.2.9). Such generalised equations are derived from equations (3.2.3)-(3.2.6),

$$g^{\mu\nu}\nabla^+_\mu\nabla^-_\nu\theta_g(x,y) = 0 \tag{3.2.3}$$

$$\Rightarrow g^{\mu\nu}\nabla_\mu\omega\left(\theta_{g,\nu}\right)(x) = 0 \tag{3.2.4}$$

$$(\Box^+ + \Box^-)\theta_g(x,y) = -\Big(4m^2 - 2\xi R(x) - 2\xi R(y)\Big)\theta_g(x,y) + 4C(x,y) \tag{3.2.5'}$$

$$\Rightarrow \Box\,\omega\left(\theta_g\right)(x) = -\,\omega\left(\theta_{g,}{}^{\nu}{}_{\nu}\right)(x) - 4(m^2 - \xi R(x))\omega\left(\theta_g\right)(x) + 4C(x) \tag{3.2.6'}$$

by applying the relations from lemma 3.2.5. As such equations are derived using only the Hadamard property of the states, they are a good starting point for a refinement of the LTE condition.

The principal input to these equations that specialises to LTE states and thus makes the fulfilment of these equations nontrivial and expressive, is a sequence of trace relations like (3.1.11) and (3.2.2),

$$\Theta^\mu_{\mu\boldsymbol{\nu}} = \sum_{\boldsymbol{\alpha}\cup\boldsymbol{\lambda}=\boldsymbol{\nu}} C_{m^2,\xi,|\boldsymbol{\nu}|,\boldsymbol{\alpha}}\Theta_{\boldsymbol{\lambda}} \tag{3.4.1}$$

However, assuming that (conformal) KMS states are LTE states for models where they exist and just comparing (3.1.11) and (3.2.2) no general rule for the form of such trace relations is apparent. It is possible to calculate trace relations whenever there is a suitable class of thermal reference states, however it would be very unsatisfactory to restrict to such models. The least one would want are trace relations for any free scalar field on conformally flat spacetimes. Assuming the trace relation (3.1.11) to be general for static spacetimes one may combine it with (3.2.2) to conjecture

$$\widetilde{\Theta}^{\mu}_{\mu} = \frac{-4}{\Omega^4}\left(m^2 - \xi\widetilde{R} + \frac{1}{2}\left(g^{\mu\nu}\frac{\partial_\mu\Omega\partial_\nu\Omega}{\Omega^2} - \frac{\Box\Omega}{\Omega}\right)\right)\widetilde{\Theta} + C \tag{3.4.2}$$

where we follow the notation of section 3.2 and C is the generic curvature term that stems from the Hadamard renormalisation. Analogous relations could be assumed for the traces of higher order observables. However, guessing a general trace relation is somewhat problematic without additional physical input and the predictions of such a model will have to be treated with some caution.

In fact the trace conditions are indeed the only ingredient making the equations LTE specific, so in fact requiring the trace relations is equivalent to requiring the equations to be fulfilled. However, as the observables involved in the trace relations are of higher order, the equations may still be easier to check in many cases. Furthermore, some physically meaningful results have been derived from the dynamic equations in the case of Minkowski spacetime by [12], therefore stating the refined LTE condition in terms of these equations seems preferable.

Assuming the dynamic equations for the thermal observables as defining of LTE yields a condition that is compatible with the KMS condition on static spacetimes and the conformal KMS condition on conformally static spacetimes. It is also compatible with the setting of local covariance, as the equations are formulated in a covariant manner, in contrast to the extrinsic LTE condition. From the covariant form of the thermodynamic equations of state one can derive the "standard" form of the equations of state using the non-covariant classic thermal observables, which leads to the occurrence of geometric terms. Therefore, the fact that the dynamical equations are dependent on the geometry of spacetime is to be expected.

If the two-point function of a state is given, it can be straight forwardly checked whether the thermal observables fulfil the dynamic equations. Thus, the condition suggested here is easier to check than the original LTE condition, especially for massive fields and on curved spacetimes. Although equations (3.2.5')-(3.2.6') are quite painstaking to generalise to higher order balanced derivatives as seen in 3.2 and finding appropriate trace relations remains problematic, taking the dynamical equations for the thermal observables as starting point addresses the requirements (b) and (c) with some success.

3.4.3. Positivity Inequalities

The question investigated in this subsection is, which additional conditions are necessary to fulfil requirement (a). The dynamic equations on Minkowski spacetime are fulfilled by any translation invariant state and these do not all have a reasonable thermal interpretation. As an illustrative example of what can go wrong, one can define positive two-point functions for certain indefinite normalised premeasures that induce a "pseudomixture" of temperatures. An explicit example of such a state for a massless field on Minkowski spacetime is given in the following lemma

Lemma 3.4.1.
The bidistribution

$$\mathscr{W}_2^{sign} := \int \Big(2\delta(\beta-\alpha) - \delta(\beta - 2\alpha)\Big)\mathscr{W}_2^{\beta} d\beta$$

defines a Gaussian Hadamard state ω_{sign} for the massless scalar field.

Proof.
As the Hadamard property follows straight forwardly and the Klein-Gordon equation is satisfied in both arguments, only positivity of the two-point function remains to be shown. It suffices to examine the symbolic form

$$\begin{aligned}\mathscr{W}_2^{\mathrm{sign}}(x,y) = &\int \frac{1}{(2\pi)^3 2p}\Bigg(2\Big(\frac{2}{e^{\alpha p}-1} - \frac{1}{e^{2\alpha p}-1}\Big)\cos\Big((x^0-y^0)p - (\vec{x}-\vec{y})\vec{p}\Big) \\ &+ e^{-i(x^0-y^0)p + i(\vec{x}-\vec{y})\vec{p}}\Bigg)d^3p \\ = &\int \frac{1}{(2\pi)^3 2p}\Bigg(2\Big(\frac{1}{e^{\alpha p}-1} + \frac{e^{\alpha p}}{e^{2\alpha p}-1}\Big)\cos\Big((x^0-y^0)p - (\vec{x}-\vec{y})\vec{p}\Big) \\ &+ e^{-i(x^0-y^0)p + i(\vec{x}-\vec{y})\vec{p}}\Bigg)d^3p\end{aligned}$$

As $\forall \vec{p} \in \mathbb{R}^3 : \frac{1}{e^{\alpha p}-1} + \frac{e^{\alpha p}}{e^{2\alpha p}-1} > 0$ the two-point function is clearly positive. This proves the claim. □

But the expectation values of the thermal observables are

$$\begin{aligned}12\omega_{\mathrm{sign}}(\theta) =& \frac{2}{\alpha^2} - \frac{1}{4\alpha^2} = \frac{7}{4\alpha^2} \\ -\frac{120}{\pi^2}\omega_{\mathrm{sign}}(\theta_{00}) =& \frac{2}{\alpha^4} - \frac{1}{16\alpha^4} = \frac{31}{16\alpha^2}\end{aligned}$$

which obviously violates the necessary condition $(12\Theta)^2 \leq -\frac{120}{\pi^2}\Theta_{00}$ shown in equation (2.2.17). The fact that ω_{sign} is Gaussian while generic mixtures of KMS states are non-Gaussian plays no role here, as we are only interested in thermality with respect to the thermal observables derived from the two-point function. To restrict to sensible mixtures of KMS states, such situations must be excluded. This means we have to impose positivity inequalities on the thermal macroobservables. As even for the massless field the thermal macroobservables for mixtures of rKMS states present a special case of a multidimensional moment problem, no positivity inequalities are readily available. For the massive field the situation is even more complicated, because the macroobservables corresponding to the balanced derivatives are not simple functions of the inverse temperature.

Lemma 3.4.2.
For rKMS states of the massless scalar field let

$$f_a(\beta_0, \beta) := \frac{1}{(2a-1)!}\partial_{\beta_0}^{(2a-2)}\frac{1}{\beta_0^2 - \beta^2} \propto \Theta_{\underbrace{0\ldots0}_{2a-2}}$$

These functions fulfil

$$\forall a \in \mathbb{N},\, \beta_0 > \beta: \; f_{a+1}^a(\beta_0, \beta) \geq f_a^{a+1}(\beta_0, \beta) \tag{3.4.3}$$

Proof. The proof is done in appendix A.3. □

Using Jensen's inequality as in equation (2.2.17) we can extend these inequalities to mixtures of rKMS states and thus get a necessary condition for LTE states. As this is only a necessary condition for mixtures of rKMS states, it can be improved and we conjecture the stricter inequality $f_{a+1}^a \geq f_a^{a+1} + f_1^{a^2} f_a - f_1^{a^2+a}$, which is however still not a sufficient condition. Finding a sufficient condition is a problem related to the multidimensional moment problem, so this problem in the general case of mixtures of rKMS states is far beyond the scope of the present work. However, a necessary condition alone still yields a definite exclusion principle. If a state does not fulfil these inequalities it is definitely not thermal.

For mixtures not of rKMS states but KMS states for the massless field the proved and conjectured inequalities are identical and equivalent to the usual positivity inequalities of the one-dimensional moment problem. The solution to the one-dimensional moment problem states that the inequalities are necessary and sufficient in this case. This does not imply, however, that whenever one of the sets of inequalities is fulfilled, the state can be understood as a mixture of KMS states, because for mixtures of rKMS states there need not be a reference frame, for which all non-diagonal components of the higher order balanced derivatives vanish.

For the massive field, it is more difficult to prove necessary conditions even for KMS states. The present work will only consider the simpler case of KMS states. This implies that any balanced derivative has only one independent component. We pick the following representation of this components

$$\theta_{2n}(z) := \lim_{\zeta\to 0}(\triangle^{\zeta})^n \theta(z+\zeta, z-\zeta)$$

which means for a KMS state

$$\begin{aligned}\theta_{\beta,2n} &= \lim_{\zeta\to 0}(\triangle^{\zeta})^n \int \frac{\cos\left(2\zeta^0\omega_p - 2\vec{\zeta}\vec{p}\right)}{(2\pi)^3\omega_p\left(e^{\beta\omega_p}-1\right)} d^3p \\ &= \int_0^\infty \frac{(-4)^n p^{2n+2}}{2\pi^2\sqrt{p^2+m^2}\left(e^{\beta\sqrt{p^2+m^2}}-1\right)} dp \\ &= \frac{1}{\beta^{2n+2}} \int_0^\infty \frac{(-4)^n \rho^{2n+2}}{2\pi^2\sqrt{\rho^2+m^2\beta^2}\left(e^{\sqrt{\rho^2+m^2\beta^2}}-1\right)} dp\end{aligned}$$

This motivates

$$g_a(m,\beta) = \frac{1}{\beta^{2a}} \int_0^\infty \frac{q^{2a}}{\left(e^{\sqrt{q^2+m^2\beta^2}}-1\right)\sqrt{q^2+m^2\beta^2}} dq \propto \Theta_{\beta,2a-2}$$

and we state the following

Conjecture 3.4.3.

$$\forall a \in \mathbb{N}: \quad \left(\frac{g_a(m,\beta)}{g_a(0,\beta)}\right)^{a+1} \leq \left(\frac{g_{a+1}(m,\beta)}{g_{a+1}(0,\beta)}\right)^{a} \tag{3.4.4}$$

This claim is not straight forward to prove, as the integrals involved cannot be solved analytically in general. Some considerations towards a proof of this inequality and supplementary inequalities can be found in appendix A.4. Numerical calculations indicate the correctness of these relations as illustrated below. In the following illustrations

$$h_n(m\beta) := \frac{g_n^{n+1}(m,\beta)}{g_{n+1}^n(m,\beta)}$$

will be plotted for some n and it can be seen that the functions appear to decay monotonously. If one takes the numeric results for granted, the graphics given here together with the considerations in appendix A.4 suffice to prove conjecture 3.4.3.

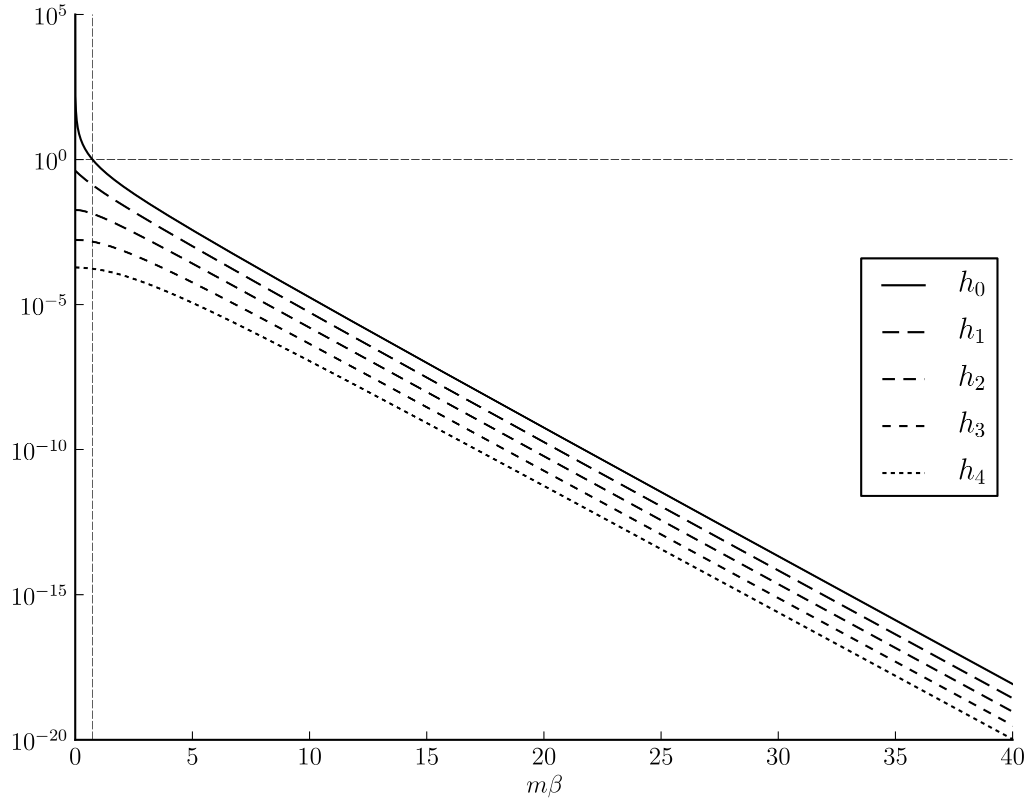

Figure 3.2.: Graphs of h_n for some n

For the more general case of a free scalar field with arbitrary mass and coupling to curvature on a conformally static spacetime, no general recipe for a derivation of adequate “positivity” inequalities is apparent. For static spacetimes a strategy similar to the one pursued for the massive field may work and for conformally static spacetimes rescaling of the thermal observables with different powers of the scale factor may lead to reasonable inequalities.

It is not a priori clear that positivity inequalities are preserved under the dynamics of the thermal observables. Indeed the result of [12] that the region of definition of LTE states is always a future light cone implies that the dynamic equations can have a past bounded domain of definition. In the simple example of the heat bang states discussed in [11] the thermal observables diverge on the boundary of the domain of LTE.

Two open questions in this context are, whether there must always be a singularity of some sort on the boundary of the domain of LTE for nontrivial ∞-LTE states and whether the domain of LTE can be future bounded. An investigation of these questions would be of some relevance to the assessment of the results for extrinsic LTE states in section 3.2. In this case the domain of LTE can be future bounded but no singularities occur, as the states are Hadamard states defined on the whole spacetime.

The difficulties in deriving suitable inequalities in a more general setting are closely linked to the difficulties concerning the macroobservable interpretation. If explicit representations in terms of series of balanced derivatives which correspond to macroobservables which are simple (inverse) powers of β can be given, these series have to fulfil the inequalities for the massless field in Minkowski spacetime. However it is not clear whether such powers are contained in a suitably extended set of thermal observables, which is the prerequisite for the existence of convergent series approximating them.

3.4.4. Macroobservable Interpretation

Another interesting question needs to be pointed out. The interpretation of the proposed refined LTE condition in terms of macroobservables is not clear in general. This can be understood as a scale problem in the sense that the relation between macroscopic and microscopic theory is unclear. The problem can partly be blamed on the fact that the foundation of thermodynamics in curved spacetimes is much less understood than it is in flat spacetime. This makes it difficult to decide whether thermodynamic relations that emerge from a macroobservable interpretation on a curved spacetime are thermodynamically acceptable.

The extrinsic LTE condition implies a macroobservable interpretation for the microobservables as the expectation values of microobservables on Minkowski spacetime bear a macroobservable interpretation by definition (2.2.3). However, it was illustrated in the previous sections of this chapter that this macroobservable interpretation comes with some serious questions. Also the macroobservables corresponding to the balanced derivatives for the massive field in Minkowski spacetime are not straight forward to interpret and an extended set of thermal observables is necessary to derive physically meaningful results as done in [23].

Recalling the considerations in section 3.1 it seems not reasonable to transfer macroobservable interpretation between spacetimes with different geometry or at least topology of the Cauchy surface. Thus on static spacetimes it seems reasonable to extract the macroobservable interpretation from KMS states. For the conformally static spacetimes the results of section 3.2 seem somewhat peculiar at first. Plugging the trace relation (3.2.2) into equation (3.2.6) the resulting equation for a spatially homogeneous and isotropic state in the case of conformal coupling is

$$\ddot{\Theta} + 3H\dot{\Theta} + 2H^2\Theta = 4C$$

which yields the result

$$\Theta = A_2 e^{-2Ht} + A_1 e^{-Ht} + \frac{C}{2H^2}.$$

This in conjunction with the solution of equation (3.2.14) suggests setting $A_1 = 0$ and interpreting $\Theta - \frac{C}{2H^2} \propto \frac{1}{\beta^2}$ for the massless conformally coupled field. However, the non-vanishing trace (3.2.2) also implies that the macroobservable interpretation cannot be simply carried over from Minkowski spacetime, unless the trace is accounted for, e.g. by taking $\varepsilon_{\mu\nu} - \frac{1}{4} g_{\mu\nu} \varepsilon_\lambda^\lambda$ as the microobservable to identify with the $\varepsilon_{\mu\nu}$ macroobservable on Minkowski spacetime. If this is done, consistency of such identifications with the dynamic equations must be checked. As noted above a full consideration of the macroobservable interpretation is beyond the scope of this work. For sake of illustration the case of the thermal energy-momentum tensor of a conformally coupled massless field in de Sitter spacetime will be investigated in the following section.

As a general remark, one should note that the equations derived from equations (3.2.3) and (3.2.4) are valid for all Hadamard states and are in their final form without further input. Equations (3.2.5') and (3.2.6') on the other hand require trace relations, which are encoded in the macroobservable interpretation if one exists. This means that the quest for a macroobservable interpretation suffers from the difficulties of identifying suitable trace relations. Part of the difficulty identifying suitable trace relations is that these relations are assumed for the whole domain of definition of the state, which requires them to be compatible with dynamics in a suitable sense.

Section 3.2 as well as this subsection can be understood as an investigation into the question what constitutes compatibility with dynamics, where the focus lies on states resembling KMS states in the sense that they are spatially homogeneous. Of course the trace relation that was proposed as potentially compatible with dynamics very probably encompasses also spatially inhomogeneous states, however we refrain from identifying an example here.

3.5. An Application

In this section we will apply the LTE-equations and positivity inequalities to check whether the final state of the massive field found in section 3.3 corresponds to a well defined mixture of KMS states. However, as checking the positivity inequalities meets the same technical difficulties as the proof of said inequalities, only graphical evidence will be given.

For the model at hand let

$$g_a(\epsilon, m, \rho, \beta) = \frac{1}{\beta^{2a}} \int_0^\infty \frac{q^{2a}}{\sqrt{q^2 + m^2\beta^2}} \left(\frac{2B(q, \epsilon, m, \rho) + 1}{e^{\sqrt{q^2+\epsilon^2 m^2 \beta^2}} - 1} + B(q, \epsilon, m, \rho) \right) dq \propto \Theta_{\beta, 2a-2}$$

$$B(q, \epsilon, m, \rho) = \frac{\sinh^2\left(\frac{\pi(\sqrt{q^2+m^2\beta^2} - \sqrt{q^2+\epsilon^2 m^2\beta^2})}{2\beta\rho}\right)}{\sinh\left(\frac{\pi\sqrt{q^2+m^2\beta^2}}{\beta\rho}\right)\sinh\left(\frac{\pi\sqrt{q^2+\epsilon^2 m^2\beta^2}}{\beta\rho}\right)}$$

Defining $r := \beta\rho$ and $M := \beta m$ the parameter β is eliminated in the inequalities and only three free parameters remain.

Again one meets considerable technical difficulties if one tries to check inequalities (3.4.4). Therefore only numerical evidence will be presented here to indicate whether these inequalities are probably fulfilled or violated. For the numerics to be meaningful some remarks about appropriate orders of magnitude of the model parameters seem in order.

If one is interested in an inflationary scenario, one may pick $\epsilon = 10^{-30}$, implying an expansion by 30 orders of magnitude. To gauge which order of magnitude is reasonable to choose for the other parameters, recall that the inverse temperature before inflation is given by $\epsilon\beta$. If one assumes the temperature before inflation to be reasonably below the Planck scale, for example at the supposed GUT scale, one is lead to $\epsilon\beta \sim 10^3$, i.e. $\beta \sim 10^{33}$ in Planck units. In SI units the temperature before inflation is thus of the order of magnitude $T_{\text{in}} \sim 10^{29}$K, which would correspond to a temperature after inflation of the order of magnitude of $T_{\text{out}} \sim 0.1$K if the field were massless. If one assumes a mass $m \sim 10^{-17}$, which is the order of magnitude of the Higgs mass $m \sim 100GeV/c^2$, one is lead to $M \sim 10^{16}$. The choice of r determines the range of the Hubble parameter. In the present model the Hubble parameter during the expansion starts out as $H_{\max} \sim \frac{r}{\epsilon\beta}$ and decreases to $H_{\min} \sim \frac{r}{\beta}$. As the time scale for inflation is usually assumed to be smaller or equal to $\Delta t \sim 10^{14}$ in Planck units or $\Delta t \sim 10^{-30}s$ in SI units, and the order of magnitude of inflation is assumed above $\epsilon^{-1} \gtrsim 10^{30}$ one may assume $H_{\min} \sim (\epsilon\Delta t)^{-1} \gtrsim 10^{16}$ in Planck units, which implies $r \gtrsim 10^{49}$.

In the numerical calculations the parameters will be chosen near the orders of magnitude described above. In the following illustrations

$$h_n(M, \epsilon, r) := \frac{g_n^{n+1}(\epsilon, m, \rho, \beta)}{g_{n+1}^n(\epsilon, m, \rho, \beta)}$$

is plotted for $n = 1$ and $n = 2$ for two parameter sets. It can be seen that all the curves are monotonously increasing, in contrast to the behaviour seen in figure 3.2.

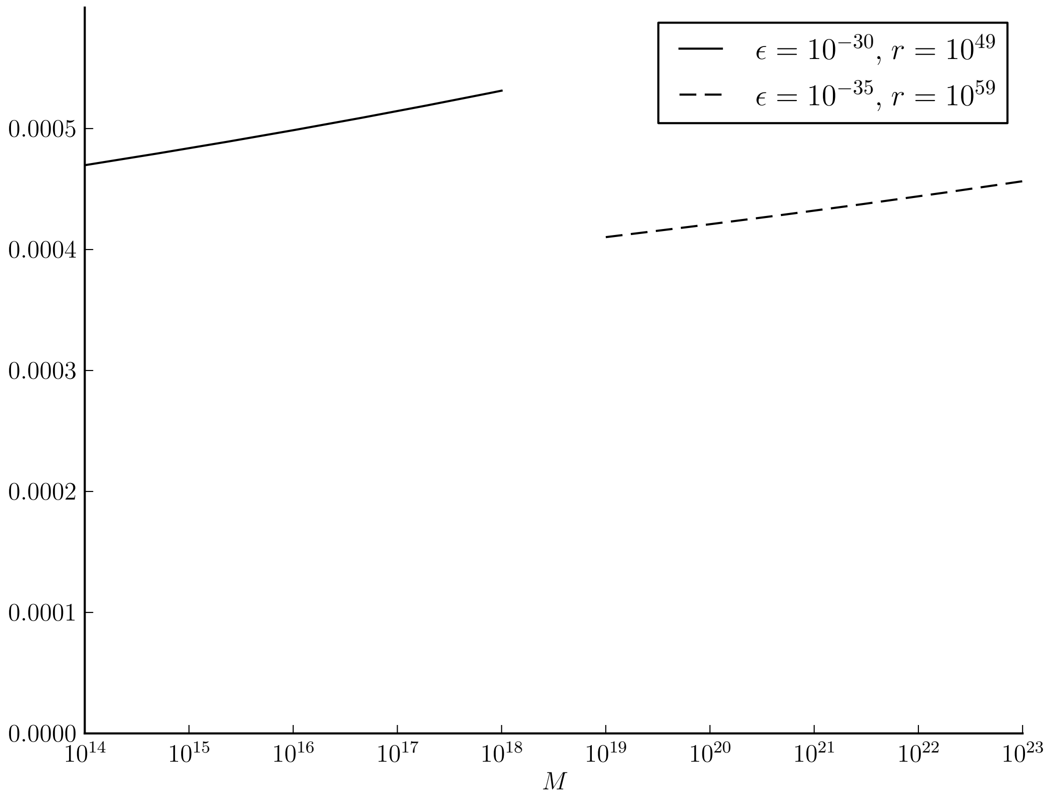

Figure 3.3.: Plot of h_1 for two different sets of parameters

The numerics thus seem to indicate that the resulting states at late times of the model investigated in section 3.3 may not be valid mixtures of KMS states as they apparently violate (A.4.2) from which the positivity requirement (3.4.4) follows, which might consequently be violated at least for some range of values for M. This result is very peculiar, as it indicates that a simple mass term may be sufficient to destroy thermality under some geometric circumstances, not only in the sense that a mixture of thermal states emerges but really leading to a state that has no valid thermal interpretation.

In the context of cosmological particle creation this may be interpreted in the sense that the particles that are created by the expansion of spacetime are, in general, not in thermal equilibrium and even destroy thermal equilibrium states for certain ranges of the $\frac{m}{T_{\text{out}}}$-ratio. As the effect seems to occur for a large ratio, corresponding

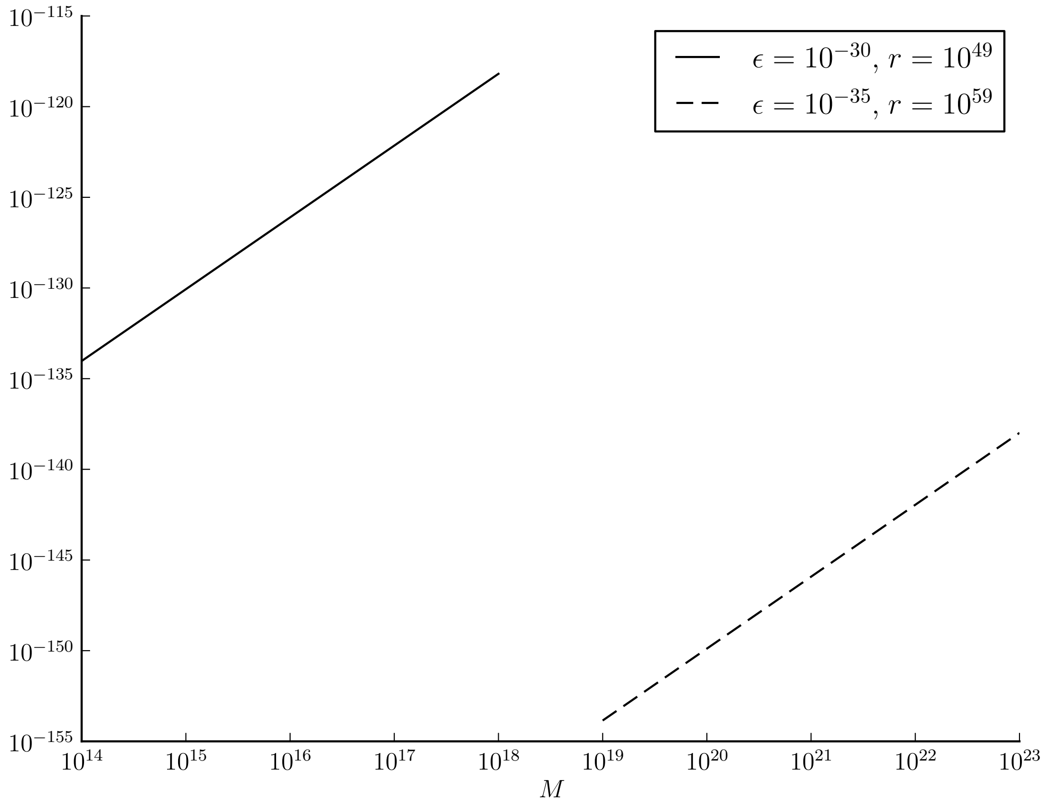

Figure 3.4.: Plot of h_2 for two different sets of parameters

to "low temperature", this effect is not very surprising. It is however interesting in a physical sense that for standard inflaton models the $\frac{m}{T_{\text{out}}}$-ratio is to be considered "large" as the above estimate illustrates and therefore this effect can be expected to play a role for the inflaton field. This is due to the fact that the true temperature for early times in the model considered here is $T_{\text{in}} = \frac{1}{\epsilon\beta}$, which means that many orders magnitude of inflation require a small β, which in turn leads to a large M.

It may be interesting to investigate more realistic inflation models in a similar thermal context to see how generic the described effect is.

4. Cosmological Perturbation Theory

In this chapter, some points in the context of cosmological perturbation theory are discussed in the light of a more rigorous approach to quantum field theory. The focus of this investigation lies on the derivation of the cosmic microwave background's spectrum of temperature inhomogeneities.

As was explained in section 2.3 three relevant epochs are to be distinguished for this derivation. The first relevant epoch is the inflationary universe, which is assumed to present the origin of the inhomogeneities which give rise to perturbations of the background temperature. The second epoch is the phase of tight coupling, which is mostly relevant for the coupling of the photon fluid to the dark matter distribution, thus giving rise to the matter inhomogeneities that lead to cosmological structure formation. Furthermore, fluid dynamic interactions, especially sound waves in the coupled fluid, are responsible for the spectrum of temperature inhomogeneities of the photon background at small angles. For the spectrum at large angles only the distribution of inhomogeneities and the interactions in the time shortly before recombination are relevant, as discussed in 2.3.5. The last relevant epoch is the time of free streaming, which is the time span from recombination until present day, within which the mean free path of the photons is approximated to be infinite.

Of these phases the first and third can be straight forwardly approached from the point of view of algebraic quantum field theory, whereas the second phase cannot be treated in a fully rigorous way with existing methods, because it involves field interactions. Even for the treatment of the other phases there is however one caveat. As the spacetime in algebraic quantum field theory is assumed a classical entity, whose dynamics are determined by the matter content of the spacetime, a full quantum treatment is impossible in this theoretical framework. The dynamics of spacetime are treated in a semiclassical setting. A semiclassical approach is implicit to cosmological perturbation theory, in the sense that the background quantities are assumed classical.

This chapter consists of two sections. In the first section, the quantisation of the field perturbation in the inflationary phase will be investigated. The second section discusses the derivation of the perturbation spectrum in the phase of free streaming in the context of the LTE framework.

4.1. Dynamics of Perturbations in Inflation

In this section the coupled dynamical system of the field and metric perturbation in the era of inflation are investigated under the principal angle of the quantisation of perturbations. As the dynamical system includes a constraint, the treatment of this constraint is a recurring topic of this section. The treatment in the present work takes a straight forward approach and does not make contact with existing literature on quantisation of dynamical systems with constraints.

The first subsection of this investigation is a review of the dynamical system in a spatial mode setting. Taking a naive approach, which ignores the question of appropriate treatment of the constraint, an ambiguity in the choice of quantisation is found and discussed.

In the second subsection the dynamical system of the modes is discussed in the context of symplectic geometry. Especially the impact of the constraint equation on the symplectic structure is investigated. The result of this investigation is discussed in the context of the quantisation ambiguity, where the quantisation procedure sticks rather close to the concept of generic Dirac quantisation.

The last subsection briefly reviews the previous analysis from the point of view of algebraic quantum field theory. However, this investigation remains closely tied to the quantisation procedure discussed in the preceding subsections, so the more intricate questions related to quantum systems with constraints, such as existence of fundamental solutions and the likes, will not play a role here.

4.1.1. CCR Quantisation is Ambiguous

In this subsection the dynamical system consisting of equations (2.3.3), (2.3.4) and (2.3.2) is recast in a spatial mode setting. The first objective is to simplify and unify the notation of the equations.

The dynamical system for the gauge invariant field perturbation χ and the Bardeen potential Ψ is

$$
\begin{aligned}
&\Psi'' - \triangle\Psi + 2\left(\mathcal{H} - \frac{\phi_0''}{\phi_0'}\right)\Psi' + 2\left(\mathcal{H}' - \frac{\phi_0''}{\phi_0'}\mathcal{H}\right)\Psi = 0 \\
&\chi'' - \triangle\chi + \quad 2\mathcal{H}\chi' + \quad V_{,\phi\phi}\, a^2\chi = 4\phi_0'\Psi' - 2V_{,\phi}\, a^2\Psi \\
&\qquad\qquad\qquad \Psi' + \quad \mathcal{H}\Psi = 4\pi G\phi_0'\chi
\end{aligned}
$$

For simplified and homogeneous display of the equations, the following calculations use the parameter $z = \frac{a\phi_0'}{\mathcal{H}}$ and the slow-roll parameters ε and δ as defined in (2.3.7) and (2.3.8). With the additional use of of the Klein-Gordon equation (2.3.1)

$$\phi_0'' + 2\mathcal{H}\phi_0' + V_{,\phi}(\phi_0)a^2 = 0$$

for the background field ϕ_0, a number of useful relations can be shown.

$$\frac{z'}{z} = (1+\varepsilon-\delta)\mathcal{H} \qquad \frac{z''}{z} = \left(2 + 2\varepsilon - 3\delta + 2\varepsilon^2 - 3\varepsilon\delta + \delta^2 - \frac{\delta'}{\mathcal{H}}\right)\mathcal{H}^2$$

$$\frac{\mathcal{H}'}{\mathcal{H}} = (1-\varepsilon)\mathcal{H} \qquad \frac{\mathcal{H}''}{\mathcal{H}} = (2 - 4\varepsilon + 2\varepsilon\delta)\,\mathcal{H}^2$$

$$\frac{\phi_0''}{\phi_0'} = (1-\delta)\mathcal{H} \qquad \frac{\phi_0'''}{\phi_0'} = \left(2 - \varepsilon - 3\delta + \varepsilon\delta + \delta^2 - \frac{\delta'}{\mathcal{H}}\right)\mathcal{H}^2$$

$$V_{,\phi}\, a^2 = -(3-\delta)\frac{\mathcal{H}^2 z}{a} \qquad V_{,\phi\phi}\, a^2 = \left((3-\delta)(\varepsilon+\delta) + \frac{\delta'}{\mathcal{H}}\right)\mathcal{H}^2$$

$$\frac{\varepsilon'}{\varepsilon} = 2(\varepsilon-\delta)\mathcal{H}$$

These relations can be used to unify the notation for the dynamical system such that only a, $\mathcal{H}$, δ, ε and z are used.

$$\Psi'' - \triangle\Psi + 2\delta\mathcal{H}\Psi' + 2(\delta-\varepsilon)\mathcal{H}^2\Psi = 0 \tag{4.1.1}$$

$$\chi'' - \triangle\chi + 2\mathcal{H}\chi' + \left((3-\delta)(\varepsilon+\delta) + \frac{\delta'}{\mathcal{H}}\right)\mathcal{H}^2\chi = 4\frac{\mathcal{H}z}{a}\Psi' + 2(3-\delta)\frac{\mathcal{H}^2 z}{a}\Psi \tag{4.1.2}$$

$$\Psi' + \mathcal{H}\Psi = \frac{\varepsilon\mathcal{H}a}{z}\chi \tag{4.1.3}$$

The aim is now, to eliminate the dependence on Ψ from equation (4.1.2). To achieve this, firstly equation (4.1.3) is inserted into equation (4.1.2) and equation (4.1.1) is inserted into the derivative of equation (4.1.3). This yields

$$\chi'' - \triangle\chi + 2\mathcal{H}\chi' + \left(-\varepsilon + 3\delta - \varepsilon\delta - \delta^2 + \frac{\delta'}{\mathcal{H}}\right)\mathcal{H}^2\chi = 2(1-\delta)\frac{\mathcal{H}^2 z}{a}\Psi \tag{4.1.4}$$

$$\triangle\Psi + (1-2\delta)\mathcal{H}\Psi' + (1+\varepsilon-2\delta)\mathcal{H}^2\Psi = \frac{\varepsilon\mathcal{H}a}{z}(\chi' + (1-\delta)\mathcal{H}\chi) \tag{4.1.5}$$

Now Ψ' is eliminated from equation (4.1.5) using equation (4.1.3), which leads to

$$\triangle\Psi + \varepsilon\mathcal{H}^2\Psi = \frac{\varepsilon\mathcal{H}a}{z}(\chi' + \delta\mathcal{H}\chi) \tag{4.1.6}$$

Applying the operator $\triangle + \varepsilon\mathcal{H}^2$ in equation (4.1.4) and inserting equation (4.1.6) yields an equation for χ only

$$(\triangle + \varepsilon\mathcal{H}^2)\chi'' + 2\mathcal{H}(\triangle + \varepsilon\delta\mathcal{H}^2)\chi' + \left(-\triangle^2 + \left(-2\varepsilon + 3\delta - \varepsilon\delta - \delta^2 + \frac{\delta'}{\mathcal{H}}\right)\mathcal{H}^2\triangle\right.$$
$$\left. + \left(-\varepsilon + \delta - \varepsilon\delta + \delta^2 + \frac{\delta'}{\mathcal{H}}\right)\varepsilon\mathcal{H}^4\right)\chi = 0 \tag{4.1.7}$$

This equation is a fourth order partial differential equation but it nevertheless tractable using the Fourier transformation. Considering the mode decomposition of the field, the equation reduces to a second order ODE which can be interpreted as a Klein-Gordon mode equation with additional inverse powers of the mode number in the "effective mass term" of the modes. The full system of equations in the mode setting is

$$\Psi_k'' + 2\delta\mathcal{H}\Psi_k' + \left[2(\delta - \varepsilon)\mathcal{H}^2 + k^2\right]\Psi_k = 0 \tag{4.1.8}$$

$$\chi_k'' + 2\mathcal{H}\frac{k^2 - \varepsilon\delta\mathcal{H}^2}{k^2 - \varepsilon\mathcal{H}^2}\chi_k' + \left[k^4 + \left(-2\varepsilon + 3\delta - \varepsilon\delta - \delta^2 + \frac{\delta'}{\mathcal{H}}\right)\mathcal{H}^2k^2\right.$$
$$\left. + \left(\varepsilon - \delta + \varepsilon\delta - \delta^2 - \frac{\delta'}{\mathcal{H}}\right)\varepsilon\mathcal{H}^4\right]\frac{1}{k^2 - \varepsilon\mathcal{H}^2}\chi_k = 0 \tag{4.1.9}$$

$$\Psi_k' + \mathcal{H}\Psi_k = \frac{\varepsilon\mathcal{H}a}{z}\chi_k \tag{4.1.10}$$

Lemma 4.1.1.
Ψ and χ cannot both fulfil ordinary CCR.

Proof.
For the proof of this lemma it is easiest to investigate equal time CCR. We will start from the CCR for Ψ in the form

$$[\Psi(x), \Psi(y)]\Big|_{x^0=y^0} = [\Psi'(x), \Psi'(y)]\Big|_{x^0=y^0} = 0$$

$$[\Psi(x), \Psi'(y)]\Big|_{x^0=y^0} = i\delta(\vec{x} - \vec{y})$$

To calculate the commutation relations of χ we derive from equations (4.1.3) and (4.1.5) the relation

$$\chi' = -\frac{\delta z}{\varepsilon a}\Psi' + \frac{z\Big(\triangle + (\varepsilon - \delta)\mathcal{H}^2\Big)}{\varepsilon \mathcal{H} a}\Psi \tag{4.1.11}$$

which can then be used to compute the commutation relations

$$\begin{aligned}
[\chi(x), \chi(y)]\Big|_{x^0=y^0} &= 0 \\
[\chi'(x), \chi'(y)]\Big|_{x^0=y^0} &= \frac{z^2\Big(\triangle^x + (\varepsilon - \delta)\mathcal{H}^2\Big)\Big(\triangle^y + (\varepsilon - \delta)\mathcal{H}^2\Big)}{(\varepsilon a)^2\mathcal{H}}\,[\Psi(x), \Psi(y)]\Big|_{x^0=y^0} \\
&\quad - \frac{\delta z^2\Big(\triangle^y + (\varepsilon - \delta)\mathcal{H}^2\Big)}{(\varepsilon a)^2\mathcal{H}}\,[\Psi'(x), \Psi(y)]\Big|_{x^0=y^0} \\
&\quad - \frac{\delta z^2\Big(\triangle^x + (\varepsilon - \delta)\mathcal{H}^2\Big)}{(\varepsilon a)^2\mathcal{H}}\,[\Psi(x), \Psi'(y)]\Big|_{x^0=y^0} \\
&= 0 \\
[\chi(x), \chi'(y)]\Big|_{x^0=y^0} &= \frac{z^2\Big(\triangle^y + (\varepsilon - \delta)\mathcal{H}^2\Big)}{(\varepsilon \mathcal{H} a)^2}\,[\Psi'(x), \Psi(y)]\Big|_{x^0=y^0} \\
&\quad - \frac{\delta z^2}{(\varepsilon a)^2}\,[\Psi(x), \Psi'(y)]\Big|_{x^0=y^0} \\
&= -i\frac{z^2\Big(\triangle^x + \varepsilon\mathcal{H}^2\Big)}{(\varepsilon \mathcal{H} a)^2}\delta(\vec{x} - \vec{y})
\end{aligned}$$

This proves the claim. □

As a direct corollary it is not possible for Ψ and χ to both be in a Hadamard state. As χ does not fulfil a normal Klein-Gordon equation but a dynamic equation of fourth order, it is not to be expected that the CCR or the Hadamard condition are of any significance in this case. The field Ψ however fulfils a Klein-Gordon type equation, so at first glance it seems reasonable to assume standard CCR for this field as a means of quantisation and treating χ as a derived field whose commutation relations as derived from the CCR for Ψ bear no significance.

However, in the standard approach, quantisation is done by assuming CCR for the field $u = a\chi + z\Psi$ defined in equation (2.3.5). As u also fulfils a Klein-Gordon type equation, this approach is equally valid from the simplistic point of view taken in this subsection. However, this approach leads to an inequivalent quantisation, as shown in the following lemma, which also makes more explicit what the CCR quantisation of u implies for the commutation relations of Ψ.

Lemma 4.1.2.
If standard CCR for u *and* $[\Psi(x), \Psi(y)]\Big|_{x^0=y^0} = [\Psi'(x), \Psi'(y)]\Big|_{x^0=y^0} = 0$ *are imposed,*

$$[\Psi(x), \Psi'(y)]\Big|_{x^0=y^0} = i\frac{\varepsilon^2\mathcal{H}^2}{4\pi z^2}\frac{1}{|\vec{x}-\vec{y}|}$$

Proof.
The commutation relations for Ψ are derived in an indirect way. Using equation (4.1.3) the following relations can be derived

$$u = \frac{z}{\varepsilon\mathcal{H}}\Psi' + \frac{1+\varepsilon}{\varepsilon}z\Psi$$

$$u' = \frac{z}{\varepsilon\mathcal{H}}\triangle\Psi + (1+\varepsilon-\delta)\mathcal{H}u$$

$$[u(x), u'(y)]\Big|_{x^0=y^0} = -\frac{z^2}{\varepsilon^2\mathcal{H}^2}\triangle_y[\Psi(y), \Psi'(x)]\Big|_{x^0=y^0} \tag{4.1.12}$$

Now the last relation can be recast in the form

$$\frac{iz^2}{\varepsilon^2\mathcal{H}^2}\triangle_y[\Psi(y), \Psi'(x)]\Big|_{x^0=y^0} = \delta(\vec{x}-\vec{y}) = \delta(\vec{y}-\vec{x})$$

which is the distributional differential equation for the fundamental solution of the Laplacian. This is straight forward to solve and yields

$$[\Psi(x), \Psi'(y)]\Big|_{x^0=y^0} = \frac{i\varepsilon^2\mathcal{H}^2}{4\pi z^2}\frac{1}{|\vec{x}-\vec{y}|}$$

which implies the claim. □

It is obvious that commutation relations for Ψ are quite different from the CCR and even non-local. Thus, if u is quantised with standard CCR, this implies that Ψ cannot be interpreted as a local scalar quantum field at the same time. This means that CCR quantisation for Ψ and u yield inequivalent quantum field theories. The following subsection investigates the classical dynamical system in some depth to control this ambiguity.

It is also interesting to note that, if there is an argument that favours the choice of u as the variable to canonically quantise, the fields Ψ and χ, which bear well-defined physical meaning, have to be interpreted as non-local. Such a situation may point to an underlying non-commutativity of spacetime, leading to non-locality. This point will be referred to in the outlook in chapter 5.

4.1.2. Canonical Symplectic Form

In this subsection the dynamical system of the modes is reviewed from the angle of symplectic geometry. To this avail, the dynamical system has to be cast in Hamiltonian form, which implies the identification of the Darboux coordinates of the symplectic form. To achieve this, it is necessary to use the action presented e.g. in [7] and derive the corresponding Hamiltonian system. Then the impact of the constraint on the symplectic structure is discussed.

For the treatment of a dynamical system with second class constraints several methods exist. The dynamical variables, including the Lagrange multipliers, may be combined into a reduced set of dynamical variables in such a way that the resulting Lagrangian contains no constraints and only depends on the new variables. This is the strategy which is pursued in the standard literature on cosmological perturbations during inflation. However, finding an appropriate reduced set of dynamical variables is not a straight forward task and is usually done by simply choosing the appropriate ansatz to begin with. As the resultant dynamical system is a generic Hamiltonian system, quantisation is straight forward.

A second method consists in the straight forward construction of a Hamiltonian containing the Lagrange multipliers and the subsequent application of a standard procedure to eliminate the Lagrangian multipliers. This procedure does not lead to an obvious reduction of phase space, however it can be seen that the phase space is not symplectic and the maximally symplectic subspace whose complement has a dimension which is identical to the number of constraints. This procedure has the disadvantage that the geometry of the phase space is unclear and therefore quantisation of the dynamical system is not straight forward.

Yet another method consists in ignoring the constraints at first, to produce an "unconstrained Hamiltonian" with a corresponding canonical symplectic form. Then the constraints are used to derive the so-called Dirac bracket from the Poisson bracket of the unconstrained system. The tensor corresponding to the Dirac bracket will be called the "Dirac form" in the present treatment. The Dirac form is degenerate in a number of dimensions corresponding to the number of constraints and symplectic in the remaining dimensions. The present treatment will pursue the derivation of the Dirac bracket to shed some light on the quantisation of the system. The classic reference for this method is [14] but it is treated to varying degree of detail in many standard textbooks.

As a first step it is convenient to rescale the fields Ψ and χ so they have the same dimension. Therefore we define the rescaled fields

$$\boldsymbol{\psi} := z\Psi \qquad \lambda := a\chi$$

The Lagrangian given in [7], equation (10.68) is given here in terms of the rescaled variables, suppressing the total divergences and simplifying by setting $\Phi = -\Psi$ and $L := 4\triangle(B - E')$ (note the different notation). From the treatment in [7] it is clear that the terms introduced by switching to gauge invariant variables cancel out.

$$\begin{aligned}\mathscr{L} = &\frac{1}{2\varepsilon}\left[-3(\boldsymbol{\psi}')^2 + 6(\varepsilon-\delta)\mathcal{H}\boldsymbol{\psi}'\boldsymbol{\psi} + (\varepsilon - 3\varepsilon^2 + 6\varepsilon\delta - 3\delta^2)\mathcal{H}^2\boldsymbol{\psi}^2 + \boldsymbol{\psi}\triangle\boldsymbol{\psi}\right]\\ &+\frac{1}{2}\left[(\lambda')^2 - 2\mathcal{H}\lambda'\lambda + \left(1 - 3\varepsilon - 3\delta + \varepsilon\delta + \delta^2 - \frac{\delta'}{\mathcal{H}}\right)\mathcal{H}^2\lambda^2 + \lambda\triangle\lambda\right]\\ &+ 4\mathcal{H}\boldsymbol{\psi}'\lambda + 2(1-2\varepsilon+\delta)\mathcal{H}^2\boldsymbol{\psi}\lambda + zL\left[-\frac{1}{\varepsilon}\boldsymbol{\psi}' + \frac{\varepsilon-\delta}{\varepsilon}\mathcal{H}\boldsymbol{\psi} + \mathcal{H}\lambda\right]\end{aligned}$$

The next step in the treatment is to consider the "unconstrained Lagrangian", thus setting $L = 0$. We will additionally switch to a "mode Lagrangian".

$$\begin{aligned}\mathscr{L}_{0,k} = &\frac{1}{2\varepsilon}\left[-3(\boldsymbol{\psi}_k')^2 + 6(\varepsilon-\delta)\mathcal{H}\boldsymbol{\psi}_k'\boldsymbol{\psi}_k + [(\varepsilon - 3\varepsilon^2 + 6\varepsilon\delta - 3\delta^2)\mathcal{H}^2 - k^2]\boldsymbol{\psi}_k^2\right]\\ &+\frac{1}{2}\left[(\lambda_k')^2 - 2\mathcal{H}\lambda_k'\lambda_k + \left[\left(1 - 3\varepsilon - 3\delta + \varepsilon\delta + \delta^2 - \frac{\delta'}{\mathcal{H}}\right)\mathcal{H}^2 - k^2\right]\lambda_k^2\right]\\ &+ 4\mathcal{H}\boldsymbol{\psi}_k'\lambda_k + 2(1-2\varepsilon+\delta)\mathcal{H}^2\boldsymbol{\psi}_k\lambda_k\end{aligned}$$

Note that the mode Lagrangian is not the Fourier transform of the Lagrangian, as a Fourier transformation would not map products of functions to products of their Fourier transforms but to convolutions. The Lagrangian for the modes is instead designed to produce the correct dynamic equations for the modes.

From the mode Lagrangian one calculates the canonical momentum modes

$$\Pi_k = \frac{\partial\mathscr{L}_{0,k}}{\partial\boldsymbol{\psi}_k'} = -\frac{3}{\varepsilon}\boldsymbol{\psi}_k' + 3\frac{\varepsilon-\delta}{\varepsilon}\mathcal{H}\boldsymbol{\psi}_k + 4\mathcal{H}\lambda_k$$

$$\Leftrightarrow \quad \boldsymbol{\psi}_k' = -\frac{\varepsilon}{3}\Pi_k + (\varepsilon-\delta)\mathcal{H}\boldsymbol{\psi}_k + \frac{4}{3}\varepsilon\mathcal{H}\lambda_k$$

$$\kappa_k = \frac{\partial \mathscr{L}_{0,k}}{\partial \lambda'_k} = \lambda'_k - \mathcal{H}\lambda_k$$

$$\Leftrightarrow \lambda'_k = \kappa_k + \mathcal{H}\lambda_k$$

which allows the derivation of the unconstrained Hamiltonian for the modes

$$\begin{aligned} \mathscr{H}_{0,k} = & -\frac{\varepsilon}{6}\Pi_k^2 + (\varepsilon - \delta)\mathcal{H}\Pi_k \boldsymbol{\psi}_k + \left(-\frac{1}{2}\mathcal{H}^2 + \frac{1}{2\varepsilon}k^2\right)\boldsymbol{\psi}_k^2 \\ & + \frac{1}{2}\kappa_k^2 + \mathcal{H}\kappa_k\lambda_k + \left[\frac{1}{6}\left(-7\varepsilon + 9\delta - 3\varepsilon\delta - 3\delta^2 + 3\frac{\delta'}{\mathcal{H}}\right)\mathcal{H}^2 + k^2\right]\lambda_k^2 \\ & + \frac{4}{3}\varepsilon\mathcal{H}\Pi_k\lambda_k - 2(1-\delta)\mathcal{H}^2\boldsymbol{\psi}_k\lambda_k \end{aligned}$$

As the canonical variables of the unconstrained Hamiltonian are the Darboux coordinates of the canonical symplectic form on the unconstrained phase space, the symplectic form corresponding to the Poisson bracket takes the standard form.

$$\forall \eta : \ (\omega^{\alpha\beta})_{\alpha,\beta}(\eta) = \begin{pmatrix} 0_2 & \mathbb{1}_2 \\ -\mathbb{1}_2 & 0_2 \end{pmatrix}$$

The constraint equation implies a projection to a subspace of the phase space. Contrary to the projection to an energy hypersurface this projection constrains the accessible phase space for all solutions of the dynamical system so it can be interpreted as a genuine reduction of phase space. The primary constraint given by equation (4.1.10) in canonical variables reads

$$\mathcal{C}_1 = \Pi_k - \mathcal{H}\lambda_k = 0 \tag{4.1.13}$$

and a secondary constraint can be derived as

$$\mathcal{C}_2 := -\frac{1}{\mathcal{H}}\{\mathcal{C}_1, \mathscr{H}_{0,k}\} - \frac{1}{\mathcal{H}}\frac{\partial \mathcal{C}_1}{\partial \eta} = \kappa_k - \frac{\varepsilon\mathcal{H}^2 - k^2}{\varepsilon\mathcal{H}}\boldsymbol{\psi}_k + \delta\mathcal{H}\lambda_k = 0 \tag{4.1.14}$$

using the first constraint. The tertiary constraint vanishes

$$\mathcal{C}_3 = \{\mathcal{C}_2, \mathscr{H}_{0,k}\} + \frac{\partial \mathcal{C}_2}{\partial \eta} = 0$$

applying the first two constraints, so there are exactly two geometrically independent constraints, which means that the phase space dimension is reduced by two. It is worth emphasising that these constraints are fulfilled by all valid solutions of the dynamical system, so all solutions of the dynamical system can be described as living on a two dimensional reduced phase space.

For the treatment of constraints it is of great importance, whether they are first or second class constraints. In the case discussed here, only second class constraints occur, due to the following lemma.

Lemma 4.1.3.
The constraints (4.1.13) *and* (4.1.14) *are second class constraints for* $k \neq 0$*.*

Proof.
To fix notation let $(M_{ab})_{a,b}$ denote the matrix with components M_{ab}. If the constraint matrix $(C_{ab})_{a,b} := \Big(\{\mathcal{C}_a, \mathcal{C}_b\}\Big)_{a,b}$ is invertible, the constraints are second class constraints. Using the definition of the Poisson bracket

$$\{f, g\} := \frac{\partial f}{\partial \boldsymbol{\psi}_k}\frac{\partial g}{\partial \Pi_k} + \frac{\partial f}{\partial \lambda_k}\frac{\partial g}{\partial \kappa_k} - \frac{\partial f}{\partial \Pi_k}\frac{\partial g}{\partial \boldsymbol{\psi}_k} - \frac{\partial f}{\partial \kappa_k}\frac{\partial g}{\partial \lambda_k}$$

one gets

$$C_{12} = \{\mathcal{C}_1, \mathcal{C}_2\} = \frac{\varepsilon\mathcal{H}^2 - k^2}{\varepsilon\mathcal{H}} - \mathcal{H} = -\frac{k^2}{\varepsilon\mathcal{H}}$$

which yields, due to antisymmetry

$$(C_{ab})_{a,b} = \frac{k^2}{\varepsilon\mathcal{H}}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

which is invertible as long as $k \neq 0$. □

First class constraints usually occur in the context of gauge theories so one might expect that a full treatment of scalar perturbation theory, not using gauge invariant variables might be significantly more complicated, especially when it comes to quantisation. Such a more extensive investigation is not attempted in the present work.

In the present case, the constraints are first class constraints for the zero mode $k = 0$. This implies, that the physical phase space for the zero mode has dimension zero, as primary constraints reduce the dimension by two each, and not only by one, as second class constraints. In the present work, no separate treatment of the zero mode is performed. A complete formulation of the Dirac bracket on the full phase space of all modes is nevertheless possible, as will be seen below.

The Dirac bracket is derived from the Poisson bracket and the constraint matrix as

$$\{f, g\}_{\mathrm{D}} := \{f, g\} - \{f, \mathcal{C}_i\}(C^{-1})_{ij}\{\mathcal{C}_j, g\}$$

and a straight forward calculation yields the mode Dirac form

$$(\omega^{\alpha\beta}_{\mathrm{D},k})_{\alpha,\beta} = \begin{pmatrix} 0 & \frac{\varepsilon\mathcal{H}}{k^2} & \frac{\varepsilon\mathcal{H}^2}{k^2} & -\frac{\varepsilon\delta\mathcal{H}^2}{k^2} \\ -\frac{\varepsilon\mathcal{H}}{k^2} & 0 & 0 & 1 - \frac{\varepsilon\mathcal{H}^2}{k^2} \\ -\frac{\varepsilon\mathcal{H}^2}{k^2} & 0 & 0 & \mathcal{H} - \frac{\varepsilon\mathcal{H}^3}{k^2} \\ \frac{\varepsilon\delta\mathcal{H}^2}{k^2} & -1 + \frac{\varepsilon\mathcal{H}^2}{k^2} & -\mathcal{H} + \frac{\varepsilon\mathcal{H}^3}{k^2} & 0 \end{pmatrix} \tag{4.1.15}$$

which obviously diverges for $k \to 0$. The Dirac bracket on all modes is defined as

$$\left\{ \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix}, \begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \end{pmatrix} \right\}_{\mathrm{D}} := \int \left\{ \begin{pmatrix} f_1(\vec{k}) \\ f_2(\vec{k}) \\ f_3(\vec{k}) \\ f_4(\vec{k}) \end{pmatrix}, \begin{pmatrix} g_1(\vec{k}) \\ g_2(\vec{k}) \\ g_3(\vec{k}) \\ g_4(\vec{k}) \end{pmatrix} \right\}_{\mathrm{D},k} d^3k \tag{4.1.16}$$

where all the functions f_i and g_i are Schwartz functions in k. As the mode Dirac form given in equation (4.1.15) behaves like k^{-2} for $k \to 0$ and the volume element of the integral in equation (4.1.16) gives a factor of k^2 the limit of the integrand for $k \to 0$ is finite. Thus the integrand is a Schwartz function and the integral is well defined. In the remainder of this subsection the treatment is performed in terms of modes but for the following subsection the full Dirac form will play a role.

It is straight forward to check that in coordinates[1]

$$f_1 := \boldsymbol{\psi}_k + \frac{\varepsilon\delta\mathcal{H}}{k^2 - \varepsilon\mathcal{H}^2}\Pi_k + \frac{\varepsilon\mathcal{H}}{k^2 - \varepsilon\mathcal{H}^2}\kappa_k \qquad f_2 := \lambda_k - \frac{1}{\mathcal{H}}\Pi_k$$

$$f_3 := \frac{1}{\mathcal{H}}\Pi_k \qquad f_4 := \frac{k^2}{k^2 - \varepsilon\mathcal{H}^2}\kappa_k$$

the mode Dirac form is of standard form

$$(\tilde{\omega}^{\alpha\beta}_{\mathrm{D},k})_{\alpha,\beta} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

which conforms to the expectation that there are two dynamical degrees of freedom in the system at hand. This implies that it suffices to canonically quantise one appropriate pair of canonically conjugate variables. These variables can be chosen freely and only need to fulfil the requirement $\{X, P\}_{\mathrm{D}} = 1$. This freedom implies the application of the constraints as well as symplectomorphisms. To make a connection to the previous subsection, the possible canonically conjugate variables P for $X = u_k = \boldsymbol{\psi}_k + \lambda_k$ and for $X = \frac{1}{z}\boldsymbol{\psi}_k$ will be the centre of attention here.

Considering $X = u_k$ the corresponding conjugate variable has to fulfil

$$-\frac{\varepsilon\mathcal{H}}{k^2}\frac{\partial P}{\partial \boldsymbol{\psi}_k} + \frac{\varepsilon\mathcal{H}}{k^2}\frac{\partial P}{\partial \lambda_k} + \frac{\varepsilon\mathcal{H}^2}{k^2}\frac{\partial P}{\partial \Pi_k} + \frac{k^2 - \varepsilon\mathcal{H}^2 - \varepsilon\delta\mathcal{H}^2}{k^2}\frac{\partial P}{\partial \kappa_k} = 1$$

[1]The coordinate singularity for $k^2 = \varepsilon\mathcal{H}^2$ can be circumvented by picking other coordinates; the coordinates given here serve only as an example.

which is indeed fulfilled by

$$P = u_k' = (\varepsilon - \delta)\mathcal{H}\boldsymbol{\psi}_k + \left(1 + \frac{4}{3}\varepsilon\right)\lambda_k - \frac{\varepsilon}{3}\Pi_k + \kappa_k$$

which implies that the standard quantisation procedure is indeed justified.

For $X = \frac{1}{z}\boldsymbol{\psi}_k$ the corresponding conjugate variable has to fulfil

$$\frac{\varepsilon\mathcal{H}}{zk^2}\frac{\partial P}{\partial\lambda_k} + \frac{\varepsilon\mathcal{H}^2}{zk^2}\frac{\partial P}{\partial\Pi_k} - \frac{-\varepsilon\delta\mathcal{H}^2}{zk^2}\frac{\partial P}{\partial\kappa_k} = 1$$

which can be fulfilled by

$$P = \alpha X' = -\frac{\alpha\mathcal{H}}{z}\boldsymbol{\psi}_k + \frac{4}{3}\frac{\alpha\varepsilon\mathcal{H}}{z}\lambda_k - \frac{\alpha\varepsilon}{3z}\Pi_k$$

namely if $\alpha = \frac{z^2k^2}{\varepsilon^2\mathcal{H}^2}$. This result is peculiar in that it includes a prefactor of k^2. A comparison with equation (4.1.12) shows that the treatment of this subsection reproduces the result of the previous subsection with respect to the relation of the commutators (or in the classical setting Dirac brackets). However, the treatment in the present subsection allows to take the point of view that the standard treatment of quantising u is canonical in the sense of Dirac quantisation, while the straightforward CCR quantisation of Ψ is not.

As a closing remark for this subsection, we would like to consider the general solution to $X = A\boldsymbol{\psi}_k + B\lambda_k$ and $P = X'$. These requirements lead to the equation

$$\frac{\varepsilon\mathcal{H}}{k^2}(AB' - A'B) + \frac{k^2 - \varepsilon\mathcal{H}^2}{k^2}B^2 + (1-\varepsilon)\frac{\varepsilon\mathcal{H}^2}{k^2}AB + \frac{\varepsilon^2\mathcal{H}^2}{k^2}A^2 = 1$$

$$\varepsilon\mathcal{H}(AB' - A'B) + (k^2 - \varepsilon\mathcal{H}^2)B^2 + (1-\varepsilon)\varepsilon\mathcal{H}^2AB + \varepsilon^2\mathcal{H}^2A^2 = k^2$$

Demanding that A and B do not depend on k, the k-dependent terms can be treated separately and yield $B^2 = 1$. If A and B are additionally required to be real, the only solutions to this equation are $B = 1$ and $B = -1$. This yields

$$A' \mp \varepsilon\mathcal{H}A^2 - (1-\varepsilon)\mathcal{H}A \pm \mathcal{H} = A' \mp (A \mp 1)(A\varepsilon \pm 1)\mathcal{H} = 0$$

which can be cast in a simpler form using $D := A \mp 1$

$$D' \mp D(D\varepsilon \pm (1+\varepsilon))\mathcal{H} = 0$$

such that one receives a Bernoulli differential equation. This type of equation is solvable with trivial solution $D = 0$ and a nontrivial solution which can be found by using $E = \frac{1}{D}$ leading to

$$E' + (1+\varepsilon)\mathcal{H}E = \mp\varepsilon\mathcal{H}$$

a readily solvable linear equation. The solution for A is

$$A = \pm \left(1 - \frac{a^2}{\mathcal{H}} \left(\int\limits_{\eta_0}^{\eta} \varepsilon(\eta') a^2(\eta')\, d\eta' + K \right)^{-1} \right)$$

where K and η_0 account for one free constant. The standard choice of dynamical variable amounts to picking the trivial solution $A = B = 1$, however the present treatment suggests that there is a one-parameter family of possible choices. All these possible choices imply the same classical dynamics, as different choices of dynamical variables are related by symplectomorphisms on phase space. Therefore all choices lead to the same quantum system in terms of the algebra of observables. As there is no obvious mechanism at the current stage of development to justify a particular choice of dynamical variables from the one-parameter family, it is an interesting problem to investigate the dynamical systems these potential variables fulfil. In the context of the dynamic equations for the different fields one can then consider whether they suggest preferred states, whether these preferred states are equal and whether the corresponding two-point functions have the same infrared asymptotics. This seems to be an interesting investigation in its own right, however these questions will not be investigated in the present work.

4.1.3. The Algebraic Point of View

In this subsection the results of this section will be reviewed in the context of algebraic quantum field theory. The general pattern that will be followed is the same as in the previous subsections. First the system without constraint[2] is considered and then the impact of the constraint on this system is investigated. The present subsection does not provide additional information on the dynamical system but clarifies the impact of the constraint on the level of algebraic quantum field theory.

As we will deal with the quantum system here and not the classical system, the question whether quantisation commutes with reduction comes into play. In the present setting, reduction on the classical level can be split up into two parts. First the Poisson bracket on phase space is replaced by the Dirac bracket, which induces a presymplectic form, and in the second step a projection to the symplectic subspace is performed. It is not clear how the first part of the reduction procedure should be implemented on the quantum level, while the second part of the reduction procedure gives rise to a well defined algebraic procedure, such that quantisation commutes with the second part of reduction by construction.

[2]We speak only of one constraint here, as the second constraint is derived from this constraint as a secondary constraint.

Starting out from the dynamical system for Ψ and χ is unsuitable for a consideration from the point of view of algebraic quantum field theory as the system contains coupling of the fields, which undermines a completely rigorous treatment with current methods. Instead it would be preferable to start from a system of two independent free scalar fields. To achieve this, it is necessary to apply the constraints to arrive at a dynamical system for $\boldsymbol{\Psi} = \frac{a^2}{\mathcal{H}z}\Psi$ and u.

$$\boldsymbol{\Psi}'' - \triangle\boldsymbol{\Psi} + \left(-2\varepsilon + \delta + \varepsilon\delta - \delta^2 - \frac{\delta'}{\mathcal{H}}\right)\mathcal{H}^2\boldsymbol{\Psi} = 0 \tag{4.1.17}$$

$$u'' - \triangle u + \left(-2 - 2\varepsilon + 3\delta - 2\varepsilon^2 + 3\varepsilon\delta - \delta^2 + \frac{\delta'}{\mathcal{H}}\right)\mathcal{H}^2 u = 0 \tag{4.1.18}$$

and the constraint takes the form

$$\boldsymbol{\Psi}' + (1 + \varepsilon - \delta)\mathcal{H}\boldsymbol{\Psi} = \frac{\varepsilon a^2}{z^2}u = 4\pi G u \tag{4.1.19}$$

Ignoring the constraint, $\boldsymbol{\Psi}$ and u are free scalar fields and the symplectic space $\mathscr{P}$ of their modes is straight forward. Now in the present treatment the reduction of phase space is done in two steps. First the Poisson bracket is replaced by the degenerate Dirac bracket, leading to a space $\mathscr{D}$ with a symplectic subspace. Then a projection to the maximal symplectic subspace is performed by factoring out the primary and secondary constraint, leading to a symplectic space $\mathscr{D}/\mathcal{C}$.

To tackle the problem of quantisation, it is useful to take the spatial Fourier transform of the fields, as this allows to make direct contact with the previous treatment. In this context, the Dirac form is defined as in equation (4.1.16), where the mode Dirac form is of course different from the one given in equation (4.1.15), as we are working with different coordinates on the symplectic space here. However, it can be expected that the limit $k \to 0$ should be of the same order of divergence as in equation (4.1.15) because the coordinates are related by a k-independent linear transformation. Therefore the integral can be expected to exist. The constraint in mode form is

$$\mathcal{C}_{1,k} := \widetilde{\boldsymbol{\Psi}}'_k + (1 + \varepsilon - \delta)\mathcal{H}\widetilde{\boldsymbol{\Psi}}_k - 4\pi G\widetilde{u}_k = 0$$

and the Dirac bracket of the constraint with an arbitrary initial value set is

$$\left\{ \begin{pmatrix} f \\ (1 + \varepsilon - \delta)\mathcal{H}f \\ 0 \\ -4\pi G f \end{pmatrix}, \begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \end{pmatrix} \right\}_{\mathrm{D}} = 0 \tag{4.1.20}$$

The algebras of observables for $\boldsymbol{\Psi}$ and u, the Weyl algebras $\mathfrak{A}_{\boldsymbol{\Psi}/u}$, can be constructed in the standard way. The algebra of the full system is then given as the tensor product algebra $\mathfrak{A} = \mathfrak{A}_{\boldsymbol{\Psi}} \otimes \mathfrak{A}_u$. Now the constraint cannot be simply interpreted as a relation in this algebra that has to be factored out to restrict to the constrained system, because it is incompatible with the commutation relations. As discussed above, applying the constraint is not very complicated on the level of field modes; on the level of the Weyl algebra the Weyl relations have to be replaced with the modified relations derived from the mode Dirac forms, profoundly changing the algebra.

For the thus acquired algebra $\mathfrak{A}_{\mathscr{D}}$ corresponding to $\mathscr{D}$ the constraint defines a non-trivial ideal, as the Dirac form is constructed to be degenerate in exactly this sense. This is in contrast to $\mathfrak{A}$ which, as a Weyl-Algebra corresponding to a non-degenerate Poisson form, is simple. The Weyl operators are defined with respect to a set of mode initial values

$$\widehat{W}(\widetilde{\boldsymbol{\Psi}}', \widetilde{\boldsymbol{\Psi}}, \tilde{u}', \tilde{u})$$

and the Dirac-Weyl relation is

$$\begin{aligned}&\widehat{W}(f_1, f_2, f_3, f_4)\widehat{W}(g_1, g_2, g_3, g_4)\\ &= \exp\left(\frac{i}{2}\left\{\begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix}, \begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \end{pmatrix}\right\}_{\mathrm{D}}\right)\widehat{W}(f_1+g_1, f_2+g_2, f_3+g_3, f_4+g_4) \qquad (4.1.21)\end{aligned}$$

This makes it possible to formulate the constraint on the level of the Dirac-Weyl algebra $\mathfrak{A}_{\mathscr{D}}$ as

$$\forall f \in \mathscr{S}(\mathbb{R}^3): \quad \widehat{W}(f, (1+\varepsilon-\delta)\mathcal{H}f, 0, -4\pi G f) = \mathbb{1}$$

where $\mathscr{S}(\mathbb{R}^3)$ denotes the space of Schwartz functions. The constraint is compatible with the Dirac-Weyl relation (4.1.21) by virtue of equation (4.1.20). The secondary constraint can be calculated and cast into a similar form on the level of the algebra. The constraint relations defined two ideals on the algebra and are factored out. The resultant algebra is denoted as $\mathfrak{A}_{\mathscr{D}}/\mathcal{C}'$ and corresponds by construction to the reduced phase space $\mathscr{D}/\mathcal{C}$. This is illustrated in the following diagram, where it should be noted, that the connection between $\mathfrak{A}$ and $\mathfrak{A}_{\mathscr{D}}$ is not clear on the purely algebraic level. Instead $\mathfrak{A}_{\mathscr{D}}$ is constructed using results on the classical level.

$$\begin{array}{ccccc}
\mathscr{P} & \xrightarrow{\text{Dirac}} & \mathscr{D} & \xrightarrow{\text{Reduction}} & \mathscr{D}/\mathcal{C} \\
\downarrow{\scriptstyle\text{Quantisation}} & & \downarrow{\scriptstyle\text{Quantisation}} & & \downarrow{\scriptstyle\text{Quantisation}} \\
\mathfrak{A} & \overset{?}{\dashrightarrow} & \mathfrak{A}_{\mathscr{D}} & \xrightarrow{\text{Reduction}} & \mathfrak{A}_{\mathscr{D}}/\mathcal{C}'
\end{array}$$

States from the state space $\mathcal{S}$ of the tensor product algebra $\mathfrak{A}$ can be freely chosen, for instance it is possible to pick states which have the Hadamard property for both fields. The simplest states of this kind are simply tensor products of Hadamard states for the single field algebras $\mathfrak{A}_{\boldsymbol{\Psi}/u}$. When the constraint $\mathcal{C}'$ is applied, the resultant algebra $\mathfrak{A}_{\mathscr{D}}/\mathcal{C}'$ has a very different state space $\mathcal{S}_{\mathrm{c}}$. In the construction applied here, the isomorphism $\mathfrak{A}_{\mathscr{D}}/\mathcal{C}' \simeq \mathfrak{A}_u$ is implied, which permits a canonical injective, unit preserving C^*-homomorphism $\alpha : \mathfrak{A}_{\mathscr{D}}/\mathcal{C}' \to \mathfrak{A}$. The dual map to this homomorphism is a positive map $\alpha' : \mathcal{S} \to \mathcal{S}_{\mathrm{c}}$ which means that states on $\mathfrak{A}$ give rise to states on $\mathfrak{A}_{\mathscr{D}}/\mathcal{C}'$ by simply restricting to their action to $\mathfrak{A}_u \subset \mathfrak{A}$.

The explicit form of the relations between states in $\mathcal{S}$ and states in $\mathcal{S}_{\mathrm{c}}$ is greatly simplified by our choice of dynamical variables. If one chooses different dynamical variables, like Ψ and χ, the construction of a corresponding algebra $\mathfrak{A}'$ is much more troublesome and a simple relation between $\mathfrak{A}'$ and $\mathfrak{A}'_{\mathscr{D}}/\mathcal{C}' \simeq \mathfrak{A}_{\mathscr{D}}/\mathcal{C}'$ need not exist.

4.2. LTE States in Cosmology

In the present section, the post-inflationary evolution of large scale perturbations mainly during the epoch of free streaming is treated. For simplicity of the treatment polarisation is ignored such that the photon fluid can be modelled by a Klein-Gordon field model. In this context the extrinsic LTE concept can be used to describe thermal properties of the fluid. The first part of this section will show some limitation of the extrinsic LTE concept for the description of temperature fluctuations in terms of cylindrical modes. The second part highlights another limitation of the LTE concept, which prevents a description of the Sachs-Wolfe effect by LTE states.

4.2.1. The Link to Fluid Dynamics

The temperature fluctuations are described by the angular spectrum of the autocorrelation of the background rescaled bolometric phase space density Λ as introduced in (2.3.11). If one attempts to describe the temperature fluctuations in terms of LTE states it is thus desirable to express the cylindric moments of Λ in terms of thermal observables. As the concept of extrinsic LTE, defined in subsection 2.2.4, has been established only with a very limited set of thermal observables, only the three moments of lowest order can be linked to thermal observables. However, even taking the extrinsic LTE concept for granted for all balanced derivative, it is not straight forward to define the cylindric moments in terms of the balanced derivatives.

To link the first three cylindric moments of Λ to LTE observables it is useful to consider the energy-momentum tensor of a perturbed fluid, express the Fourier transforms of its components in terms of cylindric moments and compare it to the energy-momentum tensor of a scalar field in an extrinsic LTE state. In the following, conformal gauge is used for simplicity. To convert to gauge free notation the components of the energy-momentum tensor have to be replaced by their gauge invariant counterparts.

The general form of the energy-momentum tensor of a fluid with phase space density $f(\eta, \vec{x}, p, \hat{p})$ is [16][47]

$$T^{\overline{\mu}}{}_{\overline{\nu}}(\eta, \vec{x}) = \int p^{\overline{\mu}} p_{\overline{\nu}} f(\eta, \vec{x}, p, \hat{p}) \frac{d^3p}{p^{\overline{0}}(\vec{p})}$$

where $p^{\overline{\mu}} = p \cdot \hat{p}^{\overline{\mu}}$. For the massless case and using $f(\eta, \vec{x}, p, \hat{p}) = f_0(\eta, p) + \delta f(\eta, \vec{x}, p, \hat{p})$ this yields

$$T^{\overline{\mu}}{}_{\overline{\nu}}(\eta, \vec{x}) = \int \hat{p}^{\overline{\mu}} \hat{p}_{\overline{\nu}} d\Omega_p \int_0^\infty f_0(\eta, p) p^3 dp + \int \hat{p}^{\overline{\mu}} \hat{p}_{\overline{\nu}} \int_0^\infty \delta f(\eta, \vec{x}, p, \hat{p}) p^3 dp d\Omega_p$$

The background part fulfils the equation of state for a fluid of massless particles $p_0 = \frac{1}{3}\rho_0$. The linear perturbation of this quantity can now be Fourier transformed to be comparable to the moments of

$$\Lambda = \frac{\int_0^\infty \delta f q^3 dq}{4 \int_0^\infty f_0 q^3 dq} \tag{2.3.11'}$$

The linear perturbation of the energy-momentum tensor in terms of Λ is

$$\widetilde{\delta T}^{\overline{\mu}}{}_{\overline{\nu}}(\eta, \vec{k}) = 4 \frac{(T_0)^{\overline{0}}{}_{\overline{0}}}{4\pi} \int \hat{p}^{\overline{\mu}} \hat{p}_{\overline{\nu}} \Lambda(\eta, \vec{k}, \hat{p}) d\Omega_p$$

where one uses $\hat{p}^{\overline{0}} = 1$, which holds in the massless case.

Now one can restrict to perturbations of scalar type, implying $\Lambda(\eta, \vec{k}, \hat{p}) = \Lambda(\eta, \vec{k}, \mu)$ which yields the components

$$\widetilde{\delta T}^{\overline{0}}{}_{\overline{0}}(\eta, \vec{k}) = 4 \frac{(T_0)^{\overline{0}}{}_{\overline{0}}}{4\pi} \int \Lambda(\eta, \vec{k}, \mu) d\Omega_p = 4 (T_0)^{\overline{0}}{}_{\overline{0}} \lambda_0(\eta, \vec{k})$$

$$\hat{k}^{\overline{i}} \widetilde{\delta T}^{\overline{0}}{}_{\overline{i}}(\eta, \vec{k}) = -4 \frac{(T_0)^{\overline{0}}{}_{\overline{0}}}{4\pi} \int \mu \Lambda(\eta, \vec{k}, \mu) d\Omega_p = i \frac{4}{3} (T_0)^{\overline{0}}{}_{\overline{0}} \lambda_1(\eta, \vec{k})$$

$$\begin{aligned} \left(\hat{k}_{\overline{i}} \hat{k}^{\overline{j}} \widetilde{\delta T}^{\overline{i}}{}_{\overline{j}}(\eta, \vec{k}) - \frac{1}{3} \widetilde{\delta T}^{\overline{0}}{}_{\overline{0}}(\eta, \vec{k}) \right) &= 4 \frac{(T_0)^{\overline{0}}{}_{\overline{0}}}{4\pi} \int \left(\mu^2 - \frac{1}{3} \right) \Lambda(\eta, \vec{k}, \mu) d\Omega_p \\ &= -\frac{8}{15} (T_0)^{\overline{0}}{}_{\overline{0}} \lambda_2(\eta, \vec{k}) \end{aligned}$$

As explained in [16][47] the scalar perturbations of the energy-momentum tensor of a fluid have the form

$$\widetilde{\delta T}^{\bar{0}}{}_{\bar{i}} = i\hat{k}_{\bar{i}} k\widetilde{A} \quad \Leftrightarrow \quad \delta T^{\bar{0}}{}_{\bar{i}} = A_{|i}$$

$$\widetilde{\delta T}^{\bar{i}}{}_{\bar{j}}(\eta, \vec{k}) = -\delta^{\bar{i}}{}_{\bar{j}}\widetilde{\delta p} + \left(-\hat{k}^{\bar{i}}\hat{k}_{\bar{j}} + \frac{1}{3}\delta^{\bar{i}}{}_{\bar{j}}\right) k^2 \widetilde{B}$$

$$\Leftrightarrow \quad \delta T^{\bar{i}}{}_{\bar{j}}(\eta, \vec{x}) = -\delta^{\bar{i}}{}_{\bar{j}}\delta p + B^{|\bar{i}}{}_{|\bar{j}} - \frac{1}{3}\delta^{\bar{i}}{}_{\bar{j}}\triangle B$$

Interpreting $\delta p = \frac{1}{3}\delta T^{\bar{0}}{}_{\bar{0}}$ and using "rescaled" Fourier transforms as in [47]

$$\lambda_l(\eta, \vec{x}) := \int e^{i\vec{k}\vec{x}} \frac{\lambda_l(\eta, \vec{k})}{(-k)^l} d^3k$$

one can thus derive using $\hat{k}^{\bar{i}}\hat{k}_{\bar{i}} = -1$

$$T^{\bar{0}}{}_{\bar{0}}(\eta, \vec{x}) = 4(T_0)^{\bar{0}}{}_{\bar{0}}\lambda_0(\eta, \vec{x}) \tag{4.2.1}$$

$$-k\widetilde{A} = \frac{4}{3}(T_0)^{\bar{0}}{}_{\bar{0}}\lambda_1(\eta, \vec{k}) \qquad \Rightarrow \quad \delta T^{\bar{0}}{}_{\bar{i}}(\eta, \vec{x}) = \frac{4}{3}(T_0)^{\bar{0}}{}_{\bar{0}}\lambda_1(\eta, \vec{x})_{|i} \tag{4.2.2}$$

$$-\frac{4}{3}k^2\widetilde{B} = -\frac{8}{15}(T_0)^{\bar{0}}{}_{\bar{0}}\lambda_2(\eta, \vec{k}) \quad \Rightarrow \quad \delta T^{\bar{i}}{}_{\bar{j}}(\eta, \vec{x}) - \frac{1}{3}\delta T^{\bar{0}}{}_{\bar{0}}(\eta, \vec{x}) \tag{4.2.3}$$

$$= \frac{2}{5}(T_0)^{\bar{0}}{}_{\bar{0}}\left(\lambda_2(\eta, \vec{x})^{|\bar{i}}{}_{|\bar{j}} - \frac{1}{3}\delta^{\bar{i}}{}_{\bar{j}}\triangle\lambda_2(\eta, \vec{x})\right) \tag{4.2.4}$$

Having expressed the perturbations in terms of moments of Λ, the next step is to compare these results to the components of the energy-momentum tensor for a suitable "perturbative LTE" model. As calculated explicitly in [43], the expectation value of the renormalised energy momentum tensor for 2-LTE states on curved spacetime is given not only by the thermal expectation values Θ and ε but depends also on the conformal anomaly Q and on renormalisation ambiguities $C_{\mu\nu}$. The explicit form is

$$\begin{aligned}\langle T_{\mu\nu}\rangle =& \varepsilon_{\mu\nu} + \left(\frac{1}{4} - \xi\right)\nabla_\mu\nabla_\nu\Theta + \xi\left(R_{\mu\nu} + (4\xi - 1)\, Rg_{\mu\nu}\right)\Theta \\ &+ \left(12\xi - \frac{5}{2}\right) Qg_{\mu\nu} + C_{\mu\nu}\end{aligned} \tag{4.2.5}$$

For the present work it is useful to split this tensor into three parts, calling $\varepsilon_{\mu\nu}$ the equilibrium contribution, $f_{\mu\nu} = \left(\frac{1}{4} - \xi\right)\nabla_\mu\nabla_\nu\Theta + \xi\left(R_{\mu\nu} + (4\xi - 1)\, Rg_{\mu\nu}\right)\Theta$ the flow contribution and $\mathbb{G}_{\mu\nu} = \left(12\xi - \frac{5}{2}\right) Qg_{\mu\nu} + C_{\mu\nu}$ the geometric contribution.

The geometric term $\mathbb{G}_{\mu\nu}$ can be heuristically interpreted as a dark energy contribution, but the only point that will be made here is that it is state independent. Because of its state independence, the geometric term may be rightfully ignored, if one is only interested in the state dependent thermal or fluid dynamic part. As the geometric term stems from quantisation and relatively contributes ever less with increasing temperature, it can be regarded as a typical quantum effect that cannot be expected to be comparable to the results of the wholly classical fluid dynamic approach, therefore it is also from a utilitarian point of view sensible to disregard this term in the present treatment.

The flow contribution will be omitted in the present treatment, implying that the fluid is assumed to be close to equilibrium.

Using the form of $\varepsilon_{\mu\nu}$ in terms of β given in equation (2.2.11), temperature perturbations around a background temperature in the LTE setting can be linked to the first two moments λ_0 and λ_1 of the photon phase space density perturbation, which are the most relevant at the end of inflation. Taking $\underline{\beta} = \begin{pmatrix} \beta_0 \\ \vec{0} \end{pmatrix} (\eta) + \begin{pmatrix} \delta\beta_0 \\ \overrightarrow{\delta\beta} \end{pmatrix} (\eta, \vec{x})$ and expanding only to first order in $\delta\beta$ we get

$$\varepsilon_{00} = \frac{\pi^2}{30} \frac{1}{\beta_0^4} \left(1 - 4 \frac{\delta\beta_0}{\beta_0} \right) \tag{4.2.6}$$

$$\varepsilon_{0i} = \frac{4}{3} \frac{\pi^2}{30} \frac{1}{\beta_0^4} \frac{\delta\beta_i}{\beta_0} \tag{4.2.7}$$

$$\varepsilon_{ij} = \frac{1}{3} \frac{\pi^2}{30} \frac{1}{\beta_0^4} \left(1 - 4 \frac{\delta\beta_0}{\beta_0} \right) \delta_{ij} \tag{4.2.8}$$

If these components are interpreted in a tetrad, the extrinsic LTE condition as proposed for tetrads in [38] can be straight forwardly applied. The tetrad components can then be compared to the stress-energy tensor for a perturbed fluid, the linear terms of which are given in equations (4.2.1)–(4.2.4). This comparison gives the following identification of quantities

$$\rho = \frac{\pi^2}{30} \frac{1}{\beta_{\bar{0}}^4} = 3p \tag{4.2.9}$$

$$\lambda_0(\eta, \vec{x}) = \frac{\delta\beta_{\bar{0}}}{\beta_{\bar{0}}} \tag{4.2.10}$$

$$\lambda_1(\eta, \vec{x})_{|\bar{i}} = \frac{\delta\beta_{\bar{i}}}{\beta_{\bar{0}}} \tag{4.2.11}$$

$$\lambda_2(\eta,\vec{x})^{|\bar{i}}{}_{|\bar{j}} = \frac{1}{3}\delta^{\bar{i}}{}_{\bar{j}}\triangle\lambda_2(\eta,\vec{x}) \tag{4.2.12}$$

One sees that, in keeping with the standard literature on cosmological perturbation theory, the reference frame is not the rest frame of the perturbed matter (which may indeed vary from point to point as the perturbation $\delta\beta$ is assumed to be position dependent as opposed to β_0) but the rest frame of the background. Additionally, one can see that in the present approach $\overrightarrow{\delta\beta}$ must be a pure gradient and thus only two scalar degrees of freedom are present. Under these circumstances it is not surprising that equation (4.2.12) implies that $\lambda_2(\eta,\vec{x})$ is spatially homogeneous in this model, as can be easily checked using the Fourier transformation, so it can be set to 0 without loss of generality.

One might expect a possibility for a nontrivial λ_2 to arise, if the flow contribution is considered, but the freedom is very limited. As all quantities involved except $\overrightarrow{\delta\beta}$ are scalar, the only non-gradient terms that could appear in $\overrightarrow{\delta\beta}$ are of the form $A(\vec{x})\overrightarrow{\delta\beta}$ or $A(\vec{x})\vec{\nabla}B(\vec{x})$. However, only the perturbation quantities are dependent on $\vec{x}$, so such terms do not occur in the linear approximation. Therefore $\overrightarrow{\delta\beta}$ is a pure gradient also in the more general setting, only two scalar degrees of freedom are allowed and thus λ_0, λ_1 and λ_2 can by no means be independent.

As an aside, this implies that the restriction to perturbations of scalar type enforces a $\underline{\beta}$ which is of scalar type.

Linking higher moments to LTE observables is not as straight forward. Let $\delta_0 := \frac{\delta\beta_0}{\beta_0}$ and $\vec{\delta} := \frac{\overrightarrow{\delta\beta}}{\beta_0}$ and consider

$$f = \frac{1}{e^{p\beta_0(1+\delta_0-\hat{p}\vec{\delta})}-1} \qquad f_0 = \frac{1}{e^{p\beta_0}-1} \qquad \delta f = f - f_0$$

Then one can gets

$$4\Lambda = \frac{\int\limits_0^\infty \delta f p^3 dp}{\int\limits_0^\infty f_0 p^3 dp} = \frac{1}{\left(1+\delta_0-\hat{p}\vec{\delta}\right)^4} - 1$$

Obviously the cylindrical moments of Λ in $\hat{p}$ are the same if we ignore the summand -1, except for the zeroth moment. This means one can simplify the task to the description of moments of $\overline{\Lambda} = \int\limits_0^\infty f p^3 dp$, if one additionally ignores prefactors which are the same for all moments.

Let $\boldsymbol{\nu}$ be a multiindex of an even number of n indices, $\hat{p}\vec{\delta} = \delta\cos\vartheta$. Then we have

$$\lambda_{\boldsymbol{\nu}} \propto \int \hat{p}_{\{\nu\}} \int\limits_0^\infty \frac{p^{n+1}}{e^{p\beta_0(1+\delta_0-\delta\cos\vartheta)}-1} dp d\Omega \propto \int \frac{\hat{p}_{\boldsymbol{\nu}}}{\beta_0^{n+2}(1+\delta_0-\delta\cos\vartheta)^{n+2}} d\Omega$$

The last form can be compared to

$$\lambda_l \propto \int \frac{P_l(\cos\vartheta)}{\beta_0^4(1+\delta_0-\delta\cos\vartheta)^4} d\Omega$$

which holds for $l > 0$ as explained above. It turns out that for $l > 2$ the moments cannot be produced in a straight forward manner in terms of LTE observables.

In reference to the argument made above, one sees that the perturbed LTE states investigated in this subsection carry, if restricting to linear perturbations, only two scalar degrees of freedom, such that there are at most two independent moments of Λ. This is a quite general feature of the LTE approach which has a significant impact on the range of applicability of the LTE concept. Mixtures of KMS states are not suited to achieve more degrees of freedom because in fact the perturbations are to be interpreted as random fields all along, which in the LTE context is modelled by a temperature mixture whose distribution can be interpreted as the distribution of the random field.

4.2.2. Incompatibility of LTE with Sachs-Wolfe Effect

In the previous subsection the limited number of degrees of freedom was identified as principal problem in the treatment of temperature fluctuations of the cosmic microwave background in terms of LTE states. The first, most obvious problem when trying to approach the development of temperature fluctuations more rigorously is the impossibility to account for scattering in the tightly coupled fluid. One may take the result of the usual semiclassical calculation for the time of last scattering for granted as an initial value for the epoch of free streaming (for which a free field treatment is adequate) but then the problem of limited degrees of freedom arises.

To show the problem in applying LTE states in the context of scalar cosmological perturbation theory, it suffices to consider the simple case of the Sachs-Wolfe effect. The usual treatment in terms of the Boltzmann-Equation will be briefly referred to and adjusted for the present treatment. A problem when trying to describe the effect by LTE states is that the extrinsic LTE concept has not been shown to be applicable to perturbed FRW spacetimes and more importantly it is not clear whether an analogue of the phase space density can be found in a suitable extended set of observables. If such an observable were identified the next problem would arise in that it would fulfil the free Boltzmann equation for Minkowski spacetime, due to the extrinsic LTE property. To tackle this problem, it will be shown that the Sachs-Wolfe spectrum, except for the integrated Sachs-Wolfe effect, can be qualitatively reproduced in a treatment without metric perturbations. The “sudden decoupling approximation” detailed in 2.3.5 can be substituted by an equivalent initial value formulation. This initial value problem allows further simplification as it is also well defined on Minkowski spacetime. This last finding allows one to use the wide range of known facts about LTE states on Minkowski spacetime.

In cosmological perturbation theory the evolution of the temperature fluctuations of the cosmological background radiation is described by the linear perturbation of the Boltzmann equation. Recalling equation (2.3.12) the linear perturbation of the Boltzmann equation with Thomson scattering is

$$(\Lambda+\Psi)'+(ik\mu+\dot{\tau})(\Lambda+\Psi)=(\Psi-\Phi)'+\dot{\tau}\left(\lambda_0+\Psi-i\mu\lambda_1-\frac{1}{10}P_2(\mu)\lambda_2\right)$$

As explained above, one would like to eliminate the metric perturbations from the equation. Simply ignoring metric perturbations yields the equation

$$\Lambda'+(ik\mu+\dot{\tau})\Lambda=\dot{\tau}\left(\lambda_0-i\mu\lambda_1-\frac{1}{10}P_2(\mu)\lambda_2\right)$$

which is qualitatively equivalent to the full Boltzmann equation except for the term $(\Psi-\Phi)'$ on the right hand side, which causes the integrated Sachs-Wolfe effect. The fact that $\Lambda+\Psi$ is substituted to Λ has a great impact on the physical interpretation of the results, even changing the sign of the measured red/blueshift. However, for an understanding of the structure of the equation and its solution this is not significant. As explained in 2.3.5 the standard treatment essentially adds Ψ to the monopole moment, which is quite close to ignoring it as a separate quantity.

The following treatment will be simplified by suppressing the metric perturbations, thus also ignoring the integrated Sachs-Wolfe effect. It should be noted that this omission is in the present context meant to have the associated physical implication, so in the following the physical scenario is that of an unperturbed FRW metric.

The solution of simplified Boltzmann equation is analogously to (2.3.14)

$$\Lambda(\eta)=\int_0^{\eta}\dot{\tau}e^{-\tau(\eta',\eta)}\left(\lambda_0(\eta')-i\mu\lambda_1(\eta')-\frac{1}{10}P_2(\mu)\lambda_2(\eta')\right)e^{ik\mu(\eta'-\eta)}d\eta'$$

where $\tau(\eta',\eta)=\int_{\eta'}^{\eta}\dot{\tau}d\eta''$ and $\dot{\tau}e^{-\tau(\eta',\eta)}$ is the visibility function. As in the standard treatment, the sudden decoupling approximation is given by $\dot{\tau}e^{-\tau(\eta',\eta)}=\delta(\eta'-\eta_*)$, where η_* is the time of decoupling. Using this approximation one gets

$$\Lambda(\eta)=\left(\lambda_0(\eta_*)-i\mu\lambda_1(\eta_*)-\frac{1}{10}P_2(\mu)\lambda_2(\eta^*)\right)e^{-ik\mu(\eta-\eta_*)} \tag{4.2.13}$$

very similar to the result of the standard treatment.

However, at this point still two obstacles hinder the application of the LTE concept. Firstly, the scattering term in the Boltzmann equation is problematic to account for in the context of axiomatic QFT. Apart from the unsolved question of summability of perturbation series, little rigorous results exist for thermodynamics in interacting theories. Secondly, even on FRW spacetimes the knowledge about existence of LTE states is quite limited and as discussed in the present work there are some open questions. Therefore it would be desirable to enable the use of the existing techniques for LTE states on Minkowski spacetime. This goal will be pursued below.

The next step is to recast the problem into a form that is tractable in the setting of axiomatic QFT and especially LTE. The sudden decoupling approximation models a situation where all photons are last scattered exactly at the time of decoupling η_*. As this last interaction of the photons is Thomson scattering, the angular spectrum of the photon fluid is given by the cross section of Thomson scattering. Afterwards the photon fluid simply streams freely without any interaction. The described situation corresponds to an initial value problem of the free Boltzmann equation

$$\Lambda' + ik\mu\Lambda = 0$$

$$\Lambda(\eta_*) = \lambda_0(\eta_*) - i\mu\lambda_1(\eta_*) - \frac{1}{10}P_2(\mu)\lambda_2(\eta^*) \tag{4.2.14}$$

Indeed (4.2.13) solves the initial value problem (4.2.14), so this reformulation of the dynamical problem is justified.

The initial value problem (4.2.14) shows no dependence on the metric. This is due to the fact that only the background Boltzmann equation is dependent on the scale parameter $a(\eta)$, while the linear perturbation part of the Boltzmann equation is only dependent on the linear perturbations of the metric. The background Boltzmann equation

$$f_0' - \mathcal{H}p\frac{\partial f_0}{\partial p} = 0$$

is solved by any function of the form

$$f_0(\eta, p) = g_0(a(\eta)p)$$

where a Planck type distribution

$$f_0 = \frac{1}{(2\pi)^3}\frac{1}{e^{\gamma a(\eta)p} - 1}$$

is to be expected for a thermal state according to the correspondence principle.

If a split of the phase space density into background part and perturbation is done in Minkowski spacetime, the background equation is simply

$$f_0' = 0$$

which allows arbitrary functions of p. For a thermal state one would expect the usual Planck spectrum

$$f_0 = \frac{1}{(2\pi)^3}\frac{1}{e^{\beta p}-1}$$

which is trivially allowed. The Boltzmann equation for the linear perturbation is exactly the same as in (4.2.14) where however Λ is to be interpreted differently from the case in curved spacetime because it is defined using the bolometric background phase space density, which differs in both cases.

Thus, the initial value problem (4.2.14) is also a valid initial value problem for the Boltzmann equation on Minkowski spacetime. This means that the angular spectrum produced by the Sachs-Wolfe effect can be reproduced in the context of an initial value problem on flat spacetime, although again the physical interpretation of the objects is changed. The extrinsic LTE concept is not immediately helpful in this context, as Λ has not been described in a QFT setting, such that its identification with a phase space density observable, if such an observable were available on FRW spacetimes, would be completely unjustified. The aim of the following investigation is to check whether the initial value problem (4.2.14) is compatible with an interpretation of Λ as the phase space density of an LTE state.

Taking $f(\eta,\vec{x},\vec{p})$ as the phase space density for a massless scalar field, the dynamic equations implied by the LTE condition are, following [12]

$$f'(\eta,\vec{x},\vec{p}) + \hat{p}^i\partial_i f(\eta,\vec{x},\vec{p}) = 0 \quad\Rightarrow\quad \tilde{f}'(\eta,\vec{k},\vec{p}) + i\hat{p}\cdot\hat{k}k\tilde{f}(\eta,\vec{k},\vec{p}) = 0$$

$$f''(\eta,\vec{x},\vec{p}) - \triangle f(\eta,\vec{x},\vec{p}) = 0 \quad\Rightarrow\quad \tilde{f}''(\eta,\vec{k},\vec{p}) - k^2\tilde{f}(\eta,\vec{k},\vec{p}) = 0$$

where the latter equation emerges from the trace relations that hold for the balanced derivatives in LTE states. If a splitting $f(\eta,\vec{x},\vec{p}) = f_0(\eta,p) + \delta f(\eta,\vec{x},\vec{p})$ is assumed, as in the case of cosmological perturbation theory it turns out that $f_0(\eta,p) = f_0(p)$ as detailed above and $f_0 = \frac{1}{(2\pi)^3}\frac{1}{e^{\beta p}-1}$ can be assumed as the cosmic microwave background is as a first approximation thermal with sharp temperature. As

$$(\Lambda+1) = \frac{\int\limits_0^\infty f p^3 dp}{4\int\limits_0^\infty f_0 p^3 dp}$$

the equations that hold for f also hold for $(\Lambda+1)$, which in turn only deviates from Λ in the monopole moment.

As in the cosmological case Λ will be assumed to be of scalar type, $\Lambda(\eta, k, \mu)$, which leads to the equations

$$(\Lambda+1)' + i\mu k(\Lambda+1) = 0 \tag{4.2.15}$$

$$(\Lambda+1)'' + k^2(\Lambda+1) = 0 \tag{4.2.16}$$

$$\Rightarrow \quad k^2(\mu^2-1)(\Lambda+1) = 0 \tag{4.2.17}$$

where the last equation can be derived from the first two equation and makes explicit the constraint nature of equation (4.2.16) stemming from the trace relations. The refined constraint equation (4.2.17) shows that the trace relations pose a serious restriction on initial conditions for the Boltzmann equation that are valid in the context of LTE. $(\Lambda+1)$ is, by equation (4.2.17), of the form

$$\begin{aligned}(\Lambda+1) &= A(\eta,k)\delta(\mu-1) + B(\eta,k)\delta(\mu+1) + C(\eta)\delta(k)\\ &= \sum_l \frac{2l+1}{2}\Big(A(\eta,k) + (-1)^l B(\eta,k)\Big) P_l(\mu) + C(\eta)\delta(k)\end{aligned} \tag{4.2.18}$$

It is obvious that this is incompatible with the initial condition $\Lambda(\eta_*) = \lambda_0(\eta_*) - i\mu\lambda_1(\eta_*) - \frac{1}{10}P_2(\mu)\lambda_2(\eta^*)$. The term $C(\eta)\delta(k)$ is homogeneous and thus can be interpreted as part of the background. The cylindric moments in the LTE setting show a peculiar pattern, in that all the even respectively odd moments are essentially equal, the greater moments even increasing in magnitude. This is obviously incompatible with the requirement from the initial value given by the Thomson cross section that the modes decrease for large l, only the first three moments being relevant. Again the LTE condition implies only two scalar degrees of freedom to be freely chosen, which is due to the fact that the temperature vector field only has two scalar degrees of freedom and determines the state completely.

This incompatibility can be assessed under different angles. On the one hand one may take the point of view that the incompatibility is not surprising as a validity of the Thomson scattering initial condition in the LTE concept would imply a compatibility with a non-interacting treatment at all times. However, the initial condition is produced by interaction, so one would not a priori expect that it can similarly be produced in a free model. On the other hand one might expect the interaction of the photon fluid to lead to a thermalisation of the fluid and therefore produce a state of at least local thermal equilibrium in the limit of vanishing cross section. Such an effect can be calculated for the classical ideal gas, where the limit of point interactions, which implies vanishing cross section, leads to an equilibrium state. However, in the case at hand the interacting fluid consists of two components, a charged plasma and a photon fluid and their interaction ends due to physical circumstances and not as a formal limit. Taking the vanishing of traces of thermal expectation values as indicative of local thermal equilibrium, in keeping with the LTE concept, one can say that there is no reason to expect the respective traces to vanish separately for two formerly interacting matter components after the interaction ends due to cooling of the ensemble by spacetime expansion.

In the present subsection an incompatibility of the LTE framework on Minkowski spacetime with a derivation of the Sachs-Wolfe effect has been shown. On a curved spacetime one may expect the constraint equation (and also the Boltzmann equation) to take a different form, if one follows the considerations of chapter 3. However, the qualitative situation of an overdetermined system remains, so one cannot expect a successful reconciliation other than by chance. The general problem of a limited number of scalar degrees of freedom persists also in modified approaches to LTE. An explicit treatment of the full system appears impossible at the current stage of development of the extrinsic LTE concept on curved spacetimes. If, however, the λ_l are assumed to be LTE observables (one could argue that in the above context all even moments are equal as well as all uneven moments, if C is assumed to vanish) the framework developed in [42] suggests directly carrying over the conclusion to curved spacetime.

To describe the Sachs-Wolfe effect, a less restrictive framework for non-equilibrium thermodynamics than LTE is needed. Especially the trace relations leading to the constraint equation (4.2.16) would need to be substituted by a weaker requirement. However, the consideration of appropriate weaker requirements is beyond the scope of the present work.

5. Conclusion and Outlook

The limitations of the LTE concept described in the present work are twofold. Firstly, in chapter 3 some evidence was presented that the extrinsic LTE concept leads to an interpretation of thermal observables which is inconsistent with interpretation connected to the intrinsic KMS condition. It was shown that the extrinsic LTE condition is unstable and its macroobservable interpretation leads to unacceptable thermodynamics even in a simple non-stationary spacetime model. Additionally it was made clear that simply ignoring the coupling of the scalar field to curvature as is done in the current state of the extrinsic LTE condition appears not reasonable as it leads to inconsistencies in both cases. Also the question of symmetrisation of balanced derivatives and the cited inconsistency in the Dirac field case found by [25] were briefly mentioned.

Therefore we concluded that the extrinsic LTE concept, despite its successes, needs to be adjusted. Some additional clues as to which properties are desirable for a modified LTE condition were found by investigating conformal KMS states and a simple model for an expanding spacetime. We drew the conclusion, that the modified thermal observables put forth in [45] provide only a partial solution to the problems identified. Therefore we proposed a stronger emphasis on the dynamical equations for LTE observables analogous to those investigated in [12] for Minkowski spacetime. We identified a hierarchy of trace relations and positivity relations as the essential missing links towards a consistent graded LTE concept as the one in Minkowski spacetime.

We proposed furthermore a tentative trace relation for conformally static spacetimes as well as a draft for positivity inequalities, however these cannot be considered satisfactory. The problem of suitable positivity inequalities is related to the multidimensional moment problem, a problem in mathematics currently not solved in a satisfactory manner, which is all the more disappointing as suitable positivity inequalities would be a welcome tool to identify mixtures of KMS states. The problem of missing trace relations occurs because no macroobservable interpretation is implied in the dynamical equations alone, as opposed to the extrinsic LTE concept which includes a built-in macroobservable interpretation.

The absence of a macroobservable interpretation of the balanced derivatives is a problem which appears in a weaker form already for the massive field in

Minkowski spacetime as the thermodynamic integrals cannot be solved analytically. If satisfactory trace and positivity relations can be identified in a model, one may pursue a path similar to the one outlined in [23] to find thermal observables with a sensible macroobservable interpretation corresponding to a certain classical thermodynamic quantity. This would imply a transition to an extended set of thermal observables where the topology needed to extend the set of thermal observables suitably can in general be expected to be at least as weak as the one considered by [23]. This is due to the fact that in the Minkowski case a stronger topology is only sufficient for the subset of measure zero of the parameter space where $m = 0$.

However, as the modified LTE concept proposed in the present work comes with at least one serious problem, namely the missing trace relations, one may expect that a further refinement of the concept would be necessary if it were not to be discarded altogether. Indeed, the second limitation of LTE illustrated in section 4.2 of the present work would affect the proposed modified LTE concept in qualitatively the same way as the standard LTE concept. A concept of local thermal equilibrium which does not encompass a state describing the temperature fluctuations of the cosmic microwave background may be regarded as too restrictive. The treatment in section 4.2 suggests that a general idea for a less restrictive concept of thermal states which stays close to LTE may be to assume the equations derived as balanced derivatives of equation (3.2.4) but substitute the second set of equations derived from equation (3.2.5') by suitable restrictions on initial values.

The source of the problem described in section 4.2 could also be traced to the fact that only the photon fluid is considered and the charged plasma is ignored. If one assumes that the interacting fluid is in local thermal equilibrium, the failure of the photon fluid to be locally thermal may be mirrored by a non-termality of the plasma such that a full treatment of the system would be compatible with local thermal equilibrium.

Additionally the backreaction of the fluid on spacetime was ignored in section 4.2, so another question which could be investigated, is whether the resulting state of the photon fluid is locally thermal an the perturbed spacetime. However, the fact that the deviation from local thermal equilibrium is not a phenomenon of large scales but occurs pointwise, it seems unlikely that the perturbations of the metric resolve this incompatibility. Heuristically speaking, one may expect the spectrum given by equation (4.2.18) to hold for local thermal equilibrium at points where the spacetime curvature vanishes. However, the spectrum enforced by Thomson scattering makes no reference to curvature such that at least in this case the incompatibility can be expected to remain.

The present work leads to some open questions related to the LTE concept on curved spacetimes. In section 2.2.3 it was shown that a finite number of balanced derivatives suffices to approximate the cumulants of a temperature distribution in case a suitable decay property holds for the sequence of cumulants. It would be interesting to investigate whether decay property like $K_n \propto \epsilon^n$ can be proved to follow from a set of physically justified conditions via the central limit theorem.

In light of section 3.1 it would be interesting to investigate the β-dependence of the expectation values of LTE observables for KMS states of the static hyperbolic spacetime $\mathbb{R} \times H^3$. If the limit of small temperatures would deviate from a β^{-2} behaviour also in that case, this would imply that the incompatibility of intrinsic KMS and extrinsic LTE condition is not only a topological effect but also has geometric roots. If one takes seriously the conformal KMS states as thermal states, their incompatibility with the extrinsic LTE condition leads to the expectation that such a deviation may occur.

As already remarked, it would be interesting to have some means to decide which boundary properties LTE states on curved spacetimes should have. On Minkowski spacetime it has been shown in [12] that the region of LTE for the massless field may be past but not future bounded. If one would regard this qualitative behaviour as a desirable feature also for the conformally invariant field on curved spacetimes, the result of section 3.2 would render the extrinsic LTE concept even more unacceptable. An interesting side question is whether LTE states always become singular on the border of the domain of LTE, as is the case for the heat bang states. The derivation of the domain property in [12] seems to hint at this. If this property indeed holds true for Minkowski spacetime and one regards it as a desirable feature also for curved spacetimes, this would further undermine the extrinsic LTE concept.

The spacetime model considered in section 3.3 does exhibit typical features expected to be found in an inflationary model, however inflation in this model is not characterised by a de Sitter phase. In order to stay closer to usual models of inflation it would be interesting to investigate the model which fulfils

$$H = \rho \frac{(1-a^2)(a^2-\epsilon^2)}{(1-\epsilon^2)a^2} \quad \Leftrightarrow \quad ds^2 = dt^2 - \left(\frac{1+\epsilon^2}{2} + \frac{1-\epsilon^2}{2}\tanh(\rho t)\right) d\vec{x}^2$$

however the Klein-Gordon equation for this model is not as straight forward to solve.

Another question which appears worthy of investigation, is whether the state of movement of the observer should be built into the LTE concept in some more detail, by taking into account non-inertial observers. As an example the Minkowski vacuum is seen as a thermal state by a uniformly accelerated observer, due to the Unruh effect. If the observer does however measure the LTE temperature at some point on his world line the generic LTE concept would have him measure zero temperature. In [41] and [42] the LTE observables were linked to inertial Unruh detectors, which should however react to non-inertial motion according to the Unruh effect. Therefore that work might give a hint on how to implement non-inertial observers. In a curved spacetime, geodesic movement takes the place of inertial movement, so one should interpret the extrinsic LTE concept and also the modified concept proposed in the present work as describing geodesic observers.

In the present work some ideas have been presented that illustrate that only some LTE observables can be reconstructed as cylindric moments of the phase space density. However, for KMS and LTE states, e.g. the heat bang states described in [12], the two-point function of the state connected to some phase space density $f(t, \vec{x}, \vec{p})$ can be constructed as

$$\mathscr{W}_2^f(x, y) = \int 2\cos\Big((x^0 - y^0)\omega_p - (\vec{x} - \vec{y})\vec{p}\Big) f\left(\frac{x^0 + y^0}{2}, \frac{\vec{x} + \vec{y}}{2}, \vec{p}\right) d^3p + \mathscr{W}_2^\infty(x, y)$$

One might tentatively extend this construction to a more general class of phase space densities not necessarily stemming from LTE states, however positivity and Hadamard property of the state have to be ensured for this construction to make sense. Positivity and exponential decay for $|\vec{p}| \to \infty$ of the phase space density are sufficient conditions to get a valid Hadamard two-point function. However, in cases where the phase space density does not satisfy the LTE constraint equation, as is the case for the Sachs-Wolfe density investigated in section 4.2, the thermal observables derived from the two-point function constructed in this manner will not fit the LTE picture in the sense that traces of thermal observables may be non-vanishing and positivity inequalities may be violated.

Other approaches to thermal quantum field theory on curved spacetimes have been and are still investigated. On Robertson-Walker spacetimes a class of states called “almost equilibrium states” have been investigated in [26] and it was found that these states include the states of low energy described by [31] as ground states. These states are designed to minimise a free energy functional and were shown to satisfy the Hadamard condition; their relation to LTE states has not been investigated.

Currently a concept developed by N. Pinamonti and R. Verch, called “local KMS states” is under investigation. As this concept is related rather closely to the KMS condition in case the spacetime admits KMS states, it is to be expected that no incompatibility analogous to the one described in section 3.1 arises. However, local KMS states for non-stationary spacetime may lead to more trouble, as the requirement that the two-point function be the real limit of a function in time which is complex analytic in a strip-shaped domain can be expected to restrict applicability to analytic spacetimes. Additionally a requirement of polynomial boundedness in time direction built into the local KMS condition might imply restrictions on the time dependence of the spacetime metric. On Minkowski spacetime local KMS states are closely related to LTE states, but their relation to extrinsic LTE states has not yet been investigated.

The present work investigates parts of the formalism of linear perturbation theory in its application to the derivation of the spectrum of temperature perturbations of the cosmic microwave background. It has been clarified in section 4.1, how the reduction of the dynamic equations of the perturbations to a single Klein-Gordon equation is justified. It was found that the field u, which is usually quantised, is among the fields for which canonical commutation relations can be assumed. This implies that Ψ and χ are non-local fields, which could be interpreted as indicating a non-commutative spacetime structure, implying non-locality of the field and thus making a connection to deformed field algebras. It would be interesting to pursue this point further, also in the context of different approaches like deformation quantisation.

Additionally, it was found that a one-parameter family of composite fields exist, which all yield conjugate pairs with their time derivatives and whose quantisation should be investigated. The classical dynamics of all fields of the family are equivalent, in the sense that they are described by the same geometric structure on phase space. However, it is not clear how picking another field than u from this family impacts the form of the dynamical equation, the identification of a "preferred state" and the infrared asymptotics of this state's two-point function.

It would be interesting to investigate a similar model of linear perturbation theory where the scalar field is not minimally coupled to curvature, for example with $V(\phi) = \widetilde{V}(\phi) - \frac{1}{2}R\phi^2$ as a simple model of a metric dependent potential. As it is not clear, which composite fields are valid under these circumstances, a Hamiltonian treatment with constraints as in section 4.1 appears reasonable. However a suitable form of the second perturbation order of the action has to be identified, which involves very tedious calculations, which are however simplified by the premise that all terms in the action can be calculated in conformal gauge, because the gauge degrees of freedom only account for the constraints, which can be easily derived from the Einstein equations. For the suitable composite fields the dynamics and especially the infrared asymptotics of the two-point function for a preferred state would be of some interest.

A. Technical proofs

A.1. Proof of Lemma 3.2.5

Following are the necessary calculations to prove lemma 3.2.5.

(a) Elementary relations

$$[\nabla^-_\alpha, \nabla^+_\beta] = [\nabla^x_\alpha - \nabla^y_\alpha, \nabla^x_\beta + \nabla^y_\beta] = [\nabla^x_\alpha, \nabla^x_\beta] - [\nabla^y_\alpha, \nabla^y_\beta]$$

$$[\nabla^-_\alpha, \nabla^-_\beta] = [\nabla^x_\alpha - \nabla^y_\alpha, \nabla^x_\beta - \nabla^y_\beta] = [\nabla^x_\alpha, \nabla^x_\beta] + [\nabla^y_\alpha, \nabla^y_\beta]$$

(b) Relations relevant for generalisation of equations (3.2.3) and (3.2.4)

$$\nabla^+_\lambda [\nabla^-_\rho, \nabla^-_\mu] \nabla^-_\nu \theta(x,y)|_{x=y} = \nabla^+_\lambda \Big(R^\alpha{}_{\nu\mu\rho}(x) \nabla^x_\alpha - R^\alpha{}_{\nu\mu\rho}(y) \nabla^y_\alpha \Big) \theta(x,y)|_{x=y}$$

$$= \Big(R^\alpha{}_{\nu\mu\rho}(x) \nabla^+_\lambda \nabla^x_\alpha - R^\alpha{}_{\nu\mu\rho}(y) \nabla^+_\lambda \nabla^y_\alpha$$

$$+ (\nabla^x_\lambda R^\alpha{}_{\nu\mu\rho}(x)) \nabla^x_\alpha - (\nabla^y_\lambda R^\alpha{}_{\nu\mu\rho}(y)) \nabla^y_\alpha \Big) \theta(x,y)|_{x=y}$$

$$= R^\alpha{}_{\nu\mu\rho} \nabla_\lambda \theta_\alpha$$

$$\nabla^-_\mu [\nabla^+_\lambda, \nabla^-_\nu] \nabla^-_\rho \theta(x,y)|_{x=y} = \nabla^-_\mu \Big(R^\alpha{}_{\rho\nu\lambda}(x) \nabla^x_\alpha + R^\alpha{}_{\rho\nu\lambda}(y) \nabla^y_\alpha \Big) \theta(x,y)|_{x=y}$$

$$= \Big(R^\alpha{}_{\rho\nu\lambda}(x) \nabla^-_\mu \nabla^x_\alpha + R^\alpha{}_{\rho\nu\lambda}(y) \nabla^-_\mu \nabla^y_\alpha$$

$$+ (\nabla^x_\mu R^\alpha{}_{\rho\nu\lambda}(x)) \nabla^x_\alpha - (\nabla^y_\mu R^\alpha{}_{\rho\nu\lambda}(y)) \nabla^y_\alpha \Big) \theta(x,y)|_{x=y}$$

$$= R^\alpha{}_{\rho\nu\lambda} \nabla_\alpha \theta_\mu$$

$$[\nabla^+_\lambda, \nabla^-_\mu]\nabla^-_\nu\nabla^-_\rho\theta(x,y)|_{x=y} = \Big(R^\alpha{}_{\nu\mu\lambda}(x)\nabla^x_\alpha\nabla^x_\rho + R^\alpha{}_{\rho\mu\lambda}(x)\nabla^x_\nu\nabla^x_\alpha$$

$$- R^\alpha{}_{\rho\mu\lambda}(x)\nabla^y_\nu\nabla^x_\alpha - R^\alpha{}_{\nu\mu\lambda}(x)\nabla^x_\alpha\nabla^y_\rho - (x \leftrightarrow y)\Big)\theta(x,y)|_{x=y}$$

$$= \Big(R^\alpha{}_{\nu\mu\lambda}(x)\nabla^x_\alpha\nabla^-_\rho + R^\alpha{}_{\rho\mu\lambda}(x)\nabla^x_\alpha\nabla^-_\nu$$

$$+ R^\alpha{}_{\nu\mu\lambda}(y)\nabla^y_\alpha\nabla^-_\rho + R^\alpha{}_{\rho\mu\lambda}(y)\nabla^y_\alpha\nabla^-_\nu\Big)\theta(x,y)|_{x=y}$$

$$= R^\alpha{}_{\nu\mu\lambda}\nabla_\alpha\theta_\rho + R^\alpha{}_{\rho\mu\lambda}\nabla_\alpha\theta_\nu$$

(c) Relations relevant for generalisation of equations (3.2.5) and (3.2.6)

$$\nabla^+_\lambda[\nabla^+_\rho, \nabla^-_\mu]\nabla^-_\nu\theta(x,y)|_{x=y} = \nabla^+_\lambda\Big(R^\alpha{}_{\nu\mu\rho}(x)\nabla^x_\alpha + R^\alpha{}_{\nu\mu\rho}(y)\nabla^y_\alpha\Big)\theta(x,y)|_{x=y}$$

$$= \Big(R^\alpha{}_{\nu\mu\rho}(x)\nabla^+_\lambda\nabla^x_\alpha + R^\alpha{}_{\nu\mu\rho}(y)\nabla^+_\lambda\nabla^y_\alpha$$

$$+ (\nabla^x_\lambda R^\alpha{}_{\nu\mu\rho}(x))\nabla^x_\alpha + (\nabla^y_\lambda R^\alpha{}_{\nu\mu\rho}(y))\nabla^y_\alpha\Big)\theta(x,y)|_{x=y}$$

$$= R^\alpha{}_{\nu\mu\rho}\nabla_\lambda\nabla_\alpha\theta + (\nabla_\lambda R^\alpha{}_{\nu\mu\rho})\nabla_\alpha\theta$$

$$\nabla^-_\mu[\nabla^+_\lambda, \nabla^-_\nu]\nabla^+_\rho\theta(x,y)|_{x=y} = \nabla^-_\mu\Big(R^\alpha{}_{\rho\nu\lambda}(x)\nabla^x_\alpha - R^\alpha{}_{\rho\nu\lambda}(y)\nabla^y_\alpha\Big)\theta(x,y)|_{x=y}$$

$$= \Big(R^\alpha{}_{\rho\nu\lambda}(x)\nabla^-_\mu\nabla^x_\alpha - R^\alpha{}_{\rho\nu\lambda}(y)\nabla^-_\mu\nabla^y_\alpha$$

$$+ (\nabla^x_\mu R^\alpha{}_{\rho\nu\lambda}(x))\nabla^x_\alpha + (\nabla^y_\mu R^\alpha{}_{\rho\nu\lambda}(y))\nabla^y_\alpha\Big)\theta(x,y)|_{x=y}$$

$$= R^\alpha{}_{\rho\nu\lambda}\theta_{\mu\alpha} + (\nabla_\mu R^\alpha{}_{\rho\nu\lambda})\nabla_\alpha\theta$$

$$[\nabla^+_\lambda, \nabla^-_\mu]\nabla^-_\nu\nabla^+_\rho\theta(x,y)|_{x=y} = \Big(R^\alpha{}_{\nu\mu\lambda}(x)\nabla^x_\alpha\nabla^x_\rho + R^\alpha{}_{\rho\mu\lambda}(x)\nabla^x_\nu\nabla^x_\alpha$$

$$- R^\alpha{}_{\rho\mu\lambda}(x)\nabla^y_\nu\nabla^x_\alpha + R^\alpha{}_{\nu\mu\lambda}(x)\nabla^x_\alpha\nabla^y_\rho + (x \leftrightarrow y)\Big)\theta(x,y)|_{x=y}$$

$$= \Big(R^\alpha{}_{\nu\mu\lambda}(x)\nabla^x_\alpha\nabla^+_\rho + R^\alpha{}_{\rho\mu\lambda}(x)\nabla^-_\nu\nabla^x_\alpha$$

$$+ R^\alpha{}_{\nu\mu\lambda}(y)\nabla^y_\alpha\nabla^+_\rho - R^\alpha{}_{\rho\mu\lambda}(y)\nabla^-_\nu\nabla^y_\alpha\Big)\theta(x,y)|_{x=y}$$

$$= R^\alpha{}_{\nu\mu\lambda}\nabla_\alpha\nabla_\rho\theta + R^\alpha{}_{\rho\mu\lambda}\theta_{\nu\alpha}$$

$$\nabla^-_\lambda [\nabla^-_\rho, \nabla^-_\mu] \nabla^-_\nu \theta(x,y)|_{x=y} = \nabla^-_\lambda \Big(R^\alpha{}_{\nu\mu\rho}(x) \nabla^x_\alpha - R^\alpha{}_{\nu\mu\rho}(y) \nabla^y_\alpha \Big) \theta(x,y)|_{x=y}$$

$$= R^\alpha{}_{\nu\mu\rho} \theta_{\lambda\alpha} + (\nabla_\lambda R^\alpha{}_{\nu\mu\rho}) \nabla_\alpha \theta$$

$$[\nabla^-_\lambda, \nabla^-_\mu] \nabla^-_\nu \nabla^-_\rho \theta(x,y)|_{x=y} = \Big(R^\alpha{}_{\nu\mu\lambda}(x) \nabla^x_\alpha \nabla^x_\rho + R^\alpha{}_{\rho\mu\lambda}(x) \nabla^x_\nu \nabla^x_\alpha$$

$$- R^\alpha{}_{\nu\mu\lambda}(x) \nabla^x_\alpha \nabla^y_\rho - R^\alpha{}_{\rho\mu\lambda}(x) \nabla^y_\nu \nabla^x_\alpha + (x \leftrightarrow y) \Big) \theta(x,y)|_{x=y}$$

$$= \Big(R^\alpha{}_{\nu\mu\lambda}(x) \nabla^x_\alpha \nabla^-_\rho + R^\alpha{}_{\rho\mu\lambda}(x) \nabla^-_\nu \nabla^x_\alpha$$

$$- R^\alpha{}_{\nu\mu\lambda}(y) \nabla^y_\alpha \nabla^-_\rho - R^\alpha{}_{\rho\mu\lambda}(y) \nabla^-_\nu \nabla^y_\alpha \Big) \theta(x,y)|_{x=y}$$

$$= R^\alpha{}_{\nu\mu\lambda} \theta_{\alpha\rho} + R^\alpha{}_{\rho\mu\lambda} \theta_{\nu\alpha}$$

A.2. Proof of Lemma 3.2.6

The calculation essentially amounts to sorting the derivatives into the desired order for each term of the symmetrised expressions and collecting the terms that arise due to interchange of covariant derivatives. We start out with the calculations necessary to get equation (3.2.8). First we note $g^{\lambda\rho} \nabla^+_\lambda \nabla^-_\rho \theta(x,y)|_{x=y} = 0$, which will simplify the calculations significantly.

$$g^{\lambda\rho} \nabla^+_\lambda \nabla^-_{(\rho} \nabla^-_\mu \nabla^-_{\nu)} \theta(x,y)|_{x=y} = \frac{1}{6} g^{\lambda\rho} \Big(\nabla^+_\lambda \nabla^-_\rho \nabla^-_\mu \nabla^-_\nu + 2 \nabla^+_\lambda \nabla^-_\mu \nabla^-_\nu \nabla^-_\rho$$

$$+ (\mu \leftrightarrow \nu) \Big) \theta(x,y)|_{x=y}$$

$$= \frac{1}{6} g^{\lambda\rho} \Big(\nabla^+_\lambda [\nabla^-_\rho, \nabla^-_\mu] \nabla^-_\nu + 3 [\nabla^+_\lambda, \nabla^-_\mu] \nabla^-_\nu \nabla^-_\rho + 3 \nabla^-_\mu [\nabla^+_\lambda, \nabla^-_\nu] \nabla^-_\rho$$

$$+ 3 \nabla^-_\mu \nabla^-_\nu \nabla^+_\lambda \nabla^-_\rho + (\mu \leftrightarrow \nu) \Big) \theta(x,y)|_{x=y}$$

$$= \frac{1}{6} g^{\lambda\rho} \Big(R^\alpha{}_{\nu\mu\rho} \nabla^+_\lambda \nabla^-_\alpha + 3 R^\alpha{}_{\nu\mu\lambda} \nabla^+_\alpha \nabla^-_\rho + 3 R^\alpha{}_{\rho\mu\lambda} \nabla^+_\alpha \nabla^-_\nu + 3 R^\alpha{}_{\rho\nu\lambda} \nabla^+_\alpha \nabla^-_\mu$$

$$+ (\mu \leftrightarrow \nu) \Big) \theta(x,y)|_{x=y}$$

As we are interested in the case of de Sitter spacetime, we can further simplify these expressions. Using $R^{\alpha}{}_{\mu\nu\rho} = H^2\Big(\delta^{\alpha}_{\rho} g_{\mu\nu} - \delta^{\alpha}_{\nu} g_{\mu\rho}\Big)$ we get

$$g^{\lambda\rho} R^{\alpha}{}_{\nu\mu\lambda} \nabla_{\alpha}\theta_{\rho} = g^{\lambda\rho} R^{\alpha}{}_{\nu\mu\rho} \nabla_{\lambda}\theta_{\alpha} = H^2\Big(g_{\mu\nu}\nabla_{\lambda}\theta^{\lambda} - \nabla_{\nu}\theta_{\mu}\Big)$$

$$g^{\lambda\rho} R^{\alpha}{}_{\rho\mu\lambda} \nabla_{\alpha}\theta_{\nu} = -3H^2 \nabla_{\mu}\theta_{\nu}$$

Using $\nabla_{\lambda}\theta^{\lambda} = 0$ we get

$$g^{\lambda\rho}\nabla^{+}_{\lambda}\nabla^{-}_{(\rho}\nabla^{-}_{\mu}\nabla^{-}_{\nu)}\theta(x,y)|_{x=y} = \frac{11}{3}\Big(\nabla^{+}_{\mu}\nabla^{-}_{\nu} + \nabla^{+}_{\nu}\nabla^{-}_{\mu}\Big)\theta(x,y)|_{x=y}$$

$$= \frac{22}{3}\Big(\nabla^{x}_{\mu}\nabla^{x}_{\nu} - \nabla^{y}_{\mu}\nabla^{y}_{\nu}\Big)\theta(x,y)|_{x=y} = 0$$

due to symmetry of $\theta(x,y)$ under exchange of x and y. This concludes the derivation of equation (3.2.8).

For the derivation of equation (3.2.9) note that $\theta^{\lambda}_{\lambda\mu\nu} = g^{\lambda\rho}\nabla^{-}_{(\lambda}\nabla^{-}_{\rho}\nabla^{-}_{\mu}\nabla^{-}_{\nu)}\theta(x,y)|_{x=y}$ and $\Box\theta_{\mu\nu} = g^{\lambda\rho}\nabla^{+}_{\lambda}\nabla^{+}_{\rho}\nabla^{-}_{\mu}\nabla^{-}_{\nu}\theta(x,y)|_{x=y}$ are two of the desired terms. Therefore we process the sum of these terms using the commutation relations for the covariant derivatives from the previous lemma. We calculate

$$g^{\lambda\rho}\nabla^{+}_{\lambda}\nabla^{+}_{\rho}\nabla^{-}_{\mu}\nabla^{-}_{\nu}\theta(x,y)|_{x=y} = \frac{1}{2} g^{\lambda\rho}\Big(\nabla^{-}_{\mu}\nabla^{-}_{\nu}\nabla^{+}_{\lambda}\nabla^{+}_{\rho} + \nabla^{+}_{\lambda}[\nabla^{+}_{\rho},\nabla^{-}_{\mu}]\nabla^{-}_{\nu}$$

$$+ [\nabla^{+}_{\lambda},\nabla^{-}_{\mu}]\nabla^{-}_{\nu}\nabla^{+}_{\rho} + \nabla^{-}_{\mu}[\nabla^{+}_{\lambda},\nabla^{-}_{\nu}]\nabla^{+}_{\rho} + (\mu \leftrightarrow \nu)\Big)\theta(x,y)|_{x=y}$$

$$= g^{\lambda\rho}\Big(\frac{1}{2}\Big(\nabla^{-}_{\mu}\nabla^{-}_{\nu} + \nabla^{-}_{\nu}\nabla^{-}_{\mu}\Big)\nabla^{+}_{\lambda}\nabla^{+}_{\rho}\theta(x,y)|_{x=y}$$

$$+ R^{\alpha}{}_{\nu\mu\lambda}\nabla_{\alpha}\nabla_{\rho}\theta + R^{\alpha}{}_{\mu\nu\lambda}\nabla_{\alpha}\nabla_{\rho}\theta + R^{\alpha}{}_{\rho\nu\lambda}\theta_{\alpha\mu} + R^{\alpha}{}_{\rho\mu\lambda}\theta_{\alpha\nu}$$

$$+ \frac{1}{2}\Big(\nabla_{\lambda}R^{\alpha}{}_{\nu\mu\rho} + \nabla_{\lambda}R^{\alpha}{}_{\mu\nu\rho} + \nabla_{\mu}R^{\alpha}{}_{\rho\nu\lambda} + \nabla_{\nu}R^{\alpha}{}_{\rho\mu\lambda}\Big)\nabla_{\alpha}\theta\Big)$$

As we are interested in the case of de Sitter spacetime, we can further simplify these expressions. Using $R^{\alpha}{}_{\mu\nu\rho} = H^2\Big(\delta^{\alpha}_{\rho} g_{\mu\nu} - \delta^{\alpha}_{\nu} g_{\mu\rho}\Big)$ we see that

$$\nabla_{\nu}R^{\alpha}{}_{\rho\mu\lambda} = 0$$

$$g^{\lambda\rho}R^{\alpha}{}_{\nu\mu\lambda}\nabla_{\alpha}\nabla_{\rho}\theta = H^2\Big(g_{\mu\nu}\Box - \nabla_{\mu}\nabla_{\nu}\Big)\theta$$

$$g^{\lambda\rho}R^{\alpha}{}_{\rho\nu\lambda}\theta_{\alpha\mu} = -3H^2\theta_{\mu\nu}$$

This finally yields

$$g^{\lambda\rho}\nabla^+_\lambda\nabla^+_\rho\nabla^-_\mu\nabla^-_\nu\theta(x,y)|_{x=y} = \frac{1}{2}\Big(\nabla^-_\mu\nabla^-_\nu + \nabla^-_\nu\nabla^-_\mu\Big)\Box^+\theta(x,y)|_{x=y}$$

$$+ 2H^2\Big(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\Big)\theta - 6H^2\theta_{\mu\nu}$$

Next we turn to the more tedious calculation of $\theta^\lambda_{\lambda\mu\nu}$

$$g^{\lambda\rho}\nabla^-_{(\lambda}\nabla^-_\rho\nabla^-_\mu\nabla^-_{\nu)}\theta(x,y)|_{x=y} = \frac{1}{12}g^{\lambda\rho}\Big(\nabla^-_\lambda\nabla^-_\rho\nabla^-_\mu\nabla^-_\nu + 2\nabla^-_\lambda\nabla^-_\mu\nabla^-_\nu\nabla^-_\rho$$

$$+ 2\nabla^-_\mu\nabla^-_\lambda\nabla^-_\nu\nabla^-_\rho + \nabla^-_\mu\nabla^-_\nu\nabla^-_\lambda\nabla^-_\rho + (\mu\leftrightarrow\nu)\Big)\theta(x,y)|_{x=y}$$

$$= \frac{1}{12}g^{\lambda\rho}\Big(\nabla^-_\lambda[\nabla^-_\rho,\nabla^-_\mu]\nabla^-_\nu + 3[\nabla^-_\lambda,\nabla^-_\mu]\nabla^-_\nu\nabla^-_\rho + 5\nabla^-_\mu[\nabla^-_\lambda,\nabla^-_\nu]\nabla^-_\rho$$

$$+ 6\nabla^-_\mu\nabla^-_\nu\nabla^-_\lambda\nabla^-_\rho + (\mu\leftrightarrow\nu)\Big)\theta(x,y)|_{x=y}$$

$$= \frac{1}{2}\Big(\nabla^-_\mu\nabla^-_\nu + \nabla^-_\nu\nabla^-_\mu\Big)\Box^-\theta(x,y)|_{x=y}$$

$$+ \frac{1}{12}g^{\lambda\rho}\Big(4R^\alpha{}_{\nu\mu\lambda}\theta_{\alpha\rho} + 4R^\alpha{}_{\mu\nu\lambda}\theta_{\alpha\rho} + 8R^\alpha{}_{\rho\nu\lambda}\theta_{\alpha\mu} + 8R^\alpha{}_{\rho\mu\lambda}\theta_{\alpha\nu}$$

$$+ \Big(\nabla_\lambda R^\alpha{}_{\nu\mu\rho} + \nabla_\lambda R^\alpha{}_{\mu\nu\rho} + 5\nabla_\mu R^\alpha{}_{\rho\nu\lambda} + 5\nabla_\nu R^\alpha{}_{\rho\mu\lambda}\Big)\nabla_\alpha\theta\Big)$$

We can again use the explicit form of the curvature tensor on de Sitter spacetime to get the result

$$g^{\lambda\rho}\nabla^-_{(\lambda}\nabla^-_\rho\nabla^-_\mu\nabla^-_{\nu)}\theta(x,y)|_{x=y} = \frac{1}{2}\Big(\nabla^-_\mu\nabla^-_\nu + \nabla^-_\nu\nabla^-_\mu\Big)\Box^-\theta(x,y)|_{x=y}$$

$$+ \frac{2}{3}H^2\Big(g_{\mu\nu}\theta^\lambda_\lambda - \theta_{\mu\nu}\Big) - 4H^2\theta_{\mu\nu}$$

Using equation (3.2.5) and specialising to our case $m^2 = 0$ we thus get

$$\Box\theta_{\mu\nu} + \theta^\lambda_{\lambda\mu\nu} = -2\Big(\nabla^-_\mu\nabla^-_\nu + \nabla^-_\nu\nabla^-_\mu\Big)\Big(12\xi H^2\theta(x,y) - C(x,y)\Big)|_{x=y}$$

$$+ 2H^2\Big(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\Big)\theta + \frac{2}{3}H^2 g_{\mu\nu}\theta^\lambda_\lambda - \frac{32}{3}H^2\theta_{\mu\nu}$$

$$= -\Big(\frac{32}{3} + 48\xi\Big)H^2\theta_{\mu\nu} + 2H^2\Big(g_{\mu\nu}\Box - \nabla_\mu\nabla_\nu\Big)\theta + \frac{2}{3}H^2 g_{\mu\nu}\theta^\lambda_\lambda + 4C_{\mu\nu}$$

A.3. Proof of Lemma 3.4.2

First we show two auxiliary results.

Lemma A.3.1.
Let

$$\begin{aligned} h_a(y) := y^{4a+2} + 3y^{4a+1} - (2a^2+a)y^{2a+3} - 3y^{2a+2} + 2(2a^2+a-1)y^{2a+1} - 3y^{2a} \\ - (2a^2+a)y^{2a-1} + 3y + 1 \end{aligned}$$

then

$$\forall a \in \mathbb{N}, y > 1 : \; h_a(y) \geq 0$$

Proof.
The proof is done by double induction in a. For the induction step it suffices to show

$$\forall a \in \mathbb{N}, y > 1 : \; j_a(y) := h_{a+1}(y) - y^4 h_a(y) \geq 0$$

which is then again done by induction, where for the induction step we show

$$\forall a \in \mathbb{N}, y > 1 : \; j_{a+1}(y) - y^2 j_a(y) \geq 0$$

Combining all this we have to show

$$h_1(y) \geq 0$$

$$h_2(y) - y^4 h_1(y) \geq 0$$

$$\forall a \in \mathbb{N}, y > 1 : \; h_{a+2}(y) - y^2 h_{a+1}(y) - y^4 h_{a+1}(y) + y^6 h_a(y) \geq 0$$

First we calculate

$$h_1(y) = y^6 - 3y^4 + 4y^3 - 3y^2 + 1 = (y^2-1)^3 + 2(y-1)^2(2y+1) \geq 0$$

and

$$\begin{aligned} h_2(y) - y^4 h_1(y) &= 3y^9 + 3y^8 - 14y^7 + 18y^5 - 4y^4 - 10y^3 + 3y + 1 \\ &= (y-1)^2(y+1)(3y^6 + 6y^5 - 5y^4 - 2y^3 + 5y^2 + 4y + 1) \geq 0 \end{aligned}$$

The proof of the last inequality is very tedious. Therefore we skip the initial sorting of terms.

$$\begin{aligned}
j_{a+1}(y) - y^2 j_a(y) &= h_{a+2}(y) - y^2 h_{a+1}(y) - y^4 h_{a+1}(y) + y^6 h_a(y) \\
&= 4ay^{2a+3}(y^2-1)^3 + y^{2a+3}(y^2-1)^2(3y^2-7) \\
&\quad + (3y+1)(y^2-1)(y^4-1) \\
&\geq y^{2a+3}(y^2-1)^2\Big(3(y^2-1) + 4(a-1)\Big) \geq 0
\end{aligned}$$

This concludes the proof of the first auxiliary result. ☐

Lemma A.3.2.

$$\begin{aligned}
\forall a \in \mathbb{N}, 0 < x < 1: \quad & \frac{1}{x} + \frac{(2a^2+a)\left((1+x)^{2a} + (1-x)^{2a}\right)}{(1+x)^{2a+1} - (1-x)^{2a+1}} \\
& \geq -\frac{2x}{1-x^2} + \frac{(2a^2+a-1)\left((1+x)^{2a-2} + (1-x)^{2a-2}\right)}{(1+x)^{2a-1} - (1-x)^{2a-1}}
\end{aligned}$$

Proof. We begin the proof by multiplying with all the denominators and setting $A := 1 + x$ and $B := 1 - x$ to get the equivalent inequality

$$\begin{aligned}
AB(A^{2a+1} - B^{2a+1})(A^{2a-1} - B^{2a-1}) \\
+\tfrac{1}{2}(2a^2+a)(A-B)AB(A^{2a} + B^{2a})(A^{2a-1} - B^{2a-1}) \\
+\tfrac{1}{2}(A-B)^2(A^{2a+1} - B^{2a+1})(A^{2a-1} - B^{2a-1}) \\
+\tfrac{1}{2}(2a^2+a-1)(A-B)AB(A^{2a-2} + B^{2a-2})(A^{2a+1} - B^{2a+1}) \geq 0
\end{aligned}$$

Expanding all the terms, dividing by B^{4a+2} and defining $y = \frac{A}{B}$ this is equivalent to

$$\begin{aligned}
y^{4a+2} + 3y^{4a+1} - (2a^2+a)y^{2a+3} - 3y^{2a+2} + 2(2a^2+a-1)y^{2a+1} - 3y^{2a} \\
-(2a^2+a)y^{2a-1} + 3y + 1 \geq 0
\end{aligned}$$

which was proved to be true $\forall a \in \mathbb{N}, y > 1$ in lemma A.3.1 where $y > 1 \quad \Leftrightarrow \quad 0 < x < 1$. This proves the claim. ☐

Now we proceed to prove Lemma 3.4.2. The statement is trivial for $\beta = 0$. For $\beta > 0$ we have, using $x = \frac{\beta}{\beta_0}$

$$
\begin{aligned}
f_a(\beta_0, \beta) &= \frac{1}{(2a-1)!}\partial_{\beta_0}^{(2a-2)} \frac{1}{\beta_0^2 - \beta^2} \\
&= \frac{(2a-2)!}{2\beta(2a-1)!}\left(\frac{1}{(\beta_0 - \beta)^{2a-1}} - \frac{1}{(\beta_0 + \beta)^{2a-1}}\right) \\
&= \frac{1}{2x(2a-1)\beta_0^{2a}}\left(\frac{1}{(1-x)^{2a-1}} - \frac{1}{(1+x)^{2a-1}}\right)
\end{aligned}
$$

This yields

$$
(2x\beta_0^{2a})^{a+1}\Big(1-x^2\Big)^{2a^2+a} f_a^{a+1}(\beta_0,\beta) = \frac{1-x^2}{(2a-1)^{a+1}}\Big((1+x)^{2a-1} - (1-x)^{2a-1}\Big)^{a+1}
$$

$$
(2x\beta_0^{2a})^{a+1}\Big(1-x^2\Big)^{2a^2+a} f_{a+1}^{a}(\beta_0,\beta) = \frac{2x}{(2a+1)^{a}}\Big((1+x)^{2a+1} - (1-x)^{2a+1}\Big)^{a}
$$

and because $\forall a \in \mathbb{N}, 0 < x < 1 : \ (2x\beta_0^{2a})^{a+1}\Big(1-x^2\Big)^{2a^2+a} > 0$ we can define

$$
\begin{aligned}
g_a(x) := & \frac{2x}{(2a+1)^a}\Big((1+x)^{2a+1} - (1-x)^{2a+1}\Big)^{a} \\
& - \frac{1-x^2}{(2a-1)^{a+1}}\Big((1+x)^{2a-1} - (1-x)^{2a-1}\Big)^{a+1}
\end{aligned}
$$

and it remains to show that $\forall a \in \mathbb{N}, 0 < x < 1 : \ g_a(x) \geq 0$.

Taking the derivative of $g_a(x)$ yields

$$
\begin{aligned}
g_a'(x) := & \left[\frac{1}{x} + \frac{(2a^2+a)\left((1+x)^{2a} + (1-x)^{2a}\right)}{(1+x)^{2a+1} - (1-x)^{2a+1}}\right] \\
& \cdot \frac{2x}{(2a+1)^a}\Big((1+x)^{2a+1} - (1-x)^{2a+1}\Big)^{a} \\
& - \left[-\frac{2x}{1-x^2} + \frac{(2a^2+a-1)\left((1+x)^{2a-2} + (1-x)^{2a-2}\right)}{(1+x)^{2a-1} - (1-x)^{2a-1}}\right] \\
& \cdot \frac{1-x^2}{(2a-1)^{a+1}}\Big((1+x)^{2a-1} - (1-x)^{2a-1}\Big)^{a+1}
\end{aligned}
$$

Due to lemma A.3.2 this implies

$$\forall a \in \mathbb{N}, 0 < x < 1: \; g_a'(x) \geq \left[\frac{1}{x} + \frac{(2a^2+a)\left((1+x)^{2a} + (1-x)^{2a}\right)}{(1+x)^{2a+1} - (1-x)^{2a+1}}\right] g_a(x)$$

As g_a is a smooth function of x with $\forall a \in \mathbb{N}: \lim_{x\to 0} g_a(x) = \lim_{x \to 0} g_a'(x) = 0$ and

$$\forall a \in \mathbb{N}, 0 < x < 1: \; \frac{1}{x} + \frac{(2a^2+a)\left((1+x)^{2a} + (1-x)^{2a}\right)}{(1+x)^{2a+1} - (1-x)^{2a+1}} \geq 0$$

this proves the claim.

A.4. Idea of Proof for Conjecture 3.4.3

First a supplementary inequality will be proved, which is of some value for certain parameter values.

A relation which can be proved for strictly non-vanishing mass $m > 0$ is

$$\forall a \in \mathbb{N}: \; \left(\frac{g_a(m,\beta)}{g_0(m,\beta)}\right)^{a+1} \leq \left(\frac{g_{a+1}(m,\beta)}{g_0(m,\beta)}\right)^{a} \tag{A.4.1}$$

which obviously holds true by Jensen's inequality, as $g_0(m,\beta) > 0$ and thus $\beta^{2a}\frac{g_a(m,\beta)}{g_0(m,\beta)}$ can be interpreted as mode integral of the probability measure

$$d\mu_{m,\beta}(q) = \frac{1}{g_0(m,\beta)\left(e^{\sqrt{q^2+m^2\beta^2}} - 1\right)\sqrt{q^2+m^2\beta^2}} dq$$

Obviously relation (3.4.4) follows from (A.4.1) if

$$g_0(m,\beta) \leq \frac{g_a^{a+1}(0,\beta)}{g_{a+1}^{a}(0,\beta)} = \frac{\left[\zeta(2a)\Gamma(2a)\right]^{a+1}}{\left[\zeta(2a+2)\Gamma(2a+2)\right]^{a}}$$

which can never hold for all a at finite m as the right hand side exponentially converges to 0 for increasing a. However, if one is only interested in a small number of moments for a sufficiently large mass of the field and low temperature of the state the estimate (A.4.1) can be usable. For example, if one is only interested in the first inequality one needs only $g_0(m,\beta) \leq \frac{5}{12}$ which is fulfilled for $\beta m > 1.5$ as can easily be checked numerically.

Now we make some remarks concerning a strategy to prove conjecture 3.4.3. Defining $M := \beta m$ it would suffice to show

$$\forall a \in \mathbb{N}: \ \frac{d}{dM}\frac{g_a^{a+1}(M,\beta)}{g_{a+1}^a(M,\beta)} \leq 0 \tag{A.4.2}$$

For the case $a = 0$ relation (A.4.2) can easily be seen to hold. Additionally the relation

$$\forall a \in \mathbb{N}, M \geq 0: \ \frac{g_a^{a+1}(M,\beta)}{g_{a+1}^a(M,\beta)} \leq \frac{g_{a-1}^a(M,\beta)}{g_a^{a-1}(M,\beta)} \tag{A.4.3}$$

holds by Jensen's inequality for the probability measure

$$d\mu_{a,m,\beta}(q) = \frac{q^{2a-2}}{g_{a-1}(m,\beta)\Big(e^{\sqrt{q^2+m^2\beta^2}}-1\Big)\sqrt{q^2+m^2\beta^2}}dq$$

One easily sees that $\lim\limits_{M\to\infty} g_0(M) = 0$ so it is sufficient to show

$$\forall a \in \mathbb{N}, M \geq 0: \ \frac{d}{dM}\frac{g_a^{a+1}(M,\beta)}{g_{a+1}^a(M,\beta)} \neq 0$$

B. Introduction to Probability Theory

This appendix will present some fundamental notions of probability theory in a very condensed form. Proofs of lemmas and theorems are omitted and can be found in standard literature. The aim of this appendix is to define expectation values and correlations of random fields in a self contained form. First the necessary spaces and structures will be introduced, then random fields are defined and last the concept of integration on measure spaces will be explained to enable the definition of expectation values.

Definition B.0.1. (σ-algebra)
Let Ω be a set and $\mathcal{P}(\Omega)$ its power set, i.e. the set of all subsets of Ω. A subset $\mathscr{F} \subset \mathcal{P}(\Omega)$ is called a σ-**algebra** if

- $\Omega \in \mathscr{F}$
- If $\mathcal{A} \in \mathscr{F}$, then $\Omega \backslash \mathcal{A} = \mathcal{A}^c \in \mathscr{F}$.
- If $\forall n \in \mathbb{N} : \mathcal{A}_n \in \mathscr{F}$, then $\bigcup\limits_{n\in\mathbb{N}} \mathcal{A}_n \in \mathscr{F}$.

The elements of $\mathscr{F}$ are called **measurable sets** and $(\Omega, \mathscr{F})$ is called a **measurable space**.

Lemma B.0.2. *(generating set)*
For every $\mathcal{C} \in \mathcal{P}(\Omega)$ there is a σ-algebra $\sigma(\mathcal{C})$ such that for any σ-algebra $\mathscr{F}$ containing $\mathcal{C}$ the relation $\mathcal{C} \subseteq \sigma(\mathcal{C}) \subseteq \mathscr{F}$ holds. $\sigma(\mathcal{C})$ can be formally defined as the intersection of all σ-algebra $\mathscr{F}$ containing $\mathcal{C}$ and is called the σ-algebra generated by $\mathcal{C}$. $\mathcal{C}$ is called a generating set for $\sigma(\mathcal{C})$.

Definition B.0.3. (Special σ-algebras)

- Let I be an index set and for all $i \in I$ let $(\Omega_i, \mathscr{F}_i)$ be a measurable space. Let $\Omega = \prod\limits_{i\in I} \Omega_i$ denote the cartesian product and $\pi_i : \Omega \to \Omega_i$ the canonical projections. Then $\bigotimes\limits_{i\in I} \mathscr{F}_i := \sigma\left(\bigcup\limits_{i\in I} \pi_i^{-1}(\mathscr{F}_i)\right)$ is a σ-algebra on Ω called the **product-σ-algebra**.

- Let $(\Omega, \mathscr{F})$ be a measurable space and $\widetilde{\Omega} \subset \Omega$. Then $\mathrm{Tr}_{\widetilde{\Omega}\subset\Omega}(\mathscr{F}) := \{\mathcal{A} \cap \widetilde{\Omega} | \mathcal{A} \in \mathscr{F}\}$ is a σ-algebra over $\widetilde{\Omega}$ and is called the **trace-σ-algebra**.
- Let $\mathcal{O}_n$ be the set of all open subsets of $\mathbb{R}^n$, then $\mathscr{B}_n := \sigma(\mathcal{O}_n)$ is called the **Borel σ-algebra**. One usually denotes $\mathscr{B}_1 =: \mathscr{B}$.

Note.
The Borel-σ-algebras are compatible with the trace- and product-σ-algebra in the sense that the relation $\bigotimes_{i=1}^{n} \mathscr{B} = \mathscr{B}_n$ and for $k < n$ the relation $\mathrm{Tr}_{\mathbb{R}^k \subset \mathbb{R}^n}(\mathscr{B}_n) = \mathscr{B}_k$ hold. These properties are very useful for the definition of integration and simplify the following treatment significantly.

Definition B.0.4. (measure, measure space, probability space)
Let $(\Omega, \mathscr{F})$ be a measurable space, $\mu : \mathscr{F} \longrightarrow [0, \infty]$ a map.

- μ is called a **measure** if it satisfies
  (a) $\mu(\emptyset) = 0$
  (b) For pairwise disjoint measurable sets $\mathcal{A}_n \in \mathscr{F}$ the property $\mu\left(\bigcup_{n\in\mathbb{N}} \mathcal{A}_n\right) = \sum_{n\in\mathbb{N}} \mu(\mathcal{A}_n)$, called σ-additivity, holds.

  $(\Omega, \mathscr{F}, \mu)$ is then called a **measure space**.
- A measure μ is called a **probability measure**, if $\mu(\Omega) = 1$. One usually denotes $\mu = \mathbb{P}$. $(\Omega, \mathscr{F}, \mathbb{P})$ is then called a **probability space**.

Notation.
- $\mathcal{A}_n \nearrow \mathcal{A} \quad \Leftrightarrow \quad \forall n \in \mathbb{N} : \mathcal{A}_n \subseteq \mathcal{A}_{n+1} \wedge \mathcal{A} = \bigcup_{n\in\mathbb{N}} \mathcal{A}_n$
- $\mathcal{A}_n \searrow \mathcal{A} \quad \Leftrightarrow \quad \forall n \in \mathbb{N} : \mathcal{A}_n \supseteq \mathcal{A}_{n+1} \wedge \mathcal{A} = \bigcup_{n\in\mathbb{N}} \mathcal{A}_n$

Lemma B.0.5. *(Properties of measures)*
Let $(\Omega, \mathscr{F}, \mu)$ be a measure space, then

(a) μ *is* **continuous** *from below and above, i.e. for $\mathcal{A}_n, \mathcal{A}, \mathcal{B} \in \mathscr{F}$*
   - $\mathcal{A}_n \nearrow \mathcal{A} \quad \Rightarrow \quad \lim_{n\to\infty} \mu(\mathcal{A}_n) = \mu(\mathcal{A})$
   - $\mathcal{A}_n \searrow \mathcal{A} \wedge \exists n \in \mathbb{N} : \mu(\mathcal{A}_n) < \infty \quad \Rightarrow \quad \lim_{n\to\infty} \mu(\mathcal{A}_n) = \mu(\mathcal{A})$

(b) μ *is sigma-***subadditive***, i.e.* $\mu\left(\bigcup_{n\in\mathbb{N}} \mathcal{A}_n\right) \leq \sum_{n\in\mathbb{N}} \mu(\mathcal{A}_n)$

(c) μ *is* **isotonous***, i.e.* $\mathcal{A} \subset \mathcal{B} \quad \Rightarrow \quad \mu(\mathcal{A}) \leq \mu(\mathcal{B})$

Definition B.0.6.
Let $(\Omega, \mathscr{F}, \mu)$ be a measure space, then μ is called **concentrated** on $\widetilde{\Omega} \in \mathscr{F}$ if $\mu(\Omega \backslash \widetilde{\Omega} = 0$.

Definition B.0.7. (Measurable map)
Let $(\Omega, \mathscr{F})$ and $(\Omega', \mathscr{F}')$ measurable spaces. $f : \Omega \longrightarrow \Omega'$ is called **measurable** if $\forall \mathcal{A} \in \mathscr{F}' : f^{-1}(\mathcal{A}) = \{\omega \in \Omega | f(\omega) \in \mathcal{A}\} \in \mathscr{F}$. A measurable map $f : (\Omega, \mathscr{F}) \longrightarrow (\mathbb{R}^n, \mathscr{B}_n)$ can be integrated using the Lebesgue integral.

Definition B.0.8. (Real valued random variable, random vector)
Let $(\Omega, \mathscr{F}, \mathbb{P})$ be a probability space, then a measurable map $X : (\Omega, \mathscr{F}) \longrightarrow (\mathbb{R}, \mathscr{B})$ is called a real valued **random variable** on Ω and a measurable map $V : (\Omega, \mathscr{F}) \longrightarrow (\mathbb{R}^n, \mathscr{B}_n)$ is called a real valued **random vector** on Ω.

Note.
A random variable is a one-dimensional random vector and due to the properties of the Borel-σ-algebras real valued random vectors can be interpreted as collections of real valued random variables. Therefore the following statements on real valued random vectors are also applicable for real valued random variables and vice versa.

Definition B.0.9. (Real vector valued stochastic process, random field)
Let $(\Omega, \mathscr{F}, \mathbb{P})$ be a probability space and T a totally ordered set, then a collection of real valued random vectors $\{V_t | t \in T\}$ is called a real vector valued **stochastic process**. If $\mathfrak{X}$ is a topological space, a collection of real valued random vectors $\{V_x | x \in \mathfrak{X}\}$ is called a real vector valued **random field**. A stochastic process is a special case of a random field, therefore random fields are used in the following for generality. In the following all random variables, random vectors, stochastic processes and random fields will be real valued thus this will no longer be explicitly mentioned.

Definition B.0.10. (Distribution of a random vector)
Let $(\Omega, \mathscr{F}, \mathbb{P})$ be a probability space and V a random vector on Ω, then the probability measure $\mathbb{P}_V := \mathbb{P} \circ V^{-1}$ on $(\mathbb{R}^n, \mathscr{B}_n)$ is called the **distribution** of the random vector. The existence of the distribution is guaranteed by the fact that the random vector is a measurable map.

Note.
For applications it usually suffices to characterise a random vector V by its distribution $\mathbb{P}_V$ and the probability space $(\mathbb{R}^n, \mathscr{B}_n, \mathbb{P}_V)$. From this point of view, the underlying probability space $(\Omega, \mathscr{F}, \mathbb{P})$ is no longer of interest and two random vectors V and W of the same dimension are called distributionally equivalent, if their distributions coincide $\mathbb{P}_V = \mathbb{P}_W$, even if their underlying probability spaces are different. This is particularly interesting for the integration theory.

Definition B.0.11. (Expectation value, correlation)
All random variables in this definition are defined on the probability space $(\Omega, \mathscr{F}, \mathbb{P})$.

- Let X be a random variable, $d\mathbb{P}_X$ its distribution, then its **expectation value** is defined as

$$\langle X \rangle := \int_{\Omega} X(\omega) d\mathbb{P}(\omega) = \int_{\mathbb{R}} x d\mathbb{P}_X(x)$$

  if this integral exists. It is obvious, that the expectation values coincide for distributionally equivalent random variables.

- Let V be a random vector, $d\mathbb{P}_V$ its distribution and $V_1, \ldots, V_n$ its components, then the **correlation**[1] of the components is defined as

$$\langle V_1 \ldots V_n \rangle := \int_{\Omega} X_1(\omega) \ldots X_n(\omega) d\mathbb{P}(\omega) = \int_{\mathbb{R}^n} x_1 \ldots x_n d\mathbb{P}_V(x_1, \ldots, x_n)$$

  if this integral exists.

- Let X be a random field whose parameter space $\mathfrak{X}$ is a Lie group, $\mathcal{A}_z \subseteq \mathfrak{X}$ a subset containing the neutral element of the group and $\mathcal{A}_y \subseteq \mathfrak{X}$ a subset of finite volume $\int_{\mathcal{A}_y} d_{\mathfrak{X}} y < \infty$. Using the indicator function $\mathbb{1}_{\mathcal{A}_y}$, the function

$$\mathcal{A}_z \to \mathbb{R}$$

$$z \mapsto \left(\int_{\mathcal{A}_y} \mathbb{1}_{\mathcal{A}_y}(y * z) d_{\mathfrak{X}} y \right)^{-1} \int_{\mathcal{A}_y} \langle X_y X_{y*z} \rangle \, \mathbb{1}_{\mathcal{A}_y}(y * z) d_{\mathfrak{X}} y$$

  is called the **autocorrelation**[2] function of X on $\mathcal{A}_y$, if it exists.

Note.
In general, for a random vector V with components $V_1, \ldots, V_n$ on a probability space $(\Omega, \mathscr{F}, \mathbb{P})$,

$$\langle V_1 \ldots V_n \rangle \neq \int_{\mathbb{R}^n} x_1 \ldots x_n d\mathbb{P}_{V_1}(x_1) \ldots d\mathbb{P}_{V_n}(x_n)$$

thus the knowledge of the distributions of the individual random variables is not sufficient but the distribution of the random vector is needed for the definition of the correlation.

[1] As is common in the literature on cosmological perturbation theory, we use the term "correlation" as it is used in signal processing and not as it is used in stochastics.

[2] The term "autocorrelation" is also defined as used in signal processing and not as used in stochastics.

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Acknowledgements

I would like to thank Professor Rainer Verch for giving me the opportunity to work on this topic that makes contact with a diverse range of theories of modern physics. His advice and especially his support for working on my own ideas significantly helped shape this work into its present form.

The International Max Planck Research School supported this work financially and by offering a pleasant working environment, for which I am grateful.

Further, I would like to thank Prof. Detlev Buchholz, Dr. Jan Schlemmer, Dr. Nicola Pinamonti, Dr. Thomas-Paul Hack as well as many others for conversations, which provided a great deal of inspiration for this work and influence my view of the topic of this work. Likewise, thanks go to all the other members of the Quantum Field Theory and Gravity work group who supported this work to various degrees; especially Alexander Knospe, Falk Lindner, Thomas Ludwig, Anas Much, Adam Reichold and Jan Zschoche provided a lot of valuable creative and technical advice. I would like to particularly thank Adam Reichold and Jan Zschoche, who proof read this work and thereby helped improve countless tiny details and remedy some less tiny flaws.

Lastly, I would like to acknowledge the moral support I received from many people, notably my friends and family. Most importantly, I thank Prof. Hanno Gottschalk, who was my diploma supervisor and also encouraged me before and during my doctoral studies on several occasions. Thanks go to my friends in Leipzig, including David Dubray, Julian Hofrichter, Adam Reichold, Gesa Wilangowski and Jan Zschoche for countless, sometimes heated, discussions on a variety of serious as well as nonsensical, professional as well as trivial topics. I would like to thank my family and my friends outside Leipzig, who also provided a great deal of support and motivation. I especially thank Carina and Dario.

Correction of Lemma 3.1.2

The "two-point function" for KMS states

$$\mathscr{W}_2^\beta(f,g) = \int \sum_{n=0}^{\infty} \frac{1}{2\omega_n} \left(\frac{e^{-i\omega_n \Delta t}}{1-e^{-\beta\omega_n}} - \frac{e^{i\omega_n \Delta t}}{1-e^{\beta\omega_n}} \right) \sum_{l,m} f^*_{nlm}(t) g_{nlm}(t') dt dt' (1-\delta_{\omega_n,0})$$

that has been presented in lemma 3.1.2 is not a valid two-point function in the case $m=\xi=0$. In that case the expression

$$\mathscr{W}_2^\beta(f,f) = \int \sum_{n=1}^{\infty} \frac{1}{2\omega_n} \left(\frac{e^{-i\omega_n \Delta t}}{1-e^{-\beta\omega_n}} - \frac{e^{i\omega_n \Delta t}}{1-e^{\beta\omega_n}} \right) \sum_{l,m} f^*_{nlm}(t) f_{nlm}(t') dt dt'$$

is not necessarily positive such that the positivity requirement for states is violated. For $m=\xi=0$ no KMS states exist due to the vanishing energy of the zero mode which implies an infrared problem.

This error has been pointed out to me by Professor Fredenhagen, who reviewed this thesis.

Note that all following results of section 3.1 are unaffected by this mistake, as the special case $m=\xi=0$ is not significant for any result. Especially the incompatibility with the form of the extrinsic LTE condition considered here persists, as this condition postulates independence of the thermal functions on ξ. Therefore a restriction to the parameter space $m^2+6\xi>0$ does not undermine any of the results of section 3.1.