Local Thermal Equilibrium
on Cosmological Spacetimes

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Referat: In dieser Arbeit wird ein Kriterium für lokales, thermisches Gleichgewicht in Quantenfeldtheorien auf flacher Raumzeit von Buchholz, Ojima und Roos zunächst mit einem idealisierten Messprozess in Verbindung gebracht, dann das Kriterium auf allgemeine Raumzeiten verallgemeinert und die Konsequenzen für lokale Energiedichten in Situationen, in denen dieses Kriterium erfüllt ist, untersucht. Die Untersuchungen werden dann auf kosmologische Raumzeiten eingeschränkt und nach Entwicklung einer Methode zur Berechnung der relevanten, thermodynamischen Größen wie lokalen Temperaturen auf diesen Raumzeiten wird gezeigt, dass derartige Situationen lokalen thermischen Gleichgewichts zu einem gegebenen Anfangszeitpunkt tatsächlich in der Theorie realisiert werden können. Der Formalismus und die Zeitentwicklung der thermalen Größen werden für de Sitter-Raumzeit als Beispiel illustriert.

Contents

1 Introduction and motivation

After its initial success in predicting black-hole radiation [Haw75], a finite temperature of the vacuum for accelerated observers (the Unruh-effect) [Unr76] and “particle creation” in expanding universes [Par69], quantum field theory on curved spacetimes has by now become a standard tool in (inflationary) cosmology, where it is used to calculate the spectrum of initial density fluctuation in the early universe as a result of fluctuations of quantum fields [Muk05, Wei08, Str06]. On the other side, the discovery that quantum field theory on curved spacetimes is best formulated in the algebraic approach [Wal94], the recognition of the class of Hadamard states as basic states of physical relevance and the reformulation of their properties using microlocal analysis [Rad96b] and finally the realization that the covariance principles from general relativity can be carried over to this framework [HW01, BFV03] has lead to huge progress in the mathematically precise formulation of this theory (mainly for free and perturbatively defined fields): To name just a few highlights, the problem of defining Wick- and time-ordered products was solved [BFK96, HW01], building upon them perturbation theory was defined and investigated [BF00, HW03, Hol08], sometimes leading to interesting insights for the free theory [HW05] and Quantum Energy Inequalities [For78] were derived in many different situations [Few07a, Rom05].

However, during this mathematically rigorous (re)formulation of quantum field theory on curved spacetime it became increasingly clear that this theory allows for a huge number of quantum mechanical states, but in contrast to quantum field theory on Minkowski spacetime where there is a clear-cut interpretation of (sets of) states by their particle content, as thermal states or states approximating classical field configurations (coherent states), such a characterization is not a priori available. In recent years there has therefore been a renewed interest in finding physically motivated criteria to select states on specific spacetimes and investigate their properties and quite a few results have been achieved for the case of cosmological spacetimes [Olb07, Küs08, DMP09].

In this work we suggest one more criterion which focuses on the concept of local thermodynamic equilibrium that implicitly permeates many cosmological discussions in the form of temperature, pressure, energy densities etc. that are supposed to vary in space and time. Of course the importance of topics like thermal equilibrium, non-equilibrium, return to equilibrium etc. is well understood in cosmology and in fact the simplest, homogeneous and isotropic models with matter-content described as an ideal fluid can be seen as thermodynamic models. Also on a more advanced level, for example in the discussion of nucleosynthesis, such concepts play an important role; there Boltzmann equations are the most important tool (a standard reference is [KT90]), but these discussions, if they are not on a (semi-)classical level, mostly use quantum field theory in Minkowski spacetime or at least at some point refer to concepts (preferred states) that strictly speaking only make sense there. Whereas for some regimes this is certainly justified, for the situations where “fluctuations” of the quantum fields are the object of interest only the full quantum field theory on the cosmological background is trustworthy, so one has to formulate the criteria for the selection of states at this level. One approach where this was attempted are the states of low free-energy [Küs08] modeled after the states of low energy [Olb07]; we will briefly comment upon them later.

The criterion we want to propose here, which was basically already formulated in [BS07], is based on a notion of local thermal equilibrium (in the following often abbreviated by LTE) by Buchholz, Ojima and Roos [BOR02]. The main idea of this approach to local thermodynamic equilibrium is to perform the tasks of identification of states in local thermodynamic equilibrium and the assignment of local, thermal parameters to such states using sets of point-localized observables S_x at each spacetime point and sets of reference states whose thermal interpretation is already well known (e.g. global equilibrium states). Furthermore, as a regularity requirement, the expectation value of the point-localized observables in the reference states has to exist.

The localized observables have the interpretation of (idealized) limits of measurements of density-like thermal quantities (temperature, energy-density, pressure etc.) in smaller and smaller regions of spacetime; the physical interpretation of the observables (which observable belongs to which thermal quantity?) is done by evaluating their expectation values in the reference states; for many fields one gets for example at each x an observable whose (scalar) expectation value in global equilibrium (reference) states with temperature T is a simple function of the the temperature, so this observable has the interpretation “local thermometer”.

A states ω for which there exists a reference state ω_{ref} such that the expectation values for all observables in S_x in ω and ω_{ref} agree is then called locally thermal at x; as far as the expectation values of the thermal observables are concerned, ω and ω_{ref} are indistinguishable. Therefore it makes sense to assign the thermal parameters determined by them also to ω at this point (so ω gets e.g. assigned a temperature at x). Among these thermal parameters the same relations as in global equilibrium situations hold, so if there exists for example an equation of state relating pressure and temperature and we have thermal observables allowing the local determination of these two parameters, then the equation of state will also hold for the locally assigned pressure and temperature at points where the state is locally thermal. Finally, we get to a condition of local thermal equilibrium in spacetime regions by requiring local thermality at each point x of the region, where the reference state may depend on x, which will then lead to assignments of thermal parameters varying in space and time for states fulfilling this condition.

After introducing the necessary background in chapter 2, we start by relating the original LTE formalism on Minkowski spacetime to idealized measurements, modeled using a two-niveau system in chapter 3. This gives some *motivation* for the specific choice of the S_x-spaces that was made in the quantum field theories on Minkowski spacetime, where the formalism was already applied; since it is based on perturbation theory it is does unfortunately not (yet) *deduce* the specific choices of S_x-spaces as a consequence of these idealized measurements.

Using the concept of local covariant quantum fields [BFV03] and insights gained in the discussion of the detectors we then state our criterion of local thermality (formulated for general, globally hyperbolic spacetimes), called extrinsic local thermality. The main point in its formulation is that the formalism of local covariant quantum fields is based on an identification of observables in different space-times, and taking such observables as the generators of our S_x-spaces we can (by duality) compare states on different spacetimes as well, by comparing the expectation values the related observables are assigned to by the different states. Denoting somewhat symbolically thermal observables in the space S_x at the point x of our spacetime M as $\phi(x)$ and the related observables on Minkowski spacetime as $\phi_o(x_o)$, the criterion for a state ω of a quantum field theory on this spacetime of being locally thermal at x is formulated as: There exists a state $\omega_{\mathrm{ref,o}}$ such that

$$\omega(\phi(x)) = \omega_{\mathrm{ref,o}}(\phi_o(x))$$

for all $\phi(x) \in S_x$. As in Minkowski spacetime, once we have identified the states in local thermal equilibrium, we can then assign local, thermal properties like e.g. the temperature to them; this provides a rigorous version of the heuristic concepts of local temperature, pressure, etc. in the setting of quantum fields on curved spacetime considered here.

After fixing our LTE-criterion, in chapter 4 we then go on to discuss the relation of local thermal equilibrium to Quantum Energy Inequalities. These are important when discussing quantum field theory on a curved spacetime as semiclassical theory, i.e. when trying to solve the Einstein equations

$$G_{ab} = 8\pi T_{ab}$$

with the stress-energy tensor T_{ab} on the right-hand side given as the expectation value $\omega(T_{ab}^{\mathrm{ren}})$ of a quantum field. Quantum Energy Inequalities restrict the values this expectation value can take, providing some replacement for positivity properties that hold for stress-energy tensors from classical matter models but not for $\omega(T_{ab}^{\mathrm{ren}})$.

The existence of some relation between local thermality and the energy contents of states is plausible, since among the thermal observables there are elements $T_{ab}^{\mathrm{thermal}}$ which are closely linked to the stress-energy tensor. More precisely, the (renormalized) stress energy tensor T_{ab}^{ren} of the quantum field theory can be written as

$$T_{ab}^{\mathrm{ren}} = T_{ab}^{\mathrm{thermal}} + \mathrm{Remainder}\,,$$

where the remainder term contains another thermal observable directly related to the temperature (the scalar thermometer from above) and geometric, state independent terms, and using this we then arrive at two energy inequalities for states with bounded temperature, one along finite parts of geodesics (a so called QWEI) and the other along infinitely extended, lightlike geodesics (called ANEC). We end the chapter by a brief remark on a possible generalizations of the results.

After the formulation of the LTE-condition and the investigation of some consequences on general spacetimes we then come to the question of existence of such states in chapter 5, where we restrict the discussion to cosmological spacetimes. More specifically, we investigate the class of Robertson Walker spacetimes with flat, spatial sections; though these are highly idealized models of our universe, they are still the basis of many models in cosmology and their high degree of symmetry allows a rather thorough and explicit investigations of (linear) quantum field theories on them.

In this chapter we actually pursue two goals: One is the construction of states which are locally thermal on a Cauchy surface; the other is to explore the link between the rigorous (coordinate space) formulation of the Hadamard condition and covariant Wick products and techniques using mode-decompositions. The main problem with the coordinate space formulation is that it is only in special cases usable for concrete calculations; the methods using mode-decompositions, which are adapted to the class of spacetimes at hand, are much more suitable but often not very rigorous. While initially such an investigation was not planned, it turned out that because the criterion of local thermality requires very explicit knowledge of some expectation values of Wick products, one needs good methods to calculate them. While the ideas underlying the general procedure are long known, their discussions either mainly focus on the stress-energy tensor and predate precise formulations of the Hadamard conditions (see e.g. the book of Birrell and Davies [BD84]) or are of more general nature [LR90, JS02, Pir93], which makes them not especially suitable for the explicit calculation (and even the investigation of regularity like e.g. the Hadamard property on concrete, cosmological spacetimes).

We therefore start chapter 5 with a discussion how the calculation of concrete expectation values and (most of the) regularity question can be reduced to questions on Cauchy surfaces for the spacetimes at hand; the underlying principle is the Klein-Gordon equation which the field has to satisfy. Just as in the classical case, where the values of solutions to the Klein-Gordon equation can be deduced from values on a Cauchy surface, which consist of the value of the solution and time-derivative on this surface, we show that also here the (relevant) values of the (renormalized) two-point function $\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$, which encodes all the Wick-products and regularity properties can be obtained from its restriction and the restriction of its first time-derivatives to a Cauchy surface (strictly speaking, concerning regularity, we only give a necessary criterion for Hadamard states and sketch, how this could be turned into an equivalence).

We then go on to establish the relation between the definition of Wick products in terms of the (renormalized) two-point function on the spacetime and certain integral expressions that are obtained by "renormalizing under the integral" in the mode-decomposition of the (non-renormalized) two-point function.

Next we briefly describe, how the results obtained so far provide an alternative method to the adiabatic vacua in investigating, whether a given state is Hadamard, and briefly illustrate it on the example of de Sitter spacetime. We then return to the calculation of the expectation values of interest.

With these calculational methods in place we finally attack the problem of constructing LTE states on a Cauchy surface. The procedure used here starts from the observation that after fixing an initial state ω_{ini} on the spacetime and a Cauchy surface, different states can be obtained by modifying the initial data of the initial state on this Cauchy surface. The expectation values of the thermal observables $\phi(x)$ for points x on this Cauchy surface can then be expressed in terms of this modification as some $\Delta[\phi(x)]$

and consequently the LTE condition can be rewritten as a set of equations between the expectation values $\omega_{\mathrm{ref,o}}(\phi_o(x))$ of the thermal observables in some reference state, a term $\Phi_{\mathrm{ini}}[\phi(x)] = \omega_{\mathrm{ini}}(\phi(x))$ and $\Delta[\phi(x)]$ of the form

$$\omega_{\mathrm{ref,o}}(\phi_o(x)) = \Phi_{\mathrm{ini}}[\phi(x)] + \Delta[\phi(x)]\,.$$

For each $\phi(x)$ this gives one equation and the task is now to find a modification of the initial state and a reference state ω_{ref} such that they are simultaneously fulfilled. It turns out that the modifications of the initial state can be formulated in terms of two functions and the $\Delta[\phi(x)]$ are then given as moments of these functions; finally using the known form of the left-hand sides of this equations we show that they always have solutions for sufficiently high temperatures, i.e. if we choose on the left hand side as reference states global equilibrium states on Minkowski spacetime with sufficiently high temperature.

While this construction has the advantage of producing *states* on the *whole* spacetime (i.e. the two-point function satisfies the positivity condition on the whole spacetime and not just the Cauchy surface used in the construction), this is not true for the LTE-conditions which do not necessarily hold outside this Cauchy surface. While this is of course unpleasant, it is not completely unexpected from a physical point of view: Since the theory considered is a free field, there is no mechanism at work which thermalizes the perturbations coming from the coupling to the changing external gravitational field.

One would however intuitively expect that these perturbations are increasingly less severe as the (local) temperature of the states increases and the interaction time with the gravitational field decreases and this will be briefly commented upon after the construction of the states. We finally end the chapter by once more coming back to our example and illustrating the construction there, ending with plots giving numerical examples of the development of the thermal parameters assigned on a given Cauchy surface.

Comparing the methods and results to what has been done in the context of states of low (free-)energy, the main difference is that our criterion of local thermality is in fact a point-wise one, whereas the criterion of low (free-)energy involves integrals over test-functions. In addition, we get a procedure to locally assign thermal properties, which is closer to what is really assumed in cosmological calculations. On the other hand, we are so far only able to (strictly) control our criterion on a Cauchy surface, whereas the criterion of low (free-)energy is trivially fulfilled on the whole spacetime; nevertheless one should notice that at least a posteriori and for concrete spacetimes we can make qualitative statements about the extent to which the criterion of local thermality holds, as is illustrated by the example of de Sitter spacetime at the end of this work.

2 Technical background

In this chapter the technical background of this work will be described. We start by giving the construction of the (neutral) Klein-Gordon field on globally hyperbolic spacetimes in the algebraic approach, move on to review the concept of locally covariant quantum fields to the extent required in the following and then introduce the class of cosmological spacetimes considered in the following. Finally, for these spacetimes more concrete realizations of some of the constructions described for general globally hyperbolic spacetimes will be given. Most of the material covered is standard; exceptions are the part on regularization aspects of the Hadamard parametrix in the special coordinates chosen, the representation formulas (2.2.27) and (2.2.29), which are worked out versions of the non-Fock case of homogeneous and isotropic states only treated partially in [LR90], and the section on the specification of such states by “initial values” for the two-point function. References to the literature will be given in the individual sections. We use units where $\hbar = c = G^* = 1$.

2.1 General spacetimes

2.1.1 The Klein-Gordon field on globally hyperbolic spacetimes

Spacetime is taken here as a four-dimensional, smooth and oriented semi-riemannian manifold (M, g), where the metric tensor g has signature $(+----)$. The space of k-times continuously differentiable functions on M will be denoted by $C^k(M)$, the space of smooth function on M by $C^\infty(M)$ and the subspace of (test-)functions with compact support by $C_0^\infty(M)$. The measure induced on M by g will be denoted by μ_g; this preferred measure allows an identification of functions and densities on M and using this identification distributions on M, which following [Hör03] (see also [GKOS01] for a more detailed discussion) are at first defined as linear functional on densities, can be identified with functionals on $C_0^\infty(M)$ by composition with the identification map. In practice, this means that the (regular) distribution associated to a function $F \in C^\infty(M)$ is given by

$$C_0^\infty(M) \ni \varphi \mapsto \int_M F(x)\varphi(x)\mathrm{d}\mu_g(x)\,,$$

which formally looks exactly like on $\mathbb{R}^n$; when written in charts the volume-element $\sqrt{|\det g|}$ will however appear in addition to the usual expression on $\mathbb{R}^n$.

We will use both abstract index notation [Wal84] and decompositions with respect to specific bases; to distinguish the two different meanings of indices, we will use latin indices in the first and greek indices in the second case, furthermore Einstein summation convention is used.

The Levi-Civita connection determined by g will be denoted by ∇, concerning its curvature, Ricci-tensor R_{ab} and curvature scalar R we take the conventions [-,-,-] in the classification scheme of [MTW73], i.e. following the book of Birrell and Davies [BD84]. The wave operator $g^{ab}\nabla_a\nabla_b$ determined by g is denoted by $\Box_g$.

To be able to construct quantum field theories on M, the spacetime is furthermore assumed to be time-orientable and globally hyperbolic, which implies among other things: [BGP07], [BS05]

1. There exists a smooth function $T : M \to \mathbb{R}$, whose gradient is an everywhere non-vanishing, future-pointing vector field. The surfaces $T^{-1}(t) \subset M$ for t in the range of T are Cauchy surfaces for M.

2. The Klein-Gordon operator, defined for $m, \xi \in \mathbb{R}_0^+$ by $\mathrm{P}_{m,\xi} := \Box_g + m^2 + \xi R$, has uniquely determined retarded and advanced solution operators $\mathrm{E}^\pm$ mapping test-functions $f \in C_0^\infty(M)$ into smooth solutions to the Klein-Gordon equation satisfying

$$\begin{aligned} \mathrm{P}_{m,\xi}\mathrm{E}^\pm f = \mathrm{E}^\pm \mathrm{P}_{m,\xi} f =& f \qquad \text{for all } f \in C_0^\infty(M) \\ \operatorname{supp}\left(\mathrm{E}^\pm f\right) \subset& J^\pm\left(\operatorname{supp}(f)\right) , \end{aligned}$$

where $J^\pm(G)$ is the causal future/past set of a set $G \subset M$ [BGP07].

Using these operators, one can define an operator E as the difference $\mathrm{E}^- - \mathrm{E}^+$ and in addition the bilinear form

$$\mathscr{E}(f, f') := \int_M f(x)(\mathrm{E}f')(x)\mathrm{d}\mu_g(x) \, .$$

By definition E clearly satisfies $\mathrm{P}_{m,\xi}\mathrm{E}f = \mathrm{E}\mathrm{P}_{m,\xi}f = 0$ for all $f \in C_0^\infty(M)$ and this implies $\mathscr{E}(f, \mathrm{E}f') = 0$. Using the fact that $\int_M (\mathrm{P}_{m,\xi}f)(x)h(x)\mathrm{d}\mu_g(x) = \int_M f(x)(\mathrm{P}_{m,\xi}h)(x)\mathrm{d}\mu_g(x)$ for $f, h \in C^\infty(M)$ and one of them in addition compactly supported, we see that also $\mathscr{E}(\mathrm{P}_{m,\xi}f, f') = 0$ (this can also be deduced from the fact that $\mathscr{E}$ is antisymmetric, which is also not hard to show [Wal94]) i.e $\mathscr{E}$ is a bi-solution to the Klein-Gordon equation in the sense of distributions.

Using this data, one can now construct the *-algebra $\mathcal{A}(M, g)$ of the Klein-Gordon field as the *-algebra generated by the unit-element 1 and symbols $\phi(f)$, $f \in C_0^\infty(M)$, satisfying the additional relations ($f, f' \in C_0^\infty(M)$, $\alpha \in \mathbb{C}$)

Linearity: $\phi(\alpha f + f') = \alpha\phi(f) + \phi(f')$.

Neutral field: $\phi(f)^* = \phi(\overline{f})$.

Klein Gordon equation: $\phi(\mathrm{P}_{m,\xi}f) = 0$.

Commutator: $[\phi(f), \phi(f')] = i\mathscr{E}(f, f')1$.

($[\phi(f), \phi(f')] = \phi(f)\phi(f') - \phi(f')\phi(f)$ the commutator). Because $\mathscr{E}$ is an antisymmetric bi-solution, the commutator relation is compatible with the other three relations.

The hermitian elements in $\mathcal{A}(M,g)$ correspond to observables of the quantized system; as will turn out later we will need to enlarge this set of basic observables, i.e. pass to a larger algebra containing $\mathcal{A}(M,g)$. The other ingredient for the description of a quantized system besides the observables are the states; in the algebraic approach chosen here these are defined as functionals $\omega : \mathcal{A}(M,g) \to \mathbb{C}$ which fulfill the additional conditions

Normalization: $\omega(1) = 1$.

Positivity: $\omega(A^*A) \geq 0$ for all $A \in \mathcal{A}(M,g)$.

As already discussed in the introduction, the set of all such states for a quantum field theory is enormous and in addition contains many elements that lack regularity properties required to carry out important constructions. We will therefore restrict the set of states by several requirements, first to the set of quasifree Hadamard states and then, for the cosmological spacetimes under consideration, even further to the set of homogeneous and isotropic states.

First note that a state ω is determined by its n-point functions $\mathscr{W}_n^\omega$ defined by

$$\mathscr{W}_n^\omega : (f_1, \dots, f_n) \mapsto \omega(\phi(f_1)\dots\phi(f_n)) .$$

As a first regularity property, we demand that these n-point functions are distributions in all their arguments (and then by the kernel theorem are even distributions on M^n [RS75]). Next, looking at the properties of $\mathcal{A}(M,g)$ one notices that they are formulated in terms of algebra elements containing at most two generators $\phi(f)$. It turns out that it is possible to do something similar on the set of states; there is a set of states called quasifree states, which are uniquely determined by their two-point function, i.e. the value of the state on products of two elements[1]. Note that every monomial $\phi(f_1)\phi(f_2)\dots\phi(f_n)$ in the field-operators can be written as a sum of totally symmetric products of field operators times commutators[2]; since the commutators are multiples of the unit in $\mathcal{A}(M,g)$, it is thus sufficient to give the (totally) symmetric parts $\mathscr{W}_n^{\omega,s}$ of the n-point function in order to specify ω. (Formally) differentiating the function

$$(t_1, \dots, t_n) \mapsto (-i)^n \exp\left(-\tfrac{1}{2}\mathscr{W}_2^{\omega,s}(t_1 f_1 + \dots + t_n f_n, t_1 f_1 + \dots + t_n f_n)\right)$$

with respect to t_1, t_2, $\dots$, t_n and then setting $t_1 = t_2 = \dots = t_n = 0$[3] gives a totally symmetric expression in $f_1, \dots, f_n$ and taking this as $\mathscr{W}_n^{\omega,s}(f_1, \dots, f_n)$ defines the

[1] If one requires the state to be completely specified by its values on products of no more than two field operators, one also has to give its one-point function (the value of the zero-point function is fixed by the normalization condition). In the definition of quasifree states given here, the one-point functions are required to vanish.

[2] Replacing "contraction" of the elements A_i and A_j by $\frac{1}{2}[A_i, A_j]$ and "normal ordered product of $A_1 \dots A_k$" by "symmetrized product of $A_1 \dots A_k$" in Wick's theorem [BS80] provides a procedure for doing this.

[3] Note that this defines $\mathscr{W}_n^\omega$ by polarization [Dol03] from the $\mathscr{W}_n^{\omega,s}(f, \dots, f)$ obtained by equating the terms of order t^n in (the series expansion of) the equation $\omega\left(e^{it\phi(f)}\right) = \exp\left(-\frac{t^2}{2}\mathscr{W}_2^\omega(f,f)\right)$, which is often given as the relation defining a quasifree state.

quasifree state with two-point function $\mathscr{W}_2^\omega$. One directly sees that the symmetric part of the n-point functions for odd n all vanish. Because the expression of a product of an odd number of field-operators as a sum of totally symmetric products of field operators only contains totally symmetric products, also the full n-point functions for odd n vanish. Besides being a convenient choice, since all aspects of the state can be discussed in terms of its two-point function, the justification for the use of quasifree states is that most other physical states can be derived from those [Ver94]; furthermore the global thermal equilibrium states on Minkowski spacetime, used later as a basis for the concept of local thermal equilibrium, are of this form.

Before coming to the extension of the algebra of observables already mentioned, we need one more restriction, which can intuitively be interpreted as a restriction on the "small-distance" ↔ "high-energy" behaviour of the states and on a more technical level is a replacement for the spectrum condition on curved spacetimes. To define this condition, we first need to introduce some notation related to spacetime geometry:

Definition 2.1. For $x \in M$, denote by $\exp_x$ the exponential map at $x \in M$. A set $N \subset M$ is called geodesically starshaped with respect to $x \in N$, if there exists an open set $N' \subset T_xM$, which is starshaped wrt. $0 \in T_xM$, such that $\exp : N' \to N$ is a diffeomorphism. If N is geodesically starshaped with respect to all its points $x \in N$, it is called geodesically convex. On $N \times N$ the signed squared geodesic separation σ is defined by

$$\sigma(x, x') = -g_x(\exp_x^{-1}(x'), \exp_x^{-1}(x'))$$

($g_x : T_xM \times T_xM \to \mathbb{R}$ the metric tensor at $x \in M$).

Remark 2.2. From the definition it is clear that σ is smooth on $N \times N$ and from the definition of the exponential map it follows that σ is symmetric. Furthermore, one can show [Fri75]:

1. σ fulfills the partial differential equation

$$g^{ab}(\nabla_a\sigma)\nabla_b\sigma = -4\sigma\,. \tag{2.1.1}$$

2. For fixed x', $t^a : N \ni x \mapsto -g^{ab}\nabla_b\sigma(x, x')$ defines a vector field which at x is tangent to the (unique) geodesic through x' and x.

Concerning the existence of geodesically convex sets, it can be shown that M can be covered by such sets [O'N83], so for each $x \in N$ we have a geodesically convex neighbourhood N of x.

Using the above time function T, guaranteed to exist on globally hyperbolic spacetimes, we can now define the functions σ_ϵ as

$$\sigma_\epsilon : (x, x') \mapsto \sigma(x, x') + 2i\epsilon\,(T(x) - T(x')) + \epsilon^2\,.$$

Define the functions $\Delta^{1/2}$, v_j and $j \in \mathbb{N}$ as the solutions to the (recursive system of) partial differential equations

$$2g^{ab}(\nabla_a\sigma)\nabla_b\Delta^{1/2} + (8 + \Box_g\sigma)\Delta^{1/2} = 0 \tag{2.1.2}$$

$$2g^{ab}(\nabla_a\sigma)\nabla_b v_0 + (4 + \Box_g\sigma)v_0 = -L^2\mathrm{P}_{m,\xi}\Delta^{1/2} \tag{2.1.3}$$

$$2(j+1)g^{ab}(\nabla_a)\sigma\nabla_b v_{j+1} + (j+1)(\Box_g\sigma - 4j)v_{j+1} = -L^2\mathrm{P}_{m,\xi}v_j \tag{2.1.4}$$

with initial conditions $\Delta^{1/2}(x,x) = 1$. Using the method of characteristics and part 2. of remark 2.2, it can be shown that these equation have uniquely determined solutions remaining finite on approach to the diagonal (i.e. satisfying $\lim_{x\to x'} v_j(x,x') < \infty$) on $N \times N$ and these are in addition smooth and symmetric [BGP07, Mor99]. The regularized Hadamard-parametrix for $k \in N$ is then defined as

$$\begin{aligned} G_{k,\epsilon} :=& \frac{\Delta^{1/2}}{\sigma_\epsilon} + v^{(k)} \log\left(\tfrac{\sigma_\epsilon}{L^2}\right) \\ v^{(k)} :=& \frac{1}{L^2}\sum_{j=0}^{k} v_j \left(\frac{\sigma}{L^2}\right)^j , \end{aligned}$$

where $L \in \mathbb{R}$ is some constant (length-scale) introduced to make the argument of the logarithm dimensionless. Notice that $G_{k,\epsilon}$ is determined by the local spacetime geometry, the parameters m, ξ and a priori the time function T. With these definitions in place we can now state our regularity requirement:

Definition 2.3. A state ω is called Hadamard if for any geodesic convex neighbourhood N of any given point x_0 one can find a sequence $H_k^\omega \in C^k(N \times N)$, such that for all $f_1, f_2 \in C_0^\infty(N)$ one has

$$\mathscr{W}_2^\omega(f_1, f_2) = \lim_{\epsilon\to 0+} \frac{1}{4\pi^2}\int_{N\times N} \left(G_{k,\epsilon}(x,x') + H_k^\omega(x,x')\right) f_1(x) f_2(x') \mathrm{d}\mu_g(x)\mathrm{d}\mu_g(x') .$$

For later use, define the distribution

$$\mathcal{G}_k(f_1, f_2) = \lim_{\epsilon\to 0+} \frac{1}{4\pi^2}\int_{N\times N} G_{k,\epsilon}(x,x') f_1(x) f_2(x') \mathrm{d}\mu_g(x)\mathrm{d}\mu_g(x')$$

and denote its symmetric part $\frac{1}{2}\left(\mathcal{G}_k(f_1,f_2) + \mathcal{G}_k(f_2,f_1)\right)$ by $\mathcal{G}_k^s(f_1,f_2)$. It can be shown to be independent of the choice of time function [KW91], which is the justification for not explicitly referring to the time-function in definition 2.3. In the chapter on Quantum Energy Inequalities, we will sometimes only need that the two-point function of a state is of the form just described but not that it is quasifree; we will refer to such states as states with a two-point function of Hadamard type.

Hadamard states are extendable to a larger algebra containing in addition to the observables in $\mathcal{A}(M,g)$ observables like the stress energy tensor and certain density-like quantities at points that will be used to define local thermality. This extension will be the topic of the next section.

2.1.2 Locally covariant quantum fields and Wick products

In the original LTE-formalism by Buchholz, Ojima and Roos [BOR02], the observables used to define local thermality are chosen as special Wick products of the field and its derivatives. On Minkowski spacetime their definition for free fields via normal-ordering is standard (and normal ordering is usually already introduced when defining the Hamiltonian of the theory) and also in the more abstract, algebraic formulation of (interacting) quantum field theory there is a worked out framework to define them [Bos00]. These definitions, however, rely on the existence of a vacuum state, singled out by its behaviour under spacetime symmetries. When trying to generalize them to quantum field theory on a general curved spacetime, there are two questions that come up:

- Given a state ω and a representation $(H_\omega, \pi_\omega, \Omega_\omega)$ associated to it via the GNS-construction [Wal94, Chap. 4], is it possible to define observables by some generalization of the normal ordering prescription and what is their domain of definition, or formulated in the algebraic approach: By making use of ω, is it possible to enlarge the algebra $\mathcal{A}(M, g)$ and which states can be continued to this larger algebra?
- If this works for different ω: How do we find out which one is the "right" construction, or put in terms of observables: how do we identify the observables in the larger algebra obtained in this way ?

In answering the first question, the notion of Hadamard states comes up: Using a reformulation of the Hadamard condition in the language of wave-front sets of distributions [Rad96b], which makes the tools of microlocal analysis available [Hör03], it was noted that the same construction as in Minkowski spacetime, namely defining normal ordering recursively as ($\phi_\omega(f) := \pi_\omega(\phi(f))$ the representor of $\phi(f)$ in the GNS-representation of $\mathcal{A}(M, g)$)

$$\begin{aligned} :\!\phi_\omega(f)\!:_\omega &= \phi_\omega(f) \\ :\!\phi_\omega(f_1)\dots\phi_\omega(f_{n+1})\!:_\omega &= \,:\!\phi_\omega(f_1)\cdots\phi_\omega(f_n)\!:_\omega \phi_\omega(f_{n+1}) \\ &\quad - \sum_{l=1}^{n+1} :\!\phi_\omega(f_1)\cdots\phi_\omega(f_{l-1})\phi_\omega(f_{l+1})\cdots\phi_\omega(f_n)\!:_\omega \mathscr{W}_2^\omega(f_l, f_{n+1}) \end{aligned}$$

and then restricting these operators (e.g. by restricting the vector valued distributions $:\!\phi_\omega(f_1)\dots\phi_\omega(f_n)\!:\,\Psi$ on M^n, Ψ a vector from (a dense subset of) the common, dense invariant domain of the $\phi_\omega(f)$) to the "diagonal" by composition with the diagonal map $\delta : M \ni x \mapsto (x, \dots, x) \in M^n$ is well defined[BFK96, HW01]. As a result, one indeed obtains an algebra $\mathcal{W}(M, g) \supset \mathcal{A}(M, g)$ containing "Wick products" (for details see below) and it turns out that the algebras constructed using different Hadamard states ω, ω' are isomorphic. Furthermore, states with a two-point function of Hadamard form and smooth truncated n-point functions can be continued to $\mathcal{W}(M, g)$ [HR02], which answers the first question rather completely.

The second question however remains, and as there are very many Hadamard states [Ver94], leading to different candidates for Wick products, this is indeed a serious problem. In fact, on a more elementary level this problem was already encountered earlier in the definition of (the expectation values of) the stress-energy tensor in quantum field theory on curved spacetime. There, a solution was achieved by Wald by transferring concepts, known for classical fields in general relativity, into quantum field theory [Wal77]. The most important input was a notion of "local dependence" of the renormalization prescription on the spacetime geometry (there called causality); this was then developed into the concept of locally covariant quantum fields [HW01], [BFV03]. As only a small part of this formalism will be used in the following, the concepts required will be introduced in a rather concrete way; for the formulation emphasizing the conceptual aspects see [BFV03]. In this paper, quantum field theory and quantum fields are described using concepts from category-theory and this has proven a very useful approach in other investigations [Few07b, BR07].

First, note that the construction of $\mathcal{A}(M,g)$ works on every globally hyperbolic spacetime (M,g) and since on each $\mathcal{A}(M,g)$ there exist Hadamard states [Wal94], we also have for each globally hyperbolic spacetime (M,g) an algebra $\mathcal{W}(M,g)$. Consider now the case of a globally hyperbolic spacetime (N,g') isometrically embedded into (M,g) via the map $\psi : N \to M$. ψ is further assumed to be orientation and time-orientation preserving and causal in the sense that for $x, x' \in N$ all causal curves γ connecting $\psi(x)$ and $\psi(x')$ (in M) lie entirely in $\psi(N)$. Using ψ^{-1}, defined on the image of ψ, an algebra homomorphism between the algebra $\mathcal{A}(N,g')$ and $\mathcal{A}(M,g)$ is defined by setting $\alpha_\psi(\phi'(f')) := \phi(f' \circ \psi^{-1})$ for the generators, where $f' \in C_0^\infty(N)$, $\phi'(f') \in \mathcal{A}(N,g')$. Basically the same construction also works for the algebras $\mathcal{W}(M,g)$ [HW01]; for each isometric, causal imbedding $\psi : (N,g') \to (M,g)$ we get an algebra homomorphism $\tilde{\alpha}_\psi : \mathcal{W}(N,g') \to \mathcal{W}(M,g)$.

While the discussion so far has been on the level of algebras of observables, we now want to get to individual observables. The first important point is that a quantum field is seen as an object defined on *all* globally hyperbolic spacetimes, more precisely, for each (M,g) one has a map $\Phi[M,g] : C_0^\infty \to \mathcal{W}(M,g)$. The notion of local covariance is then formulated as the requirement

$$\alpha_\psi(\Phi[N,g'](f')) = \Phi[M,g](f' \circ \psi^{-1}) \,.$$

If we consider as fields $\Phi[M,g](f)$ the generators $\phi(f)$ of the field algebra $\mathcal{A}(M,g) \subset \mathcal{W}(M,g)$ themselves, they obviously are locally covariant quantum fields; in contrast defining the Wick product as above by the normal ordering procedure $:\cdot:_\omega$, using a Hadamard state $\omega(M,g)$ for each globally hyperbolic spacetime (M,g), one does *not* get a locally covariant quantum field [HW01]. Using in the normal-ordering procedure instead of the two-point function of a state ω the Hadamard-parametrix $\mathcal{G}_n$, one obtains a version of the Wick product, denoted in the following by $:\phi_1 \dots \phi_k:_{\mathrm{SHP}}$ and called SHP-Wick product, where $\phi_1, \dots, \phi_k$ are field operators or their derivatives, which is a locally covariant field. At first, this seems to depend on the order n of the Hadamard parametrix, but since $\mathcal{G}_n - \mathcal{G}_{n'}$ and its derivatives for $n' > n$ agree when restricted to the diagonal if only n is chosen big enough (where the minimum value of n permissible depends on the order of the derivative considered), this is in fact not the case. Furthermore, though the $:\phi_1 \dots \phi_k:_\omega$ are not locally covariant fields, the differences $:\phi_1 \dots \phi_k:_{\mathrm{SHP}} - :\phi_1 \dots \phi_k:_\omega$ lie again in $\mathcal{W}(M,g)$ (for $:\phi^2:_{\mathrm{SHP}}$ we have e.g

$:\phi^2:_{\mathrm{SHP}} - :\phi^2:_\omega = [\mathscr{W}_2^\omega - \mathcal{G}_n]_{x=x'} \cdot 1$ with $[\cdot]_{x=x'}$ denoting the restriction to the diagonal $\{(x,x) \mid x \in M\} \subset M \times M$, so the two field operators differ only by a multiple of the identity), thus the algebras $\mathcal{W}(M,g)$ in fact contain these covariant SHP-Wick products. The remaining question is now, how much freedom there is in the choice of covariant Wick products. In [HW01] this question has been tackled by giving additional requirements a Wick product should satisfy; it turns out that the general locally covariant Wick product of two field operators (only those are used in the following) may differ from the SHP products by a (universal) function times the identity, where this function is build out of local curvature-terms and parameters of the field-theory with the right scaling behaviour under rescaling of metric, mass and curvature couplings. Furthermore, a method to derive additional relations between covariant Wick products of differentiated field-operators from perturbation theoretic principles has been suggested in [HW05]; except for their Leibniz-rule, which is automatically satisfied for the SHP Wick products, this scheme will however not be applied here.

As an upshot of the construction just sketched, on each globally hyperbolic spacetime we get Wick products $:\phi_1[M,g]\ldots\phi_k[M,g]:_{\mathrm{SHP}}$ and these Wick products are related with each other; $:\phi_1[M,g]\ldots\phi_k[M,g]:_{\mathrm{SHP}}$ and $:\phi_1[N,g']\ldots\phi_k[N,g']:_{\mathrm{SHP}}$ are "the same" observable on different spacetimes (M,g) and (N,g') in the sense that they both satisfy the requirements characterizing a Wick product and if (N,g') is isometric to a part of (M,g) they are related by the local covariance equation for this embedding. This concept of identifying observables on different spacetimes will be crucial later on in the definition of local thermal equilibrium.

Concerning the practical, calculational side of the Wick products we will need formulas for the expectation values of the SHP-product of two operators in Hadamard states; just like in Minkowski spacetime, where the Wick product even exists at a point as a quadratic form, the expectation value of the SHP-products in a Hadamard state ω is a regular distribution (this can be seen directly from the definition of Hadamard states given above) and so can be restricted to points. The value of the resulting function at a point $x \in M$ will be denoted by $\omega(:\phi_1\phi_2:_{\mathrm{SHP}}(x))$. For field operators $\phi_1 = \nabla_{\mu_1}\ldots\nabla_{\mu_k}\phi$, $\phi_2 = \nabla_{\nu_1}\ldots\nabla_{\nu_l}\phi$, this expectation value can be calculated as

$$\omega(:\phi_1\phi_2:_{\mathrm{SHP}}(x)) = \left[\nabla_{x^{\mu_1}}\ldots\nabla_{x^{\mu_1}}\nabla_{x'^{\nu_1}}\ldots\nabla_{x'^{\nu_l}}\left(\mathscr{W}_2^\omega - \mathcal{G}_n\right)(x,x')\right]_{x=x'}, \tag{2.1.5}$$

where $n \geq k+l$ and the notation for the restriction is explained below. The concrete calculations can be simplified a bit by noting that the antisymmetric part of the Hadamard parametrix actually agrees with $\frac{i}{2}\mathscr{E}$ up to C^k-terms that vanish upon restriction to the diagonal (and this is again also true for the derivatives if k is chosen big enough). This is basically due to the fact that the antisymmetric parts of the distribution $\lim_{\epsilon\to 0}\frac{1}{\sigma_\epsilon}$ and $\lim_{\epsilon\to 0}\sigma^j\log\sigma_\epsilon$ agree with the (difference of the "advanced" and "retarded") Riesz-distributions used in the construction of the local fundamental solution to $\mathrm{P}_{m,\xi}$ [BGP07]. The distribution $\frac{i}{2}\mathscr{E}$ in turn is the common, antisymmetric part of all two-point functions $\mathscr{W}_2^\omega$, so defining $\mathcal{G}_k^s$ as the symmetric part of $\mathcal{G}_k$ and $\mathcal{G}_k^{\mathrm{SHP}}$ as this distribution plus the common antisymmetric part of all states

$$\mathcal{G}_k^{\mathrm{SHP}}(f_1,f_2) = \mathcal{G}_k^s(f_1,f_2) + \frac{i}{2}\mathscr{E}(f_1,f_2),$$

the term $\mathscr{W}_2^\omega - \mathcal{G}_k$ on the right hand side of (2.1.5) can be replaced by $\mathscr{W}_{\omega,k}^{\mathrm{SHP}}$ defined by

$$\mathscr{W}_{\omega,k}^{\mathrm{SHP}}(f_1,f_2) = \mathscr{W}_2^\omega(f_1,f_2) - \mathcal{G}_k^{\mathrm{SHP}}(f_1,f_2)\,,$$

which is symmetric (and not just symmetric up to remainder terms vanishing on the diagonal) and is the expression used in [FS07].

Alternatively, introducing the symmetric part of the two-point function as

$$\mathscr{W}_2^{\omega,\mathrm{s}}(f_1,f_2) = \tfrac{1}{2}\left(\mathscr{W}_2^\omega(f_1,f_2) + \mathscr{W}_2^\omega(f_2,f_1)\right)\,,$$

this can also be written as $\mathscr{W}_2^{\omega,\mathrm{s}} - \mathcal{G}_k^s$. This will be the definition used in practical calculations, since it requires only the symmetric parts of the distributions involved.

Finally in (2.1.5) and also some of the discussion so far, restrictions to the diagonal appeared; these and also partial restrictions will again show up in the following, so a few remarks on them are in order:

Functions $M \times M \ni (x,x') \mapsto f(x,x') \in \mathbb{C}$ can be considered as functions on M only by either fixing their first or second argument. For functions with one argument fixed, one can then form tensor fields by taking covariant derivatives, raise and lower indices etc.; in index notation we will denote tensor fields obtained in such a way using unprimed indices if the second argument of f was fixed and primed arguments if the first argument was fixed. Allowing the fixed argument to take all values in M (i.e. letting it vary as a parameter over M), we end up with functions $\tilde{f} : M \times M \to T_s^r(M)$, which are sections of the tensor-bundle $T_s^r(M)$ over M with respect to the first or second argument, i.e. with $\pi : T_s^r(M) \to M$ the projection of the bundle to its basis and π_1, π_2 the projections of $M \times M$ onto the first or second factor satisfy $\pi \circ \tilde{f} = \pi_1$ or $\pi \circ \tilde{f} = \pi_2$. As a $\binom{r}{s}$-tensor field, $\tilde{f}$ is a multilinear map of r covector and s vector fields into a smooth function on M, and inserting such fields we obtain a function on $M \times M$ again, which depends linearly on all the (co-)vector fields inserted. Now fixing the other argument (for concreteness assume we fix the first to $\tilde{x}$), we can again form tensor fields by taking covariant derivatives, raising indices, etc. and obtain a $\binom{r'}{s'}$-tensor field, i.e. a multilinear map of r'-covector and s'-vector fields into a smooth map. If we consider this map at $\tilde{x}$, it depends linearly on the values of all the (co-)vector fields at $\tilde{x}$ inserted in the previous step and also linearly on the values of the $r'+s'$ (co-)vector fields we can insert into the multilinear map just obtained, so it is in fact a $\binom{r+r'}{s+s'}$-tensor at $\tilde{x}$. Since we can do this for all $\tilde{x} \in M$, we obtain in this way a a multilinear map sending $r+r'$ co-vector and $s+s'$ vector fields into a smooth function, i.e. a $\binom{r+r'}{s+s'}$-tensor field. When expressed using indices with respect to bases that respect the product structure (e.g. coordinate-bases of product-coordinates), this just means that we have expressions involving two sets of indices (primed and unprimed); all tensor operations proceed as usual, but may only involve one type of indices and the order of operations involving primed and unprimed indices does not matter; finally when restricting to the diagonal $\{(x,x) \mid x \in M\}$ the distinction between indices of different type is dropped.

To denote this last step of restriction to the diagonal we use brackets, so e.g

$$[\nabla_a \nabla_{b'} f]_{x=x'}$$

is supposed to mean the $\binom{0}{2}$ tensor field mapping two vector fields X, Y in a bilinear way into a smooth function, obtained by first fixing the second argument of f and calculating for the resulting map $f_{x'}$ the $\binom{0}{1}$ tensor field $(\mathrm{d}f_{x'}) = \nabla_\mu f_{x'} \mathrm{d}x^\mu$, then inserting X and calculating for the map $\tilde{f}_X : x' \mapsto \mathrm{d}f_{x'}(X)$ the $\binom{0}{1}$ tensor field $\mathrm{d}\tilde{f}_X = \nabla_{\nu'} \tilde{f}_X \mathrm{d}x^{\nu'}$ that finally maps Y to $\mathrm{d}\tilde{f}_X(Y)$.

For the Robertson-Walker spacetimes introduced in the next section we have global coordinates $(\eta, \mathbf{x})$, $\mathbf{x} \in \mathbb{R}^3$; functions f in two arguments at $(x, x') \in M \times M$ we will denote as $f(\eta, \mathbf{x}, \eta', \mathbf{x}')$ and their restriction to $\{(\eta, \mathbf{x}, \eta', \mathbf{x}') \mid \eta = \eta'\} \subset M \times M$, the "partial diagonal", we will denote as $[f]_{\eta=\eta'}$.

2.2 Robertson Walker spacetimes

2.2.1 Some geometric properties

The class of spacetimes considered in the part on existence of LTE states will be the Robertson Walker spacetimes and among them more specifically the ones with flat spatial section. While their relevance in cosmology was briefly discussed in the introduction, here we will come to the more technical aspects and first discuss some geometric properties needed in the following (mainly some consequences of their symmetry and relations to Minkowski spacetime, which are due to the fact that these spacetimes are conformally flat).

Mathematically, (spatially flat) Robertson Walker spacetimes are given as warped products $I \times_a \mathbb{R}^3$[O'N83] of an open interval $I =]t_i, t_f[$ ($t_i = -\infty$ and $t_f = +\infty$ are permissible) and $\mathbb{R}^3$ with a positive warping function $a : I \to \mathbb{R}^+$. This means that $M = I \times \mathbb{R}^3$, with the metric tensor g given in the coordinate bases of the standard coordinates (t, x, y, z) as

$$g = \mathrm{diag}(1, -a^2, -a^2, -a^2)$$

($I \times \mathbb{R}^3$ is an open subset of $\mathbb{R}^4$, so the identity map provides a global, canonical chart used here and in the following)[4]. In these coordinates, the curves $\tau \mapsto (\tau, x_0, y_0, z_0)$ are worldlines of non-accelerated observers for all constant $(x_0, y_0, z_0) \in \mathbb{R}^3$; they are furthermore orthogonal to the surfaces of constant t which are Cauchy surfaces [BEE96, thm 3.69] and in models filled with an ideal fluid they are the flowlines of this fluid. One can therefore interpret t as some "global cosmological time" on which all the observers co-moving with the matter background can agree. Even though this chart is in this sense singled out by physical requirements, we will use an alternative time coordinate, specified by

$$\eta(t) = \int_{t_0}^{t} \frac{\mathrm{d}t'}{a(t')} \,,$$

where $t_0 \in I$ is some fixed time. Since this is monotonically increasing, ∂_η is still future pointing, we still have a global chart now with range $\hat{I} \times \mathbb{R}^3$, $\hat{I} =]\eta_i, \eta_f[$ and the surfaces of constant η are still Cauchy-surfaces (actually the same surfaces as before, but labeled

[4] M as a subset of $\mathbb{R}^4$ is oriented by taking the induced orientation; it is time oriented by taking ∂_t to be future pointing.

in a different way). Introducing the function C by the relation $C(\eta(t)) = a^2(t)$, we can express the metric tensor with respect to this new coordinates $(\eta, x, y, z) =: (\eta, \mathbf{x})$ as $g = C(\eta)\,\mathrm{diag}(1, -1, -1, -1)$. Since this is just a multiple of the Minkowski metric, the spacetime considered is seen to be conformally flat. Because it is this choice of time coordinate which makes the conformal flatness of the spacetime apparent, we will call η "conformal time"; using η as time coordinate, this property is most easily exploited, which is the reason why we will do so exclusively when dealing with Robertson Walker spacetimes in the following. The (spatially-flat) Robertson Walker spacetime, uniquely specified by the interval I and the warping function a respectively, using conformal time, the interval $\hat{I}$ and the function C, we will denote from now on as $M_{\mathrm{RW}}(\hat{I}, C)$

Denote by $E(3) = \mathbb{R}^3 \rtimes SO(3)$ the symmetry group of 3-dimensional euclidean space. Due to the warped-product structure of $M_{\mathrm{RW}}(\hat{I}, C)$ it is also the symmetry group for every spatial slice $\mathcal{S}_{\eta_0} = \{(\eta, \mathbf{x}) \mid \eta = \eta_0,\, \mathbf{x} \in \mathbb{R}^3\}$. Denote with $\rho_{\mathrm{RW}}(g)$ the group action on $M_{\mathrm{RW}}(\hat{I}, C)$ defined by $\rho_{\mathrm{RW}}(g)(\eta, \mathbf{x}) := (\eta, g\mathbf{x})$. For functions on $(M_{\mathrm{RW}}(\hat{I}, C))^n$ a natural symmetry requirement is symmetry with respect to a simultaneous transformation of all its arguments with the same element from the symmetry group by this group action. We will repeatedly encounter functions and distributions of two argument with this symmetry, which however are only defined on subsets of $(M_{\mathrm{RW}}(\hat{I}, C))^2$, so we will first introduce domains compatible with this symmetry and then describe the functions and distributions with this symmetry.

Let the open set $D \subset (M_{\mathrm{RW}}(\hat{I}, C))^2$ be such that all its spatial slices are invariant under $E(3)$, i.e.

$$\forall g \in E(3) \forall (\eta, \mathbf{x}, \eta', \mathbf{x}') \in N : (\eta, g\mathbf{x}, \eta', g\mathbf{x}') \in D\,.$$

The following lemma introduces notation and collects two well known representation statements for functions on an invariant domain and distributions on $\mathbb{R}^3$, invariant under the action $\rho_{\mathrm{RW}}(\cdot)$, respectively of $E(3)$ on $\mathbb{R}^3$.

Lemma 2.4. *Let $f : D \to \mathbb{C}$ be a function on an invariant domain $D \subset (M_{\mathrm{RW}}(\hat{I}, C))^2$ satisfying $f(\eta, g\mathbf{x}, \eta', g\mathbf{x}')$ for all $g \in E(3)$ and $(\eta, \mathbf{x}, \eta', \mathbf{x}') \in D$. Then f can be written as*

$$f(\eta, \mathbf{x}, \eta', \mathbf{x}') = \tilde{f}(\eta, \eta', \|\mathbf{x} - \mathbf{x}'\|)\,, \tag{2.2.1}$$

where $\tilde{f} : D^{\mathrm{red}} \subset \hat{I} \times \hat{I} \times \mathbb{R} \to \mathbb{C}$ is an even function of its last argument, and conversely every smooth function $\tilde{f} : D^{\mathrm{red}} \subset \hat{I} \times \hat{I} \times \mathbb{R} \to \mathbb{C}$ which is even w.r.t. its last argument determines an f with the above symmetry properties by (2.2.1) *and smoothness of f is equivalent to smoothness of $\tilde{f}$.*

Furthermore, if we define for $f \in C_0^\infty(\mathbb{R}^3)$ and $g \in E(3)$ the functions f_g by

$$f_g(\mathbf{x}) := f(g\mathbf{x})\,,$$

then a distribution T on such test-functions which satisfies $T(f_g, f'_g) = T(f, f')$ for all $g \in E(3)$ can be written as

$$\begin{aligned} T(f, f') &= \tilde{T}(f * f')\,, \qquad \textit{with} \quad \tilde{T} \in C_0^\infty(\mathbb{R}^3)' \\ (f * f')(\mathbf{x}) &:= \int_{\mathbb{R}^3} f(\mathbf{y}) f'(\mathbf{x} - \mathbf{y}) \mathrm{d}\mathbf{y} \end{aligned} \tag{2.2.2}$$

and the distribution $\tilde{T}$ is radially symmetric in the sense that for

$$\langle f\rangle_{S^2}(\mathbf{x}) := \frac{1}{4\pi^2}\int_{S^2} f(\|\mathbf{x}\|\,\zeta)\mathrm{d}\omega(\zeta)\,,$$

S^2 the unit sphere and ω the induced measure on it, we have $\tilde{T}(\langle f\rangle_{S^2}) = \tilde{T}(f)$, so $\tilde{T}$ is already determined on radially symmetric test-functions. Conversely, such a distribution $\tilde{T}$ defines via (2.2.2) *a distribution satisfying $T(f_g, f'_g) = T(f, f')$ for all $g \in E(3)$.*

Proof. For each fixed η, η' the function $(\mathbf{x}, \mathbf{x}') \mapsto f(\eta, \mathbf{x}, \eta', \mathbf{x}')$ is an $E(3)$ invariant function on (a subset of) $\mathbb{R}^3$ and using that such functions can be written as smooth, symmetric functions of $\|\mathbf{x} - \mathbf{x}'\|$ we get the claimed representation.

The statement for the distributions can be combined from the statements on translationally [RS75] and rotationally invariant [Zie80] distributions. The inverse direction is clear. □

We will denote the set of such invariant functions defined on an invariant domain by $C^\infty_{\mathrm{hi}}(D)$, denote the function associated to $f \in C^\infty_{\mathrm{hi}}(D)$ by (2.2.1) as $\tilde{f}$ and refer to it as the "symmetry-reduced function"; similarly, we will refer to the distribution $\tilde{T}$ associated to an $E(3)$-invariant distribution T by (2.2.2) as the "symmetry-reduced distribution".

Because the spacetime is conformally flat and $(\eta, \mathbf{x})$ are global conformal coordinates, the set $V_\ell \subset (M_{\mathrm{RW}}(\hat{I}, C))^2$ of points which are lightlike related is contained in

$$V := \{(\eta, \mathbf{x}, \eta', \mathbf{x}') \in (M_{\mathrm{RW}}(\hat{I}, C))^2 \mid (\eta - \eta')^2 - \|\mathbf{x} - \mathbf{x}'\|^2 = 0\}$$

(locally, e.g. for N a geodesically convex neighbourhood $V \cap (N \times N) = V_\ell \cap (N \times N)$ holds). Introducing the function $\rho : (M_{\mathrm{RW}}(\hat{I}, C))^2 \ni (\eta, \mathbf{x}, \eta', \mathbf{x}') \mapsto \|\mathbf{x} - \mathbf{x}'\|^2 - (\eta - \eta')^2$, we have $V = \rho^{-1}(0)$ and the following lemma for functions $f \in C^\infty_{\mathrm{hi}}(D)$ vanishing for points on V:

Lemma 2.5. *Let $f \in C^\infty_{\mathrm{hi}}(D)$ with $f|_{D\cap V} = 0$. Then the function*

$$\frac{f}{\rho} : D \setminus (V \cap D) \ni (\eta, \mathbf{x}, \eta', \mathbf{x}') \mapsto \frac{f(\eta, \mathbf{x}, \eta', \mathbf{x})}{\|\mathbf{x} - \mathbf{x}'\|^2 - (\eta - \eta')^2}$$

can be uniquely extended to a smooth function on D.

Proof. By the above, the statement is equivalent to the smooth extendability of

$$\tilde{h} : D^{\mathrm{red}} \setminus \{(\eta, \eta', r) \in D^{\mathrm{red}} \mid (\eta - \eta')^2 - r^2 = 0\} \ni (\eta, \eta', r) \mapsto \frac{\tilde{f}(\eta, \eta', r)}{\tilde{\rho}(\eta, \eta', r)}$$

to D^{red} and introducing $\overline{\eta}, \xi, \zeta$ by

$$\begin{pmatrix} \overline{\eta} \\ \xi \\ \zeta \end{pmatrix} = \begin{pmatrix} \frac{\eta+\eta'}{2} \\ r + (\eta - \eta') \\ r - (\eta - \eta') \end{pmatrix} =: A \begin{pmatrix} \eta \\ \eta' \\ r \end{pmatrix}$$

and setting $\tilde{\tilde{\rho}} := \tilde{\rho} \circ A^{-1} \Rightarrow \tilde{\tilde{\rho}}(\overline{\eta}, \xi, \zeta) = \xi\zeta$, this is also equivalent to the extendability statement for $\tilde{\tilde{h}} := \tilde{h} \circ A^{-1}$ from $A(D^{\mathrm{red}}) \setminus (\tilde{\tilde{\rho}}^{-1}(0) \cap A(D^{\mathrm{red}}))$ to $A(D^{\mathrm{red}})$. Setting $\tilde{\tilde{f}} := \tilde{f} \circ A^{-1}$ we have $\tilde{\tilde{f}}(\overline{\eta}, \xi, \zeta) = 0$ for $\xi = 0$ or $\zeta = 0$. Now as is easily checked

$$(\overline{\eta}, \xi, \zeta) \mapsto \begin{cases} \frac{\tilde{\tilde{f}}(\overline{\eta},\xi,\zeta)}{\xi\zeta} \text{ for } \xi \neq 0 \text{ and } \zeta \neq 0 \\ \frac{\partial_\xi \tilde{\tilde{f}}(\overline{(\eta)},0,\zeta)}{\zeta} \text{ for } \xi = 0, \zeta \neq 0 \\ \frac{\partial_\zeta \tilde{\tilde{f}}(\overline{(\eta)},\xi,0)}{\xi} \text{ for } \zeta = 0, \xi \neq 0 \\ \partial_\xi \partial_\zeta \tilde{\tilde{f}}(\overline{\eta}, 0, 0) \text{ for } \xi = \zeta = 0 \end{cases}$$

provides the required smooth extension of $\tilde{\tilde{h}}$ (uniqueness follows from the required continuity of the extension). □

We first want to apply this to the signed squared geodesic separation σ. First σ is only defined on sets $N \times N$, where N is a geodesically convex set, but using translations from $E(3)$ it can be consistently extended to an $E(3)$ invariant domain D by symmetry, since geodesics get mapped into geodesics by spacetime symmetries. As argued above, σ vanishes on $D \cap V$; applying lemma 2.5 the function $q := \frac{\sigma}{\rho} : D \setminus (D \cap V) \to \mathbb{R}$ can be smoothly extended to D, so on D the squared geodesic distance can be written as $\sigma = q\rho$.

Furthermore, the property

$$[\partial_{\mu\nu'} \sigma(x, x')]_{x'=x} = 2g_{\mu\nu}$$

for σ [Fri75] implies

$$\begin{aligned} [\partial_{rr} \tilde{\sigma}(\eta, \eta', r)]_{\eta'=\eta, r=0} &= [(2\tilde{q}(\eta, \eta', r) + 4r\partial_r \tilde{q}(\eta, \eta', r) + \rho(\eta, \eta', r)\partial_{rr}\tilde{q}(\eta, \eta', r))]_{\eta=\eta', r=0} \\ &= 2C(\eta) \\ \Rightarrow \tilde{q}(\eta, \eta, 0) &= C(\eta) > 0 \end{aligned} \tag{2.2.3}$$

and by the smoothness of q this implies that q is positive in a whole neighbourhood of $x = x'$. Summing up, one can write σ as

$$\sigma = \rho q \,, \tag{2.2.4}$$

where q is positive in a neighbourhood N_D of $x = x'$.

Introducing $\overset{o}{\nabla}_\mu$ by $\overset{o}{\nabla}_0 = \partial_\eta$, $\overset{o}{\nabla}_1 = \partial_x$, $\overset{o}{\nabla}_2 = \partial_y$, $\overset{o}{\nabla}_3 = \partial_z$ and denoting the metric tensor of Minkowski spacetime for the moment by $\epsilon = \mathrm{diag}(1, -1, -1, -1)$, we get from the equation

$$g^{ab} \nabla_a \sigma \nabla_b \sigma = \frac{1}{C} \epsilon^{\mu\nu} \overset{o}{\nabla}_\mu (\rho q) \overset{o}{\nabla}_\nu (\rho q) = -4\rho q = -4\sigma$$

for σ the equation

$$2q\epsilon^{\mu\nu} \overset{o}{\nabla}_\mu \rho \overset{o}{\nabla}_\nu q + 4q(C - q) + \rho \epsilon^{\mu\nu} (\overset{o}{\nabla}_\mu q) \overset{o}{\nabla}_\nu q = 0 \tag{2.2.5}$$

for q, where the initial condition (as already derived above) is $[q]_{(\eta,\mathbf{x})=x=x'} = C(\eta)$. Using this, one can determine the small distance asymptotics of q by inserting (for the symmetry reduced $\tilde{q}$)

$$\tilde{q}(\eta,\eta',r) = C(\eta') + q_{10}(\eta-\eta') + q_{20}(\eta-\eta')^2 + q_{02}r^2 + q_{30}(\eta-\eta')^3 + q_{12}(\eta-\eta')r^2 + \dots$$

into (2.2.5); equating equal powers, $\tilde{q}$ up to fourth order is obtained as

$$\begin{aligned}
\tilde{q}(\eta,\eta',\rho) =& C(\eta') + \frac{C'(\eta')}{2}(\eta-\eta') + \frac{C''(\eta')}{6}(\eta-\eta')^2 \\
&+ \frac{C'''(\eta')}{24}(\eta-\eta')^3 + \frac{C''''(\eta')}{120}(\eta-\eta')^4 \\
&+ \Bigg\{ (C'(\eta'))^2 + \left[C'(\eta')C''(\eta') - \frac{(C'(\eta'))^3}{2C(\eta')} \right](\eta-\eta') \\
&\qquad + \left[\frac{(C'(\eta'))^4}{4C^2(\eta')} - \frac{2}{3}\frac{(C'(\eta'))^2 C''(\eta')}{C(\eta')} + \frac{4}{15}(C''(\eta'))^2 \right. \\
&\qquad\qquad \left. + \frac{3}{10}C'''(\eta')C'(\eta') \right](\eta-\eta')^2 \Bigg\} \frac{\rho}{48C(\eta')} \\
&+ \left\{ \frac{C''(\eta')}{5} - \frac{(C'(\eta'))^2}{6C(\eta')} \right\} \frac{(C'(\eta'))^2}{192\,C^2(\eta')}\rho^2 + \dots
\end{aligned} \tag{2.2.6}$$

2.2.2 Regularization of $\mathcal{G}_k$ on Robertson Walker-spacetimes

To calculate expectation values of Wick squares, the restriction of $\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$ to the diagonal $\eta' = \eta$, $\mathbf{x} = \mathbf{x}'$ (the coincidence limit) will be the object of interest; the strategy pursued here is to perform this restriction in two steps, making use of the fact that $\mathscr{W}_2^{\omega,\mathrm{s}}$ and $\mathcal{G}_k^s$ can be restricted individually as distributions to the "partial diagonal" $\eta = \eta$. The obtained difference of the distributions $[\mathcal{G}_k^s]_{\eta=\eta'}$ and $[\mathscr{W}_2^{\omega,\mathrm{s}}]_{\eta=\eta'}$ is then rewritten before the second part of the coincidence limit (setting $\mathbf{x} = \mathbf{x}'$) is performed. We thus need expressions for $[\mathcal{G}_k^s]_{\eta=\eta'}$. Furthermore, we also need the coincidence limits of the η and η'-derivatives (up to second order) of $\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$ and as the derivatives on the terms in $\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$ obviously have to be performed before the restriction to the partial diagonal, we also need expressions for those.

It will later turn out, that besides being the obvious terms appearing in the calculation of the expectation values that enter the LTE-condition, they actually are sufficient to calculate the coincidence limit for arbitrary derivatives of $\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$, since higher η or η' derivatives can be reduced to spatial derivatives using the equation of motion.

By definition, $\mathcal{G}_k^s$ is built from the symmetric parts $\left[\frac{1}{\sigma_+}\right]^s$, $[\log(\sigma_+)]^s$ of the distributions $\lim_{\epsilon\to 0}\frac{1}{\sigma_\epsilon}$ and $\lim_{\epsilon\to 0}\log(\sigma_\epsilon)$. We already know from section 2.2.1 that σ can be written as $q\rho$ where ρ is (except for a renaming of the variables) the Minkowskian signed squared separation. Lemma 2.7 shows, that the distributions $\tilde{q}\left[\frac{1}{\tilde{\sigma}_+}\right]^s$ is identical to the corresponding distribution $\left[\frac{1}{\tilde{\sigma}_+^o}\right]^s$ on Minkowski spacetime, so this relation between Robertson Walker spacetime in conformal coordinates and Minkowski spacetime also holds for the distributional expressions. Furthermore, it gives explicit expressions for the restrictions of the distribution and its first and second η-derivative to the partial diagonal; lemma 2.8 does the same for $[\log(\tilde{\sigma}_+)]^s$.

We first need a convergence statement, before we come the proof of these two lemmas:

Lemma 2.6. *Let $\rho : \mathbb{R} \times \mathbb{R}^+ \ni (\Delta\eta, r) \mapsto r^2 - (\Delta\eta)^2$ and $q : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{R}$ be bounded from below by $1/Q_{max} > 0$. Then $(r, \Delta\eta) \mapsto \log\left(\left(\rho(r,\Delta\eta) + \frac{\epsilon^2}{q(r,\Delta\eta)}\right)^2 + 4\epsilon^2 \frac{(\Delta\eta)^2}{q^2(r,\Delta\eta)}\right)$ converges in L^1_{loc} to $(r,\Delta\eta) \mapsto \log(\rho^2(\Delta\eta, r))$.*

Proof. See appendix. □

With the help of this lemma, we can now reduce the problem to the Minkowskian case by basically the same strategy as Kay and Wald [KW91, Appendix B] and then work out the restrictions; the details are contained in the following:

Lemma 2.7. *Let the distribution $\left[\frac{1}{\sigma_+}\right]^s : C_0^\infty(\hat{I} \times \hat{I} \times \mathbb{R}^3) \to \mathbb{C}$ be given by*

$$\begin{aligned}\left[\frac{1}{\tilde{\sigma}_+}\right]^s(f) = \lim_{\epsilon\to 0}\int_{\hat{I}}\int_{\hat{I}}\int_{\mathbb{R}^3} \frac{1}{2\tilde{q}(\eta,\eta',\|\mathbf{x}\|)}&\left[\frac{1}{\mathbf{x}^2 - (\eta-\eta')^2 + \frac{2i\epsilon(\eta-\eta')}{\tilde{q}(\eta,\eta',\|\mathbf{x}\|)} + \frac{\epsilon^2}{\tilde{q}(\eta,\eta',\|\mathbf{x}\|)}}\right.\\ &\left. + \frac{1}{\mathbf{x}^2 - (\eta-\eta')^2 + \frac{2i\epsilon(\eta'-\eta)}{\tilde{q}(\eta,\eta',\|\mathbf{x}\|)} + \frac{\epsilon^2}{\tilde{q}(\eta,\eta',\|\mathbf{x}\|)}}\right]\\ &\ldots \times f(\eta,\eta',\mathbf{x})\, \mathrm{d}\mathbf{x}\, C^2(\eta)\mathrm{d}\eta\, C^2(\eta')\mathrm{d}\eta'\,.\end{aligned} \tag{2.2.7}$$

Then $\left[\frac{1}{\tilde{\sigma}_+}\right]^s$ can be written as

$$\left[\frac{1}{\tilde{\sigma}_+}\right]^s = \int_{\hat{I}}\int_{\hat{I}} \tilde{\sigma}^{-1}_{\eta-\eta'}\left(\frac{f(\eta,\eta',\cdot)}{\tilde{q}(\eta,\eta',\|\cdot\|)}\right) C^2(\eta)\mathrm{d}\eta\, C^2(\eta')\mathrm{d}\eta'\,, \tag{2.2.8}$$

where the function $\Delta\eta \mapsto \tilde{\sigma}^{-1}_{\Delta\eta}(h)$ is (for fixed $h \in C_0^\infty(\mathbb{R}^3)$) twice continuously differentiable with

$$\tilde{\sigma}^{-1}_{\Delta\eta}(h)|_{\Delta\eta=0} = \lim_{\epsilon\to 0}\int_{\mathbb{R}^3} \frac{h(\mathbf{x})}{\mathbf{x}^2+\epsilon^2}\,\mathrm{d}\mathbf{x} =: \frac{1}{r_+^2}(h) \tag{2.2.9}$$

$$\partial_{\Delta\eta}\left(\tilde{\sigma}^{-1}_{\Delta\eta}(h)\right)|_{\Delta\eta=0} = 0 \tag{2.2.10}$$

$$\partial_{\Delta\eta\Delta\eta}\left(\tilde{\sigma}^{-1}_{\Delta\eta}(h)\right)|_{\Delta\eta=0} = \lim_{\epsilon\to 0}\int_{\mathbb{R}^3} \frac{\Delta h(\mathbf{x})}{\mathbf{x}^2+\epsilon^2}\mathrm{d}\mathbf{x} =: \frac{2}{r_+^4}(h)\,. \tag{2.2.11}$$

Proof. Due to the rotational symmetry of $\mathbb{R}^3 \in \mathbf{x} \mapsto \frac{1}{\mathbf{x}^2-(\eta-\eta')^2 \pm \frac{2i\epsilon(\eta-\eta')}{\tilde{q}(\eta,\eta',\|\mathbf{x}\|)} + \frac{\epsilon^2}{\tilde{q}(\eta,\eta',\|\mathbf{x}\|)}}$, one can restrict to test-functions f which are given as $f(\eta,\eta',\mathbf{x}) = \tilde{f}(\eta,\eta',\|\mathbf{x}\|)$, where the function $\tilde{f} : \hat{I} \times \hat{I} \times \mathbb{R}_0^+ \to \mathbb{C}$ is smooth, has bounded supported and satisfies $\left[\partial_r^{2k+1}\tilde{f}(\eta,\eta',r)\right]_{r=0} = 0$ for all $k \in \mathbb{N}_0$.

Introduce now the functions

$$\begin{aligned}
p^s(\eta,\eta',r) =& \frac{2r\tilde{q}(\eta,\eta',r) - \epsilon^2 \frac{\partial_r \tilde{q}(\eta,\eta',r)}{\tilde{q}(\eta,\eta',r)}}{\left(2\tilde{q}(\eta,\eta',r) - \epsilon^2 \frac{\partial_r \tilde{q}(\eta,\eta',r)}{r\tilde{q}(\eta,\eta',r)}\right)^2 + 4\epsilon^2(\eta-\eta')^2 \left(\frac{\partial_r \tilde{q}(\eta,\eta',r)}{r\tilde{q}(\eta,\eta',r)}\right)^2} \\
p^a(\eta,\eta',r) =& \frac{2(\eta-\eta')\frac{\partial_r \tilde{q}(\eta,\eta',r)}{\tilde{q}(\eta,\eta',r)}}{\left(2\tilde{q}(\eta,\eta',r) - \epsilon^2 \frac{\partial_r \tilde{q}(\eta,\eta',r)}{r\tilde{q}(\eta,\eta',r)}\right)^2 + 4\epsilon^2(\eta-\eta')^2 \left(\frac{\partial_r \tilde{q}(\eta,\eta',r)}{r\tilde{q}(\eta,\eta',r)}\right)^2} \\
p^\pm(\eta,\eta',r) =& \frac{r}{2\tilde{q}(\eta,\eta',r) \mp 2i\epsilon(\eta-\eta')\frac{\partial_r \tilde{q}(\eta,\eta',r)}{r\tilde{q}(\eta,\eta',r)} - \epsilon^2 \frac{\partial_r \tilde{q}(\eta,\eta',r)}{r\tilde{q}(\eta,\eta',r)}} = p^s(\eta,\eta',r) \pm i\epsilon p^a(\eta,\eta',r)\,.
\end{aligned}$$

Again due to the (spatial) symmetry of the spacetimes considered, $\lim_{r\to 0}\partial_r q = 0$, and $(\Delta\eta, \Delta\eta', r) \mapsto \frac{\partial_r \tilde{q}(\eta,\eta',r)}{r\tilde{q}(\eta,\eta',r)}$ is a smooth function of η, η', r in neighbourhoods of $r = 0$, $\eta = \eta'$. This shows that on such neighbourhoods p^s, p^a and $p^\pm$ are well defined and can (for ϵ small enough) be bounded by an ϵ-independent constant. Moreover, this also holds for their r-derivative and the functions converge (together with their r-derivatives) uniformly on such sets to the expressions obtained by setting $\epsilon = 0$.

Going over to the variables $\overline{\eta} = \frac{\eta+\eta'}{2}$ and $\Delta\eta = \eta - \eta'$, introducing the intervals $\Delta I(\overline{\eta}) := \{\Delta\eta \mid \left|\overline{\eta} - \frac{\eta_i+\eta_f}{2}\right| + |\Delta\eta| \leq \frac{\eta_f-\eta_i}{2}\}$ and denoting for functions $f : \hat{I}\times\hat{I}\times\mathbb{R}^+ \to \mathbb{C}$ by $f_{\overline{\eta}}$ the function $f_{\overline{\eta}} : (\Delta\eta, r) \mapsto f(\overline{\eta}+\Delta\eta, \overline{\eta}-\Delta\eta, r)$, (2.2.7) can be written as

$$\begin{aligned}
\left[\frac{1}{\tilde{\sigma}_+}\right]^s(f) =& \lim_{\epsilon\to 0}\int_{\hat{I}}\int_{\Delta I(\overline{\eta})}\int_{\mathbb{R}^+}\frac{1}{2}\left[\frac{2r - 2i\epsilon\Delta\eta\frac{\partial_r\tilde{q}_{\overline{\eta}}(\Delta\eta,r)}{\tilde{q}^2_{\overline{\eta}}(\Delta\eta,r)} - \epsilon^2\frac{\partial_r\tilde{q}_{\overline{\eta}}(\Delta\eta,r)}{\tilde{q}^2_{\overline{\eta}}(\Delta\eta,r)}}{r^2 - (\Delta\eta)^2 + 2i\epsilon\frac{\Delta\eta}{\tilde{q}_{\overline{\eta}}(\Delta\eta,r)} + \frac{\epsilon^2}{\tilde{q}_{\overline{\eta}}(\Delta\eta,r)}}p^+_{\overline{\eta}}(\Delta\eta,r)\tilde{f}_{\overline{\eta}}(\Delta\eta,r)\right. \\
&\left. + \frac{2r + 2i\epsilon\Delta\eta\frac{\partial_r\tilde{q}_{\overline{\eta}}(\Delta\eta,r)}{\tilde{q}^2_{\overline{\eta}}(\Delta\eta,r)} - \epsilon^2\frac{\partial_r\tilde{q}_{\overline{\eta}}(\Delta\eta,r)}{\tilde{q}^2_{\overline{\eta}}(\Delta\eta,r)}}{r^2 - (\Delta\eta)^2 - 2i\epsilon\frac{\Delta\eta}{\tilde{q}_{\overline{\eta}}(\Delta\eta,r)} + \frac{\epsilon^2}{\tilde{q}_{\overline{\eta}}(\Delta\eta,r)}}p^-_{\overline{\eta}}(\Delta\eta,r)\tilde{f}_{\overline{\eta}}(\Delta\eta,r)\right]\mathrm{d}r\mathrm{d}\Delta\eta\mathrm{d}\overline{\eta} \\
=& \lim_{\epsilon\to 0}\int_{\hat{I}}\int_{\Delta I(\overline{\eta})}\int_{\mathbb{R}^+} -\frac{1}{2}\left[\log\left(\rho + 2i\frac{\epsilon\Delta\eta}{\tilde{q}_{\overline{\eta}}(\Delta\eta,r)} + \frac{\epsilon^2}{\tilde{q}_{\overline{\eta}}(\Delta\eta,r)}\right)\partial_r(p^+_{\overline{\eta}}(\Delta\eta,r)\tilde{f}_{\overline{\eta}}(\Delta\eta,r))\right. \\
&\left. + \log\left(\rho - 2i\frac{\epsilon\Delta\eta}{\tilde{q}_{\overline{\eta}}(\Delta\eta,r)} + \frac{\epsilon^2}{\tilde{q}_{\overline{\eta}}(\Delta\eta,r)}\right)\partial_r(p^-_{\overline{\eta}}(\Delta\eta,r)\tilde{f}_{\overline{\eta}}(\Delta\eta,r))\right]\mathrm{d}r\mathrm{d}\Delta\eta\mathrm{d}\overline{\eta}\,,
\end{aligned}$$

where a partial integration with respect to r was performed. Since the integrand in (2.2.7) is symmetric with respect of exchange of η and η' except for the test function f and the integration is with respect to η and η', wlog f can also be assumed to be symmetric with respect to exchange of η and η'. Using this, $\left[\frac{1}{\tilde{\sigma}_+}\right]^s$ is given by

$$\begin{aligned}\left[\frac{1}{\tilde{\sigma}_+}\right]^s(f) = &\lim_{\epsilon\to 0} -\frac{1}{2}\int_{\hat{I}}\int_{\Delta I(\overline{\eta})}\int_{\mathbb{R}^+} \log\left(\left(\rho + \tfrac{\epsilon^2}{\tilde{q}_{\overline{\eta}}(\Delta\eta,r)}\right)^2 + \tfrac{4(\Delta\eta)^2}{q^2(\Delta\eta,r)}\right)\\ &\quad \ldots \times \partial_r\left(p^s_{\overline{\eta}}(\Delta\eta,r)\tilde{f}_{\overline{\eta}}(\Delta\eta,r)\right)\mathrm{d}r\mathrm{d}\Delta\eta\mathrm{d}\overline{\eta}\\ &+\lim_{\epsilon\to 0}\epsilon\int_{\hat{I}}\int_{\Delta I(\overline{\eta})}\int_{\mathbb{R}^+}\arg\left(\rho + 2i\tfrac{\epsilon\Delta\eta}{\tilde{q}_{\overline{\eta}}(\Delta\eta,r)} + \tfrac{\epsilon^2}{\tilde{q}_{\overline{\eta}}(\Delta\eta,r)}\right)\\ &\quad \ldots \times \partial_r\left(p^a_{\overline{\eta}}(\Delta\eta,r)\tilde{f}_{\overline{\eta}}(\Delta\eta,r)\right)\mathrm{d}r\mathrm{d}\Delta\eta\mathrm{d}\overline{\eta}\,. \end{aligned} \tag{2.2.12}$$

Since the argument function arg is bounded and the same holds, with bounds independent of $\overline{\eta}$, for $\partial_r(p^a_{\overline{\eta}}\tilde{f}_{\overline{\eta}})$, the second summand goes to zero.

The first summand is an integral over a bounded set of a product of two functions which converge (by the preceding lemma and the discussion after the introduction of p^a and p^s; the appearance of the additional variable in $\tilde{q}$ is not of significance, since in the proof of the lemma only the boundedness of $\tilde{q}$ from below was needed, which holds uniform wrt. $\overline{\eta}$) in L^1_{loc} respectively uniformly to integrable respectively bounded limit functions. The limit can therefore be performed inside the integral, establishing (2.2.8) with

$$\tilde{\sigma}^{-1}_{\eta-\eta'}(f(\eta,\eta',\cdot)) = -\frac{1}{4}\int_{\mathbb{R}^+}\log\left((r^2-(\eta-\eta')^2)^2\right)\partial_r\left(r\tilde{f}(\eta,\eta',r)\right)\mathrm{d}r\,. \tag{2.2.13}$$

Starting from this equation, by repeated partial integration and application of the theorem on differentiable parameter-dependence for (Lebesgue) integrals the statements concerning differentiability and restrictions to the partial diagonal are derived rather straightforwardly: Integrating (2.2.13) twice with respect to r we get for a radially symmetric $h \in C_0^\infty(\mathbb{R}^3)$:

$$\begin{aligned}\tilde{\sigma}^{-1}_\tau(\tilde{h}) = &-\frac{1}{2}\int_{\mathbb{R}^+}\underbrace{\left[\frac{(r+\tau)^2}{2}\log|r+\tau| + \frac{(r-\tau)^2}{2}\log|r-\tau| - \frac{3}{2}r^2 - \tau^2\log|\tau|\right]}_{=:J_1(\tau,r)}\\ &\ldots\times\partial_{rrr}(r\tilde{h}(r))\mathrm{d}r\,.\end{aligned}$$

Differentiating with respect to τ we get

$$\partial_\tau J_1(\tau,r) = (r+\tau)\log|r+\tau| - (r-\tau)\log|r-\tau| - 2\tau\log|\tau|\,,$$

and since $x \mapsto x\log|x|$ is bounded in modulus on any compact interval we can take multiples of characteristic functions as majorants for the integrand which implies that $\tau \mapsto \tilde{\sigma}^{-1}_\tau(h)$ is continuously differentiable with derivative given by

$$\partial_\tau\tilde{\sigma}^{-1}_\tau(h) = -\frac{1}{2}\int_{\mathbb{R}^+}\left[(r+\tau)\log|r+\tau| - (r-\tau)\log|r-\tau| - 2\tau\log|\tau|\right]\partial_{rrr}(r\tilde{h}(r))\mathrm{d}r\,, \tag{2.2.14}$$

but setting $\tau = 0$ this vanishes showing (2.2.10). Note that in (2.2.14) the term $\tau \log|\tau|$ can be dropped, since the integral over $r \mapsto \partial_{rrr}(r\tilde{h}(r))$ from zero to infinity is just $-\left[\partial_{rr}(r\tilde{h}(r))\right]_{r=0}$, but since $\tilde{h}$ is symmetric this vanishes.

Since we now know that $\tau \mapsto \tilde{\sigma}_\tau^{-1}(h)$ is continuous, setting $\tau = 0$ in the equation (2.2.13) for $\tilde{\sigma}_\tau^{-1}(h)$ we get

$$\begin{aligned}\tilde{\sigma}_0^{-1}(h) &= -\frac{1}{2}\int_{\mathbb{R}^+} \log(r^2)\partial_r(r\tilde{h}(r))\mathrm{d}r = -\frac{1}{2}\lim_{\epsilon\to 0}\int_{\mathbb{R}^+} \log(r^2+\epsilon^2)\partial_r(r\tilde{h}(r))\mathrm{d}r \\ &= \lim_{\epsilon\to 0}\int_{\mathbb{R}^+} \frac{r^2\tilde{h}(r)}{r^2+\epsilon^2}\mathrm{d}r\end{aligned}$$

which is the claim (2.2.9). To calculate the second derivative, we again perform a partial integration, this time starting from (2.2.14) (without the $\tau\log|\tau|$-term) and get

$$\partial_\tau\tilde{\sigma}_\tau^{-1}(h) = \frac{1}{2}\int_{\mathbb{R}^+}\left[\frac{(r+\tau)^2}{2}\log|r+\tau| - \frac{(r-\tau)^2}{2}\log|r-\tau| - r\tau\right]\partial_{rrrr}(r\tilde{h}(r))\mathrm{d}r\,.$$

Differentiating wrt. τ under the integral leads to

$$\partial_{\tau\tau}\tilde{\sigma}_\tau^{-1}(h) = \frac{1}{2}\int_{\mathbb{R}^+}\left[(r+\tau)\log|r+\tau| + (r-\tau)\log|r-\tau|\right]\partial_{rrrr}(r\tilde{h}(r))\mathrm{d}r\,,$$

which is again permissible by the same argument as above, showing that $\tau \mapsto \tilde{\sigma}_\tau^{-1}(h)$ is at least C^2. Setting $\tau = 0$, performing two partial integrations in the opposite direction (inserting the ϵ^2 term by majorized convergence before the second) and using the relation $\Delta h = \partial_{rr}\tilde{h} + \frac{2}{r}\partial_r\tilde{h}$ for the application of the Laplace operator to radially symmetric h, one arrives at (2.2.11). . ☐

A corresponding result holds for the distributions $[\log(\tilde{\sigma}_+)]^s$:

Lemma 2.8. *Let the distribution* $[\log\tilde{\sigma}_+]^s : C_0^\infty(\hat{I}\times\hat{I}\times\mathbb{R}^3) \to \mathbb{C}$ *be given by*

$$\begin{aligned}\left[\log(\tilde{\sigma}_+)\right]^s(f) = \lim_{\epsilon\to 0}\int_{\hat{I}}\int_{\hat{I}}\int_{\mathbb{R}^3}\Bigg(&\log(\tilde{q}(\eta,\eta',\|\mathbf{x}\|)) \\ &+\frac{1}{2}\Bigg[\log\left(\mathbf{x}^2-(\eta-\eta')^2+\tfrac{2i\epsilon(\eta-\eta')}{\tilde{q}(\eta,\eta',\|\mathbf{x}\|)}+\tfrac{\epsilon^2}{\tilde{q}(\eta,\eta',\|\mathbf{x}\|)}\right) \\ &\quad+\log\left(\mathbf{x}^2-(\eta-\eta')^2-\tfrac{2i\epsilon(\eta-\eta')}{\tilde{q}(\eta,\eta',\|\mathbf{x}\|)}+\tfrac{\epsilon^2}{\tilde{q}(\eta,\eta',\|\mathbf{x}\|)}\right)\Bigg]\Bigg)f(\eta,\eta',\mathbf{x})\,\mathrm{d}\mathbf{x}\mathrm{d}\eta\mathrm{d}\eta'\,.\end{aligned}$$

Then $[\log(\tilde{\sigma}_+)]^s$ *can be written as*

$$[\log(\tilde{\sigma}_+)]^s = \int_{\hat{I}}\int_{\hat{I}}\int_{\mathbb{R}^3}\log\left(\tilde{q}(\eta,\eta',\|\mathbf{x}\|)\right)f(\eta,\eta',\mathbf{x})\mathrm{d}\eta\mathrm{d}\eta'\mathrm{d}\mathbf{x} + \int_{\hat{I}}\int_{\hat{I}}\tilde{\mathrm{lo}}_{\eta-\eta'}\left(f(\eta,\eta',\cdot)\right)\,\mathrm{d}\eta\mathrm{d}\eta'\,, \tag{2.2.15}$$

where the function $\Delta\eta \mapsto \tilde{\mathrm{lo}}_{\Delta\eta}(h)$ is (for fixed $h \in C_0^\infty(\mathbb{R}^3)$) twice continuously differentiable with

$$\tilde{\mathrm{lo}}_{\Delta\eta}(h)|_{\Delta\eta=0} = \int_{\mathbb{R}^3} \log\left(\mathbf{x}^2\right) h(\mathbf{x})\,\mathrm{d}\mathbf{x} \tag{2.2.16}$$

$$\partial_{\Delta\eta}\left(\tilde{\mathrm{lo}}_{\Delta\eta}(h)\right)|_{\Delta\eta=0} = 0 \tag{2.2.17}$$

$$\partial_{\Delta\eta\Delta\eta}\left(\tilde{\mathrm{lo}}_{\Delta\eta}(h)\right)|_{\Delta\eta=0} = -2\lim_{\epsilon\to 0}\int_{\mathbb{R}^3}\frac{h(\mathbf{x})}{\mathbf{x}^2+\epsilon^2}\mathrm{d}\mathbf{x} \tag{2.2.18}$$

Proof. Again picking wlog. radially symmetric functions test functions f symmetric with respect to interchange of η and η', we get for $\log[(\tilde{\sigma}_+)]^s$ the expression

$$\begin{aligned}
[\log(\tilde{\sigma}_+)]^s(f) = &\int_{\hat{I}}\int_{\hat{I}}\int_{\mathbb{R}^3}\log(\tilde{q}(\eta,\eta',\|\mathbf{x}\|))f(\eta,\eta',\mathbf{x})\mathrm{d}\mathbf{x}\mathrm{d}\eta\mathrm{d}\eta' \\
&+\lim_{\epsilon\to 0}\frac{1}{2}\int_{\hat{I}}\int_{\Delta I(\overline{\eta})}\int_{\mathbb{R}^+}\log\left(\left(\rho+\tfrac{\epsilon^2}{\tilde{q}_{\overline{\eta}}(\Delta\eta,r)}\right)^2+\tfrac{4(\Delta\eta)^2}{q^2(\Delta\eta,r)}\right)\tilde{f}_{\overline{\eta}}(\Delta\eta,r)r^2\mathrm{d}r\mathrm{d}\Delta\eta\mathrm{d}\overline{\eta} \\
&-\lim_{\epsilon\to 0}\epsilon\int_{\hat{I}}\int_{\Delta I(\overline{\eta})}\int_{\mathbb{R}^+}\arg\left(\rho+2i\tfrac{\epsilon\Delta\eta}{\tilde{q}_{\overline{\eta}}(\Delta\eta,r)}+\tfrac{\epsilon^2}{\tilde{q}_{\overline{\eta}}(\Delta\eta,r)}\right)\tilde{f}_{\overline{\eta}}(\Delta\eta,r)r^2\mathrm{d}r\mathrm{d}\Delta\eta\mathrm{d}\overline{\eta}\,.
\end{aligned} \tag{2.2.19}$$

By the same arguments as in the last lemma, the limit involving the arg-function vanishes and the other limit can be performed inside the integral, establishing (2.2.15) with

$$\tilde{\mathrm{lo}}_{\eta-\eta'}(f(\eta,\eta',\cdot)) = +\frac{1}{4}\int_{\mathbb{R}^+}\log\left(\left(r^2-(\eta-\eta')^2\right)^2\right)r^2\tilde{f}(\eta,\eta',r)r^2\mathrm{d}r\,.$$

But since this expression is completely analogous to the one obtained for $\tilde{\sigma}^{-1}_{\eta-\eta'}$ in the proof of the preceding lemma, the statements about differentiability and restrictions can also be established along the same lines as there (even requiring less partial integrations). □

2.2.3 Quasifree homogeneous and isotropic states

After having clarified the regularization aspects of the Hadamard-parametrix on Robertson Walker spacetimes to the extent required in the following, we next come to (quasifree) states of the quantum field with maximal symmetry on them. One way to define such states would be to require a two-point function which is invariant under a simultaneous action of $\rho_{\mathrm{RW}}(g)$ on both its arguments. Lüders and Roberts [LR90], whose results we use here, actually discuss the quantum field in terms of its field algebras defined on a Cauchy surface; the requirement of homogeneity and isotropy then means that the two-point function has to be invariant under replacements of the (pairs of) test-functions (f,h), (f',h') that enter the two-point function by (f_g,h_g), (f'_g,h'_g) for all $g \in E(3)$, where the group-transformed test-functions f_g, h_g, etc. are defined as in lemma 2.4. Under an additional continuity assumption on the group-action, they then show that such quasifree homogeneous and isotropic states on Robertson Walker spacetimes are given by states with a two-point function of the form[5]

$$\mathscr{W}_2^\omega(f_1,f_2) = \int_{\mathbb{R}^3} \begin{pmatrix} \overline{\widehat{(E\overline{f}_1)}}(\eta_0,\mathbf{p}) & \overline{\partial_{\eta_0}\widehat{(E\overline{f}_1)}(\eta_0,\mathbf{p})} \end{pmatrix} \mathrm{S}(p) \begin{pmatrix} \widehat{(Ef_2)}(\eta_0,\mathbf{p}) \\ \partial_{\eta_0}\widehat{(Ef_2)}(\eta_0,\mathbf{p}) \end{pmatrix} C(\eta_0)\mathrm{d}\mathbf{p} \tag{2.2.20}$$

$$\mathrm{S}(p) = \begin{pmatrix} \alpha(p) & \frac{i}{2}+\gamma(p) \\ -\frac{i}{2}+\gamma(p) & \beta(p) \end{pmatrix},$$

where here an in the following $p = \|\mathbf{p}\|$ and for $f \in C_0^\infty(\hat{I}\times\mathbb{R}^3)$ we denote by $\widehat{f}$ the Fourier-transform of f wrt. the "spatial variables", i.e.

$$\widehat{f}(\eta,\mathbf{p}) = \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3} f(\eta,\mathbf{x})e^{-i\mathbf{p}\mathbf{x}}\mathrm{d}\mathbf{x}\,,$$

the expression on the rhs. of (2.2.20) is independent of η_0 and the functions $\alpha,\beta>0$, γ satisfy the relation

$$\gamma^2 \le \alpha\beta - \frac{1}{4} \tag{2.2.21}$$

and are polynomially bounded.

Inserting the expression (A.1.6) from the appendix for the commutator distribution Ef into the two-point function one is left with

$$\mathscr{W}_2^\omega(f_1,f_2) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} w_{p,p'}(f_1,f_2)e^{i(\mathbf{p}-\mathbf{p}')\mathbf{x}}\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{p}'\,\mathrm{d}\mathbf{x} \tag{2.2.22}$$

$$w_{p,p'}(f_1,f_2) = \int_{\mathbb{R}}\int_{\mathbb{R}} \begin{pmatrix} \overline{G_p}(\eta_0,\eta) & \partial_{\eta_0}\overline{G_{p'}}(\eta_0,\eta) \end{pmatrix} \begin{pmatrix} \alpha(p) & \frac{i}{2}+\gamma(p) \\ \gamma(p)-\frac{i}{2} & \beta(p) \end{pmatrix} \begin{pmatrix} G_{p'}(\eta_0,\eta') \\ \partial_{\eta_0}G_{p'}(\eta_0,\eta') \end{pmatrix}$$

$$\ldots \times \overline{\hat{\overline{f}}}_1(\eta,\mathbf{p})\hat{f}_2(\eta',\mathbf{p}')C^2(\eta)\mathrm{d}\eta\,C^2(\eta')\mathrm{d}\eta'$$

where G_p is given in terms of the function V_p satisfying the ordinary differential equation

$$V_p'' + \left[p^2 + Q_{m,\xi}\right]V_p = 0 \tag{2.2.23}$$
$$Q_{m,\xi} = (m^2 + (\xi - 1/6)R)C$$

and the Wronski-determinant condition[6]

$$\overline{V_p}V_p' - \overline{V_p}'V_p = i \tag{2.2.24}$$

as

$$G_p(\eta_0,\eta) = i\,\frac{V_p(\eta_0)\overline{V_p}(\eta) - \overline{V_p}(\eta_0)V_p(\eta)}{\sqrt{C(\eta_0)C(\eta)}}\,.$$

[5] This is a translation of their result into the setup used here using the commutator distribution as discussed in [Wal94].

[6] Unfortunately, there seems to be disagreement which sign to pick in the Wronski-determinant condition. Since here the results from [LR90] are used, the sign chosen is also the same as theirs; note that this differs from [BD84] and [JS02]. A different sign here leads to V_p and $\overline{V_p}$ being interchanged in all the formulas involving two-point functions etc.

Consider now a family V_p of solutions to (2.2.23) satisfying (2.2.24) with polynomially bounded initial value functions $\mathbf{p} \mapsto V_p(\eta_0)$ and $\mathbf{p} \mapsto V_p'(\eta_0)$. Defining for each $p \geq 0$ the function

$$E_p : \eta \mapsto \frac{1}{2} \left| V_p'(\eta) \right|^2 + \frac{p^2 + Q_{m,\xi}^2(\eta)}{2} \left| V_p(\eta) \right|^2 ,$$

$p \mapsto E_p(\eta_0)$ is again polynomially bounded. For a compact interval $I_0 := [\eta_1, \eta_2]$ we furthermore have for each p and $\tilde{\eta} \in I_0$

$$\begin{aligned} E_p'(\tilde{\eta}) &= \tfrac{Q'_{m,\xi}(\tilde{\eta})}{2} \left| V_p(\tilde{\eta}) \right|^2 \\ \Rightarrow \left| \, E_p(\tilde{\eta}) \right| &\leq \left| E_p(\eta_0) + \int_{\eta_0}^{\tilde{\eta}} \tfrac{Q'_{m,\xi}(\eta)}{2} \left| V_p(\eta) \right|^2 \mathrm{d}\eta \right| \leq \left| E_p(\eta_0) \right| + \tfrac{|\tilde{\eta} - \eta_0|}{2} \left\| Q'_{m,\xi} \left| V_p \right|^2 \right\|_\infty \\ \text{with} \qquad & \left\| Q'_{m,\xi} \left| V_p \right|^2 \right\|_\infty := \sup_{\tilde{\eta} \in I_0} \left| Q'_{m,\xi}(\tilde{\eta}) \left| V_p(\tilde{\eta} \right|^2 \right| . \end{aligned}$$

For $\tilde{\eta} \in I_0$ we have $\frac{\left| p^2 + Q_{m,\xi}(\tilde{\eta}) \right|}{2} \left| V_p(\tilde{\eta}) \right|^2 \leq \left| E_p(\tilde{\eta}) \right|$ and taking the supremum over I_0, we get

$$\left(\frac{\left\| p^2 + Q_{m,\xi} \right\|_\infty}{2} - \left| \eta' - \eta_0 \right| \left\| Q'_{m,\xi} \right\|_\infty \right) \left\| V_p \right\|_\infty \leq \left| E_p(\eta_0) \right| ,$$

which however implies that $p \mapsto \|V_p\|_\infty$ is polynomially bounded. This in turn implies the polynomial boundedness of $p \mapsto \|E_p\|_\infty$ and because of $\left| V_p'(\tilde{\eta}) \right|^2 \leq 2 \left| E_p(\tilde{\eta}) \right|$ we get that also $p \mapsto \left\| V_p' \right\|_\infty$ is polynomially bounded and therefore $w_{p,p'}(f_1, f_2)$ is rapidly decaying in p and p'. We can then switch the order of integration in (2.2.22), integrate first over $\mathbf{x}$ and then $\mathbf{p}'$ and are left with

$$\mathscr{W}_2^\omega(f_1, f_2) = \int_{\mathbb{R}^3} w_{p',p'}(f_1, f_2) \mathrm{d}\mathbf{p}' .$$

Inserting the definition of G_p into the integrand of $w_{p,p}(f_1, f_2)$ we get

$$\begin{aligned}
&\begin{pmatrix}\overline{G_p}(\eta_0,\eta) & \partial_{\eta_0}\overline{G_p}(\eta_0,\eta)\end{pmatrix}\begin{pmatrix}\alpha(p) & \frac{i}{2}+\gamma(p)\\ \gamma(p)-\frac{i}{2} & \beta(p)\end{pmatrix}\begin{pmatrix}G_{p'}(\eta_0,\eta')\\ \partial_{\eta_0}G_p(\eta_0,\eta')\end{pmatrix}\overline{\hat{f}}_1(\eta,\mathbf{p})\hat{f}_2(\eta',\mathbf{p}')\\
&=\Bigg\{\underbrace{\begin{pmatrix}\frac{\overline{V_p}(\eta_0)}{\sqrt{C(\eta_0)}} & \partial_{\eta_0}\frac{\overline{V_p}(\eta_0)}{\sqrt{C(\eta_0)}}\end{pmatrix}\begin{pmatrix}\alpha(p) & \frac{i}{2}+\gamma(p)\\ \gamma(p)-\frac{i}{2} & \beta(p)\end{pmatrix}\begin{pmatrix}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}\\ \partial_{\eta_0}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}\end{pmatrix}}_{A_1(p)}\frac{V_p(\eta)\overline{V_p}(\eta')}{\sqrt{C(\eta)C(\eta')}}\\
&\quad-\underbrace{\begin{pmatrix}\frac{\overline{V_p}(\eta_0)}{\sqrt{C(\eta_0)}} & \partial_{\eta_0}\frac{\overline{V_p}(\eta_0)}{\sqrt{C(\eta_0)}}\end{pmatrix}\begin{pmatrix}\alpha(p) & \frac{i}{2}+\gamma(p)\\ \gamma(p)-\frac{i}{2} & \beta(p)\end{pmatrix}\begin{pmatrix}\frac{\overline{V_p}(\eta_0)}{\sqrt{C(\eta_0)}}\\ \partial_{\eta_0}\frac{\overline{V_p}(\eta_0)}{\sqrt{C(\eta_0)}}\end{pmatrix}}_{A_2(p)}\frac{V_p(\eta)V_p(\eta')}{\sqrt{C(\eta)C(\eta')}}\\
&\quad-\underbrace{\begin{pmatrix}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}} & \partial_{\eta_0}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}\end{pmatrix}\begin{pmatrix}\alpha(p) & \frac{i}{2}+\gamma(p)\\ \gamma(p)-\frac{i}{2} & \beta(p)\end{pmatrix}\begin{pmatrix}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}\\ \partial_{\eta_0}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}\end{pmatrix}}_{A_3(p)}\frac{\overline{V_p}(\eta)\overline{V_p}(\eta')}{\sqrt{C(\eta)C(\eta')}}\\
&\quad+\underbrace{\begin{pmatrix}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}} & \partial_{\eta_0}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}\end{pmatrix}\begin{pmatrix}\alpha(p) & \frac{i}{2}+\gamma(p)\\ \gamma(p)-\frac{i}{2} & \beta(p)\end{pmatrix}\begin{pmatrix}\frac{\overline{V_p}(\eta_0)}{\sqrt{C(\eta_0)}}\\ \partial_{\eta_0}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}\end{pmatrix}}_{A_4(p)}\frac{\overline{V_p}(\eta)V_p(\eta')}{\sqrt{C(\eta)C(\eta')}}\Bigg\}\\
&\qquad\qquad\qquad\qquad\ldots\times\overline{\hat{f}}_1(\eta,\mathbf{p})\hat{f}_2(\eta',\mathbf{p}')\,.
\end{aligned}$$

Except for the condition (2.2.24) and the polynomial boundedness of the initial values (wrt p) the V_p have not yet been further specified. Take the initial values now as

$$V_p(\eta_0) =\sqrt{\frac{\beta(p)}{2}}\frac{1}{\sqrt[4]{\alpha(p)\beta(p)-\gamma^2(p)}} \tag{2.2.25}$$

$$\sqrt{C(\eta_0)}\partial_{\eta_0}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}} =\frac{1}{\sqrt{2\beta(p)}}\left(i\sqrt[4]{\alpha(p)\beta(p)-\gamma^2(p)}-\frac{\gamma(p)}{\sqrt[4]{\alpha(p)\beta(p)-\gamma^2(p)}}\right) \tag{2.2.26}$$

By (2.2.21) we have $\alpha\beta \geq \alpha\beta-\gamma^2 \geq \frac{1}{4}$ which implies that $\sqrt[4]{\alpha\beta-\gamma^2} \geq \frac{1}{\sqrt{2}}$ so the function $p \mapsto |V_p(\eta_0)|$ is finite and polynomially bounded and using $\frac{1}{\sqrt{\beta}} \leq 2\alpha$ it follows that also $p \mapsto |V_p(\eta_0)|$ is polynomially bounded. Furthermore, the condition (2.2.24) is satisfied and for these initial values A_2 and A_3 vanish, whereas A_1 and A_4 are given by

$$\begin{aligned}
A_1 &=\frac{\sqrt{\alpha\beta-\gamma^2}-\frac{1}{2}}{C(\eta_0)}\\
A_4 &=\frac{\sqrt{\alpha\beta-\gamma^2}+\frac{1}{2}}{C(\eta_0)}\,,
\end{aligned}$$

so the two-point function can be written as

$$\mathscr{W}_2^{\omega}(f_1,f_2) = \int_{\mathbb{R}^3}\int_{\hat{I}}\int_{\hat{I}}\Big[\Big(\sqrt{\alpha(p)\beta(p)-\gamma^2(p)}-\tfrac{1}{2}\Big)V_p(\eta)\overline{V_p}(\eta') + \Big(\sqrt{\alpha(p)\beta(p)-\gamma^2(p)}+\tfrac{1}{2}\Big)\overline{V_p}(\eta)V_p(\eta')\Big] \dots \times \overline{\hat{f}_1(\eta,\mathbf{p})}\hat{f}_2(\eta',\mathbf{p})C^{3/2}(\eta)\mathrm{d}\eta\, C^{3/2}(\eta')\mathrm{d}\eta'\,\mathrm{d}\mathbf{p} \quad (2.2.27)$$

Now for α,β,γ satisfying the above restrictions, we get Im $(V_p(\eta_0)) = 0$, Re $(V_p(\eta_0)) > 0$, Im $\left(\sqrt{C(\eta_0)}\partial_{\eta_0}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}\right) = \frac{1}{2V_p(\eta_0)}$ and conversely for $V_p(\eta_0)$, $\sqrt{C(\eta_0)}\partial_{\eta_0}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}$ satisfying these conditions, we can invert the equations (2.2.25) and (2.2.26) to obtain

$$\beta(p) = \frac{V_p^2(\eta_0)}{C(\eta_0)\left|\partial_{\eta_0}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}\right|^2}\alpha(p)$$

$$\gamma(p) = \left[\frac{i}{2C\left|\partial_{\eta_0}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}\right|^2} - \frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}\partial_{\eta_0}\frac{\overline{V_p}(\eta_0)}{\sqrt{C(\eta_0)}}}\right]\alpha(p)\,.$$

Inserting this back into $\sqrt{\alpha\beta-\gamma^2}$ we get

$$\sqrt{\alpha\beta-\gamma^2} = \frac{\alpha}{2C(\eta_0)\left|\partial_{\eta_0}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}\right|^2}\,. \quad (2.2.28)$$

General initial values $\tilde{V}_p(\eta_0)$, and $\sqrt{C(\eta_0)}\partial_{\eta_0}\frac{\tilde{V}_p(\eta_0)}{\sqrt{C(\eta_0)}}$ can be written as $e^{i\varphi_p(\eta_0)}V_p(\eta_0)$ and $e^{i\varphi_p(\eta_0)}\sqrt{C(\eta_0)}\partial_{\eta_0}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}$ with $\varphi_p(\eta_0)$ real valued[7]; they do however lead to the same results in (2.2.27) and (2.2.28) as the more restricted ones considered so far. This shows that instead of specifying the state by α, β and γ, one can also pick initial values for V_p, $\sqrt{C}\partial_\eta\frac{V_p}{\sqrt{C}}$ such that (2.2.24) is satisfied and an $\alpha > 0$, and then determine the only term in (2.2.27) involving α, β and γ, namely $\sqrt{\alpha\beta-\gamma^2}$, by (2.2.28). By the above this term has to be no smaller than $\frac{1}{2}$ and this imposes the additional requirement $\alpha \geq C(\eta_0)\left|\partial_{\eta_0}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}\right|^2$.

Now looking again at the two-point function (2.2.27) as the prime object of interest, the upshot of the discussion is that an arbitrary homogeneous and isotropic quasifree state is given by (2.2.27) with V_p an arbitrary function satisfying (2.2.23) and (2.2.24)

[7] the appearance of the same phase-function $e^{i\varphi_p(\eta_0)}$ in front of both $V_p(\eta_0)$ and $\sqrt{C(\eta_0)}\partial_{\eta_0}\frac{V_p(\eta_0)}{\sqrt{C(\eta_0)}}$ is again a consequence of (2.2.24).

and $\sqrt{\alpha\beta - \gamma^2}$ replaced by a function Ξ of p, which is polynomially bounded and almost everywhere bigger or equal $\frac{1}{2}$. Its symmetric part then takes the form

$$\mathscr{W}_2^{\omega,\mathrm{s}}(f_1, f_2) = \int_{\mathbb{R}^3} \Xi(p) \left[V_p(\eta)\overline{V_p}(\eta') + \overline{V_p}(\eta)V_p(\eta')\right] \\ \ldots \times \overline{\hat{f}_1(\eta, \mathbf{p})}\hat{f}_2(\eta', \mathbf{p})C^{3/2}(\eta)\mathrm{d}\eta\, C^{3/2}(\eta')\mathrm{d}\eta'\, \mathrm{d}\mathbf{p}\,. \quad (2.2.29)$$

The special case of the pure state is obtained for the constant function $\Xi = \frac{1}{2}$.

2.2.4 Specification of states on surfaces of constant cosmological time

Yet another way to specify the two-point function, which is in spirit much closer to the classical wave equation and will be used later on in the construction of LTE states, is by giving its restriction together with the restrictions of its "time-derivatives" to a Cauchy surface, here actually a surface of constant (conformal) cosmological time η. As the antisymmetric part of $\mathscr{W}_2^{\omega}$ is given by the commutator distribution, $\mathscr{W}_2^{\omega}$ is determined once its symmetric part $\mathscr{W}_2^{\omega,\mathrm{s}}$ is specified.

Except for the factors $C^2(\eta)$ and $C^2(\eta')$, which can be identified as the volume elements of the spacetime under consideration, $\mathscr{W}_2^{\omega}$ depends on η and η' via the function V_p and a prefactor $\frac{1}{\sqrt{C(\eta)C(\eta')}} =: \frac{1}{D_{\eta\eta'}}$. This prefactor will appear frequently in the following and it turns out to be convenient to go over from the ordinary time-derivatives ∂_η and $\partial_{\eta'}$ to alternative "time-derivatives", which only act on the function remaining after dropping the prefactor $\frac{1}{D_{\eta\eta'}}$. This is achieved by introducing the operators $\mathcal{D}$ and $\mathcal{D}'$ as

$$\mathcal{D} = \partial_\eta + \frac{C'(\eta)}{2C(\eta)} \qquad \mathcal{D}' = \partial_{\eta'} + \frac{C'(\eta')}{2C(\eta')}\,.$$

We then have for an $f \in C^k\left((M_{\mathrm{RW}}(\hat{I}, C))^2\right)$:

$$\mathcal{D}\frac{f(\eta, \mathbf{x}, \eta', \mathbf{x}')}{D_{\eta\eta'}} = \frac{\partial_\eta f(\eta, \mathbf{x}, \eta', \mathbf{x}')}{D_{\eta\eta'}} \qquad \mathcal{D}'\frac{f(\eta, \mathbf{x}, \eta', \mathbf{x}')}{D_{\eta\eta}} = \frac{\partial_{\eta'} f(\eta, \mathbf{x}, \eta', \mathbf{x}')}{D_{\eta\eta'}}$$

and from $\mathcal{D}f$, $\mathcal{D}'f$ and f the ordinary η and η' derivatives of f can be recovered by

$$\partial_\eta = \mathcal{D} - \frac{C'(\eta)}{2C(\eta)}\,, \qquad \partial_{\eta'} = \mathcal{D}' - \frac{C'(\eta')}{2C(\eta')}\,.$$

Since the summand $\frac{C'(\eta)}{2C(\eta)}$ appearing in $\mathcal{D}$ only depends on η, the $\mathcal{D}$ and $\mathcal{D}'$-derivative commute with each other and with spatial derivatives like the ordinary η and η'-derivatives.

Looking now at the symmetric part (2.2.29) of the two-point (bi-)distribution, it is seen that $\mathscr{W}_2^{\omega,\mathrm{s}}$, $\mathcal{D}\mathscr{W}_2^{\omega,\mathrm{s}}$ and $\mathcal{D}\mathcal{D}'\mathscr{W}_2^{\omega,\mathrm{s}}$ (the derivatives taken in the sense of distributions) can be restricted to the surface $\eta = \eta'$ and these restrictions are given by

$$[\mathscr{W}_2^{\omega,\mathrm{s}}]_{\eta=\eta'}(f_1, f_2) = \frac{1}{C(\eta)} \int_{\mathbb{R}^3} 2\Xi(p) \left|V_p(\eta)\right|^2 \overline{\hat{f}}_1(\mathbf{p}) \hat{f}_2(\mathbf{p}) C^4(\eta) \mathrm{d}\mathbf{p} \tag{2.2.30}$$

$$[\mathcal{D}\mathscr{W}_2^{\omega,\mathrm{s}}]_{\eta=\eta'}(f_1, f_2) = \frac{1}{C(\eta)} \int_{\mathbb{R}^3} 2\Xi(p) \mathrm{Re}\left(V_p'(\eta)\overline{V_p(\eta)}\right) \overline{\hat{f}}_1(\mathbf{p}) \hat{f}_2(\mathbf{p}) C^4(\eta) \mathrm{d}\mathbf{p} \tag{2.2.31}$$

$$[\mathcal{D}\mathcal{D}'\mathscr{W}_2^{\omega,\mathrm{s}}]_{\eta=\eta'}(f_1, f_2) = \frac{1}{C(\eta)} \int_{\mathbb{R}^3} 2\Xi(p) \left|V_p'(\eta)\right| \overline{\hat{f}}_1(\mathbf{p}) \hat{f}_2(\mathbf{p}) C^4(\eta) \mathrm{d}\mathbf{p}\,, \tag{2.2.32}$$

where $\hat{f}_1$ and $\hat{f}_2$ are the ordinary Fourier transforms of $f_1, f_2 \in C_0^\infty(\mathbb{R}^3)$. As the state is by assumption homogeneous and isotropic, these restrictions are according to the results cited in lemma 2.4 determined by distributions $\tilde{W}^{()}$, $\tilde{W}^{(\eta)}$ and $W^{\widetilde{(\eta\eta')}}$ and using the fact that the Fourier-transform maps convolutions into products[8], these $\tilde{W}^{()}$, $\tilde{W}^{(\eta)}$ and $\tilde{W}^{(\eta\eta')}$ are seen to be up to factors of $C(\eta)$, which come from the volume element, and a factor $\frac{1}{(2\pi)^{3/2}}$ Fourier back-transforms in the sense of distributions of the functions

$$\hat{w}^{()} : p \mapsto 2\Xi(p) \left|V_p(\eta)\right|^2 \tag{2.2.33}$$

$$\hat{w}^{(\eta)} : p \mapsto \Xi(p) \left(V_p'(\eta)\overline{V_p(\eta)} + V_p(\eta)\overline{V_p'(\eta)}\right) \tag{2.2.34}$$

$$\hat{w}^{(\eta\eta')} : p \mapsto 2\Xi(p) \left|V_p'(\eta)\right|^2 . \tag{2.2.35}$$

Once we know the restrictions of $\mathscr{W}_2^{\omega,\mathrm{s}}$, $\mathcal{D}\mathscr{W}_2^{\omega,\mathrm{s}}$ and $\mathcal{D}\mathcal{D}'\mathscr{W}_2^{\omega,\mathrm{s}}$ to $\eta = \eta'$ we thus know $\hat{w}^{()}$, $\hat{w}^{(\eta)}$ and $\hat{w}^{(\eta\eta')}$, but from these $\Xi(p)$, $V_p(\eta)$ and $\partial_\eta \frac{V_p(\eta)}{\sqrt{C(\eta)}}$ can be reconstructed up to an irrelevant, p-dependent phase factor: As already used above taking $V_p(\eta)$ as positive, the Wronski-determinant condition (2.2.24) for V_p gives $\mathrm{Im}\,(\chi'(\eta)) = \frac{1}{2V_p(\eta)}$. From (2.2.34) we get $\mathrm{Re}\left(V_p'(\eta)\right) = \frac{\hat{w}^{(\eta)}(p)}{2\Xi(p)V_p(\eta)}$ and inserting these two relations into (2.2.35) and expressing $V_p(\eta)$ by $\hat{w}^{()}(p)$ using (2.2.33) the function $\Xi(p)$ follows as

$$\Xi(p) = \sqrt{\hat{w}^{()}(p)\hat{w}^{(\eta\eta')}(p) - (\hat{w}^{(\eta)}(p))^2}\,,$$

which implies for $V_p(\eta)$

$$V_p(\eta) = \frac{\sqrt{\hat{w}^{()}(p)}}{\sqrt{2}\sqrt[4]{\hat{w}^{()}(p)\hat{w}^{(\eta\eta')}(p) - (\hat{w}^{(\eta)}(p))^2}}$$

and $V_p'(\eta)$:

$$V_p'(\eta) = \frac{\hat{w}^{(\eta)}(p)}{\sqrt{2\hat{w}^{()}}\sqrt[4]{\hat{w}^{()}(p)\hat{w}^{(\eta\eta')}(p) - (\hat{w}^{(\eta)}(p))^2}} + i\frac{\sqrt[4]{\hat{w}^{()}(p)\hat{w}^{(\eta\eta')}(p) - (\hat{w}^{(\eta)}(p))^2}}{\sqrt{2\hat{w}^{()}(p)}}$$

[8] With our convention for the prefactor of the Fourier-transform we have $\widehat{f \star h} = (2\pi)^{3/2}\hat{f}\hat{h}$.

For $\hat{w}^{()}(p)\hat{w}^{(\eta\eta')}(p) - (\hat{w}^{(\eta)}(p))^2 \geq \frac{1}{4}$ the condition $\Xi(p) \geq \frac{1}{2}$ is satisfied; the Wronski-determinant condition (2.2.24) is always satisfied. If $\hat{w}^{()}$, $\hat{w}^{(\eta)}$ and $\hat{w}^{(\eta\eta')}$ are in addition polynomially bounded, this shows together with the results of the preceding section that there exists a homogeneous and isotropic quasifree state with a two-point function $\mathscr{W}_2^{\omega,\mathrm{s}}$ satisfying (2.2.30)–(2.2.32). On the other hand, as already argued at the end of the preceding section, allowing for $V_p(\eta)$ not anymore restricted by the condition of positivity leads to the same state, so the the state is also uniquely specified by (2.2.30)–(2.2.32) and we have the following

Lemma 2.9. *Let $\tilde{W}$, $\tilde{W}^{(\eta)}$, $\tilde{W}^{(\eta\eta')}$ be tempered, radially symmetric distributions on $\mathbb{R}^3$ with Fourier transforms $\hat{w}^{()}$, $\hat{w}^{(\eta)}$ and $\hat{w}^{(\eta\eta')}$ satisfying $\hat{w}^{()}(p) > 0, \hat{w}^{(\eta\eta')}(p) > 0$, $\hat{w}^{(\eta)}(p)$ real valued and $\hat{w}^{()}(p)\hat{w}^{(\eta\eta')}(p) - (\hat{w}^{(\eta)}(p))^2 \geq \frac{1}{4}$ for almost all $p = \|\mathbf{p}\|$. Then there exists a unique homogeneous and isotropic state ω of the free Klein-Gordon field, such that the symmetric part $\mathscr{W}_2^{\omega,\mathrm{s}}$ of its two-point function satisfies*

$$\begin{aligned} \left[\mathscr{W}_2^{\omega,\mathrm{s}}\right]_{\eta=\eta'}(f_1, f_2) =& C^3(\eta)\tilde{W}^{()}(f_1 * f_2) \\ \left[\mathcal{D}\mathscr{W}_2^{\omega,\mathrm{s}}\right]_{\eta=\eta'}(f_1, f_2) =& C^3(\eta)\tilde{W}^{(\eta)}(f_1 * f_2) \\ \left[\mathcal{D}\mathcal{D}'\mathscr{W}_2^{\omega,\mathrm{s}}\right]_{\eta=\eta'}(f_1, f_2) =& C^3(\eta)\tilde{W}^{(\eta\eta')}(f_1 * f_2)\,. \end{aligned}$$

Intuitively, this lemma says that the two-point function of an isotropic and homogeneous states, which is a bi-solution of the Klein-Gordon equation, is uniquely determined by the expected data, namely its value and combinations of first time-derivatives wrt the two arguments on a Cauchy surface, where due to symmetry only one of the terms $[\mathcal{D}\mathscr{W}_2^{\omega,\mathrm{s}}]_{\eta=\eta'}$, $[\mathcal{D}'\mathscr{W}_2^{\omega,\mathrm{s}}]_{\eta=\eta'}$ is required. It should however be noted that there is an inequality between the initial values, which has to be satisfied in order to guarantee positivity of the state so defined; furthermore if we require the state to be a Fock-state, i.e. Ξ to be equal to $1/2$, the function $\hat{w}^{(\eta)}$ is determined as $\hat{w}^{(\eta)} = \sqrt{\hat{w}^{()}\hat{w}^{(\eta\eta')} - \frac{1}{4}}$ from $\hat{w}^{()}$ and $\hat{w}^{(\eta\eta')}$. In this case only these two functions, corresponding to the initial data $V_p(\eta_0)$ and $V_p'(\eta_0)$ for the solutions V_p of the mode-equation (2.2.23), have to be given.

3 Condition of local thermality and detectors

In this chapter we will discuss the concept of local thermal equilibrium used in the following two chapters. We will start by very briefly reviewing the situation of global thermal equilibrium on Minkowski spacetime to the extend needed in the following, then proceed with a section motivating the specific choice of observables used to determine local thermal properties by relating them to idealized measurements (not yet completely rigorous) and finally present the concept of (extrinsic) local thermal equilibrium on curved spacetimes. The results linking detectors and thermal observables were published as a preprint [Sch07]; the parts on local thermal equilibrium mostly follow [BOR02, Buc03]; the concept of (extrinsic) local thermal equilibrium is also contained in the publication [SV08].

3.1 Global equilibrium states on Minkowski spacetime

Since the global equilibrium states of the massive Klein-Gordon field on Minkowski spacetime ($M = \mathbb{R}^4, g = \eta = \mathrm{diag}(1, -1, -1, -1)$) will enter our criterion of local thermality below, we briefly collect their properties to the extent required in the following.

To formulate the notion of global thermal equilibrium, we first need a notion of time-evolution relating observations made in some given spacetime region to the same observations made some time t later. As the notion of (global) thermal equilibrium is formulated for very large systems (mathematically usually for the limit of infinite system size), this has to be a global concept which also encodes the observer (reference system) chosen. Mathematically, we need a one-parameter family α_t of isomorphisms of the field algebra $\mathcal{A}(\mathbb{R}^4, \eta)$ acting on the $\phi(f)$ as $\alpha_t(\phi(f)) := \phi(f_{\chi_t})$, where $f_{\chi_t}(x) := f(\chi_t^{-1}(x))$ and all χ_t are spacetime isometries encoding the observer(s) as their proper-time parametrized flowlines (i.e. α_t is required to act geometrically). Here, we are interested in global thermal equilibrium for non-accelerated observers with wordline $\tau \mapsto x_0 + \tau e_0$, where e_0 is some timelike unit vector and $x_0 \in \mathbb{R}^4$ specifies the position of the observer at some reference time. The χ_t are then given by $\chi_t^{e_0} : \mathbb{R}^4 \ni x \mapsto x + te_0$; the corresponding algebra-automorphism is denoted by $\alpha_t^{e_0}$. Using the algebraic approach to quantum field theory, global equilibrium states are most conveniently described by the KMS-condition [HHW67, BR97], which generalized the concept of Gibbs states[1] and allows a direct treatment of the global equilibrium situation for infinitely extended systems (without

[1] It can also be derived directly as a consequence of other assumptions, which on physical grounds should be characteristic for global equilibrium situations [PW78, HTP77].

using boxes and a thermodynamic limits) by giving a condition singling out the states on $\mathcal{A}(\mathbb{R}^4, \eta)$ (as defined in chapter 2), which are in global equilibrium:

Definition 3.1. Let $\mathcal{A}$ be a *-algebra and α_t a one-parameter group of isomorphisms acting on $\mathcal{A}$ and denote for $\beta > 0$ by S_β the strip

$$S_\beta := \{z \in \mathbb{C} \mid 0 < \mathrm{Im}\,(z) < \beta\}$$

and $\overline{S_\beta}$ its closure. Then a state ω_β is said to be a KMS-state at inverse temperature[2] $\beta = \frac{1}{k_B T}$, if for each $A, B \in \mathcal{A}$ there exist a continuous function $F_{AB} : \overline{S_\beta} \to \mathbb{C}$ analytic in S_β and satisfying for all $t \in \mathbb{R}$:

$$\omega(B(\alpha_t A)) = F_{AB}(t) \quad , \qquad \omega((\alpha_t A)B) = F_{AB}(t + i\beta)\,.$$

For the neutral, massive Klein-Gordon field there is for each $\alpha^{e_0}_{\cdot}$ and $\beta > 0$ a unique, quasifree[3] KMS-state [BOR02, Hüb05]. Furthermore, states for different β or e_0 never agree, so a convenient labeling for the global equilibrium states is obtained by combining β and e_0 into the timelike four-vector $\boldsymbol{\beta} =: \beta e_0$ and denoting the KMS state for the isomorphism group $t \mapsto \alpha^{e_0}_t$ with inverse temperature β by $\omega^{\boldsymbol{\beta}}$. By the definition of $\chi^{\eta_0}_{\cdot}$, $\omega^{\boldsymbol{\beta}}$ is an equilibrium state for an observer with rest-frame specified by a tetrad (e_0, e_1, e_2, e_3) and the discussion so far implies that equilibrium states are *not* Lorentz-invariant but rather distinguish rest-frames in relative motion to each other. This is however very sensible from a physical point of view, since it is entirely possible to determine by physical procedures whether one is at rest with respect to a typical thermodynamic system like a gas, or moving relative to it with high speed (in contrast, relative movement with respect to the vacuum, which is modeled by a Lorentz invariant state, can not be detected).

For the free field considered here, the KMS-states can be calculated using a Fourier transformed version of the KMS-condition [HHW67, Haa96] from the commutator distribution; choosing coordinates (x^0, x^1, x^2, x^3) on Minkowski spacetime such that the coordinate axes are aligned with (e_0, e_1, e_2, e_3) their two-point function is given by

$$\begin{aligned}\mathscr{W}_2^{\omega^{\boldsymbol{\beta}}}(f_1, f_2) = \int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}^3} \Bigg(& e^{-i\sqrt{p^2+m^2}\,(x^0 - x'^0)} \, \frac{\overline{\hat{\hat{f}}}_1(x^0, \mathbf{p}) \hat{f}_2(x'^0, \mathbf{p})}{1 - e^{-\beta p}} \\ & - e^{i\sqrt{p^2+m^2}(x^0 - x'^0)} \frac{\overline{\hat{\hat{f}}}_1(x^0, \mathbf{p}) \hat{f}_2(x'^0, \mathbf{p})}{1 - e^{\beta p}} \Bigg) \frac{\mathrm{d}\mathbf{p}}{2\sqrt{p^2 + m^2}} \mathrm{d}x_0 \mathrm{d}x'_0 \,, \quad (3.1.1)\end{aligned}$$

where the notation introduced in chapter 2 for states on Robertson Walker spacetimes was used, i.e. $\hat{f}$ denotes the spatial Fourier-transform

$$\hat{f}(x^0, \mathbf{p}) := \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{-i(x^1 p^1 + x^2 p^2 + x^3 p^3)} f(x) \mathrm{d}x^1\, \mathrm{d}x^2\, \mathrm{d}x^3\,.$$

[2] Here k_B denotes the Boltzmann constant.

[3] By the above definition of quasifree states this in particular means a vanishing one-point function ("gauge-invariance") ruling out things like phase-transitions that would be reflected in non-uniqueness. Furthermore, this also means that the n-point functions are in fact distributions; in general this is an additional condition one has to impose in the (*-algebraic) formulation of the KMS condition.

As mentioned in the introduction, the formalism of local thermal equilibrium of Buchholz, Ojima and Roos [BOR02], introduced in a modified formulation for curved spacetimes in this chapter, relies on spaces S_x of local thermal observables at each point x, physically interpreted as idealization of measurements of (intensive) thermal quantities in smaller and smaller regions of spacetime. The question of how this leads to the specific choice of the balanced derivatives as the generators of the S_x spaces in the concrete case of the Klein-Gordon field is however not discussed in more detail in their paper (although there are arguments that the set of thermal observables chosen is big enough to separate the set of reference states). Here, the specific choice is motivated by looking at a simple model of a detector interacting with the field and implementing the physical idea of measurements in successively smaller spacetime regions for this model detector. This is done in the context of Minkowski spacetime, since this is the context in which one imagines the calibration of the observables to take place.

As a model for the measurement process some kind of Unruh-de Witt detector [Unr76], [DeW79], in this case a two-level system moving along a given trajectory in spacetime and interacting with the given quantum-field, is used. For large interaction-times and time-invariant states the (suitably normalized) probability for the transition of the detector system from its initial (ground- or excited state) to its respective other state due to interactions with the quantum field, calculated in first order perturbation theory, can be used to determine thermal properties of the quantum field. Namely, by the principle of detailed balancing in a thermal state one expects the transition rates from the ground- to the excited and from the excited- to the ground-state to be related by a Boltzmann factor $e^{-\beta E/\hbar}$, if the state of the field is a thermal state at inverse temperature β and E is the energy difference between the two levels of the detector system. In fact, such a relation between the two transition rates for all two-level monopole detector at rest wrt. the thermal state exactly corresponds to the KMS condition for this state [Tak86]. More generally, the dependence of the transition probabilities on $E/\hbar$ corresponds to "spectral properties" of the field, with the principle of detailed balancing as a relation between the rates for E and $-E$ as a special case.

Now in order to be able to proceed to measurements taking place in a short time-interval, the idea is first not to look at the absolute transition probabilities but rather at their differences to those in a common reference state (i.e. to "remove the vacuum fluctuations"), and secondly to consider instead of the transition probabilities as function of E the sequence of moments of this function. When proceeding to arbitrarily short measurement times (while increasing the interaction coupling suitably) these moments will, in general, still diverge; however, starting from the zeroth moment, which stays finite, one can subtract from the higher moments "perturbations" by the lower moments in such a way that the resulting (modified) moments all stay finite when sending the duration of measurement to zero. In this limit, the modified moments are exactly what is measured by the balanced derivatives "in timelike direction", i.e. by the balanced derivatives with ζ tangential to the trajectory of the detector. At this point, some potential problem has to be mentioned: Since all the calculations are based on a treatment of the interaction of the quantum system and the detector in first order perturbation theory, it is not clear, whether in the limit of a short interaction with big couplings they are still trustworthy. This point will taken up once more at the end of the discussion of detectors.

Finally it will be shown that although these balanced derivatives do not span the whole S_x-spaces at first, in fact all the balanced derivatives can be recovered when considering detectors in different states of motion, and even though part of the discussion before that point might not be physically relevant due to the above mentioned problems with the perturbative approach, at this point one gains some insight concerning the relation of balanced derivatives and detector velocities that is not very strongly dependent on the precise mechanism of detector-field interaction and therefore can be expected to also hold if (some potentially modified) balanced derivatives can be related to idealized measurements in a more rigorous setup.

3.2 Thermal observables

3.2.1 Specification of the detector-model

The physical picture of the measurements considered here is the following: An ensemble of quantum-mechanical detectors (two-level systems) moves along a (common, classical) trajectory γ, parametrized by proper time τ, with each member initially in its ground-states. At some time the detectors are (smoothly) switched on, interact with the field for some time and are then switched off again. Finally the number of detectors in the excited state is determined, which yields the transition probability for a single detector (which is of course the same as the expectation value of the transition rate times the interaction duration).

Mathematically, the free two-level detector system is described in the Heisenberg picture by a two-dimensional complex Hilbert-Space $(\mathcal{H}_D, < \cdot, \cdot >_D)$ spanned by the two orthonormal states ψ_g and ψ_e of the detector. These two states are assumed to be eigenstates with eigenvalues zero and ϵ of the detector-Hamiltonian H_D and furthermore the existence of a (time-dependent) self-adjoint operator $\tau \mapsto M(\tau) := e^{i\tau H_D} M_0 e^{-i\tau H_D}$ such that $|< \psi_e, M_0 \psi_g >| \neq 0$ is assumed.

For a given state ω of the quantum field, the coupled detector-field system is described in the interaction picture in the Hilbert-space $\mathcal{H}_\omega \otimes \mathcal{H}_D$ where $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ denotes the GNS representation [Wal94, Chap. 4] of $\mathcal{A}(\mathbb{R}^4, \eta)$ belonging to ω. The initial state Φ of the coupled system is taken to be $\Omega_\omega \otimes \psi_g$ and the time evolution of this state is determined by

$$i\partial_\tau \Phi(\tau) = H_{int}(\tau)\Phi(\tau) := [\chi(\tau)\phi(\gamma(\tau)) \otimes M(\tau)]\, \Phi(\tau)\,,$$

where $\gamma : \mathbb{R} \to \mathbb{R}^4$ is the detector-trajectory as described above, $\chi \in \mathscr{S}(\mathbb{R})$ is the detector switching function (real-valued and normalized by the requirement $\int_{\mathbb{R}} \chi(\tau)\mathrm{d}\tau = 1$) and $\mathbb{R}^4 \ni x \mapsto \phi(x)$ is related to $\pi_\omega(\phi(f))$ by $\pi_\omega(\phi(f)) = \int \phi(x) f(x)\mathrm{d}x$ in the sense of quadratic forms on (a subset of) H_ω.

Even though we are in a quantum mechanical setup, one would expect that measurement with a physical detector should not lead to huge back-reaction effects, so following [Tak86, BD84], the field-detector interaction is calculated perturbatively; in weak coupling situations such a procedure can be rigorously justified [DBM06], for further discussion of the situation encountered here see below.

To first order perturbation-theory, the state of the detector-field system at time τ is given by

$$\Phi(\tau) = \Omega_\omega \otimes \psi_g - i \int_{-\infty}^{\tau} \chi(\tau') \ \left(\phi(\gamma(\tau'))\Omega_\omega\right) \otimes \left(M(\tau')\psi_g\right) \mathrm{d}\tau' .$$

For the probability of finding the detector in the excited state ψ_e and the field in a state Ψ_n at large times, one then has

$$\begin{aligned} |\langle \Psi_n \otimes \psi_e, \Phi(\infty)\rangle|^2 \quad &= \quad \int_{\mathbb{R}} \int_{\mathbb{R}} \langle \chi(\tau')\phi(\gamma(\tau'))\Omega_\omega \otimes M(\tau')\psi_g, \Psi_n \otimes \psi_e\rangle \times \ldots \\ \ldots \quad & \times \langle \Psi_n \otimes \psi_e, \chi(\tau'')\phi(\gamma(\tau''))\Omega_\omega \otimes M(\tau'')\psi_g\rangle \mathrm{d}\tau' \mathrm{d}\tau'' \end{aligned}$$

and by summing over a complete set of Ψ_n in $\mathcal{H}_\omega$ and using

$$< \psi_e, M(\tau)\psi_g > = < \psi_e, e^{i\tau H} M_0 e^{-i\tau H} \psi_g > = e^{i\epsilon\tau} < \psi_e, M_0 \psi_g >$$

the probability of finding the detector in the excited and the field in any state is

$$\begin{aligned} P_\omega(\epsilon) \quad &= \quad |< \psi_e, M_0\psi_g >|^2 \int_{\mathbb{R}} \int_{\mathbb{R}} \chi(\tau')\chi(\tau'') e^{-i\epsilon(\tau'-\tau'')} \times \ldots \\ \ldots \quad & \times < \phi(\gamma(\tau'))\Omega_\omega, \phi(\gamma(\tau''))\Omega_\omega > \mathrm{d}\tau' \mathrm{d}\tau'' \\ &= \quad m \int_{\mathbb{R}} \int_{\mathbb{R}} \chi(\tau')\chi(\tau'') e^{-i\epsilon(\tau'-\tau'')} \omega(\phi(\gamma(\tau'))\phi(\gamma(\tau''))) \mathrm{d}\tau' \mathrm{d}\tau'' , \end{aligned}$$

where the constant of proportionality $m := |< \psi_e, M_0\psi_g >|^2$ depends on details of the detector but not on the field configuration.

Now instead of comparing directly the transition probabilities $P_\omega(\epsilon)$ and $P_{\omega_\beta}(\epsilon)$ in two states, one can in principle compare their difference to the transition probability $P_{\omega_{ref}}$ in a common reference state. Choosing ω_∞ as ω_{ref} this amounts heuristically to “removing the vacuum fluctuations” and the resulting (difference in) transition probability is then

$$\begin{aligned} P_\omega^{\mathrm{ren}}(\epsilon) \quad &= \quad m \int_{\mathbb{R}} \int_{\mathbb{R}} e^{-i\epsilon s} F_\omega(\tau, s) \chi\left(\tau + s/2\right) \chi\left(\tau - s/2\right) \mathrm{d}s \mathrm{d}\tau \qquad (3.2.1) \\ F_\omega(\tau, s) \quad &:= \quad \omega\left(\phi\left(\gamma\left(\tau + s/2\right)\right) \phi\left(\gamma\left(\tau - s/2\right)\right)\right) - \ldots \\ & \qquad \ldots - \omega_\infty\left(\phi\left(\gamma\left(\tau + s/2\right)\right) \phi\left(\gamma\left(\tau - s/2\right)\right)\right) . \end{aligned}$$

Assuming ω to be a Hadamard state, the integrand is smooth and compactly supported and therefore $\epsilon \mapsto P_\omega^{\mathrm{ren}}(\epsilon)$ is a rapidly decreasing, smooth function. Thus all moments of this function are defined and we turn to the analysis of these moments in order to obtain a means for local investigation of states.

3.2.2 Convolution and moments

As already mentioned above, in the case of global equilibrium and for χ approaching a constant function, the dependence of the transition probabilities on ϵ approaches a function that gives information about the thermal properties of the state under consideration. Disregarding for a moment the τ-integration in (3.2.1), more rapid switching of the detector can be seen to disturb this function by convolution with a function that becomes wide as χ becomes narrow, as is of course to be expected due to time-energy uncertainty. There is however a way to get around this, if one is only interested in the moments of this function and knows the moments of χ.

To see this, consider two rapidly decaying functions $f, h \in \mathscr{S}(\mathbb{R})$. Denote the k-th moment of a function $f \in \mathscr{S}(\mathbb{R})$ by

$$\mathcal{M}^k[f] := \int_{\mathbb{R}} t^k f(t) \mathrm{d}t$$

and assume $\mathcal{M}^0[h] = 1$ (i.e. the integral over h is one). Then by a direct computation one has for the convolution $f * h$:

$$\mathcal{M}^k[f * h] = \sum_{j=0}^{k} \binom{k}{j} \mathcal{M}^j[f] \mathcal{M}^{k-j}[h] \,. \tag{3.2.2}$$

For the special case $k = 0$ this relation gives $\mathcal{M}^0[f * h] = \mathcal{M}[f]$, so the zeroth moment of f is always known once the zeroth moment of $f * h$ is known. Noting that on the rhs of equation (3.2.2) the k-th moment of f is multiplied by one and the further terms involve only lower moments of f, one can therefore determine the moments of f from those of $f * h$ and h by the recursion

$$\mathcal{M}^k[f] = \mathcal{M}^k[f * h] - \sum_{j=0}^{k-1} \binom{k}{j} \mathcal{M}^j[f] \mathcal{M}^{k-j}[h] \tag{3.2.3}$$

starting from $\mathcal{M}^0[f]$.

3.2.3 Modified moments of transition rates and elements of S_x

Now returning to (3.2.1), for general χ the application of the idea of the preceding section to the transition-probability is complicated by the τ-integration. This problem can however be overcome by choosing χ to be a Gaussian of width σ centered at τ_0:

$$\chi_{\sigma,\tau_0} : \tau \mapsto \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(\tau-\tau_0)^2}{2\sigma^2}} \,.$$

Then $\chi_{\sigma,\tau_0}(\tau + s/2)\, \chi_{\sigma,\tau_0}(\tau - s/2)$ factorizes into $\chi_{\sigma/\sqrt{2},\tau_0}(\tau)\chi_{\sqrt{2}\sigma,0}(s)$ and the moments of $\epsilon \mapsto P^{\mathrm{ren}}_{\omega}(\epsilon)$ are:

$$\mathcal{M}^k[P^{\mathrm{ren}}_{\omega}] = m \int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}} F_{\omega}(\tau, s) \chi_{\sigma/\sqrt{2},\tau_0}(\tau) \mathrm{d}\tau \; e^{-i\epsilon s} \chi_{\sqrt{2}\sigma,0}(s) \mathrm{d}s \epsilon^k \mathrm{d}\epsilon \,.$$

Identifying the Fourier transform of $s \mapsto \sqrt{2\pi} \int_{\mathbb{R}} F_{\omega}(\tau, s) \chi_{\sigma/\sqrt{2}}(\tau) \mathrm{d}\tau$ with f and the Fourier transform of $\sqrt{2\pi}\chi_{\sqrt{2}\sigma}$ with h, this is the situation of the preceding section and by the recursive procedure described there, one can obtain the k-th moments of f which will be called $\mathcal{P}^k_\omega$. Explicitly they are given by

$$\mathcal{P}^k_\omega = m\int_{\mathbb{R}}\int_{\mathbb{R}} F_\omega(\tau,s)\chi_{\sigma/\sqrt{2},\tau_0}(\tau)\mathrm{d}\tau e^{-i\epsilon s}\mathrm{d}s\epsilon^k\mathrm{d}\epsilon\,.$$

By partial integration using the decay-properties of χ_{σ,τ_0} and the regularity of F_ω this can be expressed as

$$\mathcal{P}^k_\omega = m\int_{\mathbb{R}}(-i\partial_s)^k F_\omega(\tau,s)|_{s=0}\chi_{\sigma/\sqrt{2},\tau_0}(\tau)\mathrm{d}\tau\,. \tag{3.2.4}$$

For this expression one can proceed to the limit $\sigma \to 0$, which shows that the $\mathcal{P}^k_\omega$ are objects which can be measured over arbitrarily short time-intervals. In the limit one has

$$\begin{aligned}\lim_{\sigma\to 0}\mathcal{P}^k_\omega &= m(-i\partial_s)^k F_\omega(\tau_0,s)|_{s=0}\\ &= m(-i/2)^k\partial_s^k(\omega-\omega_\infty)\left(\phi(\gamma(\tau_0+s))\phi(\gamma(\tau_0-s))\right)|_{s=0}\end{aligned} \tag{3.2.5}$$

Defining for a (sufficiently differentiable) function $f : \mathbb{R}^4\times\mathbb{R}^4 \to \mathbb{R}$ and $u_1,\dots,u_k \in \mathbb{R}^4$ the *balanced derivative* $[\eth^{(u_1,\dots,u_k)}f](x)$ by

$$[\eth^{(u_1,\dots,u_k)}f](x) = \partial_{t_1}\dots\partial_{t_k} f\Big(x+\sum_{i=1}^k t_i u_i\ ,\ x-\sum_{j=1}^k t_j u_j\Big)|_{t_1=\dots=t_n=0} \tag{3.2.6}$$

one can rewrite (3.2.5) for inertial detectors with $\gamma(\tau_0) = x$ and $\dot\gamma(\tau_0) = u$ as

$$\begin{aligned}\lim_{\sigma\to 0}\mathcal{P}^k_\omega &= m(-i/2)^k\ \eth^{(u,\dots,u)}w(x)\\ w(x,y) &:= \omega(\phi(x)\phi(y)) - \omega_\infty(\phi(x)\phi(y)) \quad \text{in the sense of distributions.}\end{aligned}$$

The definition (3.2.6) slightly generalizes the definition for $\eth^{(\mu_1,\dots,\mu_k)}$ from [BOR02] which is recovered by choosing $u_i = \eta^{\mu_i\mu_i}e_{\mu_i}$ with $e_0,\dots,e_3$ the basis vectors of $\mathbb{R}^4$, so the expectation values of elements $m(-i/2)^k\ \eth^{(0,\dots,0)}\ {:}\phi^2{:}_{\omega_\infty}$ from the S_x-spaces in the state ω used there can be interpreted as measurements of $\mathcal{P}^k_\omega$ in the limit of arbitrarily short interaction of detector and field. A prominent example from this class is the Wick-square itself, which gives the expectation-value of the local temperature squared.

3.2.4 Moving detectors and the full S_x-space

As calculated in the last section, measurement of balanced derivatives $\eth^{(u,\dots,u)}\ {:}\phi^2(x){:}_{\omega_\infty}$ can be described by a limiting process involving measurements carried out on an ensemble of detectors moving through the spacetime point x with a four-velocity u. As they stand, these balanced derivatives only generate a subset of the S_x-spaces used in the formalism of local thermal equilibrium on Minkowski spacetime [BOR02, Buc03] and important (local thermal) observables like the (thermal) stress-energy tensor are not among them.

As already mentioned, global equilibrium states on Minkowski spacetime are not invariant under the full Poincaré group but single out a set of inertial frames that only differ by rotations and translations. Physically, they correspond to the observers being at rest with respect to the "gas" described by the thermal state. As thermality properties, like the principle of detailed balancing, hold only for those systems coupled to the field which are at rest in these inertial frames, for the investigation of an equilibrium state with an unknown associated rest frame one should use not one detector, but detectors with all possible velocities smaller than the velocity of light relative to a given one. The detector behaving according to the principle of detailed balancing then indicates the rest frame of the given state, and starting from this one can then check, whether the readings of the other detectors are compatible with the interpretation of being in relative motion to a thermal state.

Whereas for a global equilibrium state, whose rest-frame is usually known a priori this discussion might sound rather odd, the hydrodynamical description of gases by a velocity field varying in space and time can be rephrased as the statement that at each point the state looks like a thermal state, with reference frames at different points being in relative motion to each other. As this dependence of the frames on space-time is not known a priori but rather one piece of information an LTE-formalism should yield, it seems therefore sensible to not just consider one detector with a worldline passing through a spacetime point x, but the set of all detectors passing through it.

By the above procedure, one then obtains as local thermal observables the balanced derivatives $\eth^{(u,\dots,u)} :\phi^2:_{\omega_\infty} (x)$ for *all* timelike unit vectors u. Continuing this for the k-th balanced derivative (i.e. with u appearing k-times in $\eth^{(u,\dots,u)}$) to (nonzero) $\tilde{u}$ of non-unit length by inserting $u = \frac{\tilde{u}}{\sqrt{\tilde{u}^a \tilde{u}_a}}$ and multiplying the result by $(\tilde{u}^a \tilde{u}_a)^{k/2}$, we get the balanced derivatives with $u_1 = \dots = u_k = \tilde{u}$ for arbitrary timelike vectors $\tilde{u}$. If we had this results for arbitrary $u \in \mathbb{R}^4$, using the fact that $f_\eth : u \mapsto \omega(\eth^{(u,\dots,u)} :\phi^2:_{\omega_\infty})$ is homogeneous of degree k and smooth for Hadamard states, it would again follow that we could get back the (totally symmetric) balanced derivative for arbitrary $u_1, \dots, u_k$ as[4]

$$\frac{1}{k!} \partial_{t_1} \dots \partial_{t_k} f_\eth (t_1 u_1 + \dots + t_k u_k)|_{t_1 = \dots = t_k = 0}$$

(again the concept of polarization). This can however also be applied to the case when u is only allowed to be timelike: Replacing $t_1 u_1 + \dots + t_k u_k$ by $\xi + t_1 u_1 + \dots + t_k u_k$, where ξ is a timelike vector, the $t_1, \dots, t_k$-derivatives of $f_\eth$ can be calculated for $t_1, \dots, t_k$ in a neighbourhood of zero using only values of $f_\eth$ on timelike vectors, resulting for $t_1 = \dots = t_k = 0$ in a totally symmetric form in $u_1, \dots, u_k$, which still depends on ξ; but again by the smoothness of $f_\eth$ for $\xi \to 0$ we get back the desired, arbitrary balanced derivative.

Though this argument, showing that all balanced derivatives can be recovered from the special ones related to detector measurements, relies on limits, it should be noted that interesting cases of general balanced derivatives can be expressed in terms of the special ones using purely algebraic relations; one example are the second balanced derivatives,

[4]This was first pointed out to me by Detlev Buchholz

which can be expressed as

$$\begin{aligned}
\frac{1}{4}\eth^{(e_j,e_j)} :\phi^2:_{\omega_\infty} &= \eth^{\left(e_0+\frac{1}{2}e_j,e_0+\frac{1}{2}e_j\right)} :\phi^2:_{\omega_\infty} + \eth^{\left(e_0-\frac{1}{2}e_j,e_0-\frac{1}{2}e_j\right)} :\phi^2:_{\omega_\infty} - \eth^{(e_0,e_0)} :\phi^2:_{\omega_\infty} \\
2\eth^{(e_0,e_j)} :\phi^2:_{\omega_\infty} &= \eth^{\left(e_0+\frac{1}{2}e_j,e_0+\frac{1}{2}e_j\right)} :\phi^2:_{\omega_\infty} - \eth^{\left(e_0-\frac{1}{2}e_j,e_0-\frac{1}{2}e_j\right)} :\phi^2:_{\omega_\infty} \\
\eth^{(e_j,e_k)} :\phi^2:_{\omega_\infty} &= \eth^{\left(e_0+\frac{1}{2}e_j+\frac{1}{2}e_k,e_0+\frac{1}{2}e_j+\frac{1}{2}e_k\right)} :\phi^2:_{\omega_\infty} - \eth^{\left(e_0+\frac{1}{2}e_j-\frac{1}{2}e_k,e_0+\frac{1}{2}e_j-\frac{1}{2}e_k\right)} :\phi^2:_{\omega_\infty} \\
&\quad - \eth^{\left(e_0+\frac{1}{2}e_k,e_0+\frac{1}{2}e_k\right)} :\phi^2:_{\omega_\infty} + \eth^{\left(e_0-\frac{1}{2}e_k,e_0-\frac{1}{2}e_k\right)} :\phi^2:_{\omega_\infty} ,
\end{aligned}$$

where $k \neq j, k, j = 1, 2, 3$ and $e_0, \ldots, e_3$ are the basis-vectors of $\mathbb{R}^4$.

3.2.5 On the perturbative aspect of the calculation

The calculation so far has been a first order perturbation theoretic calculation, which in most cases might seem appropriate for a (small) detector system interacting with the (big) system under investigation. The problem here is that one in the end wants to consider very short measurements, which implies that the cut-off functions χ, who are interpreted as couplings, get big (though their area remains constant during this process). The question of the validity of the perturbation-theoretic discussion can then be split up into two parts:

1. Does the perturbation series converge or are there at least error estimates for calculations in finite order perturbation theory ?
2. Does the regularization procedure (taking the relative transition probabilities, reconstructing the balanced derivatives recursively from moments) still survive the limit of arbitrarily short interactions when using exact or higher order expressions for the transition probabilities ?

Whereas for the first question, rough calculations seem to indicate that this is not a serious problem, the second question is much more severe: First the construction of the modified moments used implicitly the simple structure of (expectation values) of Wick products of two field operators to establish the existence of all moments for the relative transition rate.

When calculating the transition probabilities to higher order perturbation theory, expectation values of products of more field-operators and time-ordering appears, so it is not clear whether for the relative transition rates all the moments exist, which in turn of course makes the second step impossible. Whether this is really the case and whether there are ways out by for example replacing the relative transition probabilities and/or the moments by some other construction are interesting questions, they have however so far not been investigated.

Another way to approach this problem would be not to proceed all the way to point-limits, but to pick χ_{σ,τ_0} with a sufficiently large width (i.e. σ) that the calculation of the transition rates in first order perturbation theory is still sufficiently accurate (potentially only up to some maximum energy $E_{\max}$, if there is trouble with convergence of the moments), and then use the moments for this finite value of σ as approximations for the balanced derivatives. From (3.2.4) one sees, that this results in balanced derivatives smeared with $\chi_{\sigma/\sqrt{2},\tau_0}$, so instead of the idealized, point-localized measurements one would get some coarse-graining scale that depends on the detail of the field-theory and the measurement process.

At first, from (3.2.4) it looks as this would actually work for balanced derivatives of arbitrary order with the same coarse graining scale, but although candidates for their expectation values can of course be calculated, due to the recursive nature of the calculation involving subtraction of lower moments, the initial difference between the transition probabilities calculated in first order perturbation theory and the true transition probabilities will most likely lead to quickly increasing errors in the higher moments, so by this approach one can only hope to get the first few balanced derivatives, smeared over a part of a geodesic. Still, since we use only the zeroth and second balanced derivative in the next chapters, at current this seems the best one can say about the physical relevance of the formal relation between detectors and balanced derivatives in first order calculation theory. To make this second approach to the problem more rigorous, one would first need error-estimates relating the first-order perturbational calculation to the true transition rates (taking care of the problem of existence of moments) and then one would need to check, how these errors propagate in the recursive calculation of the expectation values of the (smeared) balanced derivatives.

As a last remark, it should be pointed out that the discussion of moving detectors does not depend very strongly on the specific detector-model and the precise way the balanced derivatives are defined, justifying to some extent its use as a guiding principle in the definition of the balanced derivative.

3.3 The criterion of extrinsic, local thermality

Using the linear spaces S_x generated by the balanced derivatives $\eth^{\boldsymbol{\mu}} :\!\phi^2\!:$, $\boldsymbol{\mu}$ a multiindex, the criterion of local thermality of a state ω at a spacetime-point $x \in \mathbb{R}^4$ is formulated in [BOR02] as follows[5]

Definition 3.2. A state ω is called S_x-thermal if there exists a KMS-state ω_β such that for all $\phi(x) \in S_x$ there holds

$$\omega(\phi(x)) = \omega_\beta(\phi(x))\,. \tag{3.3.1}$$

This means that the state ω can not be distinguished from ω_β on the thermal observables in S_x. Thermality in an open set $\mathcal{O} \subset \mathbb{R}^4$ is then defined as thermality at each point $x \in \mathcal{O}$, where the reference state on the right hand side of (3.3.1) may depend on x.

Attempts to generalize this definition to curved spacetime face two problems:

- What should be the replacement for the balanced derivatives generating the spaces S_x ?

[5]More precisely, the definition given here is the special case of local-thermality with a sharp (inverse) temperature; in [BOR02] on the right hand side of (3.3.1) a state from a set of reference states, including also mixtures of KMS-states for different temperatures and rest-frames, is allowed

- What should be put in place of the global equilibrium states ω_β ?

As it turns out, the formalism of locally covariant quantum field suggests an answer to both questions.

First, in the discussion of the recovery of generalized balanced derivatives we used the ideas of detectors in different states of motion, characterized by their velocity u at x. Heavy use was made of the fact that the detector-velocities are elements of some linear space at x to deduce totally symmetric tensors, the balanced derivatives. In addition to their velocity at x, the additional requirement fixing the worldlines of the detectors was that they move freely (i.e. along geodesics). But the velocities of different observers at a point x in a general spacetime M are still from a linear space, namely the tangent space T_xM, and if we assume that also in curved spacetime the detector response depends in a similar way upon properties of the state, encoded in a function $W : M \times M \to \mathbb{C}$ replacing $(x, x') \mapsto m(-i/2)^k(\omega - \omega_\infty)(\phi(x)\phi(x'))$ along its trajectory, the right hand side of (3.2.5) gets replaced by

$$\partial_\tau^k W(\gamma_u(\tau), \gamma_u(-\tau))|_{\tau=0} \,.$$

By the definition of the exponential map $\exp_x$ at x this can be rewritten as

$$\partial_\tau^k W(\exp_x(\tau u), \exp(-\tau u))|_{\tau=0}$$

and if we take the point of view that we extract the observed values for the thermal observables from this function of $u \in T_xM$ by the above procedure, we end up with the balanced derivative (still denoted by $\eth^{(u_1,\dots,u_k)}$) defined as

$$[\eth^{(u_1,\dots,u_k)}W](x) := \\ \partial_{t_n} \dots \partial_{t_k} W\left(\exp_x(t_1u_1 + \dots + t_ku_k), \exp(-t_1u_1 - \dots - t_ku_k)\right)|_{t_1=\dots=t_k} \,. \tag{3.3.2}$$

This might at first look a bit odd from a geometrical point of view, but since it uses only the geometrically defined exponential map as an input, this is a totally symmetric, n-linear map on T_xM and allowing x to vary over the domain of definition $N \subset M \times M$ of a smooth function W, we can associate to n vector-fields $U_1, \dots, U_k$ a smooth function defined for $x \in M$ as $[\eth^{(U_1(x),\dots,U_k(x))}W](x)$. This depends only on the values of $U_1, \dots, U_k$ at $x \in M$ and is linear in each entry, so the balanced derivative in fact defines a $\binom{0}{k}$-tensor field, denoted in abstract index notation as $[\eth_{a_1,\dots,a_k}W]$.
If W is a symmetric function, the balanced derivatives so defined vanishes for odd n; using the geodesic equation and once more the symmetry of W, the first non-trivial balanced derivative is calculated as

$$\begin{aligned}[\eth_{ab}W](x) =& [\nabla_a\nabla_bW]_{x=x'} - [\nabla_a\nabla_{b'}W]_{x=x'} - [\nabla_{a'}\nabla_bW]_{x=x'} + [\nabla_{a'}\nabla_{b'}W]_{x=x'} \\ =& 2\,[\nabla_a\nabla_bW]_{x=x'} - 2\,[\nabla_a\nabla_{b'}W]_{x=x'} \,.\end{aligned} \tag{3.3.3}$$

This second balanced derivative can also be defined in a slightly different way using parallel transports [SV08]; due to the fact that the Levi-Civita connection is torsion free the two definitions coincide.

As a next step, we need to find a replacement for the Wick-products, defined on Minkowski spacetime by normal-ordering with respect to the vacuum state. Since the idea behind the whole formalism is to use observables that correspond to (idealized) measurements of specific thermal quantities, we would like to take observables modeling the measurements of the same quantities as generators of the S_x-spaces on each spacetime, so we would e.g. like to have Wick-products $:\phi(M,g)^2:(x)$ that on each spacetime M correspond to the measurement of (a simple function of) the temperature at point x. The direct way would now be to try and identify observables by their properties (expectation values in states with known interpretation, etc.), for example by generalizing the discussion of detectors from the preceding sections to general spacetimes, but there are immediate problems arising in this approach. For example, to check whether an observable is sensitive to thermal properties of the system under investigation one needs a notion of equilibrium situation, and while global equilibrium states as defined by the KMS conditions do not exist on general spacetimes without time-translation isometries, local equilibrium is precisely what we want to define and therefore cannot be used in such an investigation either. Like in classical physics we can however take covariance principles as a guiding principle in defining observables in general relativity; here this is the concept of a locally covariant quantum fields from section 2.1.2. Since the idealized, pointwise measurements are mathematically realized as linear spaces (not algebras) S_x of point-localized observables, we only need to define the expectation values of the covariant derivatives of the Wick square and this is done in the following

Definition 3.3. Let ω be a Hadamard state on $\mathcal{A}(M,g)$. Then the expectation value of the (n-th order) covariant, balanced derivative $\eth_{a_1\dots a_n} :\phi^2:_{\text{SHP}}(x)$ in the state ω is

$$\omega(\eth_{a_1\dots a_n} :\phi^2:_{\text{SHP}}(x)) := [\eth_{a_1\dots a_n}\mathscr{W}^{\text{SHP}}_{\omega,k}](x)\,.$$

This is independent of k due to the fact that for $k'>k$, $\mathcal{G}_k-\mathcal{G}_{k'}$ and all its derivatives of order no higher than k vanish when restricting to the diagonal $x=x'$; since $\mathscr{W}^{\text{SHP}}_{\omega,k}$ is symmetric, the odd balanced derivatives are all zero.

Concerning possible choices in the definition of the covariant balanced derivatives, because these are in the end just sums of Wick products of derivatives of (two) field operators (with the same scaling degree for each summand), the same ambiguity as for the definition of those arise. There are at least three possible ways to reduce these ambiguities:

1. Use the formalism of [HW05] to establish relations between the balanced derivatives of different order induced from corresponding relations between Wick products of differentiated fields.

2. Use the fact that these ambiguities take the form of (locally constructed) geometric terms with the right scaling behaviour multiplied with the undetermined parameters, which have to be the same for *all* spacetimes. Now pick a few spacetimes with non-trivial curvature on which there still exist one-parameter families of timelike isometries that lead to KMS-states which are in a suitable sense isotropic

and homogeneous (e.g. Einstein static universes [HE73] or de Sitter for a special (inverse) temperature). These states should correspond physically to global equilibrium states and their thermal properties are known. Calculate for each spacetime the expectation values of the covariant balanced derivatives in these global equilibrium states and try to adjust the parameters in such a way that the observables have the expected values. Since the parameters have to be fixed to the same value for all spacetime, for each additional spacetime this gives (potentially) more restrictions on them. A first example for an application of this procedure is the massless scalar field on de Sitter spacetime, where the free parameter c_1 in front of the ambiguity $c_1 R \cdot 1$ was fixed by the requirement that for de Sitter KMS-states $:\phi^2:_{\mathrm{SHP}}$ should, like in Minkowski spacetime, give (up to a proportionality constant) the square of the temperature of the KMS-state[6] [BS07].

3. One could try to fix the parameters by requiring that the Quantum Energy Inequalities in the next chapter are "optimal" in a suitable sense.

Here we will take the more pragmatic approach of simply sticking to the SHP-Wick products and when relevant carry a term encoding the renormalization ambiguities along. This is justified by the fact that most results do not really depend on the precise form of the ambiguity (an exception is ANEC in the next chapter; see the discussion there for more details); however all three procedures are well worth further investigation, especially since one could encounter incompatible requirements for the parameters that would point to problems in this approach to local equilibrium.

Note that the SHP Wick products differ on Minkowski spacetime from the Wick products obtained by normal ordering with respect to the vacuum-state by a multiple of the unit-operator; for the Wick-square and the second order balanced derivative the relations are given by[7]

$$:{\phi_o}^2:_{\mathrm{SHP}}(x_o) = :{\phi_o}^2:_{\omega_\infty}(x_o) + c_{0,m}1 \tag{3.3.4}$$

$$\eth_{\mu\nu}:{\phi_o}^2:_{\mathrm{SHP}}(x_o) = \eth_{\mu\nu}:{\phi_o}^2:_{\omega_\infty}(x_o) + c_{2,m}\eta_{\mu\nu}1\,. \tag{3.3.5}$$

The constants $c_{0,m}$ and $c_{2,m}$ depend on the mass of the field and the length-scale L appearing in the definition of the Hadamard parametrix (see [HW01], [Mor03] for a discussion of their relation to the concept of local covariance); in the chapter on Quantum Energy Inequalities and for the construction of LTE-states it will be set to one, again since this is considered part of the (geometric) renormalization ambiguity. The constants $c_{0,m}$, $c_{2,m}$ can be calculated as a special case of the technique explained in chapter 5 as

$$c_{0,m} = \frac{m^2}{(4\pi)^2}\left[2\gamma + \log\left(\frac{m^2}{4}\right) - 1\right]$$

$$c_{2,m} = -\frac{m^4}{(4\pi)^2}\left[2\gamma + \log\left(\frac{m^2}{4}\right) - \frac{5}{2}\right]\,.$$

[6] These states are not homogeneous and isotropic (i.e. when considered on a part of de Sitter which can be regarded as a Robertson Walker spacetime) and this is seen on higher balanced derivatives; for the (scalar) Wick square this does however not matter.

[7] ϕ_o is the field on Minkowski spacetime; see below for the reason for this notation

We can now take the space $S_x^{(n)}$ as the linear spaces generated by the covariant, balanced derivatives of $:\phi^2:_{\mathrm{SHP}}$ of order no higher than n; in the following we will restrict to the rather small space $S_x^{(2)}$, which is however still big enough to contain energy-like observables.

Finally, we need to address the problem of reference states in the LTE condition. As the formalism of locally covariant quantum fields is based on an identification of observables on different spacetimes, this suggest that the observables so identified could be used to compare states in quantum field theories on *different* spacetimes. Since the global equilibrium situation is well understood on Minkowski spacetime, the states of quantum fields on Minkowski spacetime will be taken as reference states, which also has the advantage that the results derived for the LTE-formalism there can be used[8].

To make this idea precise, we need to compare tensorial quantities at the point $x \in M$ with tensorial quantities in Minkowski spacetime. To be able to do that, we need an isometric isomorphism between (M_o, η) and $(T_x M, g)$. Here, a convenient way to proceed is by first fixing an orthonormal basis in Minkowski spacetime once and for all and only take KMS-states with rest-frame specified by the timelike vector of this basis as reference states. The balanced derivative with respect to this basis we denote as above by $\eth_{\mu\nu} :{\phi_o}^2:_{\mathrm{SHP}} (x_o)$, where x_o is some reference point in M_o (by translation-invariance of $\omega_o^{\beta e}$, the particular choice of x_o is irrelevant). The isomorphism is then specified by giving a tetrad $(e_0, \dots, e_3)$ at $x \in M$ (e_0 timelike and future-pointing) to which this basis is mapped.

With this preparations we can now define our condition of local thermality:

Definition 3.4. Let ω be a Hadmard-state for the quantized linear scalar field ϕ on a globally hyperbolic spacetime (M, g) and let ϕ_o denote the quantized linear scalar field, with the same parameters as ϕ, on Minkowski spacetime M_o.

a) We say that ω is $S_x^{(2)}$-*thermal* at a point $x \in M$ if, with some orthonormal tetrad $e = (e_0, e_1, e_2, e_3)$ at x such that e_0 is timelike and future-pointing, there is a thermal equilibrium state $\omega_o^{\beta e}$ of ϕ_o so that the equalities

$$\begin{aligned} \omega(:\phi^2:_{\mathrm{SHP}} (x)) &= \omega_o^{\beta e}(:{\phi_o}^2:_{\mathrm{SHP}} (x_o)) \qquad (3.3.6)\\ &= \omega_o^{\beta e}(:{\phi_o}^2:_{\omega_\infty} (x_0)) + c_{0,m} \\ v^a w^b \omega(\eth_{ab} :\phi^2:_{\mathrm{SHP}} (x)) &= v^\mu w^\nu \omega_o^{\beta e}(\eth_{\mu\nu} :{\phi_o}^2:_{\mathrm{SHP}} (x_o)) \qquad (3.3.7)\\ &= v^\mu w^\nu \omega_o^{\beta e}(\eth_{\mu\nu} :{\phi_o}^2:_{\omega_\infty} (x_o)) + c_{2,m} v^\mu w^\nu \eta_{\mu\nu} \end{aligned}$$

hold for all vectors $v, w \in T_x M$ with coordinates $v^\mu e_\mu = v$, $w^\nu e_\nu = w$.

b) Let N be a subset of M. We say that ω is $S_N^{(2)}$-*thermal* if $\omega(:\phi^2:_{\mathrm{SHP}} (x))$ and $\omega(\eth_{ab} :\phi^2:_{\mathrm{SHP}} (x))$ are continuous in $x \in N$ and if, for each $x \in N$, ω is $S_x^{(2)}$-thermal at x.

[8] To clearly distinguish the quantities on Minkowski spacetime from those on (M, g), they will be denoted with a sub- or superscript index $_o$ respectively ^{o}; following this logic Minkowski spacetime itself will be denoted M_o.

Introducing for the right hand sides appearing in (3.3.6) and (3.3.7) the abbreviations

$$\begin{aligned}\vartheta^o(\beta) =& \omega^{\beta e_0}(:{\phi_o}^2:_{\mathrm{SHP}}(x_o))\\ \varepsilon^o_{\mu\nu}(\beta) =& -\frac{1}{4}\omega^{\beta e_0}(\eth_{\mu\nu} :{\phi_o}^2:_{\mathrm{SHP}}(x_o))\end{aligned}$$

and using the explicit expression for the two-point-function of the KMS-state at inverse temperature β from equation (3.1.1) we have

$$\vartheta^o(\beta) =\frac{1}{\beta^2}\chi(m\beta) + c_{0,m} \tag{3.3.8}$$

$$\varepsilon^o_{00}(\beta) =\frac{1}{\beta^4}\chi_{tt}(m\beta) + c_{2,m} \tag{3.3.9}$$

$$\varepsilon^o_{jj}(\beta) =\frac{1}{\beta^4}\chi_{xx}(m\beta) - c_{2,m} \qquad j \in \{1,2,3\}\,, \tag{3.3.10}$$

where

$$\begin{aligned}\chi(\xi) =& \frac{1}{2\pi^2}\int_{\mathbb{R}^+} \frac{\rho^2}{e^{\sqrt{\rho^2+\xi^2}}-1}\,\frac{\mathrm{d}\rho}{\sqrt{\rho^2+\xi^2}}\\ =& \frac{1}{2\pi^2}\int_{\mathbb{R}^+}\left(\frac{\rho}{\sqrt{\rho^2+\xi^2}}\,\frac{e^\rho-1}{e^{\sqrt{\rho^2+\xi^2}}-1}\right)\frac{\rho\,\mathrm{d}\rho}{e^\rho-1}\end{aligned} \tag{3.3.11}$$

$$\begin{aligned}\chi_{tt}(\xi) =& \frac{1}{2\pi^2}\int_{\mathbb{R}^+} \frac{\sqrt{\rho^2+\xi^2}}{e^{\sqrt{\rho^2+\xi^2}}-1}\,\rho^2\mathrm{d}\rho\\ =& \frac{1}{2\pi^2}\int_{\mathbb{R}^+}\left(\frac{\sqrt{\rho^2+\xi^2}}{\rho}\,\frac{e^\rho-1}{e^{\sqrt{\rho^2+\xi^2}}-1}\right)\frac{\rho^3\,\mathrm{d}\rho}{e^\rho-1}\end{aligned} \tag{3.3.12}$$

$$\begin{aligned}\chi_{xx}(\xi) =& \frac{1}{6\pi^2}\int_{\mathbb{R}^+} \frac{\rho^4}{e^{\sqrt{\rho^2+\xi^2}}-1}\,\frac{\mathrm{d}\rho}{\sqrt{\rho^2+\xi^2}}\\ =& \frac{1}{6\pi^2}\int_{\mathbb{R}^+}\left(\frac{\rho}{\sqrt{\rho^2+\xi^2}}\,\frac{e^\rho-1}{e^{\sqrt{\rho^2+\xi^2}}-1}\right)\frac{\rho^3\,\mathrm{d}\rho}{e^\rho-1}\,.\end{aligned} \tag{3.3.13}$$

From these expressions it follows that the relation

$$\varepsilon^{o\,\mu}_{\mu}(\beta) = \tfrac{m^2}{\beta^2}\chi(m\beta) - c_{2,m}\,, \tag{3.3.14}$$

relating the trace of $\varepsilon^o_{\mu\nu}$ to χ, holds.

Since the ϑ^o and $\varepsilon^o_{\mu\nu}$ are (except for the constants $c_{0,m}$ and $c_{2,m}$) thermal functions that already appeared in previous investigations of the LTE-condition on Minkowski spacetime [Buc03, Hüb05] and their thermal interpretation was there determined as a scalar thermometer reading $(k_bT)^2\chi\left(\frac{m}{k_BT}\right)$ at temperature T and the thermal part of the stress-energy tensor respectively, for an $S^{(2)}_x$-thermal state we can now assign at x these two thermal functions to ω; they will be denoted as

$$\vartheta^\omega(x) =\omega(:\phi^2:_{\mathrm{SHP}}(x)) \tag{3.3.15}$$

$$\varepsilon^\omega_{ab}(x) =\omega(\eth_{ab} :\phi^2:_{\mathrm{SHP}}(x))\,. \tag{3.3.16}$$

This assignment gives the local temperature and energy density which, as explained in the introduction, are some of the quantities that one wants to define rigorously in an LTE approach to quantum field theory in curved spacetime.

4 Energy inequalities

After having fixed our notion of local thermality, as a first application we now investigate its relation to the (expectation values) of the energy density of the field. In Minkowski spacetime, the second balanced derivative as the most elementary, non-scalar thermal observable is closely related to the stress energy tensor of the theory [BOR02] and by definition is a function of temperature for LTE-states; the difference is interpreted as being due to energy-fluxes which show up in the full stress energy tensor, but not in the second balanced derivative, which as its "thermal part" should be a density-like quantity. Assuming that the same holds true on general spacetime and that energy-fluxes in LTE states with bounded (local) temperature are themselves bounded, one therefore expects to be able to derive bounds on the energy densities in LTE-states with bounded (local) temperature. In this chapter we will derive such bounds, showing that these intuitive ideas are in fact true; we will start by giving a brief review of the concept of energy inequalities for quantum fields and put the results obtained in the following into perspective, then proceed to define the stress-energy tensor for the quantum fields considered here and finally derive two quantum energy inequalities, where for the second the question of renormalization ambiguities will once more appear. We end with a comment on possible generalizations of the results obtained here. The results presented in this chapter are published in a joint paper with Rainer Verch [SV08].

One of the interesting features of the expectation value of stress energy is that the energy density seen by an observer traveling on a timelike geodesic γ with tangent vector v^a at x, $\omega(T_{ab}(x))v^a v^b$, is unbounded above *and* below as ω ranges over the set of all states ω (for which the expectation value of stress-energy at any spacetime point x can be reasonably defined). This is a long known feature of quantum field theory (see [EGJ65]) and is in contrast to the behaviour of macroscopic matter which can usually be assumed to satisfy one of the classical energy conditions, like the weak energy condition, which means $T_{ab}^{class}(x)v^a v^b \geq 0$, i.e. the energy density seen by any observer is always positive at any spacetime point x. Energy positivity conditions like the (pointwise) weak energy conditions play an important role in the derivation of singularity theorems [HE73, Wal84]. One consequence of energy positivity conditions when plugged into Einstein's equations is that gravitational interaction is always attractive. Negative energies, in contrast, would be affected by a repelling gravitational interaction. This could, a priori, lead to solutions of Einstein's equations exhibiting very strange spacetime geometries, such as spacetimes with closed timelike curves, wormholes or "warpdrive scenarios" [MTY88, Alc94]. Moreover, concentration of a vast amount of negative energies and their persistence over a long duration could lead to violations of the second law of thermodynamics.

Motivated by the latter point, L. Ford has proposed that physical states of quantum fields in generic spacetimes should not permit arbitrary concentration of large amounts of negative energy over a long duration [For78]. Such limitations on physical quantum field states have come to be called *quantum energy inequalities (QEIs).* Let us explain this concept in greater detail. Let $\mathcal{L}$ be a set of states of the quantum field such that the expectation value of the stress-energy tensor, $\omega(T_{ab}(x))$, is defined for each $\omega \in \mathcal{S}$ at each spacetime point x. We will furthermore suppose that this quantity is continuous in x for each $\omega \in \mathcal{L}$. Under these assumptions, we say that the set of quantum field states $\mathcal{L}$ fulfills a QEI with respect to γ if

$$\int h^2(t)\omega(T_{ab}(\gamma(t)))\dot{\gamma}^a(t)\dot{\gamma}^b(t)\,\mathrm{d}t \geq q(\gamma, h) \tag{4.0.1}$$

holds for all smooth (or at least C^2) real functions h having compact support on the (open) curve domain, with a constant $q(\gamma, h) > -\infty$; the constant may depend on the curve γ and the weighting function h, but is required to be independent of the choice of state $\omega \in \mathcal{L}$.

In principle this concept makes sense for arbitrary (C^1 and causal) curves γ, in practice one however usually restricts the class of curves to timelike (or lightlike) geodesics. Such a limiting case of a QEI is the following: If γ is a complete (lightlike or null) geodesic, then one says that a set of states $\mathcal{L}$ fulfills the averaged null energy condition (ANEC) if

$$\liminf_{\lambda \to 0+} \int h^2(\lambda t)\dot{\gamma}^a(t)\dot{\gamma}^b(t)\,\omega(T_{ab}(\gamma(t)))\,\mathrm{d}t \geq 0$$

holds for all states $\omega \in \mathcal{L}$. Conditions of such form (and related conditions, see (4.3.1)), if valid for all complete null geodesics, allow conclusions about focusing of null geodesics for solutions to the semiclassical Einstein equations similar to that resulting from a pointwise null energy condition [Tip78, Bor87, Rom88, WY91]. (See also the beginning of section 4.3). Thus, the ANEC is a key property for deriving singularity theorems for solutions to the semiclassical Einstein equations.

Quantum energy inequalities have been investigated extensively for quantum fields subject to linear field equations in the recent years, and there is now a wealth of results in this regard. We refer to the reviews by Fewster and by Roman [Rom05, Few07a] for representative lists of references. Important to mention, however, is the fact that for many linear fields, like the minimally coupled scalar field, the Dirac field and the electromagnetic field, it could be shown that the set of Hadamard states fulfills a QEI with respect to timelike curves γ in generic globally hyperbolic spacetimes [Few00, FV02, FP03]. There is also an intimate relation between QEIs, the Hadamard condition and thermodynamic properties of linear quantum fields [FV03]. It has been shown that QEIs put strong limitations on the possibility of solutions to the semiclassical Einstein's equations to allow exotic spacetime scenarios such as wormholes or warpdrive [FR96, FR05, PF97]. It is also worth mentioning two other recent results. First, it has been shown that the non-minimally coupled linear scalar field on any spacetime violates QEIs for the class of Hadamard states; nevertheless, the class of Hadamard states fulfills in this case weaker bounds, called "relative QEIs", cf. [FO08] for results and discussion. Secondly, one is interested in lower bounds $q_\gamma(h)$ which depend (apart from renormalization constants entering the definition of expectation value of the stress energy tensor) only on the underlying spacetime geometry in a local and covariant manner, and one also aims at making this dependence as explicit as possible. Considerable progress on this issue, for the case of the minimally coupled linear scalar field on globally hyperbolic spacetimes, has been achieved in [FS07]. We will derive QEI-like bounds on sets of LTE-states of the non-minimally coupled linear scalar field $\phi(x)$ on generic globally hyperbolic spacetimes. More precisely, we consider LTE states ω whose thermal function $\vartheta^\omega(x) = \omega(:\phi^2:(x))$ is bounded by some constant $\mathtt{T}_0^2$ (corresponding to a maximal squared temperature) and we will show that there are upper and lower bounds for the averaged energy density

$$\int_{-\infty}^{\infty} \eta(\tau) v^a v^b \omega(T_{ab}(\gamma(\tau)))\, \mathrm{d}\tau\,,$$

averaged against a C^2-weighting function $\eta \geq 0$ with compact support along any causal geodesic γ with affine parameter τ and tangent $v^a = \dot{\gamma}^a$. The lower bound depends only on $\mathtt{T}_0^2$, the geodesic γ and η, while the upper bound depends additionally on local tetrads entering into the definition of LTE states. The lower bound is therefore state-independent within each set of LTE states ω with a fixed maximal value of ϑ^ω. The bounds depend on the spacetime geometry in a local covariant manner which, together with their dependence on $\mathtt{T}_0^2$, we will make explicit. This result holds for all values of curvature coupling ξ in the Klein-Gordon operator $\mathrm{P}_{m,\xi}$, and upon averaging along causal geodesic, not only those which are timelike. Hence, the result is not immediate from know quantum energy inequalities for Hadamard states, as these are violated in general for non-minimally coupled fields [FO08], and upon averaging along null geodesics [FR03]. Furthermore, we will show that the ANEC holds for LTE states ω of the quantized linear scalar field with curvature couplings $0 \leq \xi \leq 1/4$, provided that the growth of the thermal function ϑ^ω along the null geodesics γ fulfills certain bounds. Despite the fact that we have to assume that the LTE states we consider are Hadamard states – in order to have a well-defined, local covariant expression of expected stress-energy for these states – our derivation of QEIs and ANEC makes no further use of the Hadamard property but uses only properties of LTE states. Therefore, one may expect that, in principle, similar results could be derived for LTE states of interacting quantum fields.

4.1 The stress energy tensor

Consider first the case of the classical Klein-Gordon field φ on a globally hyperbolic spacetime (M, g) with mass parameter $m \geq 0$ and curvature coupling parameter ξ, i.e. φ satisfies

$$\mathrm{P}_{m,\xi}\varphi = (\Box_g + \xi R + m^2)\varphi = 0 \tag{4.1.1}$$

If φ is a field configuration, i.e. a smooth solution to the field equation (4.1.1), then the corresponding classical stress-energy tensor is a $\binom{0}{2}$ (co-)tensor field $T_{ab}^{(\varphi)}$ given by

$$\begin{aligned} T_{ab}^{(\varphi)}(x) =& (\nabla_a\varphi(x))(\nabla_b\varphi(x)) + \frac{1}{2}g_{ab}(x)(m^2\varphi^2(x) - (\nabla^c\varphi)(\nabla_c\varphi)(x)) \\ &+ \xi(g_{ab}(x)\nabla^c\nabla_c - \nabla_a\nabla_b - G_{ab}(x))\varphi^2(x)\,, \quad x \in M \end{aligned} \tag{4.1.2}$$

where $G_{ab} = R_{ab} - \frac{1}{2} g_{ab} R$ is the Einstein tensor.

Now let ϕ be the quantized linear scalar field on (M, g), corresponding to the choice of parameters m and ξ. The stress energy tensor for this (quantum) field will be obtained by correspondence from the stress-energy tensor of the classical field with the products of the field φ and its derivatives replaced by the corresponding, covariant Wick products from section 2.1.2. Again we even want to have expectation values at points $x \in M$ which exist in states of sufficient regularity like Hadamard states. For those from (2.1.5) we get:

$$\omega(:\phi \nabla_a \phi:_{\text{SHP}}(x)) = \left[\nabla_{a'} \mathscr{W}^{\text{SHP}}_{\omega,k}\right]_{x=x'} \tag{4.1.3}$$

$$\omega(:\phi \nabla_a \nabla_b \phi:_{\text{SHP}}(x)) = \left[\nabla_{a'} \nabla_{b'} \mathscr{W}^{\text{SHP}}_{\omega,k}\right]_{x=x'} \tag{4.1.4}$$

$$\omega(:(\nabla_a \phi)(\nabla_b \phi):_{\text{SHP}}(x)) = \left[\nabla_a \nabla_{b'} \mathscr{W}^{\text{SHP}}_{\omega,k}\right]_{x=x'} \tag{4.1.5}$$

with $k \geq 2$, $x \in M$. (Note again that a and a' are identified upon taking the coincidence limit $x = x'$.) Due to the symmetry of $\mathscr{W}^{\text{SHP}}_{W,\omega} k$, one can easily check that the following Leibniz rule is fulfilled for SHP Wick-products involving derivatives:

$$\omega(\nabla_a(:\phi^2:_{\text{SHP}}(x))) = 2\omega(:\phi \nabla_a \phi:_{\text{SHP}}(x)) \tag{4.1.6}$$

$$\omega(\nabla_a(:\phi \nabla_b \phi:_{\text{SHP}}(x))) = \omega(:(\nabla_a \phi)(\nabla_b \phi):_{\text{SHP}}(x)) + \omega(:\phi \nabla_a \nabla_b \phi:_{\text{SHP}}(x))\,. \tag{4.1.7}$$

The renormalized expectation value of the stress-energy is then obtained by replacing the classical expressions $\varphi^2(x)$, $(\nabla_a \varphi(x))(\nabla_b \varphi(x))$, and so on, by $\omega(:\phi^2:_{\text{SHP}}(x))$, $\omega(:(\nabla_a \phi)(\nabla_b \phi):_{\text{SHP}}(x))$, etc. Using also the Leibniz rule for SHP Wick products, this leads to

$$\begin{aligned}
\omega(T^{\text{SHP}}_{ab}(x)) = &- \omega(:\phi \nabla_a \nabla_b \phi:_{\text{SHP}}(x)) + \frac{1}{4}\omega(\nabla_a \nabla_b :\phi^2:_{\text{SHP}}(x)) \\
&+ \left(\frac{1}{4} - \xi\right) \omega\left(\nabla_a \nabla_b :\phi^2:_{\text{SHP}}(x) - g_{ab}(x) \nabla^c \nabla_c :\phi^2:_{\text{SHP}}(x)\right) \\
&+ \frac{1}{2} g_{ab}(x) \omega\left(:\phi \nabla^c \nabla_c \phi:_{\text{SHP}}(x) + m^2 :\phi^2:_{\text{SHP}}(x)\right) \\
&- \xi G_{ab}(x) \omega(:\phi^2:_{\text{SHP}}(x))\,.
\end{aligned}$$

This expression, however, has the defect of a non-vanishing divergence. The way to cope with this problem, following Wald [Wal78, Wal94], is like this: It can be shown that $\nabla^a \omega(T^{\text{SHP}}_{ab}(x)) = \nabla_b Q(x)$, where (apart from a free constant which can be set to a preferred value depending on the mass parameter m) Q is a function which is determined by the local geometry of (M, g); in particular, Q is independent of the state ω. One may therefore subtract the term $Q(x) g_{ab}(x)$ from $\omega(T^{\text{SHP}}_{ab}(x))$ to make the resulting quantity have vanishing divergence. There remains an ambiguity in that one may still add other $\binom{0}{2}$ (co-)tensor fields C_{ab} which are determined by the local geometry of (M, g) and have vanishing divergence. We take here the same view as put forward in [FS07], namely that the specification of C_{ab} is a further datum of the underlying quantum field ϕ on (M, g), in addition to the parameters m and ξ. An alternative method has been proposed by

Moretti [Mor03], which we won't follow here mainly because we would like to maintain close contact to other works on quantum energy inequalities. This understood, we finally define the renormalized expectation value of the stress energy tensor in some Hadamard state ω of the linear scalar field ϕ on (M, g) as

$$\omega(T_{ab}^{\text{ren}}(x)) = \omega(T_{ab}^{\text{SHP}}) - Q(x)g_{ab}(x) + C_{ab}(x)\,, \quad x \in M\,. \tag{4.1.8}$$

Next, observe that for each state ω of ϕ with two-point function of Hadamard form,

$$\begin{aligned} F(x) =&\omega(:\!\phi(\nabla^a\nabla_a + m^2 + \xi R)\phi\!:_{\text{SHP}}(x)) \\ =&\omega(:\!\phi(\nabla^a\nabla_a\phi)\!:_{\text{SHP}}(x)) + (m^2 + \xi R(x))\omega(:\!\phi^2\!:_{\text{SHP}}(x)) \end{aligned}$$

is a continuous function of $x \in M$, independent of the state ω, entirely determined by the local geometry of (M, g) and the parameters m and ξ of ϕ. To see this, note that

$$\omega(:\!\phi(\nabla^a\nabla_a + m^2 + \xi R)\phi\!:_{\text{SHP}}(x)) = \left[(\nabla^{a'}\nabla_{a'} + m^2 + \xi R)\mathscr{W}_{\omega,k}^{\text{SHP}}\right]_{x=x'}\,.$$

On the other hand, by definition $\mathscr{W}_{\omega,k}^{\text{SHP}} = \mathscr{W}_2^{\omega} - \mathcal{G}_k^{\text{SHP}}$ and since $\mathscr{W}_2^{\omega}$ is a bi-solution of the Klein-Gordon equation in the sense of distributions, i.e. $\mathscr{W}_2^{\omega}(f, (\nabla^b\nabla_b + m^2 + \xi R)h) = 0$, it follows that $(\nabla^{a'}\nabla_{a'} + m^2 + \xi R)\mathscr{W}_{\omega,k}^{\text{SHP}}$ is independent of ω; furthermore as we will see more explicitly in section 5.1.1, $(\nabla^{a'}\nabla_{a'} + m^2 + \xi R)\mathcal{G}_k^{\text{SHP}}$ is a continuous function on its domain of definition and thus can be restricted to the diagonal $x = x'$. In consequence, $F(x)$ is state-independent, continuous in x, and actually it is determined by the local geometry of (M, g) since so is $\mathcal{G}_k$ (by the Hadamard recursion relations) [1].

4.2 Quantum Weak Energy Inequality

Using the Leibniz rule, we can rewrite the expression for $\omega(T_{ab}^{\text{ren}})$ as follows:

$$\begin{aligned} \omega(T_{ab}^{\text{ren}}(x)) =&\omega(-:\!\phi\nabla_a\nabla_b\phi\!:_{\text{SHP}}(x)) + \frac{1}{4}\omega\left(\nabla_a\nabla_b :\!\phi^2\!:_{\text{SHP}}(x)\right) \\ &+ \left(\frac{1}{4} - \xi\right)\omega(\nabla_a\nabla_b :\!\phi^2\!:_{\text{SHP}}(x)) \\ &+ (4\xi - 1)\left(\omega(-:\!\phi\nabla^c\nabla_c\phi\!:_{\text{SHP}}(x)) + \frac{1}{4}\omega(\nabla^c\nabla_c :\!\phi^2\!:_{\text{SHP}}(x))\right)g_{ab} \\ &+ \left(\left((1 - 4\xi)(m^2 + \xi R) - \frac{1}{2}\xi R\right)g_{ab} - \xi G_{ab}\right)\omega(:\!\phi^2\!:_{\text{SHP}}(x)) \\ &+ \left(12\xi - \frac{5}{2}\right)Q(x)g_{ab}(x) + C_{ab}(x) \end{aligned} \tag{4.2.1}$$

By (3.3.3) and once more the Leibniz rule, $\varepsilon_{ab}^{\omega}$ can also be expressed as

$$\varepsilon_{ab}^{\omega}(x) = \omega(-:\!\phi\nabla_a\nabla_b\phi\!:_{\text{SHP}}(x)) + \frac{1}{4}\omega(\nabla_a\nabla_b :\!\phi^2\!:_{\text{SHP}}(x))$$

[1] This term will reappear several times in chapter 5, where an extended version of this property will be used to reduce orders of derivatives and there also an explicit expression for it on Robertson Walker spacetimes is given.

Thus, if ω is an $S_x^{(2)}$-thermal state of ϕ, we obtain

$$\begin{aligned}\omega(T_{ab}^{\text{ren}}(x)) =& \varepsilon_{ab}^{\omega}(x) + (4\xi - 1)g_{ab}(x)\varepsilon_{c}^{\omega c}(x)\\ &+ (\frac{1}{4} - \xi)\nabla_a\nabla_b\vartheta^{\omega}(x) + (g_{ab}(x)\psi(x) - \xi R_{ab}(x))\vartheta^{\omega}(x)\\ &+ (12\xi - 5/2)Q(x)g_{ab}(x) + C_{ab}(x)\,,\end{aligned} \tag{4.2.2}$$

where we use the abbreviation

$$\psi(x) = (1 - 4\xi)(m^2 + \xi R(x))\,. \tag{4.2.3}$$

To derive bounds from this expression, we need estimates of the functions $\varepsilon^o_{\mu\nu}$ that on LTE-states by definition is related to $\varepsilon^{\omega}_{ab}(x)$ at points x where ω is locally $S_x^{(2)}$-thermal. The following lemma gives the required estimates for the functions χ_{tt} and χ_{xx}, in terms of which it is expressed by equation (3.3.9),(3.3.10). Furthermore it gives the asymptotics for those functions and in addition for the function χ, related to ϑ^o by equation (3.3.8).

Lemma 4.1. *Let $\beta > 0$ and $e = (e_0, \dots e_3)$ an orthonormal basis of Minkowski spacetime. Then for $\varepsilon^o_{\mu\nu} = -\frac{1}{4}\omega^{\beta e_0}(\eth_{\mu\nu} :\phi^2:_{\text{SHP}})$ and the functions $\chi(m\beta) := \beta^2\omega^{\beta e_0}(:\phi^2:_{\omega_\infty})$, $\chi_{tt}(m\beta) := -\frac{\beta^4}{4}\omega^{\beta e_0}(\eth_{00} :\phi^2:_{\omega_\infty})$ and $\chi_{xx}(m\beta) := -\frac{\beta^4}{4}\omega^{\beta e_0}(\eth_{11} :\phi^2:_{\omega_\infty})$ the following statements hold:*

a) For v a lightlike vector or a timelike unit vector (v^μ the components with respect to e), one has the bound

$$\frac{2\pi^2(v^0)^2}{45\beta^4} - v_\mu v^\mu \frac{c_{2,m}}{4} \geq v^\mu v^\nu \varepsilon^o_{\mu\nu} \geq \frac{(v^0)^2}{\beta^4}\chi_{tt}(m\beta) - v_\mu v^\mu \frac{c_{2,m}}{4}\,. \tag{4.2.4}$$

b) For $\xi \to \infty$ there holds

$$\lim_{\xi\to\infty} \chi(\xi) = \frac{1}{12} \tag{4.2.5}$$

$$\lim_{\xi\to\infty} \chi_{tt}(\xi) = \frac{\pi^2}{30} \tag{4.2.6}$$

$$\lim_{\xi\to\infty} \chi_{xx}(\xi) = \frac{\pi^2}{90}\,. \tag{4.2.7}$$

Proof. As already calculated in section 3.3, in the specific basis chosen $\varepsilon^o_{\mu\nu}$ is diagonal with the diagonal elements given by (3.3.9) and (3.3.10). Using the integral expressions (3.3.12) and (3.3.13), for $v^\mu v^\nu\varepsilon^o_{\mu\nu}(\beta)$ we end up with

$$v^\mu v^\nu \varepsilon^o_{\mu\nu} = \frac{1}{2\pi^2\beta^4}\int_{\mathbb{R}+} \frac{(v^0)^2(\rho^2 + m^2\beta^2) + \|\mathbf{v}\|^2\rho^2/3}{e^{\sqrt{\rho^2+m^2\beta^2}} - 1}\frac{\rho^2 \mathrm{d}\rho}{\sqrt{\rho^2 + m^2\beta^2}} + v^\mu v_\mu c_{2,m}$$

The upper bound is obtained by estimating $\|\mathbf{v}\|^2 \rho^2$ by $(v^0)^2(\rho^2 + m^2)$ using $v^0 \geq \|\mathbf{v}\|$; then using the fact that $x \mapsto \frac{x}{e^x - 1}$ is monotonically decreasing estimate

$$\frac{\sqrt{\rho^2 + m^2\beta^2}}{e^{\sqrt{\rho^2+\beta^2 m^2}}} \leq \frac{\rho}{e^\rho - 1}\,.$$

The value of the remaining integral is obtained from tables as $\frac{4}{3} \cdot \frac{\pi^2}{30}$ [Ste84, 23.2.7]; the lower bound is immediate.
For the limits in part b), we use that for fixed $\rho > 0$, the function $x \mapsto \frac{\sqrt{\rho^2+x^2}}{x} \frac{e^\rho - 1}{e^{\sqrt{\rho^2+x^2}}-1}$ is monotonously decreasing (for $x > 0$) and approaches one for $\xi \to 0$; this implies by monotone convergence (rewriting the integrands in the integrals defining χ, χ_{tt} and χ_{xx} as in equation (3.3.11)–(3.3.13)):

$$\lim_{\xi\to 0} \chi(\xi) = \frac{1}{2\pi^2} \int_{\mathbb{R}^+} \frac{\rho\, \mathrm{d}\rho}{e^\rho - 1} = \frac{1}{12} \tag{4.2.8}$$

$$\lim_{\xi\to 0} \chi_{\eta\eta}(\xi) = \frac{1}{2\pi^2} \int_{\mathbb{R}^+} \frac{\rho^3\, \mathrm{d}\rho}{e^\rho - 1} = \frac{\pi^2}{30} \tag{4.2.9}$$

$$\lim_{\xi\to 0} \chi_{xx}(\xi) = \frac{1}{3} \lim_{\xi\to 0} \chi_{\eta\eta}(\xi) = \frac{\pi^2}{90} \tag{4.2.10}$$

□

We now need to specify the class of states of bounded temperature, for which we will derive Quantum Energy Inequalities:

Definition 4.2. Let $\beta' > 0$, $x \in M$. Then we define $\mathcal{L}_{\beta'}(x)$ as the set of all $S_x^{(2)}$-thermal states ω of the linear scalar field on (M, g) fulfilling

$$\vartheta^\omega(x) \leq \frac{1}{(\beta')^2}\chi(m\beta') + c_{0,m}\,. \tag{4.2.11}$$

If $N \subset M$, we define $\mathcal{L}_{\beta'}(x)$ as the set of all $S_N^{(2)}$-thermal states so that (4.2.11) is fulfilled for all $x \in N$.

In other words, ω is in $\mathcal{L}_{\beta'}(x)$ if it is locally thermal at x with $1/\beta \leq 1/\beta'$. Now let N be an open subset of M, and let $\gamma : [\tau_0, \tau_1] \to N$, $\tau \mapsto \gamma(\tau)$ be a geodesic with affine parameter τ, and denote by $v^a = \dot{\gamma}^a$ the tangent vector field of γ. By the geodesic equation, it holds that

$$(v^a v^b \nabla_a \nabla_b \vartheta^\omega)(\gamma(\tau)) = \frac{\mathrm{d}^2}{\mathrm{d}\tau^2}\vartheta^\omega(\gamma(\tau))\,.$$

Consequently, we obtain for $\omega \in \mathcal{L}_{\beta'}(N)$ and $\eta \in C_0^2((\tau_0, \tau_1))$,

$$\begin{aligned} \left| \int \eta(\tau)(v^a v^b \nabla_a \nabla_b \vartheta^\omega)(\gamma(\tau))\mathrm{d}\tau \right| =& \left| \int \eta''(\tau)\vartheta^\omega(\gamma(\tau))\mathrm{d}\tau \right| \\ \leq& \|\eta''\|_{L^1} \left| \frac{1}{(\beta')^2}\chi(m\beta') + c_{0,m} \right|\,. \end{aligned} \tag{4.2.12}$$

Here, η'' is the second derivative of η.

With this definitions and results in place, we are now able to derive bounds on $v^a v^b \omega(T_{ab}^{\mathrm{ren}})$ for lightlike or timelike vectors v. We will treat lower bounds first.

Theorem 4.3. *Let ϕ be the quantized linear scalar field on (M, g), with parameters m, ξ and C_{ab}, and let ω be a state of ϕ having a two-point function of Hadamard type.*

a) Suppose that $\xi = 1/4$, and let v be a lightlike vector at $x \in M$, or a timelike vector at x with $v_a v^a = 1$. If ω is in $\mathcal{L}_{\beta'}(x)$, $\beta' > 0$, then

$$v^a v^b \omega(T_{ab}^{\mathrm{ren}}(x)) \geq q(x, v; \beta') \,, \tag{4.2.13}$$

where

$$\begin{aligned} q(x, v; \beta') = &- \frac{1}{4} \left| v^a v^b R_{ab}(x) \right| \left| \frac{1}{\beta'^2} \chi(m\beta') + c_{0,m} \right| \\ &+ \left(\frac{1}{2} Q(x) - \frac{1}{4} c_{2,m} \right) v_a v^a + v^a v^b C_{ab} \,. \end{aligned}$$

b) Let ξ be arbitrary, let $N \subset M$, and let $\gamma : [\tau_0, \tau_1] \to N$ be an affinely parametrized lightlike geodesic defined on a finite interval, with tangent vector field $v^a = \dot{\gamma}^a$. Suppose that η is in $C_0^2((\tau_0, \tau_1))$ with $\eta \geq 0$. If $\mathcal{L}_{\beta'}(N)$, there holds the bound

$$\int \eta(\tau) v^a v^b \omega(T_{ab}^{\mathrm{ren}}(\gamma(\tau))) \,\mathrm{d}\tau \geq q_0(\gamma, \eta; \beta') \,. \tag{4.2.14}$$

Here, writing

$$R_{[\gamma]} = \max_{\tau \in [\tau_0, \tau_1]} |\dot{\gamma}^a(\tau) \dot{\gamma}^b(\tau) R_{ab}(\gamma(\tau))| \,,$$

and defining $C_{[\gamma]}$ analogously, the bounding constant is given by

$$\begin{aligned} q_0(\gamma, \eta; \beta') = &- \left[|\xi| R_{[\gamma]} \left| \frac{1}{\beta'^2} \chi(m\beta') + c_{0,m} \right| + C_{[\gamma]} \right] ||\eta||_{L^1} \\ &- \left| \tfrac{1}{4} - \xi \right| \cdot \left| \frac{1}{\beta'^2} \chi(m\beta') + c_{0,m} \right| \cdot ||\eta''||_{L^1} \end{aligned}$$

c) Let ξ be arbitrary, let $N \subset M$, and let $\gamma : [\tau_0, \tau_1] \to N$ be an affinely parametrized timelike geodesic with tangent vector field $v^a = \dot{\gamma}^a$, so that $v^a v_a = 1$. Assume that η is in $C_0^2((\tau_0, \tau_1))$ with $\eta \geq 0$. If $\omega \in \mathcal{L}_{\beta'}(N)$, there holds the bound

$$\int \eta(\tau) v^a v^b \omega(T_{ab}^{\mathrm{ren}}(\gamma(\tau))) \,\mathrm{d}\tau \geq q_1(\gamma, \eta; \beta') \,, \tag{4.2.15}$$

where, using the notation $\psi_{[\gamma]} = \max_{\tau \in [\tau_0, \tau_1]} |\psi(\gamma(\tau))|$, and defining $Q_{[\gamma]}$ similarly, the bounding constant is given by

$$\begin{aligned} q_1(\gamma, \eta; \beta') = &- \left| \tfrac{1}{4} - \xi \right| \cdot \left| \frac{1}{\beta'^2} \chi(m\beta') + c_{0,m} \right| \cdot ||\eta''||_{L^1} \\ &- (\psi_{[\gamma]} + |\xi| R_{[\gamma]}) \cdot \left| \frac{1}{\beta'^2} \chi(m\beta') + c_{0,m} \right| \cdot ||\eta||_{L^1} \\ &- \left(|12\xi - \tfrac{5}{2}| Q_{[\gamma]} + |4\xi - 1| |c_{2,m}| + C_{[\gamma]} + \frac{|c_{2,m}|}{4} \right) \cdot ||\eta||_{L^1} \,. \end{aligned}$$

Proof. The proof of the statement consists in using the LTE-condition (3.3.6), (3.3.6) which (together with the definitions (3.3.15), (3.3.16)) relates the term $\varepsilon^{\omega}_{ab}(x)$ to $\varepsilon^{o}_{\mu\nu}$ and then inserting the estimates of Lemma 4.1 and discarding manifestly positive terms, in combination with estimate (4.2.12) for the average of the second derivatives of ϑ^{ω} along the geodesic. The term involving second derivatives of ϑ^{ω} doesn't occur for $\xi = 1/4$, which makes it possible to give a pointwise lower bound in this case. □

The central assertion of Theorem 4.3 is that the lower bound of the energy density averaged along a causal geodesic depends only on the temperatures an LTE state attains on the geodesic, and is otherwise state-independent. The bound worsens (shifts towards the left on the real axis) as the temperature increases, i.e. with increasing $1/\beta'$. This is related to the question of the sharpness of the obtained bounds. The point to notice here is that they were obtained by bounding the term $\varepsilon^{\omega}_{ab}v^a v^b$ from below by the temperature independent term $-v^a v_a|c_2|/4$. However, $\varepsilon^{\omega}_{ab}v^a v^b$ grows with temperature as can be seen from (4.2.4) and the growth is (for high temperatures) with the fourth power of temperature. As the ϑ^{ω} dependent term, which is responsible for the worsening of the bounds, grows (asymptotically) with the square of the temperature, it will be compensated for sufficiently high temperatures by the dropped term. By a more careful investigation one could therefore hope to obtain a lower bound where the temperature dependence is replaced by a dependence on the spacetime geometry and γ. Finally it should also be noted that the bounds are local covariant.

For upper bounds on the averaged energy density of LTE states, an additional state-dependence shows up: The bounds depend also on the tetrad e appearing in the condition of $S^{(2)}_x$-thermality, Def. 3.4. In this sense, the lower bounds on the averaged energy densities of LTE states are stronger than the upper bounds. This is similar to what holds for averages of energy densities for arbitrary Hadamard states of the linear scalar field [FO08].

Let $x \in M$, and let $e = (e_0, \dots, e_3)$ be an orthonormal tetrad at x with e_0 timelike and future-pointing. We define $\mathcal{L}_{\beta'}(x, e)$ as the set of all states ω in $\mathcal{L}_{\beta'}(x)$ where the $S^{(2)}_x$-thermality conditions (3.3.6) and (3.3.7) hold with respect to the given tetrad. Similarly, let N be a subset of M, and let $N \ni x \mapsto e(x)$, $e(x) = (e_0(x), \dots, e_3(x))$ be a C^0 field of orthonormal tetrads over N, with $e_0(x)$ timelike and future-pointing for all x. Then we define $\mathcal{L}_{\beta'}(N, e)$ as the set of all states ω in $\mathcal{L}_{\beta'}(N)$ such that, for each $x \in N$, ω satisfies the $S^{(2)}_x$-thermality conditions (3.3.6) and (3.3.7) with respect to $e = e(x)$. With these conventions, again using the LTE-condition and the above estimates, we obtain the following upper bounds on (averaged) energy densities.

Theorem 4.4. *Let ϕ be the quantized linear scalar field on (M, g), with parameters m, ξ and C_{ab}, and let ω be a state of ϕ having two-point function of Hadamard form.*

a) Suppose that $\xi = 1/4$, let v be a lightlike vector at $x \in M$, or a timelike vector at x with $v_a v^a = 1$, If ω is in $\mathcal{L}_{\beta'}(x, e)$, $\beta' > 0$, then

$$p(v, x; \beta', e) \geq v^a v^b \omega(T^{\mathrm{ren}}_{ab}(x)) \,, \tag{4.2.16}$$

where

$$p(v,x;\beta',e) = \frac{2\pi^2 (v^0)^2}{45\beta'^4} + \frac{1}{2}\left|v^a v^b R_{ab}\right| \left|\frac{1}{\beta'^2}\chi(m\beta') + c_{0,m}\right| + q(x,v;\beta')$$

with $v^0 = v_a(e_0)^a$.

b) *Let* ξ *be arbitrary,* $N \subset M$*, and let* $\gamma : [\tau_0, \tau_1] \to N$ *be an affinely parametrized lightlike geodesic defined on a finite interval, with tangent vector field* $v^a = \dot\gamma^a$*. Suppose that* η *is in* $C_0^2((\tau_0,\tau_1))$ *with* $\eta \geq 0$*. If* ω *is in* $\mathcal{L}_{\beta'}(N,e)$*, then*

$$p_0(\gamma,\eta;\beta',e) \geq \int \eta(\tau) v^a v^b \omega(T^{\mathrm{ren}}_{ab}(\gamma(\tau)))\mathrm{d}\tau\,, \tag{4.2.17}$$

where

$$p_0(\gamma,\eta;\beta',e) = \frac{2\pi^2}{45(\beta')^4}(v^0_{[\gamma]})^2 ||\eta||_{L^1} + |q_0(\gamma,\beta';\eta)|$$

with $v^0_{[\gamma]} = \max_{\tau\in[\tau_0,\tau_1]} \dot\gamma_a(\tau) e_0^a(\gamma(\tau))$.

4.3 Averaged Null Energy Condition (ANEC)

In this section we derive the averaged null energy condition (ANEC) for $S_N^{(2)}$-thermal states of the quantized linear scalar field ϕ on a globally hyperbolic spacetime (M,g).

The ANEC on a state ω of ϕ demands that

$$\liminf_{\tau_\pm\to\pm\infty} \int_{\tau_-}^{\tau_+} v^a v^b \omega(T^{\mathrm{ren}}_{ab}(\gamma(\tau)))\,\mathrm{d}\tau \geq 0 \tag{4.3.1}$$

for all complete lightlike geodesics γ in M with affine parameter τ and tangent $v^a = \dot\gamma^a$. If this condition holds, and if (M,g) together with ϕ and ω are a solution to the semiclassical Einstein equation in the form

$$G_{ab}(x) = 8\pi\omega(T^{\mathrm{ren}}_{ab}(x))\,, \quad x \in M\,, \tag{4.3.2}$$

then this implies that

$$\liminf_{\tau_\pm\to\pm\infty} \int_{\tau_-}^{\tau_+} v^a v^b G_{ab}(\gamma(\tau))\,\mathrm{d}\tau \geq 0 \tag{4.3.3}$$

for all complete lightlike geodesics γ. (We address the issue for the semiclassical Einstein equations with an additional contribution by a classical stress-energy tensor below.) It has been shown that this weaker form of the usual pointwise null energy condition, which demands that $\ell^a\ell^b G_{ab}(x) \geq 0$ for all lightlike vectors ℓ^a at each $x \in M$, is still sufficient to reach the same conclusions with respect to singularity theorems as obtained from the pointwise null energy condition, i.e. that congruences of geodesics will focus with expansion diverging to $-\infty$ at finite affine geodesic parameter [HE73]. The validity of (4.3.1) is therefore of importance for the properties of the spacetime structure of solutions to the semiclassical Einstein equations.

It has been argued in [WY91] that condition (4.3.1) may be replaced by the following condition:
$$\liminf_{\lambda\to 0}\int_{-\infty}^{\infty}\eta_\lambda(\tau)v^a v^b\omega(T^{\rm ren}_{ab}(\gamma(\tau)))\,{\rm d}\tau \geq 0 \tag{4.3.4}$$
for any $\eta \in C_0^2(\mathbb{R})$, $\eta \geq 0$, with $\eta(0) > 0$ and $\eta_\lambda(\tau) = \eta(\lambda\tau)$ for $\lambda > 0$. More precisely, in [WY91] it has been shown that (4.3.4) and (4.3.2) imply that the expansion of a congruence of lightlike geodesics around γ becomes singular along γ (in the sense of diverging to $-\infty$ at a finite value of the affine parameter) unless it vanishes identically on γ. (In [WY91] this argument is given for half-line geodesics, but it carries over to the case at hand as will be shown in our Appendix A.3)

Now let $\omega \in S_N^{(2)}$, and let γ be a complete lightlike geodesic in $N \subset M$ with affine parameter τ and tangent $v^a = \dot\gamma^a$. Then, from (4.2.2),
$$v^a v^b\omega(T^{\rm ren}_{ab}) = v^a v^b\varepsilon^\omega_{ab} + \left(\frac{1}{4}-\xi\right)v^a v^b\nabla_a\nabla_b\vartheta^\omega - \xi v^a v^b G_{ab}\vartheta^\omega + v^a v^b C_{ab} \tag{4.3.5}$$
holds along γ. Thus, positivity properties of the (integrated) energy density $v^a v^b\omega(T^{\rm ren}_{ab})$ depend also on the behaviour of G_{ab} and C_{ab}. The sign of the term involving G_{ab} is not known. To circumvent this difficulty, we assume that the underlying spacetime (M, g) together with ϕ and ω are solutions to the semiclassical Einstein equations (4.3.2), since it is this situation in which the ANEC is applied to deduce (4.3.3) and the ensuing statements about focusing of lightlike geodesics. Supposing that (M, g) together with ϕ and ω are solutions to the semiclassical Einstein equations, and also that ω is an $S_N^{(2)}$-thermal state, we obtain upon combination of (4.3.2) and (4.3.5) the equation
$$v^a v^b[G_{ab}(1+8\pi\xi\vartheta^\omega - 8\pi C_{ab}] = 8\pi v^a v^b\left(\varepsilon^\omega_{ab} + \left(\frac{1}{4}-\xi\right)\nabla_a\nabla_b\vartheta^\omega\right) \tag{4.3.6}$$
on N. In order to draw further conclusions, one must specify C_{ab}. We recall that C_{ab} is a datum of the linear quantum field ϕ, a priori only restricted by the requirement that $T^{\rm ren}_{ab}$ be a local covariant quantum field and divergence-free, thus C_{ab} should be locally constructed from the spacetime metric. Following Wald [Wal94], one can make the assumption that C_{ab} have canonical dimension, which leads to the form
$$C_{ab} = Ag_{ab} + BG_{ab} + \Gamma\frac{\delta}{\delta g^{ab}}S_1(g) + D\frac{\delta}{\delta g^{ab}}S_2(g)\,, \tag{4.3.7}$$
where $S_1(g) = \int_M R^2{\rm d}\mu_g$, $S_2(g) = \int_M R_{ab}R^{ab}{\rm d}\mu_g$, and $\delta/\delta g^{ab}$ means functional differentiation with respect to the metric, with constants A, B, Γ, D as remaining renormalization ambiguity for the quantum field ϕ (see [Wal94] for additional discussion). For the rest of our discussion, we will simplify matters by assuming $\Gamma, D = 0$.

Making these assumptions and observing that hence, $v^a v^b C_{ab} = Bv^a v^b G_{ab}$ for all lightlike vectors v^a, (4.3.6) assumes on N the form
$$v^a v^b G_{ab}(1+8\pi(\xi\vartheta^\omega - B)) = 8\pi v^a v^b\left(\varepsilon^\omega_{ab} + \left(\frac{1}{4}-\xi\right)\nabla_a\nabla_b\vartheta^\omega\right)\,. \tag{4.3.8}$$

The constant B is still free, and one may now try to choose B in such a way that (4.3.8) entails the ANEC for all lightlike geodesics in $N \subset M$ and an as large as possible class of $S_N^{(2)}$-thermal states ω. We will show that this is possible with different conditions on B for the cases $\xi = 1/4, 0 < \xi < 1/4, \xi = 0$.

Theorem 4.5. *Let (M, g) be a globally hyperbolic spacetime, let ϕ be the quantized linear scalar field on (M, g), with parameters m, ξ, C_{ab}, where $C_{ab} = Ag_{ab} + BR_{ab}$, with real constants A, B.*

Suppose further that ω is a quasifree Hadamard state for ϕ, that $\omega \in S_N^{(2)}$ for $N \subset M$, and that (M, g) together with ϕ and ω provides a solution to the semiclassical Einstein equation (4.3.2).

Let γ be a complete lightlike geodesic in N with affine parameter τ and tangent $v^a = \dot{\gamma}^a$, and let $\eta \in C_0^2(\mathbb{R})$, $\eta \geq 0$. Then

$$\lim_{\lambda \to 0} \int_{-\infty}^{\infty} \eta(\lambda\tau) v^a v^b \omega(T_{ab}^{\mathrm{ren}}(\gamma(\tau)))\, \mathrm{d}\tau \geq 0 \tag{4.3.9}$$

holds if any of the following groups of conditions is assumed:

1.) $\xi = 1/4$, $B < 1 + 2\pi c_{0,m}$. *In this case one even has*

$$v^a v^b \omega(T_{ab}^{\mathrm{ren}}(x)) \geq 0$$

pointwise for all $x \in M$ and all lightlike vectors v^a at x.

2.) $0 < \xi < 1/4$, $B \leq \xi c_{0,m} + 1/(8\pi)$,

$$\lambda \ln(\vartheta^\omega(\gamma(\tau/\lambda))) \to 0 \quad \textit{as} \quad \lambda \to 0 \quad \textit{for almost all} \quad \tau\,, \tag{4.3.10}$$

$$\int_s^r \lambda |\ln(\vartheta^\omega(\gamma(\tau/\lambda)))|\, \mathrm{d}\tau < k < \infty \quad \textit{for small } \lambda \quad \textit{and all } s < r \in \mathbb{R}\,. \tag{4.3.11}$$

3.) $\xi = 0$, $B < 1/8\pi$,

$$\lambda \vartheta^\omega(\gamma(\tau/\lambda)) \to 0 \quad \textit{as} \quad \lambda \to 0 \quad \textit{for almost all} \quad \tau\,, \tag{4.3.12}$$

$$\int_s^r \lambda \vartheta^\omega(\gamma(\tau/\lambda)) \mathrm{d}\tau < K < \infty \quad \textit{for small } \lambda \quad \textit{and all } s < r \in \mathbb{R}\,. \tag{4.3.13}$$

Remark 4.6. (a) If, instead of (4.3.2), the semiclassical Einstein equations are assumed to hold in the form

$$G_{ab}(x) = 8\pi(T_{ab}^{\mathrm{class}}(x) + \omega(T_{ab}^{\mathrm{ren}}(x)))$$

with a stress-energy tensor T_{ab}^{class} for classical, macroscopic matter distribution, and if it is assumed that this stress-energy tensor fulfills the pointwise null energy condition $\ell^a \ell^b T_{ab}^{\mathrm{class}}(x) \geq 0$ for all lightlike vectors ℓ^a at each point $x \in M$, then the statements of the theorem remain valid with $T_{ab}^{\mathrm{class}} + \omega(T_{ab}^{\mathrm{ren}})$ in place of $\omega(T_{ab}^{\mathrm{ren}})$.

(b) Conditions (4.3.10) and (4.3.11) say, roughly speaking, that $\vartheta^\omega(\gamma(\tau))$ should not grow faster than $\mathrm{e}^{|\tau|^{(1-\epsilon)}}$ for $|\tau| \to \infty$, while (4.3.12) and (4.3.13) say that $\vartheta^\omega(\gamma(\tau))$ should not grow faster than $|\tau|^{1-\epsilon}$ as $|\tau| \to \infty$. Since

$$\vartheta^\omega(\gamma(\tau)) = (\beta(\gamma(\tau))^{-2}\chi(m\beta(\gamma(\tau))) + c_{0,m}$$

and since

$$\chi(m\beta) \to \frac{1}{2\pi^2}\int_0^\infty \frac{\rho}{\mathrm{e}^\rho}\,\mathrm{d}\rho \quad \text{for} \quad \beta \to 0\,,$$

this means that the growth of the temperature $1/\beta(\gamma(\tau))$ at $\gamma(\tau)$ appearing in Def. 3.4 of $S^{(2)}_{\gamma(\tau)}$-thermality ω should not exceed $\mathrm{e}^{|\tau|^{(1-\epsilon)/2}}$ and $|\tau|^{(1-\epsilon)/2}$ as $|\tau| \to \infty$, respectively.

Proof of Thm 4.5.

1.) If $\xi = 1/4$, then (4.3.8) assumes the form

$$v^a v^b G_{ab}(1 + 8\pi(\vartheta^\omega/4 - B)) = 8\pi v^a v^b \varepsilon^\omega_{ab}\,. \tag{4.3.14}$$

If $B < 1 + 2\pi c_{0,m}$, then the factor $1 + 8\pi(\vartheta^\omega/4 - B)$ is strictly positive, as is the right hand side of (4.3.14). This equality holds pointwise at all $x \in M$ and for all lightlike vectors v^a, thus proving, in combination with the assumed property (4.3.2), the statement of the theorem.

2.) For $0 < \xi < 1/4, B = \xi c_{0,m} + 1/(8\pi) - \xi c$, where $c \geq 0$, (4.3.8) takes the form

$$v^a v^b G_{ab}(8\pi\xi(\vartheta^\omega - c_{0,m} + c)) = 8\pi v^a v^b \varepsilon^\omega_{ab} + 8\pi(1/4 - \xi)v^a v^b \nabla_a \nabla_b \vartheta^\omega\,. \tag{4.3.15}$$

Observing that $v^a v^b \nabla_a \nabla_b c_{0,m} = 0$, the last equation is turned into

$$v^a v^b G_{ab} = \frac{v^a v^b \varepsilon^\omega_{ab}}{\xi(\vartheta^\omega - c_{0,m} + c)} + \frac{(1/4 - \xi)v^a v^b \nabla_a \nabla_b(\vartheta^\omega - c_{0,m})}{\xi(\vartheta^\omega - c_{0,m} + c)}\,, \tag{4.3.16}$$

where it was used that $\vartheta^\omega - c_{0,m} + c > 0$. The first term on the right hand side of (4.3.16) is positive. Upon integration against a non-negative C^2_0 weighting function η along the geodesic γ we obtain, using the abbreviation

$$u(\tau) = \vartheta^\omega(\gamma(\tau)) - c_{0,m}\,,$$

the inequality

$$\int \eta(\tau)(v^a v^b G_{ab})(\gamma(\tau))\,\mathrm{d}\tau \geq \frac{1/4 - \xi}{\xi}\int \eta(\tau)\frac{u''(\tau)}{u(\tau) + c}\,\mathrm{d}\tau\,.$$

By partial integration,

$$\int \eta(\tau)\frac{u''(\tau)}{u(\tau) + c}\,\mathrm{d}\tau = \int \eta(\tau)\left(\frac{u'(\tau)}{u(\tau) + c}\right)^2\mathrm{d}\tau + \int \ln(u(\tau) + c)\eta''(\tau)\,\mathrm{d}\tau\,.$$

Thus, since the first integral on the right hand side is non-negative, $(1/4-\xi)/\xi > 0$ for the ξ considered and using the monotonicity of the logarithm together with $c \geq 0$,

$$\int \eta(\lambda\tau)(v^a v^b G_{ab})(\gamma(\tau))\,\mathrm{d}\tau \geq \frac{1/4-\xi}{\xi} \int \lambda \ln(u(\tau/\lambda))\eta''(\tau)\,\mathrm{d}\tau\,,$$

and owing to assumptions (4.3.10) and (4.3.11), the expression on the right hand side converges to 0 as $\lambda \to 0$. Equation (4.3.9) is then again implied by the assumed property (4.3.2).

3.) If $\xi = 0$, equation (4.3.8) turns into

$$v^a v^b G_{ab}(1-8\pi B) = 8\pi v^a v^b \varepsilon^{\omega}_{ab} + \frac{1}{4} v^a v^b \nabla_a \nabla_b \vartheta^{\omega}\,, \tag{4.3.17}$$

and by the condition on B, the factor $1-8\pi B$ is strictly positive. Observing again positivity of $8\pi v^a v^b \varepsilon^{\omega}_{ab}$, upon integration against a non-negative C^2_0 weighting function η along γ one obtains

$$\int \eta(\lambda\tau) v^a v^b G_{ab}(\gamma(\tau))\,\mathrm{d}\tau \geq \frac{1}{4(1-8\pi B)} \int \lambda u(\tau/\lambda)\eta''(\tau)\,\mathrm{d}\tau$$

and the right hand side converges to 0 as $\lambda \to 0$ by assumptions (4.3.12) and (4.3.13). Again (4.3.9) is deduced from the assumed validity of (4.3.2).

□

4.4 Generalized Local Thermal Equilibrium States

The notion of LTE states in [BOR02], and the related definition of $S^{(2)}_x$-thermal states, is actually more general than the definition given in section 3.3. In [BOR02] the possibility was considered that an LTE state ω coincides on S_x-observables not necessarily with a thermal equilibrium state at sharp temperature in a certain Lorentz frame, but with a mixture of such states.

In our setting, where we work with the linear scalar field, this corresponds to a modification of definition 3.4 as follows: As discussed in section 3.1, the quasifree thermal equilibrium states for different (inverse temperatures) and different rest-frames can be labeled as $\omega^{\boldsymbol{\beta}}$, where the vectors $\boldsymbol{\beta}$ take values in V^+, the set of future-directed timelike vectors in Minkowski spacetime.

Let (M,g) be a globally hyperbolic spacetime, let $V^+_x \subset T_xM$ be the set of future-directed timelike vectors at $x \in M$, and let ρ_x be a Borel measure on V^+_x supported on a compact subset $B_x \subset V^+_x$, with $\int_{B_x} d\rho_x(\boldsymbol{\beta}) = 1$. Then we say that a Hadamard state ω of the linear scalar field ϕ on (M,g) is a *generalized $S^{(2)}_x$-thermal state* if

$$\begin{aligned}
\omega(:\!\phi^2\!:_{\text{SHP}}(x)) &= \int_{B_x} \omega^{\boldsymbol{\beta}}(:\!{\phi_o}^2\!:_{\omega_\infty}(x_o))\mathrm{d}\rho_x(\boldsymbol{\beta}) + c_{0,m}\,,\\
v^a w^b \omega(\eth_{ab}:\!\phi^2\!:_{\text{SHP}}(x)) &= v^\mu w^\nu \int_{B_x} \omega^{\boldsymbol{\beta}}_o(\eth_{\mu\nu}:\!{\phi_o}^2\!:_{\omega_\infty}(x_o))\mathrm{d}\rho(\boldsymbol{\beta}) + c_{2,m} v^\mu w^\nu \eta_{\mu\nu}
\end{aligned}$$

holds for all (spacelike) vectors $v, w \in T_xM$ for some $x_o \in M_o$. Making further the assumption that $F \mapsto \int_M \int_{B_x} F(x, \boldsymbol{\beta}) \mathrm{d}\rho_x(\boldsymbol{\beta}) \mathrm{d}\mu_g(x)$, $F \in C_0^\infty(TM, \mathbb{C})$ is a distribution (on the manifold TM), such that $x \mapsto \int_{B_x} F(x, \boldsymbol{\beta}) \mathrm{d}\rho_x(\boldsymbol{\beta})$ is C^2, one can define generalized $S_N^{(2)}$-thermal states in analogy to the definition of $S_N^{(2)}$-thermal states in section 3.3.

With these conventions and assumptions, the results of the theorems 4.3, 4.4 and 4.5 extend to generalized $S_N^{(2)}$-thermal states, under identical assumptions, except that the bounds have to be corrected for the ρ_x-integrations.

5 On the existence of locally thermal states

After we motivated and formulated our condition of local thermality for states in chapter 3 and investigated the possibility to derive Quantum Energy Inequalities for states satisfying this condition in chapter 4, we now have to turn to the question of existence of such states. Even though we only consider the same, weak version of local thermality as in the chapter on Quantum Energy Inequalities, it seems rather hopeless to construct states satisfying this condition on sets of nonzero dimension in general (globally hyperbolic) spacetimes. The main problem is that the LTE condition, the equations of motion and the positivity condition are interlocked in a rather complicated way and while an investigation of the first two conditions is most easily done using the two-point functions directly (i.e. in "real space"), the positivity condition is most easily investigated by using representations in which it is "diagonalized" (on Minkowski spacetime by using Fourier transforms) and for the massive, scalar field even on Minkowski spacetime this makes the construction of nontrivial states a difficult thing [Hüb05].

In general spacetimes there is no equivalent of the Fourier transform available, so one would have to attack the positivity questions entirely without it; for the cosmological spacetimes considered here, the situation is however better insofar, as there is still a partial Fourier transform available, namely the Fourier transform on the spatial slices of constant, conformal time. The construction presented towards the end of this chapter will make heavy use of this and as a result lead to states on the *whole* spacetime, i.e. the positivity condition is fully under control. There is however a price to pay for this; the (homogeneous and isotropic) states defined in such a way are only (strictly) $S_x^{(2)}$-thermal on an initial Cauchy surface. While this of course less than one really desires, it is nevertheless some real advance in the quest for physically meaningful states in quantum field theory on cosmological spacetimes, because on the one hand the construction presented here is very explicit, giving states with well controllable regularity (in favorable conditions even Hadamard states). On the other hand, at the end of the chapter we will indicate why it is quite plausible that for the interesting regime of high temperatures one can construct states, which actually remain close to thermal equilibrium for some amount of (cosmological) time. Such states can then be physically interpreted as approximations to LTE states to the extent such a concept makes sense in a model without interactions.

Comparing the states obtained here to states obtained by other popular constructions on cosmological spacetimes, they can be seen as intermediate between the states often used in cosmology (low order adiabatic vacua) with explicitly specified mode-functions that can then be used to make concrete predictions like the CMB-spectrum [Str06], but lacking physical motivation, and the states of low (free-)energy [Olb07, Küs08] with nice motivation, which are however not easy to handle (though this is not entirely impossible, see [DV09]).

To be able to carry out this construction, we first have to introduce the formalism that connects the concepts of Wick products, defined in terms of the Hadamard parametrix as a series in the geodesic separation, to renormalized integrals over mode functions. While of course this idea is not new and in some form has been around under the name of "adiabatic renormalization" for a long time [PF74, Bir78, BD84] to calculate expectation values of the stress-energy tensor, it seems that this connection has not yet been systematically investigated[1] . This is why many of the calculations in this chapter are actually significantly more general than is required for the final construction of LTE-states; it is hoped that the formulas obtained for the computation of covariant Wick products and the statements on the general structure of Hadamard states on Cauchy surfaces, which to some extent can be seen to complement the more abstract approach in [JS02], might be of use to those using quantum fields on Robertson Walker spacetimes in more concrete settings and might convince them of the usefulness of these concepts. This is also the reason why the formulas are applied to a concrete example, namely (a part of) de Sitter spacetime (which is relevant as a simple starting point for inflationary models in cosmology [Str06]). There one discovers that the necessary conditions for Hadamard states derived can be solved explicitly to all orders, and even though the state obtained in the end is well known (it is the SO(4,1)-symmetric Hadamard state on this spacetime), this shows the usefulness of the conditions.

We start by two sections in which the structure of the spacetime under consideration is used, together with the fact that $\mathcal{G}^s_k$ is "almost" a bi-solution of the Klein-Gordon equation, to reduce the calculation of Wick products (here and in the following always involving two field operators) to Wick products only containing at most one derivative wrt. η and one wrt. η'.

Next, we investigate the relation of the functions v_j appearing in the Hadamard parametrix to those on Minkowski spacetime; the result is what one would intuitively expect (and was in fact used without comment in [Pir93]). The main result is a recursion relation which provides an alternative to the iteration procedure in the construction of adiabatic vacua, which seems to be rather simpler to use for concrete spacetimes. After a section collecting relations needed in the following, we then come to the core of the "generalized adiabatic renormalization" proposed here, namely the connection of the Hadamard parametrix restricted to a surface of constant conformal time to integrals mimicking those of the restricted two-point function. In contrast to the original adiabatic renormalization, where the functions appearing in these integrals where limited to sums of terms of the form $(A+p^2)^{-k+1/2}$ or terms obtained from the iteration procedure in the construction of adiabatic vacua, we here allow arbitrary, symmetric functions with the right *asymptotics*, which also makes it once more clear that it is really just the asymptotics of adiabatic vacua which has any significance.

Using these results, we are then in a position to make a remark on the general structure

[1] [Pir93] is an exception, but on the one hand no emphasis is put on explicit formulas for the calculations of expectation values there, on the other hand, some of the claims made there are probably wrong (at least in the given formulation).

of Hadamard states on the spacetimes considered here; at this point we will also point out an interesting question arising in the explicitly constructing of candidates of Hadamard states and then illustrate the result in the concrete example of de Sitter spacetime. After that we will return to the calculation of expectation values of Wick products, and it is here that we will introduce the functions from “conventional” adiabatic renormalization, already mentioned above, as one possible choice. For these we then work out all the formulas required to calculate the expected values of the thermal observables.

Finally, with all this technology in place, we will come to the construction of LTE states on a surface of constant cosmological time, which will again be illustrated by continuing the example of de Sitter spacetime and we will end this section by (somewhat heuristic) remarks on the behaviour of states constructed in this way for high temperatures.

5.1 Reduction of the problem using the Klein-Gordon operator

5.1.1 $\mathrm{P}_{m,\xi}$ and the Hadamard parametrix

By a direct calculation using $g^{ab}(\nabla_a\sigma)\nabla_b\sigma = -4\sigma$ from remark 2.2, one sees that the recursion relations for the v_j appearing in the definition of the Hadamard parametrix imply that on applying the Klein-Gordon operator $\mathrm{P}_{m,\xi}$ to $\mathcal{G}^s_k$ there remains a function with a singularity of the type $\sigma^k \log(\sigma)$; more precisely

$$\begin{aligned}\mathrm{P}_{m,\xi}\mathcal{G}^s_k =&\frac{\mathrm{P}_{m,\xi}v_k}{4\pi^2L^2}\left(\frac{\sigma}{L^2}\right)^k \log\left(\tfrac{\sigma}{L^2}\right) \qquad (5.1.1)\\ &+\frac{1}{4\pi^2L^4}\sum_{j=0}^{k-1}\Big(2g^{ab}(\nabla_a\sigma)\nabla_b v_{j+1} + (\Box\sigma - 8j-4)v_{j+1}\Big)\left(\frac{\sigma}{L^2}\right)^j\\ =&\underbrace{\frac{\mathrm{P}_{m,\xi}v_k}{4\pi^2L^2}\left(\frac{\sigma}{L^2}\right)^k}_{=:F_{l,\mathcal{G},k}}\log\left(\tfrac{\sigma}{L^2}\right) \underbrace{-\frac{1}{4\pi^2L^4}\sum_{j=0}^{k-1}\left(4(j+1)v_{j+1}+\frac{L^2}{j+1}\mathrm{P}_{m,\xi}v_j\right)\left(\frac{\sigma}{L^2}\right)^j}_{=:F_{f,\mathcal{G},k}}.\end{aligned}$$
(5.1.2)

Since this holds for all x' in a geodesic neighbourhood, we can differentiate wrt x' and obtain

$$\begin{aligned}\mathrm{P}_{m,\xi}\partial_{\mu'}\mathcal{G}^s_k =& \underbrace{\frac{1}{4\pi^2L^4}\left(\sigma(\mathrm{P}_{m,\xi}\partial_{\mu'}v_k)+k(\partial_{\mu'}\sigma)v_k\right)}_{=:F_{\mu',l,\mathcal{G},k}}\left(\frac{\sigma}{L^2}\right)^{k-1}\log\left(\tfrac{\sigma}{L^2}\right)\\ &+\frac{\mathrm{P}_{m,\xi}v_k}{4\pi^2L^4}(\partial_{\mu'}\sigma)\left(\frac{\sigma}{L^2}\right)^{k-1}\\ &-\frac{1}{4\pi^2L^4}\sum_{j=0}^{k-1}\Bigg[4(j+1)\partial_{\mu'}v_{j+1}+\frac{L^2}{j+1}\mathrm{P}_{m,\xi}\partial_{\mu'}v_j\\ &\qquad +j\frac{\partial_{\mu'}\sigma}{\sigma}\left(\frac{L^2}{j+1}\mathrm{P}_{m,\xi}v_j+4(j+1)v_{j+1}\right)\Bigg]\left(\frac{\sigma}{L^2}\right)^j\\ =:&F_{\mu',l,\mathcal{G},k}\left(\frac{\sigma}{L^2}\right)^{k-1}\log\left(\tfrac{\sigma}{L^2}\right)+F_{\mu',f,\mathcal{G},k}\,, \qquad (5.1.3)\end{aligned}$$

so upon applying $\mathrm{P}_{m,\xi}$ to $\partial_{\mu'}\mathcal{G}^s_k$ we end up with a term whose singularity is of type $(\partial_{\mu'}\sigma)\sigma^{k-1}\log(\sigma)$.

From this, we can also infer the result of repeated application of the Klein-Gordon operator on $\mathcal{G}^s_k$ and $\partial_{\mu'}\mathcal{G}^s_k$ for k sufficiently large, which will then be used for the translation of time-derivative to spatial derivatives.

Lemma 5.1. *Let the Hadamard parametrix $\mathcal{G}^s_k$ of order k be given as above and let $0 < n \leq k$, $n \in \mathbb{N}$. Then $\mathrm{P}^n_{m,\xi}\mathcal{G}^s_k$ and $\mathrm{P}^n_{m,\xi}\partial_{\mu'}\mathcal{G}^s_{k+1}$ can be written as*

$$\begin{aligned}\mathrm{P}^n_{m,\xi}\mathcal{G}^s_k =&F_1\sigma^{k+1-n}\log\left(\tfrac{\sigma}{L^2}\right)+F_2\\ \mathrm{P}^n_{m,\xi}\partial_{\mu'}\mathcal{G}^s_{k+1} =&F_3\sigma^{k+1-n}\log\left(\tfrac{\sigma}{L^2}\right)+F_4\end{aligned}$$

with smooth functions F_1, F_2, F_3 and F_4.

Proof. Using (5.1.2) we first get

$$\mathrm{P}^n_{m,\xi}\mathcal{G}^s_k = \mathrm{P}^{n-1}_{m,\xi}\left(F_{l,\mathcal{G},k}\left(\frac{\sigma}{L^2}\right)^k \log\left(\tfrac{\sigma}{L^2}\right) + F_{f,\mathcal{G},k}\right) \tag{5.1.4}$$

and by (5.1.3):

$$\mathrm{P}^n_{m,\xi}\partial_{\mu'}\mathcal{G}^s_{k+1} = \mathrm{P}^{n-1}_{m,\xi}\left(F_{\mu',l,\mathcal{G},k+1}\left(\frac{\sigma}{L^2}\right)^k \log\left(\tfrac{\sigma}{L^2}\right) + F_{\mu',f,\mathcal{G},k+1}\right). \tag{5.1.5}$$

We therefore need to investigate expressions of the form $\mathrm{P}^l_{m,\xi}\left(F_5\sigma^k\log\left(\tfrac{\sigma}{L^2}\right)+F_6\right)$ where $0 \leq l < k$ and F_5 and F_6 are smooth functions. Using $g^{ab}(\nabla_a\sigma)\nabla_b\sigma = -4\sigma$ we have

$$\begin{aligned}
\mathrm{P}_{m,\xi}\left(F_5\sigma^k\log\left(\tfrac{\sigma}{L^2}\right)+F_6\right) =& (\Box + m^2 + \xi R)\left(F_5\sigma^k\log\left(\tfrac{\sigma}{L^2}\right)\right) + \mathrm{P}_{m,\xi}F_6\\
=& \left[(\mathrm{P}_{m,\xi}F_5)\sigma + 2(N+1)g^{ab}(\nabla_a\sigma)\nabla_b F_5\right]\sigma^{k-1}\log\left(\tfrac{\sigma}{L^2}\right)\\
&+ F_5\left[k(\sigma\Box\sigma + (k-1)g^{ab}(\nabla_a\sigma)(\nabla_b\sigma)\right]\sigma^{k-2}\log\left(\tfrac{\sigma}{L^2}\right)\\
&+ F_5\left[\frac{\Box\sigma}{\sigma} - \frac{g^{ab}(\nabla_a\sigma)(\nabla_b\sigma)}{\sigma^2}\right]\sigma^k + \mathrm{P}_{m,\xi}F_6\\
=& \left[(\mathrm{P}_{m,\xi}F_5)\sigma + 2(k+1)(\nabla\sigma)\nabla F_5 + k(\Box\sigma - 4(k-1))\right]\\
&\ldots \times \sigma^{k-1}\log\left(\tfrac{\sigma}{L^2}\right) + F_5\left(\Box\sigma + 4\right)\sigma^{k-1} + \mathrm{P}_{m,\xi}F_6\,,
\end{aligned}$$

which is of the form $F_7\sigma^{k-1}\log\left(\tfrac{\sigma}{L^2}\right) + F_8$ with smooth functions F_7 and F_8, so by induction we get

$$\mathrm{P}^l_{m,\xi}\left(F_5\sigma^k\log\left(\tfrac{\sigma}{L^2}\right)+F_6\right) = F_1\sigma^{k-l}\log\left(\tfrac{\sigma}{L^2}\right) + F_2 \tag{5.1.6}$$

and combining this with (5.1.4) respectively (5.1.5) the claim follows. □

5.1.2 Reduction of orders

The requirement of being of Hadamard type for a quasi-free state ω involves the continuity of all the partial derivatives of the symmetric, regularized two-point functions $\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$. In this section we will show that the question of continuity of the partial derivatives can be reduced for Robertson Walker spacetimes to the investigation of partial derivatives of at most second order in η and η' by using the Klein-Gordon equation.
First we need a little lemma

Lemma 5.2. *Let $L = a_n\partial^n_\eta f + \ldots + a_1\partial_\eta + a_0$ be an n-th order differential operator in η on $M_{\mathrm{RW}}(\hat{I}, C)$, $a_k : M_{\mathrm{RW}}(\hat{I}, C) \to \mathbb{R}$ smooth functions. Then L can be written as*

$$L = \begin{cases} R_n\mathrm{P}^{n/2}_{m,\xi} + R_{n-1}\partial_\eta\mathrm{P}^{n/2-1}_{m,\xi} + \ldots + R_1\partial_\eta + R_0 & n \text{ even}\\ R_n\partial_\eta\mathrm{P}^{(n-1)/2}_{m,\xi} + R_{n-1}\mathrm{P}^{(n-1)/2}_{m,\xi} + \ldots + R_1\partial_\eta + R_0 & n \text{ odd}\end{cases}$$

where R_k is a differential operator of order $2\left\lfloor\frac{n-k}{2}\right\rfloor$[2] *in r.*

Proof. By induction: For $n = 0, 1$ the claim is evidently true with $R_0 = a_0$ and $R_0 = a_0$, $R_1 = a_1$ respectively.

<u>$n \to n+1$:</u> Using

$$
\begin{aligned}
\partial_\eta^{n-1}\left(\frac{1}{C}\partial_{\eta\eta} + \frac{C'}{C^2}\partial_\eta\right) &= \frac{1}{C}\partial_\eta^{n+1} + L_1 \\
L_1 &= \sum_{k=0}^{n-2}\binom{n-1}{k+1}\left(\partial_\eta^{k+1}\frac{1}{C}\right)\partial_\eta^{n-k} \\
&\quad + \sum_{k=0}^{n-1}\binom{n-1}{k}\left(\partial_\eta^{k}\frac{C'}{C^2}\right)\partial_\eta^{n-k} \\
\partial_\eta^{n-1}\left(\frac{1}{C}\left(\partial_{rr} + \frac{2}{r}\partial_r\right) - m^2 - \xi R\right) &= \left(\partial_{rr} + \frac{2}{r}\partial_r\right)\underbrace{\sum_{k=0}^{n-1}\binom{n-1}{k}\left(\partial_\eta^{k}\frac{1}{C}\right)\partial_\eta^{n-1-k}}_{=:L_2} \\
&\quad - \xi\underbrace{\sum_{k=0}^{n-1}\binom{n-1}{k}\left(\partial_\eta^{k}R\right)\partial_\eta^{n-1-k}}_{=:L_3}
\end{aligned}
$$

we can write L as

$$
L = C a_{n+1}\partial_\eta^{n-1}\mathrm{P}_{m,\xi} - C a_{n+1}L_1 + C a_{n+1}\left(\partial_{rr} + \frac{2}{r}\partial_r\right)L_2 - \xi C a_{n+1}L_3 + \sum_{k=0}^{n-1}a_k\partial_\eta^k\,.
$$

L_1 is a differential operator in η of order n whereas L_2 and L_3 are differential operators in η of order $n-1$ so inserting the induction hypothesis we get the claimed representation of L. $\square$

With the help of this preparation we can now show that, as far as the singular part of $\mathcal{G}_k^s$ is concerned, one can indeed reduce derivatives wrt η and η' to at maximum second order derivatives at the cost of higher order spatial derivatives. The same reduction can be done for the (symmetrized) two-point function $\mathscr{W}_2^{\omega,\mathrm{s}}$; since this is even a bi-solution of the Klein-Gordon equation the reduction works without the appearance of additional, finite terms.

From here on we will again only be concerned with the homogeneous and isotropic Hadamard parametrix $\mathcal{G}_k^s$ and two-point function $\mathscr{W}_2^{\omega,\mathrm{s}}$, by lemma 2.4 determined by distributions $\tilde{\mathcal{G}}_k^s$ and $\tilde{\mathscr{W}}_2^{\omega,\mathrm{s}}$. On these the Laplace operator $\partial_{xx} + \partial_{yy} + \partial_{zz}$ appearing in $\mathrm{P}_{m,\xi}$ acts as $\partial_{rr} + \frac{2}{r}\partial_r$. The same also holds true for the Laplace operator acting on $\mathbf{x}'$, which appears in $\mathrm{P}'_{m,\xi}$.

[2] $\lfloor\cdot\rfloor$ denotes the (lower) Gauss bracket, i.e. for $x \in \mathbb{R}$ $\lfloor x\rfloor$ is the biggest integer not greater than x

Lemma 5.3. *For $l, l', n \in \mathbb{N}$ such that $l + l' + n \leq k$ there holds*

$$\partial_\eta^l \partial_{\eta'}^{l'} \partial_r^n \tilde{\mathcal{G}}_k^s = D^{(\eta\eta')} \partial_\eta \partial_{\eta'} \tilde{\mathcal{G}}_k^s + D^{(\eta)} \partial_\eta \tilde{\mathcal{G}}_k^s + D^{(\eta')} \partial_\eta \tilde{\mathcal{G}}_k^s + D^{()} \tilde{\mathcal{G}}_k^s + \tilde{F}_{l,l',n} \tilde{\sigma} \log\left(\tfrac{\tilde{\sigma}}{L^2}\right) + \tilde{R}_{l,l',n}\,,$$

where $D^{(\eta\eta')}$, $D^{(\eta)}$, $D^{(\eta')}$ and $D^{()}$ are differential operators of order no bigger than $n + \left\lfloor \frac{l-1}{2} \right\rfloor + \left\lfloor \frac{l'-1}{2} \right\rfloor$, $n + \left\lfloor \frac{l-1}{2} \right\rfloor + \left\lfloor \frac{l'}{2} \right\rfloor$, $n + \left\lfloor \frac{l}{2} \right\rfloor + \left\lfloor \frac{l'-1}{2} \right\rfloor$ and $n + \left\lfloor \frac{l}{2} \right\rfloor + \left\lfloor \frac{l'}{2} \right\rfloor$ respectively in r and $\tilde{R}_{l,l',n}$, $\tilde{F}_{l,l',k}$ are the symmetry-reduced versions of smooth function $R_{l,l',n}$, $F_{l,l',k}$ on the convex normal set N where $\tilde{\mathcal{G}}_k^s$ is defined. Furthermore, for the symmetrized two-point function $\tilde{\mathscr{W}}_2^{\omega,\mathrm{s}}$ we have

$$\partial_\eta^l \partial_{\eta'}^{l'} \partial_r^n \tilde{\mathscr{W}}_2^{\omega,\mathrm{s}} = D^{(\eta\eta')} \partial_\eta \partial_{\eta'} \tilde{\mathscr{W}}_2^{\omega,\mathrm{s}} + D^{(\eta)} \partial_\eta \tilde{\mathscr{W}}_2^{\omega,\mathrm{s}} + D^{(\eta')} \partial_\eta \tilde{\mathscr{W}}_2^{\omega,\mathrm{s}} + D^{()} \tilde{\mathscr{W}}_2^{\omega,\mathrm{s}}\,.$$

Proof. Consider the case l, l' even and assume wlog $l \geq l'$. By the preceding lemma 5.2 we have

$$\partial_\eta^l \partial_{\eta'}^{l'} \partial_r^n \tilde{\mathcal{G}}_k^s = \partial_r^n \partial_{\eta'}^{l'} \left(R_l \mathrm{P}_{m,\xi}^{l/2} + \ldots + R_1 \partial_\eta + R_0 \right) \tilde{\mathcal{G}}_k^s\,, \tag{5.1.7}$$

which by lemma 5.1 can be written as

$$\begin{aligned}
\partial_\eta^l \partial_{\eta'}^{l'} \partial_r^n \tilde{\mathcal{G}}_k^s =& \partial_r^n \partial_{\eta'}^{l'} R_l \left(F_{l,1} \tilde{\sigma}^{k+1-l/2} \log\left(\tfrac{\tilde{\sigma}}{L^2}\right) + F_{l,2} \right) \\
&+ \partial_r^n \partial_{\eta'}^{l'} R_{l-1} \left(F_{l-1,1} \tilde{\sigma}^{k+2-l/2} \log\left(\tfrac{\tilde{\sigma}}{L^2}\right) + F_{l-1,2} \right) \\
&\vdots \\
&+ \partial_r^n R_1 \partial_{\eta'}^{l'} \partial_\eta \tilde{\mathcal{G}}_k^s + \partial_r^n R_0 \partial_{\eta'}^{l'} \tilde{\mathcal{G}}_k^s\,,
\end{aligned} \tag{5.1.8}$$

where the interchange of $\partial_{\eta'}^{l'}$ and R_1 and R_0 is permissible, since the latter only involve η and r. By the symmetry of $\tilde{\mathcal{G}}_k^s$, the relations (5.1.2) and therefore lemma 5.1 also hold for differentiation wrt the second argument, so for the terms $\partial_r^n R_1 \partial_{\eta'}^{l'} \partial_\eta \tilde{\mathcal{G}}_k^s$ and $\partial_r^n R_0 \partial_{\eta'}^{l'} \tilde{\mathcal{G}}_k^s$ we can write

$$\begin{aligned}
\partial_r^n R_1 \partial_{\eta'}^{l'} \partial_\eta \tilde{\mathcal{G}}_k^s =& \partial_r^n R_1 \left(S_{l'} (\mathrm{P}'_{m,\xi})^{l'/2} \partial_\eta + S_{l'-1} (\mathrm{P}'_{m,\xi})^{l'/2-1} \partial_\eta + \ldots + S_1 \partial_{\eta'} \partial_\eta + S_0 \partial_\eta \right) \tilde{\mathcal{G}}_k^s \\
=& \partial_r^n R_1 \left(S_{l'} \tilde{F}_{l',1} \tilde{\sigma}^{k-l'/2} \log \tilde{\sigma} + S_{l'} \tilde{F}_{l',2} \right) \\
&+ \partial_r^n R_1 \left(S_{l'-1} \tilde{F}_{l'-1,1} \tilde{\sigma}^{k+1-l'/2} \log \tilde{\sigma} + S_{l'-1} \tilde{F}_{l'-1,2} \right) \\
&\vdots \\
&+ \partial_r^n R_1 S_1 \partial_\eta \partial_{\eta'} \tilde{\mathcal{G}}_k^s + \partial_r^n R_1 S_0 \partial_\eta \tilde{\mathcal{G}}_k^s
\end{aligned} \tag{5.1.9}$$

and

$$\begin{aligned}
\partial_r^n R_0 \partial_{\eta'}^{l'} \tilde{\mathcal{G}}_k^s =& \partial_r^n R_0 \left(S_{l'} (\mathrm{P}'_{m,\xi})^{l'/2} + S_{l'-1} (\mathrm{P}'_{m,\xi})^{l'/2-1} + \ldots + S_1 \partial_{\eta'} + S_0 \right) \tilde{\mathcal{G}}_k^s \\
=& \partial_r^n R_0 \left(S_{l'} \tilde{F}_{l',1} \tilde{\sigma}^{k+1-l'/2} \log \tilde{\sigma} + S_{l'} \tilde{F}_{l',2} \right) \\
&+ \partial_r^n R_0 \left(S_{l'-1} \tilde{F}_{l'-1,1} \tilde{\sigma}^{k+2-l'/2} \log \tilde{\sigma} + S_{l'-1} \tilde{F}_{l'-1,2} \right) \\
&\vdots \\
&+ \partial_r^n R_0 S_1 \partial_{\eta'} \tilde{\mathcal{G}}_k^s + \partial_r^n R_0 S_0 \tilde{\mathcal{G}}_k^s
\end{aligned} \tag{5.1.10}$$

($\mathrm{P}'_{m,\xi}$ denotes the Klein-Gordon operator acting on x'). Setting $D^{(\eta\eta')} = \partial_r^n R_1 S_1$, $D^{(\eta)} = \partial_r^n R_1 S_0$, $D^{(\eta')} = \partial_r^n R_0 S_1$ and $D^{()} = R_0 S_0$ it remains to show that all the terms where differential operators act on products $\tilde{\sigma}^m \log\tilde{\sigma}$, $m \geq 1$ actually can be written as $f\tilde{\sigma}\log\tilde{\sigma} + h$ with smooth functions f and h. First looking at (5.1.8) we have differential operators of order no bigger than $n+l'+(l-s)$ acting on terms $\tilde{\sigma}^{k+1-\lfloor\frac{s}{2}\rfloor}\log\tilde{\sigma}$ multiplied with a smooth function for $0 \leq s \leq l$. In the equations (5.1.9), we have differential operators of order no bigger than $n+l-2+l'-s$ acting on terms $\tilde{\sigma}^{k-\lfloor\frac{s}{2}\rfloor}\log\tilde{\sigma}$ multiplied with a smooth function for $0 \leq s \leq l'$ and in (5.1.10) differential operators of order no bigger than $n+l+l'-s$ acting on terms $\tilde{\sigma}^{k+1-\lfloor\frac{s}{2}\rfloor}\log\tilde{\sigma}$ multiplied with a smooth function for $0 \leq s \leq l'$.

Since acting with a differential operator on the term $\tilde{\sigma}^k\log\tilde{\sigma}$ will lead to a term $f\tilde{\sigma}^{k-1}\log\tilde{\sigma} + f'$ with smooth functions f and f', i.e. reduces the power of $\tilde{\sigma}$ in front of the logarithm only by one, for $k \geq l+l'+n$ the logarithmic terms remaining in (5.1.8)-(5.1.10) all have a prefactor of at least $\tilde{\sigma}$, showing the first part of the claim.

Concerning the symmetrized two-point function $\tilde{\mathscr{W}}_2^{\omega,\mathrm{s}}$, replacing in (5.1.7) the symmetrized Hadamard Parametrix $\tilde{\mathcal{G}}_k^s$ by $\tilde{\mathscr{W}}_2^{\omega,\mathrm{s}}$, which is a bi-solution of the Klein-Gordon equation, we get

$$\partial_\eta^l \partial_{\eta'}^{l'} \partial_r^k \tilde{\mathscr{W}}_2^{\omega,\mathrm{s}} = R_1 \partial_\eta \partial_{\eta'}^{l'} \tilde{\mathscr{W}}_2^{\omega,\mathrm{s}} + R_0 \tilde{\mathscr{W}}_2^{\omega,\mathrm{s}}$$

Performing the same procedure with the η'-derivatives we then end up with the claimed expression for $\tilde{\mathscr{W}}_2^{\omega,\mathrm{s}}$.

For the other cases l odd l' even, l' odd l even and l, l' both odd the calculations work completely analogously. $\square$

Since we will need this term in the following and to illustrate the preceding procedure, let us calculate $\partial_{\eta\eta}\left(\tilde{\mathscr{W}}_2^{\omega,\mathrm{s}} - \tilde{\mathcal{G}}_k^s\right)$. First we have

$$\begin{aligned}
\partial_{\eta\eta} =& C(\eta)\left(\frac{\partial_{\eta\eta}}{C(\eta)} + \frac{C'(\eta)}{C^2(\eta)}\partial_\eta - \frac{1}{C(\eta)}\left(\partial_{rr} + \frac{2}{r}\partial_r\right) + m^2 + \xi R(\eta)\right) \\
& - \frac{C'(\eta)}{C(\eta)}\partial_\eta + \left(\partial_{rr} + \frac{2}{r}\partial_r\right) - C(\eta)\left(m^2 + \xi R(\eta)\right) \\
=& C(\eta)\mathrm{P}_{m,\xi} - \frac{C'(\eta)}{C(\eta)}\partial_\eta + \left(\partial_{rr} + \frac{2}{r}\partial_r\right) - C(\eta)\left(m^2 + \xi R(\eta)\right) ,
\end{aligned}$$

so the operators R_0, R_1 and R_2 are here given by

$$\begin{aligned}
R_0(\eta) =& \partial_{rr} + \frac{2}{r}\partial_r - C(\eta)\left(m^2 + \xi R(\eta)\right) \\
R_1(\eta) =& -\frac{C'(\eta)}{C(\eta)} \\
R_2(\eta) =& C(\eta) .
\end{aligned}$$

For the renormalized, symmetric part of the two-point function $\tilde{\mathscr{W}}_{\omega,k}^{\mathrm{SHP}} = \tilde{\mathscr{W}}_2^{\omega,\mathrm{s}} - \tilde{\mathcal{G}}_k^s$ this yields

$$\begin{aligned}\partial_{\eta\eta}\tilde{\mathscr{W}}^{\mathrm{SHP}}_{\omega,k} = &-\frac{C'}{C}\partial_\eta\tilde{\mathscr{W}}^{\mathrm{SHP}}_{\omega,k} + \left(\partial_{rr} + \frac{2}{r}\partial_r - C(m^2+\xi R)\right)\tilde{\mathscr{W}}^{\mathrm{SHP}}_{\omega,k} \\ &+ \frac{C}{4\pi^2 L^2}\left(4\frac{\tilde{v}_1}{L^2} + \mathrm{P}_{m,\xi}\tilde{v}_0\right) + o(1)\,, \end{aligned} \tag{5.1.11}$$

where $o(1)$ denotes terms that go to zero for $\sigma \to 0$.

Since the (local) Hadamard condition (see definition 2.3) is formulated as the requirement that in each geodesically convex domain the function $\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$ is C^k, in principle to establish that a homogeneous and isotropic state on Robertson Walker spacetime is Hadamard, one would have to check the continuity of all the functions $\partial^n_r\partial^l_\eta\partial^{l'}_{\eta'}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$. By the above and the symmetry of $\tilde{\mathscr{W}}^{\mathrm{SHP}}_{\omega,k}$ it is however sufficient to actually check the continuity of $\partial^l_r\partial_\eta\partial_{\eta'}\tilde{\mathscr{W}}^{\mathrm{SHP}}_{\omega,k}$, $\partial^l_r\partial_\eta\tilde{\mathscr{W}}^{\mathrm{SHP}}_{\omega,k}$ and $\partial^l_r\tilde{\mathscr{W}}^{\mathrm{SHP}}_{\omega,k}$ for all $l \in \mathbb{N}$.

Concerning calculations, by going over to the modified "time-derivatives" $\mathcal{D}$ and $\mathcal{D}'$ introduced in section 2.2.4 and rewriting the differential operator

$$D^{(\eta\eta')}\partial_\eta\partial_{\eta'} + D^{(\eta)}\partial_\eta + D^{(\eta')}\partial_{\eta'} + D^{()}$$

where the $D^{(\cdot)}$ are the differential-operators in r from lemma 5.3 as

$$D^{(\eta\eta')}_{\mathcal{D}}\mathcal{D}\mathcal{D}' + D^{(\eta)}_{\mathcal{D}}\mathcal{D} + D^{(\eta')}_{\mathcal{D}}\mathcal{D}' + D^{()}\,,$$

we can finally reduce the calculations of expressions $\partial^n_r\partial^l_\eta\partial^{l'}_{\eta'}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$ to the calculation of the expressions $D^{(\eta\eta')}_{\mathcal{D}}\mathcal{D}\mathcal{D}'\tilde{\mathscr{W}}^{\mathrm{SHP}}_{\omega,k}$, $D^{(\eta)}_{\mathcal{D}}\tilde{\mathscr{W}}^{\mathrm{SHP}}_{\omega,k}$ and $D^{()}_{\mathcal{D}}\tilde{\mathscr{W}}^{\mathrm{SHP}}_{\omega,k}$.

Still, a priori this needs to be checked on a family of geodesically convex normal neighbourhoods covering $M_{\mathrm{RW}}(\hat{I},C)$; by translational invariance and preservation of the Hadamard property under time-evolution [FSW78] it is sufficient to check the property in a single, geodesically convex neighbourhood N, but this is still a four-dimensional subset of M. A *necessary* condition for a state to be Hadamard is the requirement that the restrictions $\left[\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}$, $\left[\mathcal{D}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}$, $\left[\mathcal{D}\mathcal{D}'\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}$ to a (Cauchy-)surface of constant η are C^k (in intersections of N with the surface) for all k. Since this is a requirement on the initial values of the two-point function, and the two-point function is in turn determined by its values and the values of its first and second time-derivative on a Cauchy surface, one suspects that this is in fact equivalent to the Hadamard property. We now want to sketch an argument, why this should in fact be true; to turn this into a rigorous proof, more information about the precise regularity of solutions to the Klein-Gordon equation on Robertson Walker spacetimes, depending on initial values and parameters, would be needed.

First note that for a surface $S_{\eta_0} := \{\eta_0\} \times \mathbb{R}^3 \subset M_{\mathrm{RW}}(\hat{I},C)$ of constant $\eta = \eta_0$ and a geodesically convex neighbourhood N of $x \in S_{\eta_0}$, a neighbourhood $]\eta,\eta'[\times\mathbb{R}^3$ of S_{η_0} can be covered by taking (denumerably many) copies of N translated within S_{η_0} and this can even be done in such a way, that S_N is covered by translates of the sets $D(N\cap S_{\eta_0})$, with $D(\cdot)$ denoting the Cauchy development of a set [BGP07] (this is sketched in figure 5.1). By translational invariance of the state and the Hadamard parametrix, $\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$

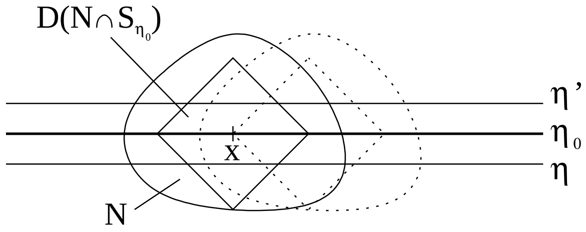

Figure 5.1: N and a translate, drawn with dashed lines

is identical on each translates of $N \times N$, so it suffices to check whether it is C^k on $D(N \cap S_{\eta 0})^2$. By the results of this section, we know that $\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$ satisfies the inhomogeneous Klein-Gordon equation $\mathrm{P}_{m,\xi}\mathscr{W}^{\mathrm{SHP}}_{\omega,k} = -\mathrm{P}_{m,\xi}\mathcal{G}^s_k$, $\mathrm{P}'_{m,\xi}\mathscr{W}^{\mathrm{SHP}}_{\omega,k} = -\mathrm{P}'_{m,\xi}\mathcal{G}^s_k$, where the right-hand side is a C^k function on N. But if we are given C^k-restrictions $\left[\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}$, $\left[\mathcal{D}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}$ and $\left[\mathcal{D}\mathcal{D}'\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}$, first for each value x of the first argument of $\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$ in $S_{\eta 0}$ we can solve the two Cauchy-problems $\mathrm{P}'_{m,\xi}\mathscr{W}^{\mathrm{SHP}}_{\omega,k} = -\mathrm{P}'_{m,\xi}\mathcal{G}^s_k$ (in the inhomogeneity, the first argument is also fixed as x) with the initial data $\left[\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}$, $\left[\mathcal{D}'\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}$ respectively $\left[\mathcal{D}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}$ and $\left[\mathcal{D}\mathcal{D}'\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}$ (on $D(N \cap S_{\eta 0})$ there exists a unique solution [BGP07]), to obtain two functions $S_{\eta 0} \times D(N \cap S_{\eta 0}) \ni (x, x') \mapsto \mathscr{W}^{\mathrm{SHP}}_{\omega,k}(x, x')$ and $S_{\eta 0} \times D(N \cap S_{\eta 0}) \ni (x, x') \mapsto \mathcal{D}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}(x, x')$. Since the initial values on $S_{\eta 0}$ and the inhomogeneities were assumed to be C^k, this should be a C^k functions in x and x'. Now considering for these functions the second argument x' as fixed, they can be used as initial data defining the Cauchy problem $\mathrm{P}_{m,\xi}\mathscr{W}^{\mathrm{SHP}}_{\omega,k} = -\mathrm{P}_{m,\xi}\mathcal{G}^s_k$ (where in the inhomogeneity now the second argument is fixed to x'); since this again has a unique solution and the initial data and the inhomogeneity where C^k, we should get for each x' a C^k-function on $D(N \cap S_{\eta 0})$ and allowing x' to vary, we get via the dependence of the initial values on x' a C^k function on $D(N \cap S_{\eta 0}) \times D(N \cap S_{\eta 0})$, which is just $\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$ on this set. We are then in the situation to apply the results from [FSW78] to conclude that the state is a (global) Hadamard state.

As a final remark, note that for the spacetimes at hand this construction can actually be made more explicit, since we can get representation formulas for solutions of the inhomogeneous Cauchy problem using the (spatial) Fourier transform similar to those for the Greens-operators from appendix A.1. The differentiability question could then be investigated using this representation.

5.2 Relation to flat spacetime

Since the spacetimes under consideration are conformally equivalent to flat spacetime, which in turn implies that the wave-operator $\Box$ is closely related to that on flat spacetime, and since the requirement that $\mathrm{P}_{m,\xi}\mathcal{G}_k$ is zero up to a term of order $\sigma^k \log \sigma$, which was used in the last section, can actually also be used to derive the relations (2.1.2)-(2.1.4), one can expect that also the functions $\Delta^{1/2}$ and v_j are closely related to those on flat spacetime. In this section it will be shown that this is indeed the case; more precisely we have

$$\frac{\Delta^{1/2}}{q} = \frac{1}{D_{\eta\eta'}}\left(1+\rho R_\Delta\right) \tag{5.2.1}$$

$$v^{(k)} = \frac{1}{D_{\eta\eta'}}\left(\sum_{j=0}^{k}\rho^j \overset{o}{v}_j + \rho^{k+1}R_v\right), \tag{5.2.2}$$

where $D_{\eta\eta'} := \sqrt{C(\eta)C(\eta')}$ and the $\overset{o}{v}_j$ are determined by a recursion relation which is almost the one determining the corresponding coefficients on flat spacetime only that the "mass-term" appearing is now η-dependent. Furthermore, the small-distance asymptotics of the function R_Δ will be given to the order needed to calculate the Wick products appearing later on.

Introducing $\overset{o}{\Box} = \partial_{\eta\eta} - \sum_{j=1}^{3}\partial_{x_jx_j}$, one calculates for an $f \in C^\infty(N)$:

$$\Box\frac{f(\eta,\mathbf{x},\eta',\mathbf{x}')}{D_{\eta\eta'}} = \frac{1}{D_{\eta\eta'}}\left(\frac{\overset{o}{\Box}}{C(\eta)} - \frac{R(\eta)}{6}\right)f(\eta,\mathbf{x},\eta',\mathbf{x}) \tag{5.2.3}$$

Using this,

$$2g^{ab}(\nabla_a\sigma)\nabla_b f + (\Box\sigma + 8)f = \Box(\sigma f) - \sigma\Box f \tag{5.2.4}$$

and introducing

$$\overset{o}{\Delta}{}^{1/2}(\eta,\eta',r) = \frac{D_{\eta\eta'}\tilde{\Delta}^{1/2}(\eta,\eta',r)}{\tilde{q}(\eta,\eta',r)}, \tag{5.2.5}$$

(2.1.2) implies

$$\overset{o}{\Box}\left(q\overset{o}{\Delta}{}^{1/2}\right) - \rho q\overset{o}{\Box}\left(\frac{\overset{o}{\Delta}{}^{1/2}}{\rho}\right) = 0\,. \tag{5.2.6}$$

Using (5.2.4) once more, this time for Minkowski spacetime and denoting the Minkowski metric again by ϵ, we end up with

$$2\epsilon^{\mu\nu}(\overset{o}{\nabla}_\mu\rho)\overset{o}{\nabla}_\nu\overset{o}{\Delta}{}^{1/2} + \frac{\rho}{q}\left(2\epsilon^{\mu\nu}(\overset{o}{\nabla}_\mu q)\overset{o}{\nabla}_\nu\overset{o}{\Delta}{}^{1/2} + (\overset{o}{\Box}q)\overset{o}{\Delta}{}^{1/2}\right) = 0\,. \tag{5.2.7}$$

Along the lightlike geodesics $\rho = 0$ (which are characteristic curves for (5.2.7)) this agrees precisely with the equation for $\Delta^{1/2}$ on Minkowski spacetime, furthermore by $\tilde{q}(\eta,\eta,0) = C(\eta)$ the initial condition $\overset{o}{\Delta}{}^{1/2}(\eta,\eta,0) = 1$ agrees with the one on Minkowski spacetime, so for $\rho = 0$ also $\overset{o}{\Delta}{}^{1/2}$ on Robertson Walker is equal to one. Therefore $\overset{o}{\Delta}{}^{1/2} - 1$ is a smooth function which vanishes on $(N\times N)\cap V$ and can thus by Lemma 2.5 be written as $\overset{o}{\Delta}{}^{1/2} = 1 + \rho R_\Delta$ where R_Δ is a smooth function on N. Inserting this into

(5.2.5) we see that $\Delta^{1/2}$ indeed has the form claimed in (5.2.1) and using (5.2.7), we obtain for R_Δ the equation

$$2\epsilon^{\mu\nu}\overset{o}{\nabla}_\mu(q\rho)\overset{o}{\nabla}_\nu R_\Delta + \left(2\epsilon^{\mu\nu}(\overset{o}{\nabla}_\mu q)\overset{o}{\nabla}_\nu\rho + \rho\overset{o}{\Box} q - 8q\right) R_\Delta = -\overset{o}{\Box} q \tag{5.2.8}$$

which yields for $x \to x'$ the identity

$$[qR_\Delta]_{(\eta,\mathbf{x})=x=x'} = C(\eta')\,[R_\Delta]_{x=x'} = \left[\frac{\overset{o}{\Box} q}{8}\right]_{x=x'}, \tag{5.2.9}$$

i.e. the initial values for R_Δ.
Since R_Δ only appears in $\Delta^{1/2}$ multiplied by a prefactor of σ, it does not contribute to the singular part of $\mathcal{G}_k$; it does however give a contribution to its finite part and therefore the asymptotic behaviour for $x \to x'$ is needed.

The small distance expansion (2.2.6) for $\tilde{q}$ can now be used together with the initial condition (5.2.9) to calculate the asymptotic expansion for R_Δ by (5.2.8). The result to second order for the symmetry-reduced function $\tilde{R_\Delta}$ is

$$\begin{aligned}\tilde{R_\Delta}(\eta, r) = &\frac{C(\eta')R(\eta')}{72} + \frac{(CR)'(\eta')}{144}(\eta-\eta') \\ &+ \left[(CR)''(\eta') - \frac{3}{4}\left(\frac{C''(\eta')}{C(\eta')}\right)^2 + \frac{C''(\eta')\,(C'(\eta'))^2}{C^3(\eta')} - \frac{3}{8}\left(\frac{C'(\eta')}{C(\eta')}\right)^4\right]\frac{(\eta-\eta')^2}{480} \\ &+ \left[\frac{15}{8}\left(\frac{C'(\eta')}{C(\eta')}\right)^4 - \frac{11}{3}\frac{C''(\eta')\,(C'(\eta'))^2}{C^3(\eta')} + \frac{3}{4}\left(\frac{C''(\eta')}{C(\eta')}\right)^2 + \frac{C'(\eta')C'''(\eta')}{C^2(\eta')}\right]\frac{r^2}{480} \\ &+ \ldots\end{aligned}$$

Concerning the v_j coefficients, introduce u_0 by

$$u_0 = D_{\eta\eta'} v_0\,.$$

Using

$$\begin{aligned}2g^{ab}(\nabla_a\sigma)\nabla_b v_0 + (4 + \Box\sigma)v_0 =&\sigma\left(\Box(v_0\log\sigma) - (\Box v_0)\log\sigma\right) \\ =&2q\epsilon^{\mu\nu}(\overset{o}{\nabla}_\mu\rho)\overset{o}{\nabla}_\nu u_0 - 4qu_0 + \rho\left(\overset{o}{\Box} q - \frac{\epsilon^{\mu\nu}(\overset{o}{\nabla}_\mu q)\overset{o}{\nabla}_\nu q}{q}\right)u_0\end{aligned}$$

and the representation (5.2.1) for $\Delta^{1/2}$ together with (5.2.6), the equation (2.1.2) for v_0 implies for u_0:

$$\epsilon^{\mu\nu}(\overset{o}{\nabla}_\mu\rho)\overset{o}{\nabla}_\nu u_0 - 4u_0 + \frac{\rho}{q}\left(\overset{o}{\Box} q - \frac{\epsilon^{\mu\nu}(\overset{o}{\nabla}_\mu q)\overset{o}{\nabla}_\nu q}{q}\right)u_0 = -L^2\left(Q_{m,\xi} + \rho\overset{o}{\mathrm{P}}_{m,\xi}R_\Delta\right), \tag{5.2.10}$$

where

$$\begin{aligned}\overset{o}{\mathrm{P}}_{m,\xi} :=&\overset{o}{\Box} + Q_{m,\xi} \\ Q_{m,\xi} :=&\left(m^2 + \left(\xi - \tfrac{1}{6}\right)R\right)C\end{aligned}$$

were introduced. The partial differential equation (5.2.10) again has geodesics as characteristic curves, so can be reduced to ordinary differential equations along these; along lightlike geodesics they precisely coincide with the equations obtained from the partial differential equation

$$\epsilon^{\mu\nu}(\overset{o}{\nabla}_\mu \rho)\overset{o}{\nabla}_\nu \overset{o}{v}_0 - 4\overset{o}{v}_0 = -L^2 Q_{m,\xi}\,. \tag{5.2.11}$$

Since the requirement of finiteness for coinciding arguments fixes u_0 uniquely this implies that u_0 agrees on V with a solution $\overset{o}{v}_0$ to (5.2.11) if $\overset{o}{v}_0$ is also required to remain finite for coinciding arguments.

Thus, defining the functions $\overset{o}{v}_j$ as the unique, bounded solutions to the recursion relations

$$2\epsilon^{\mu\nu}(\overset{o}{\nabla}_\mu \rho)\overset{o}{\nabla}_\nu \overset{o}{v}_0 - 4\overset{o}{v}_0 = -L^2 Q_{m,\xi} \tag{5.2.12}$$

$$2(j+1)\epsilon^{\mu\nu}(\overset{o}{\nabla}_\mu \rho)\overset{o}{\nabla}_\nu \overset{o}{v}_{j+1} - 4(j+1)(j+2)\overset{o}{v}_{j+1} = -L^2 \overset{o}{\mathrm{P}}_{m,\xi}\overset{o}{v}_j \tag{5.2.13}$$

and $\overset{o}{v}^{(k)}$ by

$$\overset{o}{v}^{(k)} = \frac{1}{D_{\eta\eta'}}\sum_{j=0}^{k} \rho^j \overset{o}{v}_j\,,$$

we have

$$\overset{o}{v}^{(k)}|_V = v^{(k)}|_V\,.$$

The Hadamard recursion relations (2.1.4) imply $\mathrm{P}_{m,\xi} v^{(k)} = (\mathrm{P}_{m,\xi} v_k)\sigma^k$, i.e. $v^{(k)}$ solves the Klein Gordon equation up to a term that vanishes like σ^k when approaching the “light-cone” V. On the other hand, since (5.2.12) and (5.2.13) are exactly the Hadamard recursion relations on Minkowski spacetime except for the η-dependent “mass term” $Q_{m,\xi}$, it follows by the same argument that the function $\overset{o}{\mathrm{P}}_{m,\xi}\left(\sum_{j=0}^{k} \rho^j \overset{o}{v}_j\right)$ is a term which for $\rho \to 0 \Leftrightarrow \sigma \to 0$ is of order $\rho^k \Leftrightarrow \sigma^k$. The following lemma, formulated for the spacetimes under consideration, shows that these two requirements in fact already imply that $v^{(k)}$ and $\overset{o}{v}^{(k)}$ agree up to a function that vanishes like σ^{k+1} when approaching V.

Lemma 5.4. *For functions $f_1, f_2 \in C^{2k+2}_{\mathrm{ih}}(N)$, satisfying $\mathrm{P}_{m,\xi} f_1 = r_1\sigma^k$, $\mathrm{P}_{m,\xi} f_2 = r_2\sigma^k$ and $v_1|_V = v_2|_V$ there exists a neighbourhood $U \subset N$ of the diagonal $x = x'$ and continuous function r_3 on U such that*

$$f_1 - f_2 = r_3 \sigma^{k+1}\,.$$

Proof. By induction. For $k = 0$, applying lemma 2.5 to $r_1 - r_2$, which vanishes due to the assumption $r_1|_V = r_2|_V$, we get $r_1 - r_2 = \rho\tilde{r_3}$ and by choosing $r_3 = \tilde{r_3} q$, where U is chosen such that q is positive on U (we already know that $q(x,x) > 0$) we get the claim. For the induction step, note that $\mathrm{P}_{m,\xi} f_1 = r_1\sigma^{k+1}$, $\mathrm{P}_{m,\xi} f_2 = r_2\sigma^{k+1}$ implies first by the induction hypothesis $f_1 - f_2 = \tilde{r_3}\sigma^{k+1}$ and this in turn leads to

$$\begin{aligned}\Box(f_1 - f_2) =& \sigma^{k+1}\Box\tilde{r}_3 + 2(k+1)\sigma^k g^{ab}(\nabla\sigma_a)\nabla_b\tilde{r}_3 + 2(k+1)\left[\Box\sigma - 4k\right]\tilde{r}_3\sigma^k \\ =& -(m^2 + \xi R)\tilde{r}_3\sigma^{k+1} + (r_1 - r_2)\sigma^{k+1}\,.\end{aligned}$$

Dividing by $(k+1)\sigma^k$ and restricting to V we get

$$2g^{ab}(\nabla_a\sigma)\nabla_b\tilde{r}_3 + [\Box\sigma - 4k]\,\tilde{r}_3 = 0\,.$$

By the second point of remark 2.2, $g^{ab}\nabla_b\sigma(x,x')$ is at x tangential to the light-like geodesic through x' and x and its (euclidean) modulus provides an affine parametrization of this geodesics[3], we can reduce the equation on V by the method of characteristics to the ordinary differential equation

$$-4\lambda\tilde{\tilde{r}}_3'(\lambda) + \left[\widetilde{\Box\sigma}(\lambda) - 4k\right]\tilde{\tilde{r}}_3(\lambda) = 0 \tag{5.2.14}$$

for $\tilde{\tilde{r}}_3$, $\widetilde{\Box\sigma}$ defined by $\tilde{r}_3(x,x') = \tilde{\tilde{r}}_3(\|\nabla\sigma(x,x')\|/2)$ and $(\Box\sigma)(x,x') = \widetilde{\Box\sigma}(\|\nabla\sigma(x,x')\|/2)$. Using $\Box\sigma|_V = -8$, we see that the initial values for the ODE (5.2.14) is $\tilde{\tilde{r}}_3(0) = 0$, but this leads to

$$\tilde{\tilde{r}}_3'(\lambda) = \left[\widetilde{\Box\sigma}(\lambda)/4 - k\right]\frac{\tilde{\tilde{r}}_3(\lambda) - \tilde{\tilde{r}}_3(0)}{\lambda}\,.$$

Now since $\widetilde{\Box\sigma}(0)/4 = -2$, we can choose a neighbourhood $\tilde{U}$ of 0 such that $\widetilde{\Box\sigma}/4 - k$ is negative on $\tilde{U}$ (even independent of k) and by the mean value theorem we get that $\tilde{\tilde{r}}_3$ has to be zero on $\tilde{U}$, therefore $\tilde{r}_3$ is zero on $U \cap V$, U a neighbourhood of $x = x'$, and by lemma 2.5 we can write $\tilde{r}_3$ as $\tilde{r}_3 = \sigma r_3$, i.e. $f_1 - f_2 = \sigma^{k+1}\sigma r_3$. □

This means that the functions $\Delta^{1/2}$ and $v^{(k)}$ appearing in the Hadamard parametrix can be related to functions obtained by solving the Hadamard recursion relations for the Minkowski Klein-Gordon operator with a time-dependent mass up to two remainder terms. For the first remainder term R_Δ, the short distance asymptotics can be calculated using (2.2.5) and (5.2.8); the other remainder term does not contribute to coincidence limits when k is sufficiently large. Since its regularity grows with k, it also is not relevant in discussions of regularity, so besides R_Δ only the terms $\overset{o}{\Delta}{}^{1/2}$ and $\overset{o}{v}_j$ enter into the Hadamard condition and covariant Wick products. It is thus sufficient to solve the recursion relations (5.2.12), (5.2.13) instead of the full recursion relations for $\Delta^{1/2}$ and v_j; once more making use of the methods of characteristics, it is then easily seen that the $\overset{o}{v}_j$ only depend on η and η'.

For their coincidence limits $\eta \to \eta'$ we get from (5.2.12), (5.2.13):

$$\left[\partial_\eta^l \overset{o}{v}_0(\eta,\eta')\right]_{\eta=\eta'} = \frac{L^2}{4(l+1)}\partial_\eta^l Q_{m,\xi}(\eta) \tag{5.2.15}$$

$$\left[\partial_\eta^l \overset{o}{v}_{j+1}(\eta,\eta')\right]_{\eta=\eta'} = \frac{L^2}{4(j+1)(j+2+l)}\left[\partial_\eta^{l+2}\overset{o}{v}_j(\eta,\eta') + \partial_\eta^l\left(Q_{m,\xi}(\eta)\overset{o}{v}_j(\eta,\eta')\right)\right]_{\eta=\eta'}\,. \tag{5.2.16}$$

For given C and R, these are recursion relations that allow the calculation of $\left[\partial_\eta^l\overset{o}{v}_j\right]_{\eta=\eta'}$ purely from $Q_{m,\xi}$; they get especially simple for the case of conformal coupling where $Q_{m,\xi}$ is given by $Q_{m,1/6} = m^2 C$.

[3] This can, for the spacetimes at hand, be seen by using the representation $\sigma = q\rho$ and $\partial_\eta\tilde{\rho} = -2(\eta - \eta')$, $\partial_r\tilde{\rho} = -2r$

In the following, expressions for $\left[\overset{o}{v}_0\right]_{\eta=\eta'}$, $\left[\partial_\eta \overset{o}{v}_0\right]_{\eta=\eta'}$, $\left[\partial_{\eta\eta} \overset{o}{v}_0\right]_{\eta=\eta'}$ and $\left[\overset{o}{v}_1\right]_{\eta=\eta'}$ will be needed; using the recursion relations they are calculated as

$$\left[\overset{o}{v}_0(\eta,\eta')\right]_{\eta=\eta'} = \frac{L^2 Q(\eta)}{4} \tag{5.2.17}$$

$$\left[\partial_\eta \overset{o}{v}_0(\eta,\eta')\right]_{\eta=\eta'} = \frac{L^2 Q'(\eta)}{8} \tag{5.2.18}$$

$$\left[\partial_{\eta\eta} \overset{o}{v}_0(\eta,\eta')\right]_{\eta=\eta'} = \frac{L^2 Q''(\eta)}{12} \tag{5.2.19}$$

$$\left[\overset{o}{v}_1(\eta,\eta')\right]_{\eta=\eta'} = \frac{L^2}{8}\left[\partial_{\eta\eta}\overset{o}{v}_0(\eta,\eta') + Q(\eta)\overset{o}{v}_0(\eta,\eta')\right]_{\eta=\eta'} \tag{5.2.20}$$

$$= L^4 \frac{Q''(\eta)/3 + Q^2(\eta)}{32}\,. \tag{5.2.21}$$

As a first application, we can calculate the finite term $R_{\mathrm{P}_{m,\xi}} := \frac{C}{4\pi^2 L^2}\left(4\frac{v_1}{L^2} + \mathrm{P}_{m,\xi} v_0\right)$, which appeared at the end of the preceding section in the reduction of second order η-derivatives to first order ones as:

$$R_{\mathrm{P}_{m,\xi}} = \left[-C\,\mathrm{P}_{m,\xi}\mathcal{G}^s_k\right]_{x=x'} \tag{5.2.22}$$

$$\begin{aligned} -C\mathrm{P}_{m,\xi}\mathcal{G}^s_k = & -\frac{1}{4\pi^2 D_{\eta\eta'}}\overset{o}{\mathrm{P}}_{m,\xi}\left[\frac{1}{\rho} + \frac{1}{L^2}\sum_{j=0}^{k}\left(\frac{\rho}{L^2}\right)^j \overset{o}{v}_j \log\left(\tfrac{\rho}{L^2}\right) + R_\Delta \right. \\ & \left. + \frac{1}{L^2}\sum_{j=0}^{k}\left(\frac{\rho}{L^2}\right)^j \overset{o}{v}_j \log(q) + \frac{\rho^{k+1}}{L^{2(l+2)}} R_v \log\left(\tfrac{\sigma}{L^2}\right)\right] \\ = & \frac{1}{4\pi^2 L^2 D_{\eta\eta'}}\left(4\frac{\overset{o}{v}_1}{L^2} + \overset{o}{\mathrm{P}}_{m,\xi}\overset{o}{v}_0 - L^2\overset{o}{\mathrm{P}}_{m,\xi}R_\Delta - \overset{o}{\mathrm{P}}_{m,\xi}\left(\left(\overset{o}{v}_0 + \frac{\rho}{L^2}\overset{o}{v}_1\right)\log q\right)\right) \\ & + o(1) \end{aligned} \tag{5.2.23}$$

5.3 The generalized adiabatic renormalization

5.3.1 Strategy for the introduction of “momentum-space” renormalization

The (state-dependent part) of expectation values of covariant Wick squares of the field and its derivatives in Hadamard states are given by expressions of the form

$$\left[\partial_r^k \partial_\eta^l \partial_{\eta'}^{l'} \tilde{\mathscr{W}}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta',r=0}$$

Abbreviating $\tilde{w}^{(\eta\eta')} := D^{(\eta\eta')}_{\mathcal{D}}\mathcal{D}\mathcal{D}'\tilde{\mathscr{W}}^{\mathrm{SHP}}_{\omega,k}$, $\tilde{w}^{(\eta)} := D^{(\eta)}_{\mathcal{D}}\mathcal{D}\tilde{\mathscr{W}}^{\mathrm{SHP}}_{\omega,k}$ and $\tilde{w}^{()} := D^{()}_{\mathcal{D}}\tilde{\mathscr{W}}^{\mathrm{SHP}}_{\omega,k}$, by the above discussion on Robertson Walker spacetimes their calculation can be reduced to the calculation of coincidence limit $\left[\tilde{w}^{(\eta\eta')}\right]_{\eta=\eta',r=0}$, $\left[\tilde{w}^{(\eta)}\right]_{\eta=\eta',r=0}$ and $\left[w^{()}\right]_{\eta=\eta',r=0}$. Furthermore, we can restrict $\mathcal{G}^s_k$, $\mathcal{D}\mathcal{G}^s_k$, and $\mathcal{D}\mathcal{D}'\mathcal{G}^s_k$ as distributions to the partial diagonal $\eta = \eta'$. For a Hadamard state, $\mathscr{W}_2^{\omega,\mathrm{s}}$ differs from $\mathcal{G}^s_k$ by a C^k function, so this also holds true for $\mathscr{W}_2^{\omega,\mathrm{s}}$; furthermore, since taking r-derivatives and restricting to $\eta = \eta'$ commutes, this also holds true for $w^{(\eta\eta')}$, $w^{(\eta)}$ and $w^{()}$.

The strategy to compute w^j, $j \in \{(\eta\eta'), (\eta), ()\}$ is now

1. Restrict w^j to the partial diagonal $\eta = \eta'$. One obtains a distribution in r, which is a difference of two distributions, the first given by a regularized integral and the second by a (regularized) asymptotic series expansion in r.

2. Rewrite the second term as an integral expression of a form similar to the first term plus a sufficiently often differentiable remainder term, depending on r. Combine the two integral expressions into one (which is finite for all r without regularization).

3. Now perform the r-derivatives on the obtained integral expression and the remainder term and finally set r equal to zero. One ends up with an expression of the expectation values as a sum of a one-dimensional integral and some η-dependent, finite term.

First we collect the expressions for the Hadamard parametrix and its first two “time”-derivatives restricted to a surface of constant conformal time in coordinate space.

5.3.2 Coordinate space expressions for $[\mathcal{G}_k^s]_{\eta=\eta'}$, $[\mathcal{D}\mathcal{G}_k^s]_{\eta=\eta'}$, $[\mathcal{D}\mathcal{D}'\mathcal{G}_k]_{\eta=\eta'}$

Using (5.2.1), (5.2.2) and Lemma 2.7 we get:

$$\begin{aligned}
[\mathcal{G}_k^s]_{\eta=\eta'} = \frac{1}{4\pi^2 C(\eta)}\Bigg(&\frac{1}{r_+^2} + [R_\Delta]_{\eta=\eta'} + \frac{1}{L^2}\sum_{j=0}^{k}\left(\frac{r^2}{L^2}\right)^j \left[\overset{o}{v}_j\right]_{\eta=\eta'} \ \mathrm{lo}_0 \\
&+ \frac{1}{L^2}\sum_{j=0}^{k}\left(\frac{r^2}{L^2}\right)^j \left[\overset{o}{v}_j \log(q)\right]_{\eta=\eta'} + \left[\rho^{k+1} R_v \log\sigma\right]_{\eta=\eta'}\Bigg) \\
[\mathcal{D}\mathcal{G}_k^s]_{\eta=\eta'} = \frac{1}{4\pi^2 C(\eta)}\Bigg(&\frac{1}{L^2}\sum_{j=0}^{k}\left(\frac{r^2}{L^2}\right)^j \left[\partial_\eta \overset{o}{v}_j\right]_{\eta=\eta'} \ \mathrm{lo}_0 + [\partial_\eta R_\Delta]_{\eta=\eta'} \\
&+ \frac{1}{L^2}\sum_{j=0}^{k}\left(\frac{r^2}{L^2}\right)^j \left(\left[\partial_\eta \overset{o}{v}_j \log(q)\right]_{\eta=\eta'} + \left[\overset{o}{v}_j \frac{\partial_\eta q}{q}\right]_{\eta=\eta'}\right) \\
&+ \left[\partial_\eta\left(\rho^{k+1} R_v \log\sigma\right)\right]_{\eta=\eta'}\Bigg) \\
[\mathcal{D}\mathcal{D}'\mathcal{G}_k^s]_{\eta=\eta'} = \frac{1}{4\pi^2 C(\eta)}\Bigg\{&-2\frac{1}{r_+^4} + 2\frac{\left[\overset{o}{v}_0\right]_{\eta=\eta'}}{L^2}\frac{1}{r_+^2} \\
&+ \frac{1}{L^2}\left(\sum_{j=0}^{k}\left(\frac{r^2}{L^2}\right)^j \left[\partial_\eta\partial_{\eta'}\overset{o}{v}_j\right]_{\eta=\eta'} + \frac{2}{L^2}\sum_{j=0}^{k-1}(j+1)\left(\frac{r^2}{L^2}\right)^j \left[\overset{o}{v}_{j+1}\right]_{\eta=\eta'}\right) \mathrm{lo}_0 \\
&+ \frac{2}{L^4}\sum_{j=0}^{k-1}\left(\frac{r^2}{L^2}\right)^j \left[\overset{o}{v}_{j+1}\right]_{\eta=\eta'} \\
&+ \frac{1}{L^2}\sum_{j=0}^{k}\left(\frac{2j}{L^2}\left(\frac{r^2}{L^2}\right)^{j-1}\left[\overset{o}{v}_j\right]_{\eta=\eta'} + \left(\frac{r^2}{L^2}\right)^j \left[\partial_{\eta\eta'}\overset{o}{v}_j\right]_{\eta=\eta'}\right)[\log q]_{\eta=\eta'} \\
&+ \frac{1}{L^2}\sum_{j=0}^{k}\Bigg(\left[\frac{(\partial_\eta q)\partial_{\eta'}\overset{o}{v}_j + (\partial_{\eta'} q)\partial_\eta \overset{o}{v}_j}{q}\right]_{\eta=\eta'} \\
&\qquad + \left[\left(\frac{\partial_{\eta\eta'} q}{q} - \frac{(\partial_\eta q)\partial_{\eta'} q}{q^2}\right)\overset{o}{v}_j\right]_{\eta=\eta'}\Bigg)\left(\frac{r^2}{L^2}\right)^j \\
&+ [\partial_{\eta\eta'} R_\Delta]_{\eta=\eta'} + \left[\partial_{\eta\eta'}\left(\rho^{k+1} R_v \log(\sigma)\right)\right]_{\eta=\eta'}\Bigg\}.
\end{aligned}$$

Introducing

$$\begin{aligned}
P_0^{()}(\eta) &= 1 \\
Q_j^{()}(\eta) &= \frac{\left[\overset{o}{v}_j\right]_{\eta=\eta'}}{L^2} \\
R_{\mathcal{G}_k}^{()}(\eta) &= [R_\Delta]_{\eta=\eta'} + \frac{1}{L^2}\sum_{j=0}^{k}\left(\frac{r^2}{L^2}\right)^j \left[\overset{o}{v}_j \log(q)\right]_{\eta=\eta'}
\end{aligned}$$

and

$$
\begin{aligned}
Q_j^{(\eta)}(\eta) =& \frac{\left[\partial_\eta \overset{o}{v}_j\right]_{\eta=\eta'}}{L^2} \\
R_{\mathcal{G}_k}^{(\eta)}(\eta) =& \left[\partial_\eta R_\Delta\right]_{\eta=\eta'} + \frac{1}{L^2}\sum_{j=0}^{k}\left(\frac{r^2}{L^2}\right)^j \left(\left[\partial_\eta \overset{o}{v}_j \log(q)\right]_{\eta=\eta'} + \left[\overset{o}{v}_j \frac{\partial_\eta q}{q}\right]_{\eta=\eta'}\right) \\
P_{-1}^{(\eta\eta')}(\eta) =& -2 \\
P_0^{(\eta\eta')}(\eta) =& \frac{2\left[\overset{o}{v}_0\right]_{\eta=\eta'}}{L^2} \\
Q_j^{(\eta\eta')}(\eta) =& \frac{1}{L^2}\left(\left[\partial_{\eta\eta'}\overset{o}{v}_j\right]_{\eta=\eta'} + \frac{2(j+1)}{L^2}\left[\overset{o}{v}_{j+1}\right]_{\eta=\eta'}\right) \qquad j=0,\dots,k-1 \\
Q_k^{(\eta\eta')}(\eta) =& \frac{\left[\partial_{\eta\eta'}\overset{o}{v}_k\right]_{\eta=\eta'}}{L^2} \\
R_{\mathcal{G}_k}^{(\eta\eta')}(\eta) =& \frac{1}{L^2}\left\{\frac{2}{L^2}\sum_{j=0}^{k-1}\left(\frac{r^2}{L^2}\right)^j \left[\overset{o}{v}_{j+1}\right]_{\eta=\eta'}\right. \\
& + \sum_{j=0}^{k}\left(\frac{2j}{L^2}\left(\frac{r^2}{L^2}\right)^{j-1}\left[\overset{o}{v}_j\right]_{\eta=\eta'} + \left(\frac{r^2}{L^2}\right)^j\left[\partial_{\eta\eta'}\overset{o}{v}_j\right]_{\eta=\eta'}\right)\left[\log q\right]_{\eta=\eta'} \\
& + \sum_{j=0}^{k}\left(\left[\frac{(\partial_\eta q)\partial_{\eta'}\overset{o}{v}_j + (\partial_{\eta'} q)\partial_\eta \overset{o}{v}_j}{q}\right]_{\eta=\eta'}\right. \\
& \left.\left. + \left[\left(\frac{\partial_{\eta\eta'} q}{q} - \frac{(\partial_\eta q)\partial_{\eta'} q}{q^2}\right)\overset{o}{v}_j\right]_{\eta=\eta'}\right)\left(\frac{r^2}{L^2}\right)^j\right\} \\
& + \left[\partial_{\eta\eta'} R_\Delta\right]_{\eta=\eta'}
\end{aligned}
$$

they can be written as

$$
\left[\mathcal{G}_k^s\right]_{\eta=\eta'} = \frac{1}{4\pi^2 C(\eta)}\left(\frac{P_0^{()}(\eta)}{r_+^2} + \sum_{j=0}^{k} Q_j^{()}(\eta)\left(\frac{r^2}{L^2}\right)^j \mathrm{lo}_0 + R_{\mathcal{G}_k}^{()}(\eta)\right) + o(\sigma^k) \tag{5.3.1}
$$

$$
\left[\mathcal{D}\mathcal{G}_k^s\right]_{\eta=\eta'} = \frac{1}{4\pi^2 C(\eta)}\left(\sum_{j=0}^{k} Q_j^{(\eta)}(\eta)\left(\frac{r^2}{L^2}\right)^j \mathrm{lo}_0 + R_{\mathcal{G}_k}^{(\eta)}(\eta)\right) + o(\sigma^k) \tag{5.3.2}
$$

$$
\begin{aligned}
\left[\mathcal{D}\mathcal{D}'\mathcal{G}_k\right]_{\eta=\eta'} =& \frac{1}{4\pi^2 C(\eta)}\left(\frac{P_{-1}^{(\eta\eta')}(\eta)}{r_+^4} + \frac{P_0^{(\eta\eta')}(\eta)}{r_+^2} + \sum_{j=0}^{k} Q_j^{(\eta\eta')}(\eta)\left(\frac{r^2}{L^2}\right)^j \mathrm{lo}_0 + R_{\mathcal{G}_k}^{(\eta\eta')}(\eta)\right) \\
& + o(\sigma^{k-1})\,.
\end{aligned} \tag{5.3.3}
$$

This shows, that the overall singularity structure of $[\mathcal{G}_k^s]_{\eta=\eta'}$ and $[\mathcal{D}\mathcal{G}_k^s]_{\eta=\eta'}$ agrees (with different smooth functions in front of the $\frac{1}{r_+^2}$ and $r^{2j}\mathrm{lo}_0$-terms) whereas $[\mathcal{D}\mathcal{D}'\mathcal{G}_k^s]_{\eta=\eta'}$ has the additional singular term $\frac{P_{-1}^{(\eta\eta')}}{r_+^4}$. The important observation is now, that terms with such a singularity structure can be generated by integrals resembling those appearing in the two-point function of homogeneous and isotropic states.

5.3.3 Corresponding integral expressions

To construct (regularized) integral expressions with the same singular part as (5.3.1)–(5.3.3), the following lemma is useful:

Lemma 5.5. *Let $\Omega : \mathbb{R} \to [1/m, \infty[$, $m > 0$, $z \in H_r := \{z \in \mathbb{C} \mid \mathrm{Re}\,(z) > 0\}$ and the asymptotic behaviour of Ω for $p \to \infty$ be given by:*

$$\Omega(p) = \sum_{j=-d}^{k} \frac{a_j}{p^j} + \mathcal{O}\left(\frac{1}{p^{k+1}}\right) .$$

Then for $L > 0$, $z \in H_r$, $\int_0^\infty e^{-pz}\Omega(t)\mathrm{d}p$ can be written as

$$\int_0^\infty e^{-pz}\Omega(p)\,\mathrm{d}p = \sum_{j=0}^{d} \frac{j!a_{-j}}{z^{j+1}} - E_{k-1}(z)\ln\left(\frac{z}{L}\right) + \tilde{R}_{\Omega,L}^{(k-1)}(z)$$
$$E_{k-1}(z) = \sum_{j=0}^{k-1} \frac{(-z)^j a_{j+1}}{j!}$$

where $\tilde{R}_{\Omega,L}^{(k-1)}$ is an analytic functions on H_r, such that the limit $\epsilon \to 0$ of the function $R_{\Omega,L,\epsilon}^{(k-1)} : \mathbb{R} \ni r \mapsto \tilde{R}_{\Omega,L}^{(k-1)}(\epsilon + ir)$ in the sense of distributions is given by a C^{k-1}-function $R_{\Omega,L}^{(k-1)}$ with asymptotic expansion

$$R_{\Omega,L}^{(k-1)}(r) = \sum_{l=0}^{k-1} R_l \frac{(-ir)^l}{l!} + o(r^{k-1})$$
$$R_l = \lim_{M\to\infty}\left(\int_0^M p^l\left(\Omega(p) - \sum_{j=0}^{d} a_{-j}p^j\right)\mathrm{d}p - \sum_{j=1}^{l}\frac{a_{l+1-j}}{j}M^j - a_{l+1}\log(ML)\right)$$
$$+ a_{l+1}\left(-\gamma + \sum_{n=1}^{l}\frac{1}{n}\right).$$

Proof. See appendix. □

Consider now for $\epsilon > 0$ the integral

$$W_{\Omega,\epsilon}(\mathbf{x}) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{-p\epsilon} e^{i\mathbf{px}} \Omega(p) \mathrm{d}^3\mathbf{p}$$

where $p = \|\mathbf{p}\|$. Introducing spherical coordinates in $\mathbf{x}$ direction ($r := \|\mathbf{x}\|$), this integral can be reduced to

$$4\pi^2 W_{\Omega,\epsilon}(\mathbf{x}) = \frac{1}{ir} \int_{\mathbb{R}^+} e^{-p(\epsilon - ir)} \Omega(p) p \mathrm{d}p - \frac{1}{ir} \int_{\mathbb{R}^+} e^{-p(\epsilon + ir)} \Omega(p) p \mathrm{d}p \,. \tag{5.3.4}$$

For comparison with (5.3.1)–(5.3.3), we need to look at the limits $\epsilon \to 0$ of $W_{\Omega,\epsilon}$ for Ω whose asymptotic expansion starts with the linear term in p and only contains odd powers of p. The following lemma gives the resulting limit expression in this case.

Lemma 5.6. *Let $\Omega : \mathbb{R}^+ \to \mathbb{R}$ have asymptotic behaviour*

$$\Omega(p) = \sum_{j=-1}^{k'} \frac{b_j}{p^{2j+1}} + \mathcal{O}\left(\tfrac{1}{p^{2k'+3}}\right)$$

Then for $h \in \mathbb{C}_0^\infty(\mathbb{R}^3)$ and $W_{\Omega,\epsilon}(h) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} W_{\Omega,\epsilon}(\mathbf{x}) h(\mathbf{x}) \mathrm{d}^3\mathbf{x}$ the distribution $\tilde{W}_{\Omega,+}$, defined for $h \in C_0^\infty(\mathbb{R}^3)$ as $\lim_{\epsilon\to 0} W_{\Omega,\epsilon}(h)$ is given by

$$\begin{aligned}
\tilde{W}_{\Omega,+}(h) =& \frac{1}{2\pi^2}\left(-2\frac{b_{-1}}{r_+^4}(h) + \frac{b_0}{r_+^2}(h) + V^{k'-1}\mathrm{lo}(h) + \mathcal{R}_{\Omega,L}^{(2k'-1)}(h)\right) \\
V^{k'-1}\mathrm{lo}(h) =& -\int_0^\infty \sum_{l=0}^{k'-1} \frac{b_{l+1}}{(2l+1)!} (-r^2)^l \log\left(\tfrac{r}{L}\right) h(r) r^2 \mathrm{d}r \\
\mathcal{R}_{\Omega,L}^{(2k'-1)}(h) =& \int_{\mathbb{R}^+} R_{\Omega,L}^{(2k'-1)}(r) r^2 h(r) \mathrm{d}r \,.
\end{aligned}$$

Here $R_{\Omega,L}^{(2k'-1)}$ is a $2k'-1$ times continuously differentiable function with asymptotics given by

$$\begin{aligned}
R_{\Omega,L}^{(2k'-1)}(r) =& \sum_{l=0}^{k'-1} \frac{R_{2l+1}}{(2l+1)!} (-r^2)^l + o(r^{2k'-1}) \\
R_{2l+1} =& \lim_{M\to\infty} \left(\int_0^M p^{2l+1} \Big(p\Omega(p) - b_{-1}p^2 - b_0 \Big) \mathrm{d}p - \sum_{j=1}^{l} \frac{b_{l+1-j}}{2j} M^{2j} - b_{l+1} \log(ML) \right) \\
&+ b_{l+1} \left(-\gamma + \sum_{n=1}^{2l+1} \frac{1}{n} \right)
\end{aligned}$$

Proof. By (5.3.4) and assuming wlog h to be spherically symmetric, we have

$$4\pi^2 W_{\Omega,\epsilon}(h) = \int_{\mathbb{R}^+} \left(ir \int_{\mathbb{R}^+} e^{-p(\epsilon + ir)} \Omega(p) p \mathrm{d}p - ir \int_{\mathbb{R}^+} e^{-p(\epsilon - ir)} \Omega(p) p \mathrm{d}p \right) h(r) \mathrm{d}r$$

Applying the preceding lemma with $z = \epsilon + ir$ and $z = \epsilon - ir$ we get

$$
\begin{aligned}
ir\int_{\mathbb{R}^+} e^{-p(\epsilon+ir)}\Omega(p)p\mathrm{d}p - ir\int_{\mathbb{R}^+} e^{-p(\epsilon-ir)}\Omega(p)p\mathrm{d}p = & \frac{2ib_{-1}r}{(ir+\epsilon)^3} + \frac{2ib_{-1}r}{(ir-\epsilon)^3} + \dots \\
& + \frac{ib_0 r}{ir+\epsilon} + \frac{ib_0 r}{ir-\epsilon} \\
& + ir\sum_{l=0}^{k'-1}\frac{b_{l+1}}{(2l+1)!}\left((\epsilon+ir)^{2l+1}\ln\left(\tfrac{\epsilon+ir}{L}\right) - (\epsilon-ir)^{2l+1}\ln\left(\tfrac{\epsilon-ir}{L}\right)\right) \\
& + ir(\tilde{R}^{(2k'-1)}_{\Omega,L}(\epsilon+ir) - \tilde{R}^{(2k'-1)}_{\Omega,L}(\epsilon-ir)) \\
=& 2b_{-1}\left(\frac{ir}{(ir+\epsilon)^3} + \frac{ir}{(ir-\epsilon)^3}\right) + 2b_0\frac{r^2}{r^2+\epsilon^2} \\
& + \sum_{l=0}^{k'-1}\frac{b_{l+1}}{(2l+1)!}(-r^2)^{l+1}\log\left(\frac{r^2+\epsilon^2}{L^2}\right) \\
& + r^2\epsilon^2\sum_{l=0}^{k'-1}\sum_{n=0}^{l-1}\binom{2l+1}{2n+2}\epsilon^{2n}(-r^2)^{l-n}\log\left(\tfrac{r^2+\epsilon^2}{L^2}\right) \\
& + i\epsilon r\sum_{l=0}^{k'-1}\sum_{n=0}^{l}\binom{2l+1}{2n+1}\epsilon^{2n}(-r^2)^{l-n}\log\left(\frac{\epsilon+ir}{\epsilon-ir}\right) \\
& + ir(\tilde{R}^{(2k'-1)}_{\Omega,L}(\epsilon+ir) - \tilde{R}^{(2k'-1)}_{\Omega,L}(\epsilon-ir))\,.
\end{aligned} \tag{5.3.5}
$$

Consider first the most singular term $2b_{-1}\left(\frac{ir}{(ir+\epsilon)^3} + \frac{ir}{(ir-\epsilon)^3}\right)$. For the integral against h we have by repeated partial integration

$$
\begin{aligned}
2ib_{-1}\int_{\mathbb{R}^+}\left(\frac{1}{(ir+\epsilon)^3} + \frac{1}{(ir-\epsilon)^3}\right)rh(r)\mathrm{d}r =& b_{-1}\int_{\mathbb{R}^+}\left(\frac{1}{(ir+\epsilon)^2} + \frac{1}{(ir-\epsilon)^2}\right)\partial_r(rh(r))\mathrm{d}r \\
=& -ib_1\int_{\mathbb{R}^+}\left(\frac{1}{ir+\epsilon} + \frac{1}{ir-\epsilon}\right)\partial_{rr}(rh(r))\mathrm{d}r \\
=& -2b_1\int_{\mathbb{R}^+}\frac{1}{r^2+\epsilon^2}\left(\partial_{rr}h(r) + \frac{2}{r}\partial_r h(r)\right)r^2\mathrm{d}r \\
=& -\frac{4b_{-1}}{r_+^4}(h)\,.
\end{aligned}
$$

Since for $r, \epsilon > 0$, $\left|\log\left(\frac{\epsilon+ir}{\epsilon-ir}\right)\right| < \pi$ and $\left|r^2\log\left(\frac{r^2+\epsilon^2}{L^2}\right)\right| \le r^2\left|\log(r^2/L^2)\right| + \epsilon^2$, the only other terms left after integrating against $h(r)$ and performing the limit $\epsilon \to 0$ are the next three and we are thus left with

$$
\begin{aligned}
\lim_{\epsilon\to 0} W_{\Omega,\epsilon}(h) =& -\frac{2b_1}{4\pi^2}\int_{\mathbb{R}^+}\frac{1}{r^2+\epsilon^2}\left(\partial_{rr}h(r) + \frac{2}{r}\partial_r h(r)\right)r^2\mathrm{d}r + \frac{2b_0}{4\pi^2}\int_{\mathbb{R}^+}h(r)\mathrm{d}r \\
& + \frac{1}{4\pi^2}\int_{\mathbb{R}^+}V^{(k'-1)}(r)\log\left(\frac{r^2}{L^2}\right)r^2h(r)\mathrm{d}r + \frac{1}{2\pi^2}\int_{\mathbb{R}^+}R^{(2k'-1)}_{\Omega,L}(r)r^2h(r)\mathrm{d}r\,.
\end{aligned}
$$

The statements concerning the $C^{2k'-1}$ remainder term finally follow from the statements on the limits of $\tilde{R}^{(2k'-1)}_{\Omega,L}(\epsilon \pm ir)$ for $\epsilon \to 0$ and the formula for its asymptotics, given in the preceding lemma. □

Comparing this with (5.3.1)-(5.3.3), we see that by choosing $k' = k+1$ and an Ω with the right coefficients b_j, the distribution $W_{\Omega,+}$ which has $\tilde{W}_{\Omega,+}$ as its symmetry-reduced distribution can be made to agree with $[\mathcal{G}^s_k]_{\eta=\eta'}$, $[\mathcal{D}\mathcal{G}^s_k]_{\eta=\eta'}$ or $[\mathcal{D}\mathcal{D}'\mathcal{G}^s_k]_{\eta=\eta'}$ up to a C^{2k+1}-function. More precisely, for functions $\Omega^{()}$, $\Omega^{(\eta)}$ and $\Omega^{(\eta\eta')}$[4] with asymptotic expansions as specified in lemma 5.6, where the coefficients $b^{()}_j(\eta)$, $b^{(\eta)}_j(\eta)$ and $b^{(\eta\eta')}_j(\eta)$ are given by ($b^{()}_{-1} = b^{(\eta)}_{-1} = b^{(\eta)}_0 = 0$):

$$b^{()}_0(\eta) = \frac{P^{()}_0(\eta)}{2} = \frac{1}{2} \tag{5.3.6}$$

$$b^{()}_{l+1}(\eta) = (2l+1)!(-1)^{l+1}\frac{Q^{()}_l(\eta)}{L^{2l}} = (2l+1)!(-1)^{l+1}\frac{[\overset{o}{v}_l]_{\eta=\eta'}}{L^{2(l+1)}} \tag{5.3.7}$$

$$b^{(\eta)}_{l+1}(\eta) = (2l+1)!(-1)^{l+1}\frac{Q^{(\eta)}_l(\eta)}{L^{2l}} = (2l+1)!(-1)^{l+1}\frac{[\partial_\eta \overset{o}{v}_l]_{\eta=\eta'}}{L^{2(l+1)}} \tag{5.3.8}$$

$$b^{(\eta\eta')}_{-1}(\eta) = -\frac{P^{(\eta\eta')}_{-1}(\eta)}{4} = \frac{1}{2} \tag{5.3.9}$$

$$b^{(\eta\eta')}_0(\eta) = \frac{P^{(\eta\eta')}_0(\eta)}{2} = \frac{[\overset{o}{v}_0]_{\eta=\eta'}}{L^2} \tag{5.3.10}$$

$$\begin{aligned} b^{(\eta\eta')}_{l+1}(\eta) &= (2l+1)!(-1)^{l+1}\frac{Q^{\eta\eta'}_l(\eta)}{L^{2l}} \\ &= (2l+1)!(-1)^{l+1}\left(\frac{[\partial_{\eta\eta'}\overset{o}{v}_l]_{\eta=\eta'}}{L^{2(l+1)}} + \frac{2(l+1)[\overset{o}{v}_{l+1}]_{\eta=\eta'}}{L^{2(l+2)}}\right) \end{aligned} \tag{5.3.11}$$

($l \in \{0, \ldots, k\}$), we have for $W_{\Omega^{()},+}$, $W_{\Omega^{(\eta)},+}$, $W_{\Omega^{(\eta\eta')},+}$, the distributions corresponding to the symmetry reduced distributions $\tilde{W}_{\Omega^{()}(\eta),+}$, $\tilde{W}_{\Omega^{(\eta)}(\eta),+}$, $\tilde{W}_{\Omega^{(\eta\eta')}(\eta),+}$:

$$\frac{W_{\Omega^{()},+}}{C(\eta)} - [\mathcal{G}^s_k]_{\eta=\eta'} = \frac{1}{4\pi^2 C(\eta)}\underbrace{\left(2R^{(k)}_{\Omega^{()},L} - R^{()}_{\mathcal{G}_k}(\eta)\right)}_{=:R^{()}(\eta)} + o(\sigma^k) \tag{5.3.12}$$

$$\frac{W_{\Omega^{(\eta)},+}}{C(\eta)} - [\partial_\eta\mathcal{G}^s_k]_{\eta=\eta'} = \frac{1}{4\pi^2 C(\eta)}\underbrace{\left(2R^{(k)}_{\Omega^{(\eta)},L} - R^{(\eta)}_{\mathcal{G}_k}(\eta)\right)}_{=:R^{(\eta)}(\eta)} + o(\sigma^k) \tag{5.3.13}$$

$$\frac{W_{\Omega^{(\eta\eta')},+}}{C(\eta)} - [\partial_\eta\partial_{\eta'}\mathcal{G}^s_k]_{\eta=\eta'} = \frac{1}{4\pi^2 C(\eta)}\underbrace{\left(2R^{(k)}_{\Omega^{(\eta\eta')},L} - R^{(\eta\eta')}_{\mathcal{G}_k}(\eta)\right)}_{=:R^{(\eta\eta')}(\eta)} + o(\sigma^{k-1})\,. \tag{5.3.14}$$

[4]Actually $\Omega^{(\eta)}$ depends on the conformal time η describing the surface to which we restrict; this dependence will be suppressed here, since the whole calculation takes place on one, fixed surface of constant η and the important dependence of the Ωs is that on p. In the same way we will also suppress the η-dependence of the integral kernels $K^{()}$, $K^{(\eta)}$ and $K^{(\eta\eta')}$ below, whereas for the b_j and $R^{()}$, $R^{(\eta)}$ and $R^{(\eta\eta')}$, which only depend on η, we will carry it along.

As described in chapter 2, the states under consideration are determined by a two-point function with symmetric part

$$\mathscr{W}_2^{\omega,\mathrm{s}}(f_1,f_2) = \int_{\mathbb{R}^3}\int_I\int_I \Xi(p)\left[V_p(\eta)\overline{V_p}(\eta') + \overline{V_p}(\eta)V_p(\eta')\right] \\ \ldots \times \overline{\hat{\hat{f}}}_1(\eta,\mathbf{p})\hat{f}_2(\eta',\mathbf{p})C^{3/2}(\eta)\mathrm{d}\eta\, C^{3/2}(\eta')\mathrm{d}\eta'\,\mathrm{d}\mathbf{p} \quad (5.3.15)$$

with restriction given by the formulas (2.2.30)–(2.2.32). On the other hand, for $W_{\Omega,\epsilon}(h)$, $h\in C_0^\infty(\mathbb{R}^3)$ we have

$$W_{\Omega,\epsilon}(h) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} e^{-\epsilon\|\mathbf{p}\|}e^{i\mathbf{p}\mathbf{x}}\Omega(p)h(\mathbf{x})\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{x}\,.$$

Due to the compact support of h and the decay of $e^{-\epsilon p}$ for $p\to\infty$, we can interchange the integration order and perform the limit $\epsilon\to 0$ under the integral and end up with

$$\tilde{W}_{\Omega,+}(h) = \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\check{h}(\mathbf{p})\Omega(p)\mathrm{d}\mathbf{p}\,,$$

where $\check{h}$ is the inverse Fourier transform of h, which shows that Ω is just the Fourier transform (up to the factor $\frac{1}{(2\pi)^{3/2}}$) of the symmetry reduced distribution $\tilde{W}_{\Omega,+}$, considered as a distribution on $\mathbb{R}^3$.
For the Fourier transform of $\mathcal{K} := \left[\tilde{\mathscr{W}}_2^{\omega,\mathrm{s}}\right]_{\eta=\eta'} - C^3(\eta)\tilde{W}_{\Omega^{()},+}$ in the sense of distributions this means:

$$\hat{\mathcal{K}}(h) = \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\left(2\Xi(p)\left|V_p(\eta)\right|^2 - \Omega^{()}(p)\right)C^3(\eta)h(\mathbf{p})\mathrm{d}\mathbf{p}\,.$$

To proceed, we now need some information about $\mathcal{K}$, which is an object defined on a whole surface of constant η and not just in a convex, normal neighbourhood.

As one of the first applications of the reformulation of the Hadamard condition, it was shown that two-point functions $\mathscr{W}_2^\omega$ of Hadamard states are actually smooth functions for arguments x, x', which are not spacelike related [Rad96a], so on the surfaces of constant η, which are Cauchy surfaces, except for coinciding arguments $\mathscr{W}_2^{\omega,\mathrm{s}}$ is smooth, so $\tilde{\mathscr{W}}_2^{\omega,\mathrm{s}}$ is smooth except at the origin. On the other hand, we know from lemma 5.6 that also $\tilde{W}_{\Omega^{()},+}$ is C^{2k+1} ($k=k'+1$ as above the order, to which the asymptotic condition on $\Omega^{()}$ as a function of the argument p, here suppressed, is satisfied). $\mathcal{K}$ is thus actually a C^{2k+1} function on $\mathbb{R}^3$, because the matching between $\tilde{\mathscr{W}}_2^{\omega,\mathrm{s}}$ and $\tilde{W}_{\Omega^{()},+}$ was done precisely in such a way that the singularities of the two functions at the origin cancel to this order. This implies that the limit

$$\lim_{\epsilon\to 0}\mathcal{K}\left(\frac{h(x/\epsilon)}{\epsilon}\right) = \lim_{\epsilon\to 0}\frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\check{h}(\epsilon\mathbf{p})\left(2\Xi(p)\left|V_p(\eta)\right|^2 - \Omega^{()}(p)\right)C^3(\eta)\mathrm{d}\mathbf{p} \quad (5.3.16)$$

exists for all $h\in C_0^\infty(\mathbb{R}^3)$ (this is just the value of the C^{2k+1}-function $\mathcal{K}$ at the origin), so in this weak sense the integral

$$\int_{\mathbb{R}^3} 2\Xi(p)\left|V_p(\eta)\right|^2 - \Omega(p)\mathrm{d}\mathbf{p} \quad (5.3.17)$$

exists. By differentiating $\mathcal{K}$ up to $2k+1$-times, even the limits in this sense with an additional factor p^l for $l \leq 2k+1$ in the integrand exist and define the functions $\partial_r^l \mathcal{K}$ (and this is one of the necessary condition, the restriction of the two-point function of a Hadamard state to a surface of constant η has to satisfy).

To get convergence of these integrals in the L^1-sense, we however need an additional assumption. A sufficient condition is that $\mathcal{K}$ and its derivatives are in fact L^1; we then get by the Riemann-Lebesgue lemma [Hör03] that $p^{2k+1}\left(\Xi(p)\,|V_p(\eta)|^2 - \Omega^{()}(p)\right)$ goes to zero for $p \to \infty$. Taking smooth functions $p \mapsto \Omega^{()}(p)$, decay of the term $\tilde{W}_{\Omega^{()},+}$ is guaranteed; a construction achieving this is presented in section 5.3.6, where $\Omega^{()}$ is constructed as a sum of terms $p \mapsto (A+p^2)^{-l-1/2}$, $A > 0$ and $l \in \mathbb{N}$. Relating the resulting $\tilde{W}_{\Omega^{()},+}$ to Bessel-functions by [Ste84, 9.6.25], one can even show exponential decay in this case. The L^1-condition is therefore a decay condition on the two-point function of the state at spatial separation. On Minkowski spacetime such conditions are well known and for important states they were shown to hold [AHR62, Jak98], on curved spacetimes much less seems to be known (probably also due to the fact that in cases of spacetimes with more general structure than the rather special Robertson Walker spacetimes considered here, it is hard to even formulate, what "decay for big spatial distances" is supposed to mean). Nevertheless, in calculations of the stress-energy tensor using adiabatic renormalization in the literature, it is usually assumed without comment that the integrals (5.3.17) exist (at least as improper Riemann integrals). From here on we will also assume that the integrals exist as L^1-integrals; this can be seen to be true in the example below and can (to finite order) also be achieved for the initial values of the LTE-states constructed below.

We then get

$$\left([\mathscr{W}_2^{\omega,\mathrm{s}}]_{\eta=\eta'} - \frac{W_{\Omega^{()}}}{C(\eta)}\right)(\mathbf{x},\mathbf{x}') = \frac{1}{(2\pi)^3 C(\eta)} \int_{\mathbb{R}^3} e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')} \underbrace{\left(2\Xi(p)|V_p(\eta)|^2 - \Omega^{()}(\mathbf{p})\right)}_{=:K^{()}(p)} \mathrm{d}\mathbf{p}$$

(since this is the C^{2k+1}-function evaluated at $(\mathbf{x},\mathbf{x}') \in \mathbb{R}^3 \times \mathbb{R}^3$, the terms $C^4(\eta)$ from the volume-element in the corresponding regular distributions are now missing).

First taking derivatives in the sense of distributions but otherwise proceeding in the same way, we get

$$\left([\mathcal{D}\mathscr{W}_2^{\omega,\mathrm{s}}]_{\eta=\eta'} - \frac{W_{\Omega^{(\eta)}}}{C(\eta)}\right)(\mathbf{x},\mathbf{x}') = \frac{1}{(2\pi)^3 C(\eta)} \int_{\mathbb{R}^3} e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')} \times \dots$$
$$\dots \times \underbrace{\left(\Xi(p)\left(V_p'(\eta)\overline{V_p}(\eta) + V_p(\eta)\overline{V_p'}(\eta)\right) - \Omega^{(\eta)}(p)\right)}_{=:K^{(\eta)}(p)} \mathrm{d}\mathbf{p}$$

$$\left([\mathcal{D}\mathcal{D}'\mathscr{W}_2^{\omega,\mathrm{s}}]_{\eta=\eta'} - \frac{W_{\Omega^{(\eta\eta')}}}{C(\eta)}\right)(\mathbf{x},\mathbf{x}') = \frac{1}{(2\pi)^3 C(\eta)} \int_{\mathbb{R}^3} 2e^{i\mathbf{p}(\mathbf{x}-\mathbf{x}')}$$
$$\dots \times \underbrace{\left(2\Xi(p)|V_p'(\eta)|^2 - \Omega^{(\eta\eta')}(p)\right)}_{=:K^{(\eta\eta')}(p)} \mathrm{d}\mathbf{p}\,.$$

In the calculation of expectation values of Wick products we will need the partial restrictions $\left[\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}= [\mathscr{W}^{\omega,\mathrm{s}}_2 - \mathcal{G}^s_k]_{\eta=\eta'}$, $\left[\mathcal{D}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}= [\mathcal{D}\left(\mathscr{W}^{\omega,\mathrm{s}}_2 - \mathcal{G}^s_k\right)]_{\eta=\eta'}$ and $\left[\mathcal{D}\mathcal{D}'\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}= [\mathcal{D}\mathcal{D}'\left(\mathscr{W}^{\omega,\mathrm{s}}_2 - \mathcal{G}^s_k\right)]_{\eta=\eta'}$, but using (5.3.12)–(5.3.14) they can be written as

$$
\begin{aligned}
\left[\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'} &= [\mathscr{W}^{\omega,\mathrm{s}}_2]_{\eta=\eta'} - \frac{W_{\Omega^{()}}}{C(\eta)} + \frac{R^{()}(\eta)}{4\pi^2 C(\eta)}\\
\left[\mathcal{D}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'} &= [\mathcal{D}\mathscr{W}^{\omega,\mathrm{s}}_2]_{\eta=\eta'} - \frac{W_{\Omega^{(\eta)}}}{C(\eta)} + \frac{R^{(\eta)}(\eta)}{4\pi^2 C(\eta)}\\
\left[\mathcal{D}\mathcal{D}'\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'} &= [\mathcal{D}\mathcal{D}'\mathscr{W}^{\omega,\mathrm{s}}_2]_{\eta=\eta'} - \frac{W_{\Omega^{(\eta\eta')}}}{C(\eta)} + \frac{R^{(\eta\eta')}(\eta)}{4\pi^2 C(\eta)}\,.
\end{aligned}
$$

5.3.4 Conditions on Hadamard states

As discussed in the the last section, from the fact that the distributions $\left[\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}$, $\left[\mathcal{D}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}$ and $\left[\mathcal{D}\mathcal{D}'\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{\eta=\eta'}$ are C^{2k+1} functions on $\mathbb{R}^3$, we can infer the existence of certain integrals ("improper" in the sense of equation (5.3.16)) over $p \mapsto p^{2k+1}K^{()}(p)$, $p \mapsto p^{2k+1}K^{(\eta)}(p)$ and $p \mapsto p^{2k-1}K^{(\eta\eta')}(p)$.

In the case where we have smooth $\Omega^{()}$, $\Omega^{(\eta)}$ and $\Omega^{(\eta\eta)}$ and a L^1-condition on the spatial derivatives of the restrictions of $\mathscr{W}^{\omega,\mathrm{s}}_2$, $\mathcal{D}\mathscr{W}^{\omega,\mathrm{s}}_2$ and $\mathcal{D}\mathcal{D}'\mathscr{W}^{\omega,\mathrm{s}}_2$ to the surface of constant η, the functions $p \mapsto K^{()}(p)$, $p \mapsto K^{(\eta)}(p)$ and $p \mapsto K^{(\eta\eta')}(p)$ have to be at least $o(p^{-2k-1})$ respectively $o(p^{-2k+1})$. As far as the $\Omega^{()}$, $\Omega^{(\eta)}$ and $\Omega^{(\eta\eta')}$) are concerned, only their asymptotic behaviour for $p \to \infty$ is prescribed, but this is done in a consistent way in the sense that for $\Omega^{()}(\eta)$, $\Omega^{()}{}'(\eta)$ belonging to $\mathcal{G}^s_k$ and $\mathcal{G}^s_{k'}$ with $k' > k$ there holds $[\Omega^{()}{}'(\eta) - \Omega^{()}(\eta)](p) \sim o(p^{-2k'-1})$, so the lower orders in $\frac{1}{p}$ agree. For a Hadamard state, therefore the functions $p \mapsto 2\Xi(p)|V_p(\eta)|^2$, $p \mapsto \Xi(p)\left(V'_p(\eta)\overline{V_p}(\eta) + V_p(\eta)\overline{V'_p(\eta)}\right)$ and $p \mapsto 2\Xi(p)|V'_p(\eta)|^2$ have the same asymptotics for $p \to \infty$ as the functions $\Omega^{()}$, $\Omega^{(\eta)}$ and $\Omega^{(\eta\eta')}$ respectively. By (5.3.6)–(5.3.11) this means

$$
2\Xi(p)|V_p(\eta)|^2 \sim \frac{1}{2p} + \sum_{l=0}^{\infty}(2l+1)!(-1)^{l+1}\frac{\left[\overset{o}{v}_l\right]_{\eta=\eta'}}{L^{2(l+1)}p^{2l+3}} \tag{5.3.18}
$$

$$
2\Xi(p)\mathrm{Re}\left(V'_p(\eta)\overline{V_p}(\eta)\right) \sim \sum_{l=0}^{\infty}(2l+1)!(-1)^{l+1}\frac{\left[\partial_\eta\overset{o}{v}_l\right]_{\eta=\eta'}}{L^{2(l+1)}p^{2l+3}} \tag{5.3.19}
$$

$$
\begin{aligned}
2\Xi(p)|V'_p(\eta)|^2 \sim{}& \frac{p}{2} + \frac{\left[\overset{o}{v}_0\right]_{\eta=\eta'}}{L^2 p}\\
&+ \sum_{l=0}^{\infty}\frac{(2l+1)!(-1)^{l+1}}{p^{2l+3}}\left(\frac{\left[\partial_{\eta\eta'}\overset{o}{v}_l\right]_{\eta=\eta'}}{L^{2(l+1)}} + \frac{2(l+1)\left[\overset{o}{v}_{l+1}\right]_{\eta=\eta'}}{L^{2(l+2)}}\right).
\end{aligned} \tag{5.3.20}
$$

By (5.2.15) and (5.2.16), the terms appearing in this asymptotic expansion can be calculated purely from $Q_{m,\xi}$; for $2\Xi(p)|V_p(\eta)|^2$ and $2\Xi(p)|V_p'(\eta)|^2$ the first few terms are e.g. given by

$$2\Xi(p)|V_p(\eta)|^2 \sim \frac{1}{2p} - \frac{Q_{m,\xi}(\eta)}{4p^3} + \frac{Q''_{m,\xi}(\eta) + 3Q^2_{m,\xi}(\eta)}{16p^5} - \dots \tag{5.3.21}$$

$$2\Xi(p)|V_p'(\eta)|^2 \sim \frac{p}{2} + \frac{Q_{m,\xi}}{4p} - \frac{1}{p^3}\left(\frac{Q''_{m,\xi}(\eta) + Q^2_{m,\xi}(\eta)}{16}\right) + \dots \tag{5.3.22}$$

In the cases where explicit analytic expressions for the $\overset{o}{v}_j$ for all $j \in \mathbb{N}$ can be obtained, this completely prescribes the asymptotics for Ξ and the initial values $|V_p(\eta)|^2$ and $|V_p'(\eta)|^2$. The construction of candidates for Hadamard states satisfying L^1-conditions can then be reduced to finding functions with this asymptotic behaviour for some $\eta = \eta_0$ (which one can try to tackle by using resummation techniques) and using these functions as Ξ, respectively initial values for the mode-functions V_p. But even when one is not able to obtain explicit analytic expressions for the $\overset{o}{v}_j$, this procedure still gives an easy criterion (the procedure to obtain $[\overset{o}{v}_j]_{\eta=\eta'}$ by the recursion relations (5.2.15), (5.2.16) can be implemented on computer algebra systems without much effort) for the asymptotics of the initial values for $|V_p|^2$ and $|V_p'(\eta)|^2$, which leads to states with the same regularity properties as adiabatic vacua (a bit more on that below). Compared to the adiabatic vacuum construction, (5.2.15) and (5.2.16) are however much simpler to handle; furthermore, since it is clear from the outset that only requirements on the asymptotic behaviour of Ξ and the initial value functions $V_p(\eta_0)$ and $V_p'(\eta_0)$ (for $p \to \infty$) are imposed, all questions regarding values for these functions for finite values of p are clearly separated from the outset. Adding e.g. a function of p that vanishes quicker than any inverse power of p for $p \to \infty$ will not change the asymptotics at all and a similar procedure will in fact be used to construct LTE states.

There is one interesting point which should be mentioned here, especially since its discussion also sheds some light on the relation to adiabatic vacua: a priori (5.3.18)–(5.3.20) are three independent conditions; however for a Fock state we have $\Xi = 1/2$ and since there exist Hadamard Fock states assuming that they in fact lead to absolutely convergent integrals as discussed above, it has to be possible to satisfy all *three* relations by just choosing the *two* initial-value function $p \mapsto V_p(\eta_0)$ and $p \mapsto V_p'(\eta_0)$.

Using the Wronski determinant condition (2.2.24), we get for mode functions V_p:

$$\begin{aligned}\left(V_p'\overline{V_p} + \overline{V_p}'V_p\right)^2 =& (2\overline{V_p}'V_p + i)(2V_p'\overline{V_p} - i)\\ =& 4\,|V_p|^2\,|V_p|^2 + 2i\left(V_p'\overline{V_p} - \overline{V_p}'V_p\right) + 1\\ =& 4\left|V_p'\right|^2|V_p|^2 - 1\\ \Rightarrow \left(\mathrm{Re}\,\left(V_p\overline{V_p}'\right)\right)^2 =& \left|V_p'\right|^2|V_p|^2 - \frac{1}{4}\end{aligned} \tag{5.3.23}$$

But setting $\Xi = \frac{1}{2}$ in (5.3.18)–(5.3.20), this means that the product of the rhs. of the first and third equation have to have the same asymptotics as $\frac{1}{4}$ plus the rhs. of the second equation squared. That such a relation in fact holds to the first few orders in $\frac{1}{p}$ can be checked by explicit calculation (using a computer-algebra system this was actually checked to order $\frac{1}{p^{10}}$), establishing such a relation would be interesting for the following reason: If we denote a function $|V_p|^2$ satisfying the asymptotic condition (5.3.18) up to order $\frac{1}{p^{2k+3}}$ for all $\eta \in \hat{I}$ by $w_p^{(k)}$ and set for some $\eta_0 \in \hat{I}$

$$V_p^{(k)}(\eta) = \sqrt{w_p^{(k)}(\eta)}\; e^{i\int_{\eta_0}^{\eta} \frac{\mathrm{d}\tilde{\eta}}{4w_p^{(k)}(\tilde{\eta})}} ,$$

then this function has the property:

$$V_p^{(k)\prime}(\eta) = \left(\frac{w_p^{(k)\prime}(\eta)}{2\sqrt{w_p^{(k)}(\eta)}} + \frac{i}{4\sqrt{w_p^{(k)}(\eta)}} \right) e^{i\int_{\eta_0}^{\eta} \frac{\mathrm{d}\tilde{\eta}}{4w_p^{(k)}(\tilde{\eta})}} ,$$

which implies

$$\left|V_p^{(k)\prime}(\eta)\right|^2 = \left(\frac{\left(w_p^{(k)\prime}(\eta)\right)^2}{4w_p^{(k)}(\eta)} + \frac{1}{4w_p^{(k)}(\eta)} \right)$$

Using that the rhs of (5.3.19) is obtained from (5.3.18) by taking η-derivatives (and multiplying with $\frac{1}{2}$), we get that the rhs of (5.3.19) has the same asymptotics to order k as $w_p^{(k)\prime}(\eta)/2$ and our assumed property then takes the form

$$\left|V_p^{(k)}(\eta)'\right|^2 w_p^{(k)}(\eta) - \frac{1}{4} \sim \left(w_p^{(k)\prime}(\eta)\right)^2/4 ;$$

but this implies that $\left|V_p^{(k)\prime}(\eta)\right|^2$ and $\left|V_p'(\eta)\right|^2$ have the same asymptotics, so in fact a $V_p(\eta)$ with the asymptotics required by (5.3.18)–(5.3.20) can be obtained by setting $V_p(\eta) = V_p^{(k)}(\eta)$, $V_p'(\eta) = V_p^{(k)\prime}(\eta)$, where the $V_p^{(k)}(\eta)$ is fixed by (5.3.18) *only*. One can thus reduce the problem to the specification of the single function $w_p^{(k)}(\eta)$ and its derivative $w_p^{(k)}(\eta)$ and this is precisely the first step in the approaches using adiabatic vacua (instead of $w^{(k)}$, there the function $\frac{1}{4w^{(k)}}$ is used); ultimately this is justified by the results from [JS02], in the framework presented here it is justified when working to a finite order in $\frac{1}{p^{2k+1}}$ to which the assumed property is showed. Except for the continuation of the discussion of adiabatic vacua and renormalization in section 5.3.7, these remarks will however not be used in the following.

5.3.5 An instructive example

To get a feeling how the different steps involved in this somewhat lengthy procedure interact, it is enlightening to consider de Sitter spacetime, where the above steps can be performed explicitly to arbitrary order. The part of de Sitter spacetime, which can be interpreted as spatially flat Robertson-Walker spacetime is characterized by $\eta < 0$ and its metric tensor in conformal coordinates is given by $C(\eta) = \frac{1}{H^2\eta^2}$, H the Hubble constant. The curvature then follows as $R = 12H^2$ and $Q_{m,\xi}$ is obtained as

$$Q_{m,\xi} : \eta \mapsto \left(\frac{m^2}{H^2} + 12\xi - 2 \right) \frac{1}{\eta^2} .$$

As can be checked by straightforward differentiation, the recursion relations (5.2.12), (5.2.13) are solved by

$$\overset{o}{v}_l : (\eta, \eta') \mapsto \frac{L^{2(l+1)}}{2^{2(l+1)} l!(l+1)!(\eta\eta')^{l+1}} \prod_{j=0}^{l} \left(\frac{m^2}{H^2} + 12\xi - 2 + j(j+1) \right) . \tag{5.3.24}$$

The $b_j^{()}$-coefficients then follow as

$$\begin{aligned} b_0^{()}(\eta) =& \frac{1}{2} \\ b_{l+1}^{()}(\eta) =& \frac{(2l+1)!(-1)^{l+1}}{2^{2(l+1)} l!(l+1)!} \frac{1}{\eta^{2(l+1)}} \prod_{j=0}^{l} \left(\frac{m^2}{H^2} + 12\xi - 2 + j(j+1) \right) \\ =& \frac{(2l+1)!}{2^{4(l+1)} l!(l+1)!} \frac{1}{\eta^{2(l+1)}} \prod_{j=0}^{l} \left(\mu - (2j+1)^2 \right) \\ \mu :=& 9 - 4 \left(12\xi + \frac{m^2}{H^2} \right) . \end{aligned}$$

For a Hadamard state, the asymptotics of $p \mapsto |V_p(\eta)|^2$ therefore has to be

$$|V_p(\eta)|^2 \sim \frac{\eta}{2} \cdot \frac{1}{\eta p} \left(1 + \frac{\mu - 1}{2(2\eta p)^2} + \frac{3}{4} \frac{(9-\mu)(1-\mu)}{(2\eta p)^4} + \dots \right)$$

This asymptotic expansion does not converge; comparing to the known asymptotic expansion of the absolute square of Hankel functions [Ste84, 9.2.28]

$$e^{-\pi \mathrm{Im}\,(\sqrt{\mu}/2)} |H^{(1)}_{\sqrt{\mu}/2}(x)|^2 \sim \frac{2}{\pi x} \left(1 + \sum_{l=0}^{\infty} \frac{(2l+2)!}{2^{2(l+1)}((l+1)!)^2 (2x)^{2(l+1)}} \prod_{j=0}^{l} \left(\mu - (2j+1)^2 \right) \right)$$

it is seen, that the function

$$p \mapsto \frac{-\pi\eta}{4} e^{-\pi \mathrm{Im}\,(\sqrt{\mu}/2)} |H^{(1)}_{\sqrt{\mu}/2}(-\eta p)|^2$$

has the same asymptotic expansion (for $-\eta p \to \infty$), so the symmetric part $\mathscr{W}_2^{\omega,\mathrm{s}}$ of a Hadamard state restricted to $\eta = \eta'$ is given by

$$[\mathscr{W}_2^{\omega,\mathrm{s}}]_{\eta=\eta'} = -\frac{H^2\eta^3}{(2\pi)^3}\int_{\mathbb{R}^+} e^{i\mathbf{p}\mathbf{x}}\frac{\pi}{4}e^{-\pi\mathrm{Im}\,(\sqrt{\mu}/2)}|H^{(1)}_{\sqrt{\mu}/2}(-p\eta)|^2\mathrm{d}\mathbf{p}\,.$$

The $b^{(\eta\eta')}$-coefficients follow as

$$\begin{aligned}
b_{-1}^{(\eta\eta')}(\eta) =& \frac{1}{2}\\
b_{0}^{(\eta\eta')}(\eta) =& \frac{1-\mu}{4(2\eta)^2}\\
b_{l+1}^{(\eta\eta')}(\eta) =& \frac{(2l+1)!(-1)^{l+1}}{2^{2(l+1)}l!(l+1)!\eta^{2(l+1)}}\\
&\ldots\times\left(\frac{(l+1)^2}{\eta^2}+\frac{2(l+1)}{4(l+1)(l+2)\eta^2}\left(\frac{m^2}{H^2}+12\xi-2+(l+1)(l+2)\right)\right)\\
&\ldots\times\prod_{j=0}^{l}\left(\frac{m^2}{H^2}+12\xi-2+j(j+1)\right)\\
=&\frac{(2l+1)!}{2^{2(l+1)}l!(l+1)!(2\eta)^{2(l+2)}}\left[4(l+1)^2+\frac{4(l+1)(l+2)+1-\mu}{2(l+2)}\right]\\
&\ldots\times\prod_{j=0}^{l}\left(\mu-(2j+1)^2\right)
\end{aligned}$$

and this gives for $p \mapsto |V_p'(\eta)|^2$ the asymptotics

$$\begin{aligned}
&|V_p'(\eta)|^2 \sim p\Bigg\{\frac{1}{2}+\frac{1-\mu}{4(2\eta p)^2}\\
&+\sum_{l=0}^{\infty}\frac{(2l+1)!}{2^{2(l+1)}l!(l+1)!}\frac{1}{(2\eta p)^{2(l+2)}}\left((2l+2)(2l+3)+\frac{1-\mu}{2(l+1)}\right)\prod_{j=0}^{l}\left(\mu-(2j+1)^2\right)\Bigg\}\,.
\end{aligned} \tag{5.3.25}$$

To get a candidate for $V_p'(\eta)$ with this asymptotic expansion, consider next the function

$$f:(\eta,\eta')\mapsto \mathcal{D}\mathcal{D}'\sqrt{-\eta}\sqrt{-\eta'}e^{-\pi\mathrm{Im}\,(\sqrt{\mu}/2)}\mathrm{Re}\,\left(H^{(1)}_{\sqrt{\mu}/2}(-p\eta)\overline{H^{(1)}_{\sqrt{\mu}/2}(-p\eta')}\right)\,.$$

For its restriction to $\eta' = \eta$ using [Ste84, 9.2.28] and [Ste84, 9.2.30] the asymptotics is obtained as

$$
\begin{aligned}
f(\eta,\eta) \sim \frac{1}{2\pi}\Bigg[&\frac{1}{p\eta^2}\Bigg\{1+\sum_{l=0}^{\infty}\frac{(2l+2)!}{2^{2(l+1)}((l+1)!)^2}\frac{1}{(2p\eta)^{2(l+1)}}\prod_{j=0}^{l}\left(\mu-(2j+1)^2\right)\Bigg\} \\
&-\frac{2}{p\eta^2}\Bigg\{1+\sum_{l=0}^{\infty}\frac{(2l+2)!}{2^{2(l+1)}((l+1)!)^2}\frac{1}{(2p\eta)^{2(l+1)}}\prod_{j=0}^{l}\left(\mu-(2j+1)^2\right)\Bigg\} \\
&-\frac{2}{p\eta^2}\Bigg\{1+\sum_{l=0}^{\infty}\frac{(2l+2)(2l+2)!}{2^{2(l+1)}((l+1)!)^2}\frac{1}{(2p\eta)^{2(l+1)}}\prod_{j=0}^{l}\left(\mu-(2j+1)^2\right)\Bigg\} \\
&+4p\Bigg\{1-\frac{1}{2}\frac{\mu-3}{(2\eta p)^2} \\
&\quad -\sum_{l=0}^{\infty}\frac{(2l+2)!}{2^{2l+3}(l+1)!(l+2)!}\frac{\mu-(2l+5)(2l+3)^2}{(2p\eta)^{2(l+2)}}\prod_{j=0}^{l}\left(\mu-(2j+1)^2\right)\Bigg\}\Bigg] \\
=\frac{2p}{\pi}-\frac{1}{2\pi p\eta^2}\Bigg[&1+\frac{\mu-3}{2} \\
&+\sum_{l=0}^{\infty}\frac{(2l+2)!}{2^{2(l+1)}((l+1)!)^2(2p\eta)^{2(l+1)}}\left[1+4(l+1)+\frac{\mu-(2l+5)(2l+3)^2}{2(l+2)}\right] \\
&\qquad\times\prod_{j=0}^{l}\left(\mu-(2j+1)^2\right)\Bigg]
\end{aligned}
$$

and comparing this to (5.3.25), we see that $\frac{\pi}{4}f(\eta,\eta)$ has the same asymptotics for $p\to\infty$ as $p\mapsto |V_p'(\eta)|^2$. The restriction of $\mathcal{D}\mathcal{D}'\mathscr{W}_2^{\omega,\mathrm{s}}$ of a Hadamard state is therefore given by

$$
\begin{aligned}
[\mathcal{D}\mathcal{D}'\mathscr{W}_2^{\omega,\mathrm{s}}]_{\eta=\eta'} = \frac{H^2\eta^2}{(2\pi)^3}\int_{\mathbb{R}+} e^{i\mathbf{px}}\Bigg[&\partial_\eta\partial_{\eta'}\Bigg(\frac{\pi}{4}\sqrt{-\eta}\sqrt{-\eta'}e^{-\pi\mathrm{Im}\,(\sqrt{\mu}/2)} \\
&\ldots\times\mathrm{Re}\left(H^{(1)}_{\sqrt{\mu}/2}(-p\eta)\overline{H^{(1)}_{\sqrt{\mu}/2}(-p\eta')}\right)\Bigg)\Bigg]_{\eta=\eta'}\mathrm{d}\mathbf{p}\,.
\end{aligned}
$$

Together with the expression for $[\mathscr{W}_2^{\omega,\mathrm{s}}]_{\eta=\eta'}$ and the Wronski determinant condition for V_p[5] this suggest

$$
V_p(\eta) = \frac{\sqrt{\pi}}{2}\sqrt{-\eta}\,e^{-\frac{\pi}{2}\,\mathrm{Im}\,(\sqrt{\mu}/2)}\,H^{(1)}_{\sqrt{\mu}/2}(-\eta p)
$$

as mode functions for a Hadamard state; one can however add an arbitrary function of η and p to V_p provided the asymptotics of V_p and V_p' is not changed.

[5] In this section, and this section only, we use the convention $\overline{V_p}'V_p - \overline{V_p}V_p' = i$, since we want to be able to compare the mode-functions obtained to those of [SS76] and furthermore this conventions significantly reduces the amount of complex conjugations required.

For this choice of V_p the condition (5.3.23) on $\partial_\eta |V_p(\eta)|^2$ can be explicitly checked to all orders; for the $b^{(\eta)}_{l+1}(\eta)$ we have

$$b^{(\eta)}_{l+1}(\eta) = -\frac{1}{\eta}\frac{(2l+1)!}{2^{2(l+1)}(l!)^2(2\eta)^{2(l+1)}}\prod_{j=0}^{l}\left(\mu-(2j+1)^2\right)$$

and this leads to the requirement

$$\partial_\eta |V_p(\eta)|^2 \sim -\frac{2}{\eta p}\frac{(2l+1)!}{2^{2(l+1)}(l!)^2(2\eta p)^{2(l+1)}}\prod_{j=0}^{l}\left(\mu-(2j+1)^2\right)$$

On the other hand, from [Ste84, 9.2.28] we get

$$\frac{\pi}{4}e^{-\pi \mathrm{Im}\,(\sqrt{\mu}/2)}\left(p\eta\left(|H^{(1)}_{\sqrt{\mu}/2}|^2\right)'(-p\eta) - |H^{(1)}_{\sqrt{\mu}/2}(-p\eta)|^2\right) \sim \\ -\frac{2}{\eta p}\sum_{l=0}^{\infty}\frac{(2l+1)!}{2^{2(l+1)}(l!)^2(2\eta p)^{2(l+1)}}\prod_{j=0}^{l}\left(\mu-(2j+1)^2\right) \quad (5.3.26)$$

which shows that the V_p obtained in this way indeed satisfies all the necessary conditions for mode functions defining a Hadamard state.

In this case the function $\eta \mapsto V_p(\eta)$ happens to be a solution of the mode equation $V_p'' + Q_{m,\xi}V_p = 0$ and so can be directly taken as the mode function; in general one can only expect to find for an η_0 fixed arbitrarily two functions $p \mapsto V_p(\eta_0)$ and $p \mapsto V_p'(\eta_0)$ with the required asymptotic properties, and then has to find the mode functions as solutions to the above ODE with $V_p(\eta_0)$ and $V_p'(\eta_0)$ as initial values.

Using this mode-functions and a function $p \to \Xi(p)$ which goes to $\frac{1}{2}$ for $p \to \infty$ faster than any inverse power of p, we can now define Hadamard states by (2.2.29). Choosing Ξ as constantly equal to $\frac{1}{2}$ we get a well known state; looking at the mode functions, they are nothing but the mode functions appearing in [SS76] for the Robertson Walker mode-decomposition of the (unique)de Sitter invariant state.
After this excursion into the general structure of Hadamard states and an illustrating example, we now proceed in the formalism developed so far to calculate expectation values of the Wick product and the second balanced derivative.

5.3.6 Calculation of the expectation values

To calculate the functions $w^{()} = D^{()}_{\mathcal{D}}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$, $w^{(\eta)} = D^{(\eta)}_{\mathcal{D}}\mathcal{D}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$ and $w^{(\eta\eta')} = D^{(\eta\eta')}_{\mathcal{D}}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}$ (or rather their restriction to the diagonal) by (5.3.12) – (5.3.14) (i.e. using the integral representations derived above), we need to fix functions Ω, $\Omega^{(\eta)}$ and $\Omega^{(\eta\eta')}$ with the right asymptotics. The first idea would be to choose the inverse powers $p \mapsto \frac{1}{p^{2l+1}}$ themselves; since they however diverge for $p \to 0$ (and the divergence gets increasingly worse for growing l), they have to be modified for small p. An easy way to achieve this (inspired from both the expression of the vacuum two-point function of the massive field on Minkowski spacetime as well as from the expressions for the adiabatic vacua), is to choose sums of the functions $\Omega_n : p \mapsto \left(A+p^2\right)^{-1/2-n}$, where $A>0$ is a constant. For them

$$\frac{1}{(A+p^2)^{n+1/2}} = \frac{n!}{(2n)!}\frac{1}{p^{2n+1}}\sum_{j=0}^{\infty}\frac{(2(n+j))!}{j!(n+j)!}\left(-\frac{A}{4p^2}\right)^j$$

holds, so setting

$$\Omega^{(k+1)}(p) = \sum_{n=0}^{k+1} c_n \Omega_n(p)$$

the asymptotic behaviour of $\Omega^{(k+1)}$ is given by

$$\Omega^{(k+1)}(p) = \frac{1}{p}\sum_{l=0}^{k+1}\frac{(2l)!}{l!}\left(\frac{1}{p^2}\right)^l \sum_{n=0}^{l}\frac{n!}{(2n)!}\frac{c_n}{(l-n)!}\left(-\frac{A}{4}\right)^{l-n} + \mathcal{O}\left(p^{-2k-5}\right).$$

Thus $p\mapsto p\Omega^{(k)}(p)$ has the asymptotic expansions $\sum_{l=0}^{k+1}\frac{b_l}{p^{2l}} + \mathcal{O}(p^{-2(k+1)})$ iff

$$\frac{(2l)!}{l!}\sum_{n=0}^{l}\frac{n!}{(2n)!}\frac{c_n}{(l-n)!}\left(\frac{-A}{4}\right)^{l-n} = b_l, \qquad l=0,1,\dots,k+1$$

holds. This determines c_n as

$$c_n = \sum_{j=0}^{n}\frac{(2n)!}{(2j)!}\frac{j!}{(n-j)!n!}\left(\frac{A}{4}\right)^{n-j} b_j\,. \tag{5.3.27}$$

Concerning the asymptotic expansion of $\Omega^{(\eta\eta')}$, the leading order term is $\Omega \sim b_{-1}^{(\eta\eta')}p$ and so seems not to fit into this scheme of choosing Ω, but since $p\mapsto p$ is regular at $p=0$ one can just add the term $b_{-1}^{(\eta\eta')}p$ to $\Omega^{(k+1)}$ to obtain an $\Omega^{(\eta\eta')}$ with the correct asymptotics. Using this choice of $\Omega^{(k+1)}$, the integral kernels K, $K^{()}$ and $K^{(\eta\eta')}$ follow as

$$K^{()}(p) = 2\Xi(p)|V_p(\eta)|^2 - \frac{1}{2\sqrt{A+p^2}} - \frac{A-Q_{m,\xi}(\eta)}{4\left(A+p^2\right)^{3/2}} \tag{5.3.28}$$

$$K^{(rr)}(p) = K^{()} - \frac{3(A-Q_{m,\xi}(\eta))^2 + Q''_{m,\xi}(\eta)}{16\left(A+p^2\right)^{5/2}} \tag{5.3.29}$$

$$K^{(\eta)}(p) = 2\Xi(p)\mathrm{Re}\left(V_p(\eta)\overline{V'_p(\eta)}\right) + \frac{Q'_{m,\xi}(\eta)}{8\left(A+p^2\right)^{3/2}} \tag{5.3.30}$$

$$K^{(\eta\eta')}(p) = 2\Xi(p)|V'_p(\eta)|^2 - \frac{p}{2} - \frac{Q_{m,\xi}(\eta)}{4\sqrt{A+p^2}} + \frac{Q^2_{m,\xi}(\eta) - 2AQ_{m,\xi}(\eta) + Q''_{m,\xi}(\eta)}{16\left(A+p^2\right)^{3/2}}\,. \tag{5.3.31}$$

Furthermore, one can also explicitly calculate the $\frac{R_{2l+1}}{(2l+1)!}$; the general result is

$$\begin{aligned}\frac{R_{2l+1}}{(2l+1)!} =& \frac{1}{l!}\left(-\frac{A}{4}\right)^l \Bigg[\sum_{n=0}^{\min\{l+1,k+1\}}\frac{n!}{(2n)!}\frac{\left(-\frac{A}{4}\right)^{1-n}}{(l+1-n)!}[\psi(l+1-(n-1))+\psi(l+1) \\ &\qquad - 2\log\left(\tfrac{\sqrt{A}L}{2}\right)]c_n \\ &+ (-1)^l\sum_{n=l+2}^{k+1}\frac{n!}{(2n)!}\frac{\left(\frac{A}{4}\right)^{1-n}}{l!}(n-l-2)!\,c_n\Bigg].\end{aligned} \tag{5.3.32}$$

(here ψ is the Digamma function [Ste84, 6.5]), and using this we get more concrete formulas for the $R^{()}(\eta)$, $R^{(\eta)}(\eta)$ and $R^{(\eta\eta')}(\eta)$ appearing above. In the end we need the restrictions of $R^{()}$, $\partial_{rr}R^{()}$, $R^{(\eta)}$ and $R^{(\eta\eta')}$ to the diagonal $x = x'$ and from (5.3.12)–(5.3.14), (5.3.6)–(5.3.11), (5.3.32) and (5.3.27) they follow as

$$
\begin{aligned}
\left[R_0^{()}\right]_{x=x'} =& 2\left[R^{(0)}_{\Omega^{()},L}\right]_{x=x'} - \left[R^{()}_{\mathcal{G}_0}\right]_{x=x'} \\
=& -\frac{A}{2}\left[\psi(2)+\psi(1)-2\log\left(\frac{L\sqrt{A}}{2}\right)\right]c_0^{()} \\
&+2\left(2\psi(1)-2\log\left(\frac{L\sqrt{A}}{2}\right)\right)\frac{c_1^{()}}{2} - [R_\Delta]_{x=x'} - \frac{\overset{o}{v}_0}{L^2}\left[\log(q)\right]_{x=x'} \\
=& \left(2\gamma-1+\log\left(\tfrac{AL^2}{4}\right)\right)\frac{A}{4} + \left(2\gamma+\log\left(\tfrac{AL^2}{4}\right)\right)\frac{Q_{m,\xi}(\eta)-A}{4} \\
&-\frac{C(\eta)R(\eta)}{72} - \frac{Q_{m,\xi}(\eta)}{4}\log\left(C(\eta)\right) \\
=& \left(2\gamma+\log\left(\tfrac{AL^2}{4C(\eta)}\right)\right)\frac{Q_{m,\xi}(\eta)}{4} - \frac{A}{4} - \frac{C(\eta)R(\eta)}{72}
\end{aligned}
\tag{5.3.33}
$$

$$
\begin{aligned}
\left[\partial_{rr}R_1^{()}\right]_{x=x'} =& 2\left[\partial_{rr}R^{(1)}_{\Omega^{()},L}\right]_{x=x'} - \left[\partial_{rr}R^{()}_{\mathcal{G}_1}\right]_{x=x'} \\
=& -2\left(\frac{A}{4}\right)^2\left[\psi(3)+\psi(2)-2\log\left(\frac{L\sqrt{A}}{2}\right)\right]c_0^{()} \\
&+\frac{A}{2}\left[2\psi(2)-2\log\left(\frac{L\sqrt{A}}{2}\right)\right]c_1^{()} \\
&-\frac{1}{3}\left[\psi(1)+\psi(2)-2\log\left(\frac{L\sqrt{A}}{2}\right)\right]c_2^{()} \\
&-[\partial_{rr}R_\Delta]_{x=x'} - 2\left[\frac{\overset{o}{v}_1}{L^4}\log q\right]_{\eta=\eta'} - \left[\frac{v_0}{L^2}\partial_{rr}\log(q)\right]_{x=x'} \\
=& -\frac{1}{4}\Bigg(\frac{A^2}{4}\left[5/2-2\gamma-\log\left(\tfrac{AL^2}{4}\right)\right] \\
&\quad + A\left[2-2\gamma-\log\left(\tfrac{AL^2}{4}\right)\right]\frac{Q_{m,\xi}(\eta)-A}{2} \\
&\quad + \left(\frac{(A-Q_{m,\xi}(\eta))^2}{4}+\frac{Q_{m,\xi}(\eta)}{12}\right)\left[1-2\gamma-\log\left(\tfrac{AL^2}{4}\right)\right]\Bigg) \\
&-\frac{1}{240}\left[\frac{15}{8}\left(\frac{C'(\eta)}{C(\eta)}\right)^4 - \frac{11}{3}\frac{C''(\eta)\left(C'(\eta')\right)^2}{C^3(\eta)} + \frac{3}{4}\left(\frac{C''(\eta)}{C(\eta)}\right)^2 + \frac{C'(\eta)C'''(\eta)}{C^2(\eta)}\right] \\
&-\frac{Q''_{m,\xi}(\eta)/3+Q^2_{m,\xi}(\eta)}{16}\log C(\eta) - \frac{Q_{m,\xi}}{96}\left(\frac{C'(\eta)}{C(\eta)}\right)^2
\end{aligned}
\tag{5.3.34}
$$

$$
\begin{aligned}
\left[R_0^{(\eta)}\right]_{x=x'} =& 2\left[R^{(0)}_{\Omega^{(\eta)},L}\right]_{x=x'} - \left[R^{(\eta)}_{\mathcal{G}_0}\right]_{x=x'} \\
=& -\frac{Q'_{m,\xi}(\eta)}{8}\left[2\psi(1) - 2\log\left(\frac{L\sqrt{A}}{2}\right)\right] \\
& - \left[\partial_\eta R_\Delta\right]_{x=x'} - \left[\frac{\partial_\eta \overset{o}{v}_0}{L^2}\log q\right]_{x=x'} - \left[\frac{\overset{o}{v}_0}{L^2}\frac{\partial_\eta q}{q}\right]_{x=x'} \\
=& \frac{Q'_{m,\xi}(\eta)}{8}\left(2\gamma + \log\left(\tfrac{L^2 A}{4C(\eta)}\right)\right) - \frac{(CR)'(\eta)}{144} - \frac{Q_{m,\xi}(\eta)}{4}\frac{C'(\eta)}{2C(\eta)}
\end{aligned} \tag{5.3.35}
$$

$$
\begin{aligned}
\left[R_0^{(\eta\eta')}\right]_{x=x'} =& 2\left[R^{(0)}_{\Omega^{(\eta\eta')},L}\right]_{x=x'} - \left[R^{(\eta\eta')}_{\mathcal{G}_1}\right]_{x=x'} \\
=& -\frac{A}{2}\left[\psi(2) + \psi(1) - 2\log\left(\frac{L\sqrt{A}}{2}\right)\right] c_0^{(\eta\eta')} \\
& + 2\left(2\psi(1) - 2\log\left(\frac{L\sqrt{A}}{2}\right)\right)\frac{c_1^{(\eta\eta')}}{2} - \left[\partial_{\eta\eta'} R_\Delta\right]_{x=x'} - \left[\frac{2\overset{o}{v}_1}{L^4}\right]_{\eta=\eta'} \\
& - \left[\left(\frac{\partial_{\eta\eta'}\overset{o}{v}_0}{L^2} + \frac{2\overset{o}{v}_1}{L^4}\right)\log(q)\right]_{x=x'} - \left[\frac{\partial_\eta q \partial_{\eta'}\overset{o}{v}_0 + \partial_{\eta'} q \partial_\eta \overset{o}{v}_0}{L^2 q}\right]_{x=x'} \\
& + \left[\left(\frac{\partial_\eta q \partial_{\eta'} q}{L^2 q^2} - \frac{\partial_{\eta\eta'} q}{L^2 q}\right)\overset{o}{v}_0\right]_{x=x'} \\
=& \left(2\gamma - 1 + \log\left(\tfrac{AL^2}{4}\right)\right)\frac{A Q_{m,\xi}(\eta)}{8} \\
& + \left(2\gamma + \log\left(\tfrac{AL^2}{4}\right)\right)\left(\frac{Q''_{m,\xi}(\eta) + Q^2_{m,\xi}(\eta)}{16} - \frac{A Q_{m,\xi}(\eta')}{8}\right) \\
& - \frac{1}{40}\left[\frac{(CR)''(\eta)}{9} + \frac{1}{8}\left(\frac{C''(\eta)}{C(\eta)}\right)^2 - \frac{C''(\eta)\left(C'(\eta)\right)^2}{6C^3(\eta)} + \left(\frac{C'(\eta)}{2C(\eta)}\right)^4\right] \\
& - \frac{Q''_{m,\xi}(\eta)/3 + Q^2_{m,\xi}(\eta)}{16} - \frac{Q''_{m,\xi}(\eta) + Q^2_{m,\xi}(\eta)}{16}\log(C(\eta)) - \frac{C'(\eta) Q'_{m,\xi}(\eta)}{8C(\eta)} \\
& + \left[\frac{5}{4}\left(\frac{C'(\eta)}{C(\eta)}\right)^2 - \frac{C''(\eta)}{C(\eta)}\right]\frac{Q_{m,\xi}(\eta)}{24}
\end{aligned} \tag{5.3.36}
$$

Taking this all together, we have the following result

Theorem 5.7. *For a homogeneous and isotropic Hadamard state with two-point function $\mathscr{W}_2^{\omega,\mathrm{s}}$, let the function $\mathscr{W}_{\omega,k}^{\mathrm{SHP}}$ be given by $\mathscr{W}_{\omega,k}^{\mathrm{SHP}} = \mathscr{W}_2^{\omega,\mathrm{s}} - \mathcal{G}_k^s$. Then the coincidence limits $x = x'$ of $(x,x') \mapsto \mathscr{W}_{\omega,k}^{\mathrm{SHP}}(x,x')$, $(x,x') \mapsto \partial_{rr}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}(x,x')$, $(x,x') \mapsto \mathcal{D}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}(x,x')$ and $(x,x') \mapsto \mathcal{D}\mathcal{D}'\mathscr{W}_{\omega,k}^{\mathrm{SHP}}(x,x')$, where these functions are assumed to be in $L^1(\mathbb{R}^3 \times \mathbb{R}^3)$ after partial restriction to the surface of constant $\eta = \eta'$, are given by*

$$\begin{aligned}
\left[\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'} =& \frac{1}{(2\pi)^3 C(\eta)} \int_{\mathbb{R}^3} K^{()}(p)\mathrm{d}\mathbf{p} + \frac{\left[R^{()}\right]_{x=x'}}{4\pi^2 C(\eta)} \\
\left[\partial_{rr}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'} =& \frac{1}{(2\pi)^3 C(\eta)} \int_{\mathbb{R}^3} \frac{-p^2}{3} K^{(rr)}(p)\mathrm{d}\mathbf{p} + \frac{\left[R^{(rr)}\right]_{x=x'}}{4\pi^2 C(\eta)} \\
\left[\mathcal{D}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'} =& \frac{1}{(2\pi)^3 C(\eta)} \int_{\mathbb{R}^3} K^{(\eta)}(p)\mathrm{d}\mathbf{p} + \frac{\left[R^{(\eta)}\right]_{x=x'}}{4\pi^2 C(\eta)} \\
\left[\mathcal{D}\mathcal{D}'\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'} =& \frac{1}{(2\pi)^3 C(\eta)} \int_{\mathbb{R}^3} K^{(\eta\eta')}(p)\mathrm{d}\mathbf{p} + \frac{\left[R^{(\eta\eta')}\right]_{x=x'}}{4\pi^2 C(\eta)}
\end{aligned}$$

The functions $K^{()}$–$K^{(\eta\eta')}$ and $R^{()}$–$R^{(\eta\eta')}$ are defined in (5.3.28)–(5.3.31) *and* (5.3.33)–(5.3.36)*.*

Using this information, we can finally come to the calculation of the expectation values of $:\phi^2:_{\mathrm{SHP}}$ and $\eth_{ab} :\phi^2:_{\mathrm{SHP}}$ in homogeneous and isotropic states with appropriate decay conditions. For $\omega(:\phi^2:_{\mathrm{SHP}})$ we directly get

$$\omega(:\phi^2:_{\mathrm{SHP}}) = \left[\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'} .$$

Due to the symmetry of $\mathscr{W}_{\omega,k}^{\mathrm{SHP}}$ many terms involving derivatives with respect to the spatial variables vanish; the remaining ones are $\partial_{xx}\mathscr{W}_{\omega,k}^{\mathrm{SHP}} = \partial_{yy}\mathscr{W}_{\omega,k}^{\mathrm{SHP}} = \partial_{zz}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}$ and $\partial_{xx'}\mathscr{W}_{\omega,k}^{\mathrm{SHP}} = \partial_{yy'}\mathscr{W}_{\omega,k}^{\mathrm{SHP}} = \partial_{zz'}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}$. Using the Christoffel symbols

$$\Gamma^{\eta\eta}_{\eta} = \Gamma^{\eta}_{xx} = \Gamma^{\eta}_{yy} = \Gamma^{\eta}_{zz} = \Gamma^{x}_{x\eta} = \Gamma^{y}_{y\eta} = \Gamma^{z}_{z\eta} = \frac{C'(\eta)}{2C(\eta)}$$

for $\epsilon_{ab} = -\frac{1}{4}\omega(\eth_{ab} :\phi^2:_{\mathrm{SHP}}) = \frac{1}{2}\left[\nabla_a\nabla_{b'}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'} - \frac{1}{2}\left[\nabla_a\nabla_b\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'}$ we thus get the non-vanishing components

$$\begin{aligned}
\epsilon_{\eta\eta} =& \frac{1}{2}\left[\partial_{\eta\eta'}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'} - \frac{1}{2}\left[\partial_{\eta\eta}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'} + \frac{C'(\eta)}{4C(\eta)}\left[\partial_{\eta}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'} \\
\epsilon_{xx} = \epsilon_{yy} = \epsilon_{zz} =& \frac{1}{2}\left[\partial_j\partial_{j'}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'} - \frac{1}{2}\left[\partial_{jj}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'} + \frac{C'(\eta)}{4C(\eta)}\left[\partial_{\eta}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'} \\
=& -\left[\partial_{rr}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'} + \frac{C'(\eta)}{4C(\eta)}\left[\partial_{\eta}\mathscr{W}_{\omega,k}^{\mathrm{SHP}}\right]_{x=x'}
\end{aligned}$$

By the procedure described in section 5.1.2 above, the double η-derivative can be reduced to terms containing only first derivatives; explicitly using equation (5.2.23), performing the limit $x \to x'$ and evaluating the expressions involving R_Δ, q, $\overset{o}{v}_0$ and $\overset{o}{v}_1$ we have

$$\begin{aligned}
\epsilon_{\eta\eta} =& \frac{1}{2}\left[\partial_{\eta\eta'}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{x=x'} + \frac{3C'(\eta)}{4C(\eta)}\left[\partial_\eta \mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{x=x'} - \frac{3}{2}\left[\partial_{rr}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{x=x'} \\
&+ \frac{C(\eta)\left(m^2+\xi R(\eta)\right)}{2}\left[\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{x=x'} - \frac{\left[R_{\mathrm{P}_{m,\xi}}\right]_{x=x'}}{2} \\
\left[R_{\mathrm{P}_{m,\xi}}\right]_{x=x'} =& \frac{1}{4\pi^2 C(\eta)}\left(\frac{Q''_{m,\xi}(\eta)}{8} + \frac{3}{8}Q^2_{m,\xi}(\eta) + \frac{1}{240}\left[6\left(\frac{C'(\eta)}{C(\eta)}\right)^4 - 12\frac{C''(\eta)\left(C'(\eta)\right)^2}{C^3(\eta)}\right.\right. \\
&\left. + 3\left(\frac{C''(\eta)}{C(\eta)}\right)^2 - (CR)''(\eta) + 3\frac{C'(\eta)C'''(\eta)}{C^2(\eta)}\right] - \frac{C'(\eta)Q'_{m,\xi}(\eta)}{8C(\eta)} \\
&\left. - Q_{m,\xi}(\eta)\left(\frac{C(\eta)R(\eta)}{72} + \frac{C''(\eta)}{12C(\eta)} - \frac{5}{48}\left(\frac{C'(\eta)}{C(\eta)}\right)^2\right)\right).
\end{aligned}$$

To make contact with the calculations above, we finally express the state-dependent parts of $\epsilon_{\eta\eta}$ and ϵ_{xx} as

$$\begin{aligned}
\frac{1}{2}\left[\partial_{\eta\eta'}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{x=x'} &+ \frac{3C'(\eta)}{4C(\eta)}\left[\partial_\eta \mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{x=x'} - \frac{1}{2}\left[\left(3\partial_{rr} - Q_{m,\xi}\right)\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{x=x'} \\
&= \frac{1}{2}\left[\mathcal{D}\mathcal{D}'\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{x=x'} + \frac{C'(\eta)}{4C(\eta)}\left[\mathcal{D}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{x=x'} - \frac{3}{2}\left[\partial_{rr}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{x=x'} \\
&\quad + \frac{1}{2}\left[\left(Q_{m,\xi}(\eta) + \frac{C''(\eta)}{2C(\eta)} - \frac{3}{4}\left(\frac{C'(\eta)}{C(\eta)}\right)^2\right)\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{x=x'} \\
\frac{C'(\eta)}{4C(\eta)}\left[\partial_\eta \mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{x=x'} &= \frac{C'(\eta)}{4C(\eta)}\left[\mathcal{D}\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{x=x'} - \frac{1}{8}\left(\frac{C'(\eta)}{C(\eta)}\right)^2\left[\mathscr{W}^{\mathrm{SHP}}_{\omega,k}\right]_{x=x'}
\end{aligned}$$

where $\frac{R(\eta)C(\eta)}{6} = \frac{C''(\eta)}{2C(\eta)} - \frac{1}{4}\left(\frac{C'(\eta)}{C(\eta)}\right)^2$ was used.

We can now put everything together to obtain the desired expressions for the expectation values of $:\phi^2:_{\mathrm{SHP}}$, $\eth_{\eta\eta} :\phi^2:_{\mathrm{SHP}}$ and $\eth_{xx} :\phi^2:_{\mathrm{SHP}}$ in the states of interest:

Theorem 5.8. *For a homogeneous and isotropic Hadamard state ω on a Robertson Walker spacetime with two-point function $\mathscr{W}_2^{\omega,\mathrm{s}}$ having decay properties like in the last lemma, the expectation values $\omega(:\phi^2:_{\mathrm{SHP}}(x))$, $\omega(\epsilon_{\eta\eta}(x))$ and $\omega(\epsilon_{xx}(x))$ are given by*

$$\omega(:\phi^2:_{\mathrm{SHP}}(x)) = \frac{1}{(2\pi)^3 C(\eta)} \int_{\mathbb{R}^3} K^{()}(p)\mathrm{d}\mathbf{p} + \frac{[R^{()}]_{x=x'}}{4\pi^2 C(\eta)} \tag{5.3.37}$$

$$\begin{aligned}\omega(\epsilon_{\eta\eta}(x)) =& \frac{1}{(2\pi)^3 C(\eta)} \int_{\mathbb{R}^3} \frac{K^{(\eta\eta')}(p)}{2} + \frac{C'(\eta)}{4C(\eta)} K^{(\eta)}(p) + \frac{p^2}{2} K^{(rr)}(p) \\ &+ \frac{1}{2}\left(Q_{m,\xi}(\eta) + \frac{C''(\eta)}{2C(\eta)} - \frac{3}{4}\left(\frac{C'(\eta)}{C(\eta)}\right)^2\right) K^{()}(p)\mathrm{d}\mathbf{p} \\ &+ \frac{[R^{(\eta\eta')}]_{x=x'}}{8\pi^2 C(\eta)} + \frac{C'(\eta)}{16\pi^2 C^2(\eta)}[R^{(\eta)}]_{x=x'} - \frac{3[R^{(rr)}]_{x=x'}}{8\pi^2 C(\eta)} \\ &+ \frac{1}{2}\left(Q_{m,\xi}(\eta) + \frac{C''(\eta)}{2C(\eta)} - \frac{3}{4}\left(\frac{C'(\eta)}{C(\eta)}\right)^2\right) \frac{[R^{()}]_{x=x'}}{4\pi^2 C(\eta)} - \frac{[R_{\mathrm{P}_{m,\xi}}]_{x=x'}}{2}\end{aligned} \tag{5.3.38}$$

$$\begin{aligned}\omega(\epsilon_{xx}(x)) =& \frac{1}{(2\pi)^3 C(\eta)} \int_{\mathbb{R}^3} \frac{p^2}{3} K^{(rr)}(p) + \frac{C'(\eta)}{4C(\eta)} K^{(\eta)}(p) - \frac{1}{8}\left(\frac{C'(\eta)}{C(\eta)}\right)^2 K^{()}(p)\mathrm{d}\mathbf{p} \\ &- \frac{[R^{(rr)}]_{x=x'}}{4\pi^2 C(\eta)} + \frac{C'(\eta)}{16\pi^2 C^2(\eta)}[R^{(\eta)}]_{x=x'} - \left(\frac{C'(\eta)}{C(\eta)}\right)^2 \frac{[R^{()}]_{x=x'}}{32\pi^2 C(\eta)}\end{aligned} \tag{5.3.39}$$

This is the main technical tool we will use in construction of LTE-states; before that one more brief comment on the relation of this procedure for the calculation of expectation values to adiabatic renormalization will be made in the next section.

5.3.7 Relation to adiabatic vacua and renormalization

We already discussed one aspect of adiabatic vacua in section 5.3.4; with the specific choice of the $\Omega^{()}$, $\Omega^{(\eta)}$ and $\Omega^{(\eta\eta')}$ from the last section at hand we can now finish the discussion here. As explained, the first step in this formalism is to introduce "approximate mode-functions" as

$$V_p^{(k)}(\eta) = \sqrt{w_p^{(k)}(\eta)}\; e^{i\int_{\eta_0}^{\eta} \frac{\mathrm{d}\tilde{\eta}}{4 w_p^{(k)}(\tilde{\eta})}}\,.$$

These can then either be used to specify initial values for true mode-functions (leading to an adiabatic vacuum of some order) or the expressions $\left|V_p^{(k)}(\eta)\right|^2$, $\mathrm{Re}\left(V_p^{(k)}{}'(\eta)\overline{V_p^{(k)}}(\eta)\right)$ and $\left|V_p^{(k)}{}'(\eta)\right|^2$ can be taken as the $\Omega^{()}$, $\Omega^{(\eta)}$ and $\Omega^{(\eta\eta')}$ in the integral kernels $K^{()}$, $K^{(\eta)}$, $K^{(\eta\eta')}$ (adiabatic renormalization). Focusing on the case of adiabatic renormalization and there on $K^{()}$, we see that we actually take the function $w^{(k)}$ as our $\Omega^{()}$, so the procedure of adiabatic renormalization can be seen as an alternative procedure to get an $\Omega^{()}$. The iteration procedure used there leads to an expression for $\frac{4}{w^{(k)}}$, which is nonzero for sufficiently large arguments and so can in principle be used directly as $\Omega^{()}$. Alternatively, one can write its inverse as an asymptotic series in terms $(A+p^2)^{-(l+1/2)}$, $l = 0, \ldots, k$ and this is the way adiabatic renormalization is presented in [BD84] and [Bir78]. One ends up with an expressions of the same structure as in the last section (with A now having a more complicated form involving $Q_{m,\xi}$) and the same asymptotics, so the procedure of adiabatic renormalization can be seen as a rather roundabout way to calculate the c_k from above for some specific choice of A. For $\Omega^{(\eta)}$ and $\Omega^{(\eta\eta')}$ nothing new happens, except that the expressions appearing get even more complicated.

5.4 Existence of LTE states on a Cauchy surface

5.4.1 The general construction

Coming now back to the problem of constructing states that fulfill thermality conditions at some instant of time η_0, first choose a state ω_{ini}, which according to section 2.2.3 can be specified by giving a function $\Xi \geq \frac{1}{2}$ on $\mathbb{R}^+$ and the initial values $V_p(\eta_0)$, $V_p'(\eta_0)$ for the mode functions V_p appearing in its two-point function. Since we need well-defined (finite) expectation values for $:\phi^2:_{\text{SHP}}$ and $\eth_{ab}:\phi^2:_{\text{SHP}}$ in this state, these data have to be chosen in such a way that the asymptotic conditions (5.3.18) and (5.3.19) are satisfied up to (and including) order $1/p^5$ and (5.3.20) is satisfied up to (and including) order $1/p^3$, i.e. the conditions written out in the equations (5.3.21) and (5.3.22) have to hold. For Hadamard states with decay properties this is automatically the case; explicitly constructing such states for a given spacetime is however also possible without problems (e.g. also taking the initial values as a sum of terms proportional to $(A+p^2)^{-l-1/2}$).

The restriction of the symmetric part $\mathscr{W}_2^{\omega_{\text{ini}},\text{S}}$ of the two-point function of the state ω_{ini}, together with the restrictions of $\mathcal{D}\mathscr{W}_2^{\omega_{\text{ini}},\text{S}}$ and $\mathcal{D}\mathcal{D}'\mathscr{W}_2^{\omega_{\text{ini}},\text{S}}$ to the surface at hand, then determine functions $\hat{w}_{\text{ini}}^{()}$, $\hat{w}_{\text{ini}}^{(\eta)}$ and $\hat{w}_{\text{ini}}^{(\eta\eta')}$ via (2.2.30)–(2.2.35).

Consider now the functions obtained from those as $\hat{w}^{()} = \hat{w}_{\text{ini}}^{()} + \rho_{\mu_2,\mu_4}$, $\hat{w}^{(\eta)} = \hat{w}_{\text{ini}}^{(\eta)}$ and $\hat{w}^{(\eta\eta')} = \hat{w}_{\text{ini}}^{(\eta\eta')} + N_{\tau^2}$, where N_{τ^2} is a positive, symmetric function with variance τ^2 and ρ_{μ_2,μ_4} is a symmetric function with second and fourth moment μ_2 and μ_4 respectively. Furthermore, both functions are assumed to be rapidly decaying, so that all their moments exist. Due to the positivity of ρ_{μ_2,μ_4} and N_{τ^2}, both $\hat{w}^{()}$ and $\hat{w}^{(\eta\eta')}$ are still positive and since $\hat{w}^{(\eta)}$ agrees with $\hat{w}_{\text{ini}}^{(\eta)}$ also the inequality $\hat{w}^{(\eta\eta')}\hat{w}^{()} - \left(w^{(\eta)}\right)^2 \geq \frac{1}{4}$ holds, since it is true for the initial functions $\hat{w}_{\text{ini}}^{()}$, $\hat{w}_{\text{ini}}^{(\eta)}$ and $\hat{w}_{\text{ini}}^{(\eta\eta')}$. Furthermore, the asymptotics of $\hat{w}^{()}$, $\hat{w}^{(\eta)}$, $\hat{w}^{(\eta\eta')}$ and $\hat{w}_{\text{ini}}^{()}$, $\hat{w}_{\text{ini}}^{(\eta)}$, $\hat{w}_{\text{ini}}^{(\eta\eta')}$ agree, so by lemma 2.9 they again determine a homogeneous and isotropic state $\omega_{\mu_2,\mu_4,\tau^2}$ which has the same regularity properties on the Cauchy surface as the one we started from.

Using (5.3.37)–(5.3.39), the differences of the values obtained for the thermal functions of the initial state $\omega_{\rm ini}$ and the modified $\omega_{\mu_2,\mu_4,\tau^2} =: \omega$ are given by

$$\vartheta^\omega(\eta_0) - \vartheta^{\omega_{\rm ini}}(\eta_0) = \frac{\mu_2}{4\pi^2 C(\eta_0)} \tag{5.4.1}$$

$$\begin{aligned}\varepsilon^\omega_{\eta\eta}(\eta_0) - \varepsilon^{\omega_{\rm ini}}_{\eta\eta}(\eta_0) =& \frac{\left(m^2 + (\xi - 1/6)R(\eta_0)\right) C(\eta_0) + \frac{C''(\eta_0)}{2C(\eta_0)} - \frac{3}{4}\left(\frac{C'(\eta_0)}{C(\eta_0)}\right)^2}{8\pi^2 C(\eta_0)} \mu_2 \\ &+ \frac{1}{8\pi^2 C(\eta_0)}\mu_4 + \frac{1}{8\pi^2 C(\eta_0)}\tau^2\end{aligned} \tag{5.4.2}$$

$$\varepsilon^\omega_{xx}(\eta_0) - \epsilon^{\omega_{\rm ini}}_{xx}(\eta_0) = -\frac{(C'(\eta_0))^2}{32\pi^2 C^3(\eta_0)}\mu_2 + \frac{1}{12\pi^2 C(\eta_0)}\mu_4 \,. \tag{5.4.3}$$

Being locally thermal at (sharp) inverse temperature $\beta = 1/(k_B T)$ now means that (5.4.1)–(5.4.3) hold with $\vartheta^\omega(\eta_0) = \vartheta^o(\beta) + c_{0,m}$, $\varepsilon^\omega_{\eta\eta}(\eta_0) = C(\eta_0)\left(\varepsilon^o_{00}(\beta) + c_{2,m}\right)$ and $\varepsilon^\omega_{xx}(\eta_0) = C(\eta_0)\left(\varepsilon^o_{jj}(\beta) - c_{2,m}\right)$, with the (Minkowskian) functions ϑ^o, ϵ^o_{00} and ϵ^o_{jj} from (3.3.8)–(3.3.10)[6].

Consider first the equation (5.4.1). Since $\vartheta^{\omega_{\rm ini}}$ can be positive or negative, but μ_2 and $C(\eta_0)$ are always strictly positive, it is not always solvable. However, since $\vartheta^o(\beta)$ grows with T (by the lemma 4.1 asymptotically like T^2), there is a T_0 such that the lhs of (5.4.1) is positive for all $T > T_0$ and we can then find a unique $\mu_2(T)$ such that (5.4.1) is satisfied. Moreover, using (4.2.8) and defining $f_1(T) = 4\pi^2 C(\eta_0)\left(\vartheta^o(1/(k_B T)) + c_{0,m} - \vartheta^{\omega_{\rm ini}}(\eta_0)\right)$ we have

$$\mu_2 = f_1(T) \sim \frac{\pi^2 C(\eta_0)}{3}(k_B T)^2 \,. \tag{5.4.4}$$

Consider next (5.4.3). Moving the μ_2-dependent term to the left hand side, inserting the expression just obtained for μ_2 and defining

$$f_2(T) = 8\pi^2 C(\eta_0)\left(C(\eta_0)\left(\varepsilon^o_{jj}(1/(k_B T)) + c_{2,m}\right) - \varepsilon^{\omega_{\rm ini}}_{xx}(\eta_0)\right) + \frac{1}{4}\left(\frac{C'(\eta_0)}{C(\eta_0)}\right)^2 f_1(T) \,,$$

the equation is transformed into

$$\frac{2}{3}\mu_4 = f_2(T) \,. \tag{5.4.5}$$

Again $f_2(T)$ need not be positive whereas μ_4 is, but since f_1 grows asymptotically like T^2 and ε^o_{jj} like T^4, again there is a T_1 such that f_2 is positive for $T > T_1$ and (5.4.5) can be solved, yielding a unique $\mu_4(T) = \frac{3}{2}f_2(T)$ with asymptotics $\mu_4 \sim \frac{2\pi^4}{15}(C(\eta_0)T^2)^2 \sim \frac{6}{5}\mu_2^2$. Finally regarding (5.4.2), by moving the μ_2 dependent terms to the left, inserting the expressions $\mu_2(T)$ obtained in the first step and defining

$$\begin{aligned} f_3(T) =& 8\pi^2 C(\eta_0)\left(C(\eta_0)\left(\varepsilon^o_{00}(1/(k_B T)) - c_{2,m}\right) - \varepsilon^{\omega_{\rm ini}}_{\eta\eta}(\eta_0)\right) \\ &- \left[(m^2 + (\xi - 1/6)R(\eta_0))C(\eta_0) + \frac{C''(\eta_0)}{2C(\eta_0)} - \frac{3}{4}\left(\frac{C'(\eta_0)}{C(\eta_0)}\right)^2\right] f_1(T)\end{aligned}$$

[6] The tetrad at each point $(\eta_0, \mathbf{x}) \in M_{\rm RW}(\hat{I}, C)$ appearing in the LTE-condition was taken here to consist of the vectors $\frac{1}{\sqrt{C(\eta_0)}}\partial_\eta$, $\frac{1}{\sqrt{C(\eta_0)}}\partial_x$, $\frac{1}{\sqrt{C(\eta_0)}}\partial_y$ and $\frac{1}{\sqrt{C(\eta_0)}}\partial_z$, and decomposing ε^ω_{ab} wrt. this basis we get the prefactors $C(\eta_0)$ appearing in the equations.

we are left with

$$f_3(T) = \mu_4 + \tau^2 \,. \tag{5.4.6}$$

Inserting the expression $\mu_4(T)$ obtained above, we have for $f_3(T) - \mu_4$

$$f_3(T) - \mu_4(T) \sim \frac{\pi^2 C(\eta_0)}{60}(k_B T)^4 \,, \tag{5.4.7}$$

which is again positive for T larger than some T_2. We can (for such T) find τ, such that also (5.4.2) is fulfilled. N_{τ^2} has to be a positive, symmetric, rapidly decaying function with a prescribed second moment, but taking e.g. the Gauss function with mean zero and variance τ^2, it is clear that such functions exist. But also ρ_{μ_2,μ_4} with the required properties are easily found; taking an arbitrary positive, symmetric and rapidly decaying function ψ with second and fourth moment m_2 and m_4, the function

$$p \mapsto (\mu_2/m_2)\left(\frac{\mu_2}{\mu_4/m_4}\right)^{3/2} \psi\left(\sqrt{\frac{m_4}{\mu_4}}\,\mu_2\, p\right) \tag{5.4.8}$$

has the required properties. This shows the existence of LTE-states on spatial-sections of Robertson Walker-spacetimes for sufficiently high (sharp) temperature.

Summarizing this section, we have the following existence-theorem for LTE-states:

Theorem 5.9. *Let $\{\eta_0\} \times \mathbb{R}^3 \subset M_{\mathrm{RW}}(\hat{I}, C)$ be a surface of constant, conformal time in the Robertson Walker-spacetime $M_{\mathrm{RW}}(\hat{I}, C)$. Then, for a neutral scalar Klein-Gordon field with mass $m \geq 0$ and curvature-coupling $\xi \in \mathbb{R}$ on $M_{\mathrm{RW}}(\hat{I}, C)$, there exists a temperature $T_{\min}(m, \xi, \eta_0)$, such that for all temperatures $T > T_{\min}$ there are states $\omega^{\eta_0}_{1/(k_B T)}$ of the Klein-Gordon field, which are (extrinsically) $S^{(2)}_{\{\eta_0\}\times\mathbb{R}^3}$-thermal at (sharp) inverse temperature $1/(k_B T)$.*

Inspecting once more the steps involved in the existence proof, one notices that the key point is really that for high temperatures the state-dependent terms, which (up to prefactors of C) can be brought into the form of integral expressions of the same type as in Minkowski-spacetime by the method used here, dominate the remainder terms that carry most of the dependence on the spacetime dependence. On a (more) technical level, this implies that at least for the type of existence question considered here, the precise choice of covariant Wick products does not really matter; adding a geometric term would not destroy the argument for the existence of LTE states on $\{\eta_0\} \times \mathbb{R}^3$. The dominance of these terms comes from an increase of the second and fourth moment of the absolute square of the mode functions and its derivative (as functions of p), so for higher temperatures the mode-functions with big p dominate. On a physical level one can interpret this as a dominance of the "kinetic-energy"-terms of the quantum field over "potential-energy"-terms that describe the interaction with the gravitational background in states of high energy.

5.4.2 Continuation of the example

We will again illustrate the steps involved by applying them to the example of de Sitter spacetime; to simplify the expressions appearing in this section we set $k_B = 1$, i.e. measure temperature in units of energy.

Taking the de Sitter invariant state from section 5.3.5 as ω_{ini}, one can calculate $\vartheta^{\omega_{\text{ini}}}$, $\varepsilon^{\omega_{\text{ini}}}_{\eta\eta}$ and $\varepsilon^{\omega_{\text{ini}}}_{xx}$ using the formulas (5.3.37)–(5.3.39) from theorem 5.8 (the - converging - integrals can be evaluated numerically without big problems); since for this state one even has an explicit analytic representation for the two-point function in terms of special functions [SS76],[All85] and the Hadamard parametrix can also be calculated explicitly using the symmetries of the spacetime, it is even possible to do the calculation using the expressions for $\mathscr{W}_2^{\omega,\mathrm{s}}$ and $\mathcal{G}^s_k$ directly, which also provides a check for the expressions appearing in theorem 5.8. In any case, by both methods one obtains

$$\begin{aligned}
\vartheta^{\omega_{\text{ini}}}(\eta_0) &= -\frac{H^2}{24\pi^2} - \frac{m^2 + (12\xi - 2)H^2}{16\pi^2} \\
&\qquad \ldots \times \left(1 - 2\gamma - \psi\left(\tfrac{3}{2} + \tfrac{\sqrt{\mu}}{2}\right) - \psi\left(\tfrac{3}{2} - \tfrac{\sqrt{\mu}}{2}\right) - \log\left(\tfrac{H^2L^2}{4}\right)\right) \\
\varepsilon^{\omega_{\text{ini}}}_{\eta\eta}(\eta_0) &= -\frac{1}{2\pi^2 H^2 \eta_0^2}\Bigg(\frac{17H^4}{480} + \frac{m^2 + (12\xi - 2)H^2}{48}H^2 \\
&\qquad + \frac{m^2 + (12\xi^2 - 2)H^2}{32}\left(m^2 + 12\xi H^2\right)\Bigg[\tfrac{5}{2} - 2\gamma - \psi\left(\tfrac{5}{2} + \tfrac{\sqrt{\mu}}{2}\right) \\
&\qquad\qquad - \psi\left(\tfrac{5}{2} - \tfrac{\sqrt{\mu}}{2}\right) - \log\left(\tfrac{H^2L^2}{4}\right)\Bigg]\Bigg) \\
\epsilon^{\text{ini}}_{xx}(\eta_0) &= -\,\epsilon^{\text{ini}}_{\eta\eta}(\eta_0)\,.
\end{aligned}$$

Inserting the spacetime-specific quantities into (5.4.1) we obtain for μ_2 the equation

$$\mu_2 = \frac{4\pi^2}{H^2\eta_0^2}\left(\vartheta^o(1/T) + c_{0,m} - \vartheta^{\omega_{\text{ini}}}(\eta_0)\right)\,. \tag{5.4.9}$$

The right-hand side of this equation as a function of $T = \frac{1}{\beta}$ is plotted in figure 5.2 for a few values of m, ξ and H at conformal time $\eta_0 = -1$. As used in the general construction, due to the (asymptotically) quadratic growth of the term $\vartheta^o(1/T)$ in T, the right hand side ultimately gets positive for T bigger than some T_0, which depends on the parameters H, m and ξ.

Next, inserting the scale function C into (5.4.5) and using the expression just obtained for $\mu_2(T)$, we get $\mu_4(T)$ as

$$\mu_4 = \frac{12\pi^2}{H^2\eta_0^2}\left(\frac{\varepsilon^o_{jj}(1/T) + c_{2,m}}{H^2\eta^2} - \varepsilon^{\omega_{\text{ini}}}_{xx}(\eta_0)\right) + \frac{4\pi^2}{H^4\eta_0^2}\left(\vartheta^o(1/T) + c_{0,m} - \vartheta^{\omega_{\text{ini}}}(\eta_0)\right)\,. \tag{5.4.10}$$

Again, the right-hand side can be plotted as a function of T as is done in figure 5.3, and again one sees that by the asymptotic growth like T^4 there is a T_1, such that the rhs.

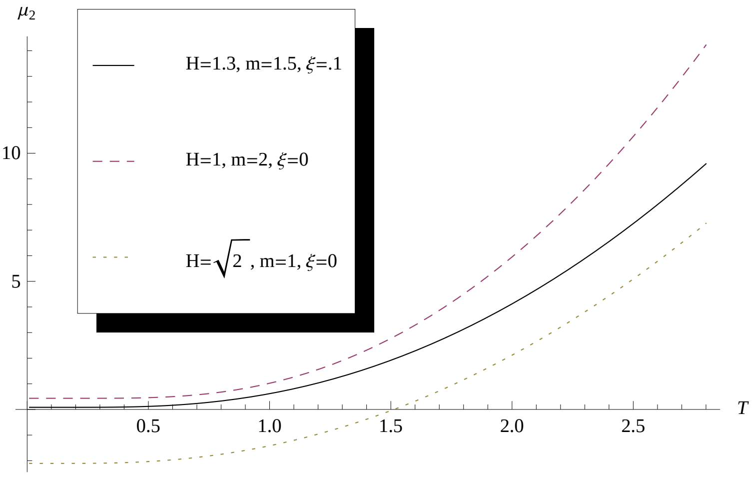

Figure 5.2: $\mu_2(T)$ on de Sitter for different values of H, m, ξ

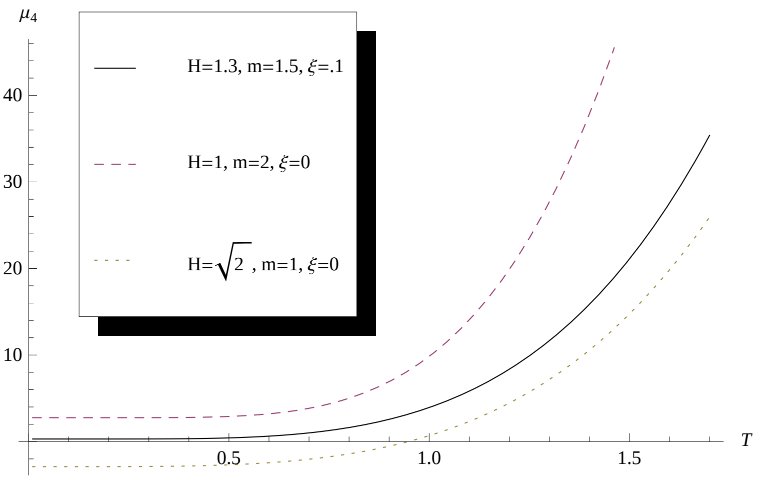

Figure 5.3: $\mu_4(T)$ on de Sitter for different values of H, m, ξ

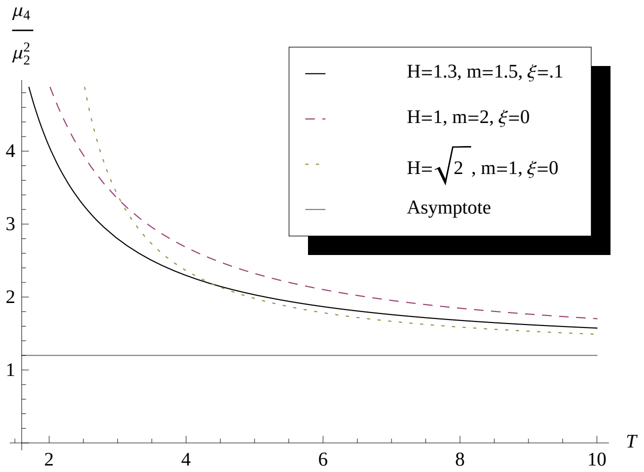

Figure 5.4: Ratio $\mu_4(T)/\mu_2^2(T)$ on de Sitter for different values of H, m, ξ

is positive for $T > T_1$. The ratio $\frac{\mu_4}{\mu_2^2}$ is also plotted in figure 5.4; this ratio is seen to approach 6/5 as it has to.

Finally there remains the equation (5.4.2) determining the third parameter τ^2, which after insertion of the scale factor into f_3 takes the form

$$\tau^2 = \frac{8\pi^2}{H^2\eta_0^2}\left(\frac{\varepsilon^o_{00}(1/T) - c_{2,m}}{H^2\eta_0^2} - \varepsilon^{\omega_{\mathrm{ini}}}_{\eta\eta}(\eta_0)\right) - \mu_4(T) - \frac{\frac{m^2}{H^2} + 12\xi - 2}{\eta_0^2}\mu_2(T)\,. \qquad (5.4.11)$$

In figure 5.5 the behaviour of the right hand side of this equation is shown in one more plot and again the positivity for T bigger than some threshold value T_2 can be seen. Summing up, for T bigger than the maximum of T_0, T_1 and T_2 the equations (5.4.9)–(5.4.11) give us positive μ_4, μ_2 and τ^2 and for large T the ratio μ_4/μ_2^2 converges to $\frac{6}{5}$; the precise form of these relations is shown in the plots above. Of course, in the end we are interested in the LTE-state for such T, and to obtain these, we next need the functions $\hat{w}$, and $\hat{w}^{(\eta\eta')}$. But by the above, we only need to fix N_{τ^2} and a ψ to obtain ρ_{μ_2,μ_4} by equation (5.4.8). Here we take for N_{τ^2} the function

$$N_{\tau^2} : p \mapsto \sqrt{\frac{\tau}{2\pi}}\exp\left(-\frac{p^2}{2\tau}\right)$$

and for ψ a Gaussian with mean zero and variance one, so we end up with functions

$$\hat{w}^{(\eta\eta')}(p) = \left[\partial_\eta\partial_{\eta'}\left(\frac{\pi}{4}\sqrt{-\eta}\sqrt{-\eta'}e^{-\pi\mathrm{Im}\,(\sqrt{\mu}/2)}\mathrm{Re}\,\left(H^{(1)}_{\sqrt{\mu}/2}(-p\eta)\overline{H^{(1)}_{\sqrt{\mu}/2}(-p\eta')}\right)\right)\right]_{\eta=\eta'=\eta_0}$$
$$+\sqrt{\frac{\tau}{2\pi}}\exp\left(-\frac{p^2}{2\tau}\right)$$

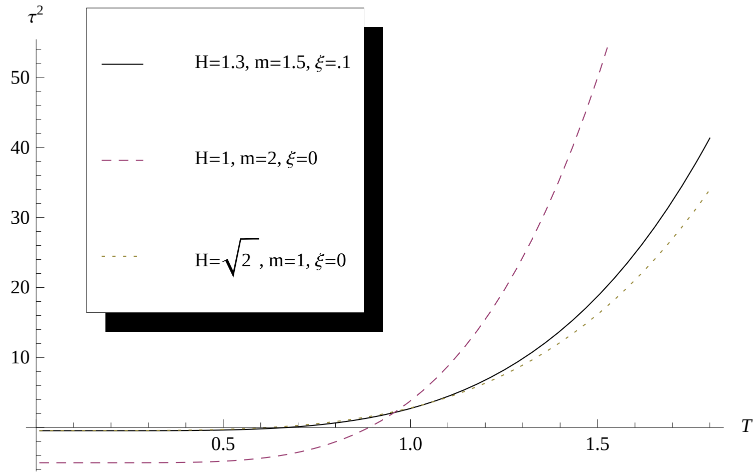

Figure 5.5: $\tau^2(T)$ on de Sitter for different values of H, m, ξ

and

$$\hat{w}^{()}(p) = -\frac{\pi\eta_0}{4} e^{-\pi \mathrm{Im}\,(\sqrt{\mu}/2)} |H^{(1)}_{\sqrt{\mu}/2}(-p\eta_0)|^2 + \frac{3^{3/2}\mu_2^{5/2}}{\sqrt{2\pi}\mu_4^{3/2}} \exp\left(-\frac{3\mu_2}{2\mu_4}p^2\right) .$$

With expressions for $\hat{w}^{()}$, $\hat{w}^{(\eta)}$ (just identical to $\hat{w}^{(\eta)}_{\mathrm{ini}}$) and $\hat{w}^{(\eta\eta')}$, the next step is to proceed to the calculation of the initial values $V_p(\eta_0)$ and $V_p'(\eta_0)$ of the mode-functions and the function Ξ. Using the results from section 2.2.4 we get

$$\begin{aligned}
\Xi(p) =& \sqrt{\frac{1}{4} + N_{\tau^2}(p)\rho_{\mu_2,\mu_4}(p) + N_{\tau^2}(p)\hat{w}^{()}_{\mathrm{ini}}(p) + \rho_{\mu_2,\mu_4}(p)\hat{w}^{(\eta\eta')}_{\mathrm{ini}}(p)} \\
V_p(\eta_0) =& \sqrt{\left|V_p^{\mathrm{ini}}(\eta_0)\right|^2 + \frac{\rho_{\mu_2,\mu_4}(p)}{2\Xi(p)}} \\
V_p'(\eta_0) =& \frac{\mathrm{Re}\,\left(V_p^{\mathrm{ini}\prime}(\eta_0)\overline{V_p^{\mathrm{ini}}(\eta_0)}\right) + \frac{i}{2}}{V_p(\eta_0)} .
\end{aligned} \tag{5.4.12}$$

These initial values can be used to calculate new mode functions $V_p = \alpha(p)V_p^{\mathrm{ini}} + \beta(p)\overline{V_p^{\mathrm{ini}}}$. Picking $T = 5$, the resulting Ξ, α and β as functions of p are shown in figure 5.6; it is seen that for $p \to \infty$ they approach $\frac{1}{2}$, one and zero respectively, as expected[7].

Finally, one can calculate for the $S^{(2)}_{\{-1\}\times\mathbb{R}^3}$-thermal state ω define by Ξ and V_p the expectation values of $\vartheta^\omega(\eta)$, $\varepsilon^\omega_{\eta\eta}(\eta)$ and $\varepsilon^\omega_{xx}(\eta)$ as functions of the (conformal) time η

[7] As can be seen in these plot, the values for α and β diverge for $p \to 0$ for the third set of parameters chosen, which might look troubling. This is however due to the fact that for such choices of parameters (low masses of the field) the initial mode functions have integrable singularities at $p = 0$. The integrals defining the two-point functions and the expectation values of the thermal observables are nevertheless well-defined.

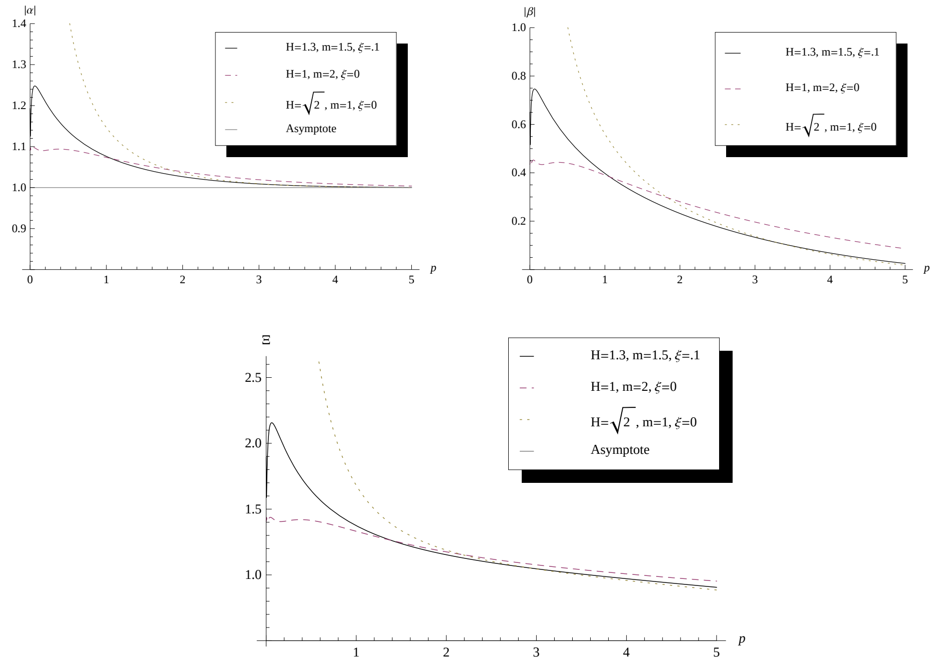

Figure 5.6: Ξ and coefficients α, β relating new and old mode-functions

using the formalism from section 5.3.6. If the state was a strict local thermal equilibrium state, a function β of η would exist, such that the three equations

$$\begin{aligned}\vartheta^{\omega}(\eta) =& \vartheta^{o}(\beta(\eta)) + c_{0,m}\\ \frac{\varepsilon^{\omega}_{\eta\eta}(\eta)}{C(\eta)} =& \varepsilon^{o}_{00}(\beta(\eta)) + c_{2,m}\\ \frac{\varepsilon^{\omega}_{xx}(\beta(\eta))}{C(\eta)} =& \varepsilon^{o}_{11}(\beta(\eta)) - c_{2,m}\end{aligned}$$

hold. To check to which extent this is true, one can calculate the function $\beta(\eta)$ appearing on the right-hand side of these equations from the left hand side by inverting ϑ^{o}, ε^{o}_{00} and ε^{o}_{11}. The result when doing this numerically for the first set of (spacetime) parameters is shown in figure 5.7

It is seen, that the three different “candidate temperatures” do not agree precisely, but start at the same point for $\eta = -1 = \eta_0$; furthermore, in this case we can also see, that the deviations between the different temperatures is not too dramatic. Furthermore it should be noted that there are some oscillations in the temperature; their significance will be discussed qualitatively in the next section. As the general message of this plot and the example, one should notice that first of all the LTE-state can be explicitly constructed; secondly one can (numerically) calculate the local thermal parameters off the initial Cauchy surface and finally these parameters are at least qualitatively in agreement with

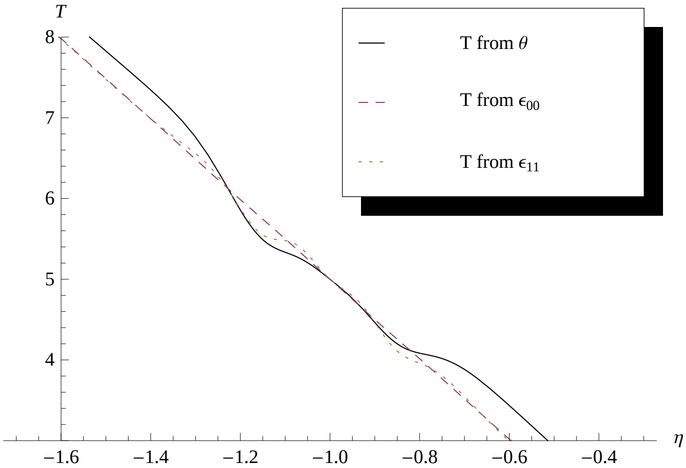

Figure 5.7: $1/\beta(\eta)$ calculated from ϑ, $\epsilon_{\eta\eta}$ and ϵ_{xx} as functions of η; $H = 1.3$, $m = 1.5$, $\xi = .1$

an interpretation of the state as a local thermal equilibrium state for some range of conformal times. They also show the expected, qualitative behaviour, namely they decreases as the universe expands.

5.5 A comment on the limit of large temperatures

Assume we fix some interval $[\eta_1, \eta_2]$ and construct by the above procedure a state which is $S^{(2)}_{\eta_0\times\mathbb{R}^3}$-thermal at some time $\eta_0 \in [\eta_1, \eta_2]$. The question is then, to what extent the state is locally thermal in the interval $[\eta_1, \eta_2]$, which one can e.g. try to quantify by comparing the three different candidates for (inverse) local temperatures $\beta(\eta)$ calculated at the end of the last section by solving each of the three equations

$$\vartheta^\omega(\eta) = \vartheta^o(\beta) + c_{0,m} \tag{5.5.1}$$
$$\varepsilon^\omega_{\eta\eta}(\eta) = C(\eta)\left(\varepsilon^o_{00}(\beta) + c_{2,m}\right) \tag{5.5.2}$$
$$\varepsilon^\omega_{xx}(\eta) = C(\eta)\left(\varepsilon^o_{jj}(\beta) - c_{2,m}\right) \tag{5.5.3}$$

for β. In this section we want to make a few remarks on the behaviour of these three functions when the (local) temperature of our state at the initial time η_0 gets big.

First, the only parts in the expressions for $\vartheta^\omega(\eta)$, $\varepsilon^\omega_{\eta\eta}(\eta)$ and $\varepsilon^\omega_{xx}(\eta)$ which are state-dependent are the terms $\hat{w}^{()}$, $\hat{w}^{(\eta)}$ and $\hat{w}^{(\eta\eta')}$ in the integral kernels $K^{()}$, $K^{(\eta)}$ and $K^{(\eta\eta')}$. Fixing the interval (i.e. the background geometry), it is thus sufficient to discuss the behaviour of the ($p-$)integrals over them. Introducing $v_p(\eta) := |V_p|(\eta)$, these terms can be written as

$$\hat{w}^{()}(p) = 2\Xi(p) v_p^2$$
$$\hat{w}^{(\eta)}(p) = 2\Xi(p) v_p v_p'$$
$$\hat{w}^{(\eta\eta')}(p) = 2\Xi(p) \left(\frac{1}{4v_p^2} + (v_p')^2 \right)$$

where relation (5.3.23) was used. Furthermore, using the same relation we also get that v_p satisfies the ordinary differential equation

$$v_p'' + (p^2 + Q_{m,\xi}) v_p = \frac{1}{4v_p^3}\,, \tag{5.5.4}$$

so in fact the whole discussion can be done in terms of this function instead of the V_p.

During the above construction of the LTE-state, the functions N_{τ^2} and ρ_{μ_2,μ_4} both get scaled in width (asymptotically their width is proportional to T^2), so starting the construction from a Fock state, we get a Ξ which deviates from its value $\frac{1}{2}$ over a wider and wider range. Furthermore, we also see from (5.4.12) that the initial values of v_p do not decrease; the precise change of v_p' is more complicated. As a result, since not the functions $\hat{w}^{()}$, $\hat{w}^{(\eta)}$ and $\hat{w}^{(\eta\eta')}$, but these functions multiplied with p^2 and p^4 enter the thermal functions, the mode-functions for larger and larger p dominate the integrals. But for large p, the time-dependent term $Q_{m,\xi}$ in the ODE (5.5.4) gets less and less important, so the situation increasingly resembles that of a field on Minkowski spacetime. The question, which is also related to the exact behaviour of v_p' from above is now, whether one can perform the above procedure for the construction of states in such a way that the obtained initial values $v_p(\eta_0)$ and $v_p'(\eta_0)$ (these are uniquely determined by $V_p(\eta_0)$, $V_p'(\eta_0)$) lead to a solution of (5.5.4) which shows little oscillation. As (5.5.4) is an equation for a (unit-mass) particle in the (time-dependent) potential $x \mapsto \frac{p^2+Q_{m,\xi}}{2} x^2 + \frac{1}{8x^2}$, the simplest way to achieve this for large p is to try and get $v_p(\eta_0)$ that are close to the bottom $x_{\min} = \frac{1}{\sqrt{2}\sqrt[4]{p^2+Q_{m,\xi}(\eta_0)}}$ of the potential and small $v_p'(\eta_0)$. Whether this is always achieved by the above construction with the specific choice of N_{τ^2} and ψ is at present not clear; what is however possible is to check for oscillations in the thermal functions for concrete situations. Looking at figure 5.7 it is seen that although oscillations are present, they are not especially large. Here it should also be pointed out that in order to simplify the construction we kept $\hat{w}^{(\eta)}$ constant; from the discussion here it seems that one should rather keep the term $V_p\overline{V_p}'$ (i.e. without the factor Ξ) constant, since it corresponds to v_p' (at least if one starts from a state with little initial oscillations in v_p like in the example of the time-invariant state on de Sitter spacetime). This will however lead to a considerable complication of the construction and so has not yet been investigated.

In any case, if the oscillations can be kept under control, the approximately constant v_p-terms will dominate the integrals giving the thermal functions and retain their initial value. They are then scaled by prefactors of $\frac{1}{C}$ and $\frac{1}{C^2}$ respectively before being compared to the Minkowskian thermal functions ϑ^o, $\varepsilon^o_{\mu\nu}$, and from the asymptotic behaviour of these functions of (inverse) temperature, it is seen that the (local) temperatures determined from (5.5.1)–(5.5.3) will then all scale with the same factor $\frac{1}{\sqrt{C}}$ for high temperatures, giving (local) temperatures that stay closely together.

As already indicated above, physically this can be understood as a concentration of the energy in kinetic degrees of freedom for high temperatures. These are little affected by the underlying spacetime geometry and the scaling of temperature with the expansion of the universe is then the same as for a massless field, as long as the thermal energy does not get too low.

A Appendix

A.1 Advanced and retarded Greens operators

On Robertson Walker spacetime, the advanced and retarded greens operators are given by

$$[\mathrm{E}^{\pm}(f)](\eta,\mathbf{x}) = \mp \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \int_{-\infty}^{\infty} \Theta(\pm(\eta-\lambda)) G_p(\eta,\lambda) \hat{f}(\lambda,\mathbf{p}) C^2(\lambda) \mathrm{d}\lambda e^{i\mathbf{px}} \mathrm{d}\mathbf{p} \tag{A.1.1}$$

$$\begin{aligned} \hat{f}(\lambda,\mathbf{p}) =& \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} f(\lambda,\mathbf{x}) e^{-i\mathbf{px}} \mathrm{d}\mathbf{x} \\ G_p(\eta,\lambda) =& i\, \frac{V_p(\eta)\overline{V_p}(\lambda) - \overline{V_p}(\eta) V_p(\lambda)}{\sqrt{C(\eta)C(\lambda)}}\,, \end{aligned}$$

where V_p is a solution to the ODE

$$V_p'' + \left[p^2 + (m^2 + (\xi - 1/6)R)C\right] V_p = 0$$

($R = 3\frac{C''}{C^2} - \frac{3}{2}\frac{(C')^2}{C^3}$ the curvature scalar) satisfying the additional condition

$$\overline{V_p}V_p' - \overline{V_p}' V_p = i$$

That (A.1.1) indeed is a Greens operator can be seen by calculating its derivatives; one gets for E^+ using that for $\varphi \in C_0^\infty(\mathbb{R})$:

$$\begin{aligned} \frac{1}{C(\eta)}\partial_\eta \left(C(\eta)\partial_\eta \int_{-\infty}^{\eta} G_p(\eta,\lambda)\varphi(\lambda)\mathrm{d}\lambda \right) =& \frac{1}{C(\eta)}\partial_\eta \Bigg(C(\eta) \underbrace{G_p(\eta,\eta)}_{=0} \varphi(\eta) \\ & + C(\eta) \int_{-\infty}^{\eta} \partial_\eta G_p(\eta,\lambda)\varphi(\lambda)\mathrm{d}\lambda \Bigg) \\ =& \partial_\eta G_p(\eta,\lambda)|_{\lambda=\eta}\varphi(\eta) + \int_{-\infty}^{\eta} \left(\frac{C'(\eta)}{C(\eta)} \partial_\eta G_p(\eta,\lambda) + \partial_{\eta\eta} G_p(\eta,\lambda) \right) \varphi(\lambda)\mathrm{d}\lambda \\ =& i \frac{V_p'(\eta)\overline{V_p(\eta)} - \bar{(}V_p(\eta))V_p(\eta)}{C(\eta)} \varphi(\eta) \\ & + i \int_{-\infty}^{\eta} \frac{\left(V_p''(\eta) - \frac{R(\eta)C(\eta)}{6} V_p(\eta)\right)\overline{V_p}(\lambda) - \left(\overline{V_p}''(\eta) - \frac{R(\eta)C(\eta)}{6}\overline{V_p}(\eta)\right) V_p(\lambda)}{\sqrt{C(\eta)C(\lambda)}} \\ & \quad \ldots \times \varphi(\lambda)\mathrm{d}\lambda \\ =& -\frac{\varphi(\eta)}{C(\eta)} - \int_{-\infty}^{\eta} (p^2 + (m^2 + \xi R(\eta))C(\eta)) G_p(\eta,\lambda)\varphi(\lambda)\mathrm{d}\lambda \end{aligned}$$

the relation

$$
\begin{aligned}
(\Box + \xi R + m^2)\left[\mathrm{E}^+(f)\right](\eta,\mathbf{x}) = \dots\\
= -\frac{1}{(2\pi)^{3/2}C(\eta)}\int_{\mathbb{R}^3}\frac{1}{C(\eta)}\partial_\eta\Bigg(C(\eta)\partial_\eta\int_{-\infty}^{\eta}G_p(\eta,\lambda)\hat{f}(\lambda,\mathbf{p})C^2(\lambda)\mathrm{d}\lambda\\
-\left[p^2+(m^2+\xi R(\eta))C(\eta)\right]\int_{-\infty}^{\eta}G_p(\eta,\lambda)\hat{f}(\lambda,\mathbf{p})C^2(\lambda)\mathrm{d}\lambda e^{i\mathbf{p}\mathbf{x}}\Bigg)\mathrm{d}\mathbf{p}\\
= \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\hat{f}(\eta,\mathbf{p})e^{i\mathbf{p}\mathbf{x}}\mathrm{d}\mathbf{p}\\
= f(\eta,\mathbf{x})
\end{aligned}
$$

and by an analogous computation also

$$
(\Box + \xi R + m^2)\left[\mathrm{E}^-(f)\right](\eta,\mathbf{x}) = f(\eta,\mathbf{x})
$$

Concerning the support properties, it is sufficient to establish that for $\mathbf{x}\mapsto f(\lambda,\mathbf{x})$ having support in the ball $B(0,r)$, the function

$$
\mathbf{x}\mapsto\frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}G_p(\eta,\lambda)\hat{f}(\lambda,\mathbf{p})e^{i\mathbf{p}\mathbf{x}}\mathrm{d}p
$$

has support in the ball $B(0,r+|\eta-\lambda|)$.

By the Paley-Wiener-Schwartz theorem, $\mathbf{p}\mapsto\hat{f}(\lambda,\mathbf{p})$ is an entire function which satisfies the growth estimate $|f(\zeta)|\leq Me^{r|\zeta|}$ for a constant $M>0$. This function is now multiplied by $G_p(\eta,\lambda)$, so we need analyticity properties and growth estimates for $G_p(\eta,\lambda)$, or equivalently $\sqrt{C(\eta)C(\lambda)}G_p(\eta,\lambda)$.

For fixed λ and $p\in\mathbb{R}$, the function $H_p:\eta\mapsto\sqrt{C(\eta)C(\lambda)}G_p(\eta,\lambda)$ satisfies the differential equation

$$
H_p''+\left(p^2+\left(m^2+\xi R\right)C\right)H_p=0 \tag{A.1.2}
$$

and has initial values

$$
H_p(\lambda)=0 \qquad H_p'(\lambda)=-1. \tag{A.1.3}
$$

Introducing $\psi_p=\frac{H_p'}{1+|p|}$ we can can rewrite the ODE for H_p as the system

$$
\begin{pmatrix}H_p'\\ \psi_p'\end{pmatrix}=\begin{pmatrix}0 & 1+|p|\\ -\frac{p^2+(m^2+(\xi-1/6)R)C}{1+|p|} & 0\end{pmatrix}\begin{pmatrix}H_p\\ \psi_p\end{pmatrix} \tag{A.1.4}
$$

On a compact interval $[\lambda,\eta]$ the smooth function $\eta'\mapsto(m^2+(\xi-1/6)R(\eta'))C(\eta')$ can be bounded in modulus by a constant M_1 and by explicitely calculating the spectral (operator) norm for the matrix appearing in (A.1.4) we get the bound:

$$\begin{aligned}&\left\|\begin{pmatrix}0 & 1+|p|\\ -\frac{p^2+(m^2+(\xi-1/6)R)C}{1+|p|} & 0\end{pmatrix}\begin{pmatrix}H_p\\ \psi_p\end{pmatrix}\right\|\\ &\leq\sqrt{\max\left\{(1+|p|)^2,\frac{|p^2+M_1|^2}{(1+|p|)^2}\right\}}\left\|\begin{pmatrix}H_p\\ \psi_p\end{pmatrix}\right\|\leq\max\left\{1,\frac{|p|^2}{1+|p|}+\frac{M_1}{1+|p|}\right\}\left\|\begin{pmatrix}H_p\\ \psi_p\end{pmatrix}\right\|,\end{aligned}\tag{A.1.5}$$

valid for all $p\in\mathbb{C}$. Taking $M_1\geq 1$, applying the Gronwall lemma to the absolute value of the integral equation corresponding to (A.1.4) and using the initial conditions for H_p and $\psi_p=\frac{H_p'}{1+|p|}$ we get

$$|H_p|\leq\left\|\begin{pmatrix}H_p\\ \psi_p\end{pmatrix}\right\|\leq e^{M_1}e^{|p||\eta-\lambda|}\left\|\begin{pmatrix}0\\ -\frac{1}{1+|p|}\end{pmatrix}\right\|\leq e^{M_1}e^{|p||\eta-\lambda|}\,.$$

On the other hand, from the theory of ODEs we get that for fixed η the solution of (A.1.2) with initial values (A.1.3) is an analytic function of p^2 since the function $(\zeta,H)\mapsto(\zeta+(m^2+(\xi-1/6)R(\eta))C(\eta))\,H$ and the functions $\zeta\mapsto 0=H_{\sqrt{\zeta}}(\lambda)$, $\zeta\mapsto -1=H'_{\sqrt{\zeta}}(\lambda)$ are analytic wrt. their arguments. Therefore, for fixed λ, η the function $\mathbf{p}\mapsto G_p(\lambda,\eta)\hat{f}(\lambda,\mathbf{p})$ is again analytic and satisfies the required growth estimate so that

$$\mathbf{x}\mapsto\frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}G_p(\eta,\lambda)\hat{f}(\lambda,\mathbf{p})e^{i\mathbf{px}}\mathrm{d}p$$

as its fourier-(back)-transform has the right support properties. Because of the Θ-(step)-function appearing in the greens operator the support of $\mathrm{E}^{\pm}$ is seen to be contained either in the past or in the future of f.

From these representations of $\mathrm{E}^{\pm}$ one directly reads of the operator $E:=\mathrm{E}^{-}-\mathrm{E}^{+}$ as

$$[E(f)]\,(\eta,\mathbf{x})=\frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\int_{-\infty}^{\infty}G_p(\eta,\lambda)\hat{f}(\lambda,\mathbf{p})C^2(\lambda)\mathrm{d}\lambda e^{i\mathbf{px}}\mathrm{d}\mathbf{p}\,.\tag{A.1.6}$$

A.2 A convergence result

Lemma A.1. *Let* $\rho:\mathbb{R}\times\mathbb{R}^+\ni(\Delta\eta,r)\mapsto r^2-(\Delta\eta)^2$ *and* $q:\mathbb{R}\times\mathbb{R}^+\to\mathbb{R}$ *be bounded from below by* $1/Q_{max}>0$*. Then* $(r,\Delta\eta)\mapsto\log\left(\left(\rho(r,\Delta\eta)+\frac{\epsilon^2}{q(r,\Delta\eta)}\right)^2+4\epsilon^2\frac{(\Delta\eta)^2}{q^2(r,\Delta\eta)}\right)$ *converges in* L^1_{loc} *to* $(r,\Delta\eta)\mapsto\log(\rho^2(\Delta\eta,r))$*.*

Proof. Let $C\subset\mathbb{R}\times\mathbb{R}^+$ bounded be given and let $\epsilon=\min\left\{\frac{1}{8\sup_{(\Delta\eta,r)\in C}(\Delta\eta)^2},\frac{1}{\sqrt{2}}\right\}$. To proof the local L^1 convergence we have to show

$$\lim_{\epsilon\to 0}\int_C\left|\log\left(\frac{\left(\rho(\Delta\eta,r)+\frac{\epsilon^2}{q(\Delta\eta,r)}\right)^2+4\epsilon^2\frac{(\Delta\eta)^2}{q^2(\Delta\eta,r)}}{\rho^2(\Delta\eta,r)}\right)\right|\mathrm{d}r\mathrm{d}\Delta\eta=0\tag{A.2.1}$$

Consider now two cases:

1. $\rho(\Delta\eta, r) > 0$ or $|\Delta\eta| > \frac{\epsilon}{2}$:

$$\frac{\left(\rho + \frac{\epsilon^2}{q}\right)^2 + 4\epsilon^2 \frac{(\Delta\eta)^2}{q^2}}{\rho^2} = 1 + \underbrace{\epsilon^2 \left(\frac{2}{\rho q} + \frac{4(\Delta\eta)^2 + \epsilon^2}{\rho^2 q^2}\right)}_{x}$$

For $\rho > 0$, $x > 0$ holds, for $|\Delta\eta| > \frac{\epsilon}{2}$ we have

$$x \geq \epsilon^2 \left(\frac{2}{\rho q} + \frac{2\epsilon^2}{(\rho q)^2}\right) = 2\epsilon^2 \left(\frac{1}{\rho q} + \frac{\epsilon^2}{(\rho q)^2}\right) \geq -\frac{1}{2}$$

since $\frac{1}{\xi} + \frac{\epsilon^2}{\xi^2} \geq -\frac{1}{4\epsilon^2}$ for all $\xi \in \mathbb{R}$. Now for $x \geq -\frac{1}{2}$ there holds $|\log(1+x)| \leq 2\log(1+|x|) \leq 2\log(1+y)$ for all y such that $y \geq |x|$. Using this, one can estimate

$$R_\epsilon := \left|\log\left(\frac{\left(\rho + \frac{\epsilon^2}{q}\right)^2 + 4\epsilon^2 \frac{(\Delta\eta)^2}{q^2}}{\rho^2}\right)\right| \leq 2\log\left(1 + \epsilon^2\left(\frac{2}{|q\rho|} + \frac{4(\Delta\eta)^2 + \epsilon^2}{|\rho q|^2}\right)\right)$$

Taking the specific choice of ϵ and $\frac{1}{q} \geq Q_{max}$ into account, this can be further estimated as

$$\begin{aligned} R_\epsilon \leq & 2\log\left(1 + \epsilon^2 \frac{2Q_{max}}{|\rho|} + \epsilon \frac{1/2 + \epsilon^2}{|\rho|^2} Q_{max}^2\right) \leq 2\log\left(1 + 2\frac{\sqrt{\epsilon}Q_{max}}{|\rho|} + \frac{\epsilon Q_{max}^2}{|\rho|^2}\right) \\ = & 4\log\left(1 + \frac{\sqrt{\epsilon}Q_{max}}{|\rho|}\right) \end{aligned} \tag{A.2.2}$$

2. $\rho(\Delta\eta, r) < 0$ and $|\Delta\eta| < \epsilon/2$:
   Because of $\rho(\Delta\eta, r) = r^2 - (\Delta\eta)^2 < 0$ this implies $r < |\Delta\eta| \leq \epsilon/2$ and also $|\rho| \leq -\epsilon^2/4$. Using $|\log x| \leq \log(x + 1/x)$ for all $x \in \mathbb{R}$, by the estimate

$$\begin{aligned} \frac{\left(\rho + \frac{\epsilon^2}{q}\right)^2 + 4\epsilon^2 \frac{(\Delta\epsilon)^2}{q^2}}{\rho^2} + & \frac{\rho^2}{\left(\rho^2 + \frac{\epsilon^2}{q^2}\right)^2 + 4\epsilon^2 \frac{(\Delta\eta)^2}{q^2}} \leq \frac{\rho^2 + \frac{\epsilon^4}{q^2} + \frac{\epsilon^4}{q^2}}{\rho^2} + \frac{\rho^2 q^2}{4\epsilon^2(\Delta\eta)^2} \\ \leq & 1 + \frac{2\epsilon^4}{\rho^2} Q_{max}^2 + \frac{Q_{max}^2 \epsilon^2}{64(\Delta\eta)^2} \end{aligned}$$

we have

$$\begin{aligned} R_\epsilon \leq & \log\left(64\rho^2(\Delta\eta)^2 + \epsilon^2 Q_{max}^2 (128\epsilon^2(\Delta\eta)^2 + \rho^2)\right) - \log\left(64\rho^2(\Delta\eta)^2\right) \\ \leq & \log(\epsilon^6(1 + Q_{max}^2(32 + 1/16))) - \log\left(64\rho^2(\Delta\eta)^2\right) \end{aligned} \tag{A.2.3}$$

Now split the integration range in (A.2.1) into the area C_1 where $0 \leq r \leq |\Delta\eta| \leq \epsilon/2$ and its complement $C \setminus C_1$. Since the rhs. in (A.2.2) is strictly positive, the integral of R_ϵ over $C \setminus C_1$ can be estimated as ($\tilde{\epsilon}^2 := \sqrt{\epsilon} Q_{max}$):

$$\begin{aligned}
\int_{C\setminus C_1} R_\epsilon(\Delta\eta, r)\mathrm{d}r\mathrm{d}\Delta\eta \leq & 4\int_{-M}^{M}\int_0^{|\Delta\eta|}\log\left(\frac{(\Delta\eta)^2 - r^2 + \tilde{\epsilon}^2}{(\Delta\eta)^2 - r^2}\right)\mathrm{d}r\mathrm{d}\eta \\
& + 4\int_{-M}^{M}\int_{|\Delta\eta|}^{\infty}\log\left(\frac{r^2 - (\Delta\eta)^2 + \tilde{\epsilon}^2}{r^2 - (\Delta\eta)^2}\right)\mathrm{d}r\mathrm{d}\eta \\
= & 8\tilde{\epsilon}^2\int_0^1\left(\int_0^{\Delta\eta}\log\left(\frac{(\Delta\eta)^2 + 1 - r^2}{(\Delta\eta)^2 - r^2}\right)\mathrm{d}r\right. \\
& \left. + \int_{\Delta\eta}^{\infty}\log\left(\frac{r^2 + 1 - (\Delta\eta)^2}{r^2 - (\Delta\eta)^2}\right)\mathrm{d}r\right)\mathrm{d}\eta \\
& + 8\tilde{\epsilon}^2\int_1^{M/\tilde{\epsilon}}\left(\int_0^{\Delta\eta}\log\left(\frac{(\Delta\eta)^2 + 1 - r^2}{(\Delta\eta)^2 - r^2}\right)\mathrm{d}r\right. \\
& \left. + \int_{\Delta\eta}^{\infty}\log\left(\frac{r^2 - (\Delta\eta)^2 + 1}{r^2 - (\Delta\eta)^2}\right)\mathrm{d}r\right)\mathrm{d}\eta \\
= & 8\tilde{\epsilon}^2\int_0^1 F_1(\Delta\eta)\mathrm{d}\eta + 8\tilde{\epsilon}^2\int_1^{M/\tilde{\epsilon}} F_2(\Delta\eta)\mathrm{d}\eta
\end{aligned}$$

where

$$\begin{aligned}
F_1(\Delta\eta) &= 2\left(\sqrt{1 - (\Delta\eta)^2}\arccos(\Delta\eta) + \sqrt{1 + (\Delta\eta)^2}\,\mathrm{Arsinh}(\Delta\eta)\right) \\
F_2(\Delta\eta) &= 2\sqrt{1 + (\Delta\eta)^2}\,\mathrm{Arsinh}(\Delta\eta) - 2\Delta\eta\log(2\Delta\eta)
\end{aligned}$$

Since both F_1 and F_2 are bounded in the regions they are integrated over, the convergence of the integral of R_ϵ over $C \setminus C_1$ to 0 follows.
Setting $\tilde{C}_1 := 6\log(32 + 1/16)$, $\tilde{C}_2 = 3\log(64)$ from (A.2.3) one has

$$R_\epsilon \leq \tilde{C}_1\log(\epsilon) + \tilde{C}_2|\log(|\rho|)|$$

Now since

$$\int_{C_1} R_\epsilon(\Delta\eta, r) = 2\int_0^{\epsilon/2}\int_0^{\Delta\eta}\log(\eta^2 - r^2)\mathrm{d}r\mathrm{d}\eta = 2\int_0^{\epsilon/2} 2\eta\log(2\eta) - 2\eta\mathrm{d}\eta = \frac{1}{4}\epsilon^2\log(\epsilon) - \frac{3}{8}\epsilon^2$$

the second integral also converges to zero for $\epsilon \to 0$ and this shows the L^1_{loc} convergence. □

A.3 A consequence of ANEC

We will present a result on real-valued solutions $\theta(t)$ of the differential equation

$$\theta'(t) + \mu\theta(t)^2 = -f(t), \quad t \in \mathbb{R}, \tag{A.3.1}$$

where $\mu > 0$ and $f \in C^1(\mathbb{R}, \mathbb{R})$, with initial condition

$$\theta(0) = \theta_0 \,. \tag{A.3.2}$$

It follows from the Picard-Lindelöf Theorem that there is an open interval (a, b) containing 0, which may be finite, semi-finite or infinite (i.e. coinciding with $\mathbb{R}$), such that this interval is the domain of the unique, inextensible C^1 solution θ of (A.3.1) satisfying the initial condition. In this case, we call θ the maximal solution of (A.3.1) defined by the initial condition, and refer to (a, b) as the maximal domain.

The following statement is a variation on a similar result in [WY91], and it uses a very similar argument, the main difference being that the assumption (A.3.3) here is slightly different from that in [WY91], where the integral is taken over a semi-axis. Note also that our parameter λ corresponds to $1/\lambda$ in the notation of [WY91].

Theorem A.2. *Suppose that $f \in C^1(\mathbb{R}, \mathbb{R})$ has the property*

$$\limsup_{\lambda \to 0} \int_{-\infty}^{\infty} f(t)\eta(\lambda t)\,\mathrm{d}t \geq 0 \tag{A.3.3}$$

for the function $\eta(t) = (1 - t^2)^4$ for $|t| < 1$, $\eta(t) = 0$ for $|t| \geq 1$.

Then either the maximal domain of θ coincides with all of the real axis and $\theta(t) = 0$ for all $t \in \mathbb{R}$, or the maximal domain (a, b) of θ is a finite or semi-finite interval. In this case, $\theta(t) \to \mp\infty$ for t approaching the finite boundary at the right/left side of the maximal domain (in the finite case this holds with the respective sign for both boundaries). In particular, this is the case if $\theta(t_0) \neq 0$ for some t_0 in the maximal domain of θ.

Proof. Consider the auxiliary differential equation

$$u''(t) + \frac{f(t)}{\mu} u(t) = 0 \tag{A.3.4}$$

For the initial values $u(0) = 1$, $u'(0) = \theta_0$ and the given f this linear differential equation has by the Picard-Lindelöf Theorem a unique, global solution $u \in C^2(\mathbb{R}, \mathbb{R})$. Furthermore, this solution is nonzero in some neighbourhood of 0. For points from this neighbourhood, one can then rewrite (A.3.4) as

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{u'(t)}{u(t)}\right) + \left(\frac{u'(t)}{u(t)}\right)^2 = -\frac{f(t)}{u(t)}$$

which implies that $\hat{\theta}(t) \equiv \frac{u'(\mu t)}{u(\mu t)}$ fulfills equation (A.3.1). Furthermore, $\hat{\theta}$ also satisfies the initial condition (A.3.2) and by the uniqueness part in the Picard Lindelöf Theorem it therefore agrees with θ. This however implies that the only way in which θ can fail to be C^1 at a boundary point $c = a$ or $c = b$ of a semi-finite interval is a zero of u at μc. At this zero u' has to differ from zero, otherwise u as a C^2-solution to (A.3.4) with initial conditions $u(\mu c) = 0, u'(\mu c) = \lim_{x \to \mu c} u'(x) = 0$ would be identically zero in contradiction to the initial values for u at 0. By continuity, u' is therefore nonzero in a neighbourhood of μc, and by (A.3.1), $\theta(t) = \frac{u'(\mu t)}{u(\mu t)}$ approaches the value $-\infty$ for $t \to c, t < c$ (right boundary point) or the value $+\infty$ for $t \to c, t > c$ (left boundary point). For proving that θ diverges at the boundary (boundaries) of a semi-finite interval it is therefore sufficient to show that θ cannot be continued as a C^1 function beyond this boundary.

With the definition of η as above, and provided that the maximal domain of θ coincides with all of $\mathbb{R}$, one has for $0 < \lambda < 1$,

$$\begin{aligned}\int_{-\infty}^{\infty} \theta'(t)\eta(\lambda t)\,\mathrm{d}t. = \int_{-\infty}^{\infty} \theta(t)\lambda\eta'(\lambda t)\,\mathrm{d}t \\ = -8\lambda \int_{-1/\lambda}^{1/\lambda} \theta(t)(\lambda t)(1-(\lambda t)^2)^3\,\mathrm{d}t \\ \geq -8\lambda \int_{-1/\lambda}^{1/\lambda} |\theta(t)|\,(1-(\lambda t)^2)^2\,\mathrm{d}t\end{aligned}$$

owing to the fact that both $|\lambda t|$ and $|(1-(\lambda t)^2)|$ are bounded by 1 on the domain of integration. Combining this with (A.3.1) and (A.3.3) leads to

$$\limsup_{\lambda\to 0}\; -8\lambda \int_{-1/\lambda}^{1/\lambda} |\theta(t)|(1-(\lambda t)^2)^2\,\mathrm{d}t + \mu \int_{-1/\lambda}^{1/\lambda} \theta(t)^2(1-(\lambda t)^2)^4\,\mathrm{d}t \leq 0\,. \tag{A.3.5}$$

Using also the Cauchy-Schwarz inequality

$$\int_{-1/\lambda}^{1/\lambda} |\theta(t)|(1-(\lambda t)^2)^2\,\mathrm{d}t \leq \left(\int_{-/\lambda}^{1/\lambda} \theta(t)^2(1-(\lambda t)^2)^4\,\mathrm{d}t\right)^{1/2} \left(\int_{-1/\lambda}^{1/\lambda} 1\,\mathrm{d}t\right)^{1/2},$$

the estimate (A.3.5) can be replaced by

$$\limsup_{\lambda\to 0}\; -\frac{8}{\mu}\sqrt{2\lambda}\left(\int_{-1/\lambda}^{1/\lambda} \theta(t)^2(1-(\lambda t)^2)^4\,\mathrm{d}t\right)^{1/2} + \int_{-1/\lambda}^{1/\lambda} \theta(t)^2(1-(\lambda t)^2)^4\,\mathrm{d}t \leq 0\,, \tag{A.3.6}$$

which shows that $\int_{-\infty}^{\infty} \theta(t)^2\,\mathrm{d}t = 0$ upon using Levi's theorem. Since θ is C^1, this implies that $\theta(t) = 0$ for all t.

We have therefore shown that the assumption of θ being C^1 on all of $\mathbb{R}$ implies $\theta(t) = 0$ for all $t \in \mathbb{R}$; if on the other hand θ is C^1 only on a maximal finite or semi-finite interval, then by the statement in the first paragraph of the proof, it will diverge at the finite boundaries of this interval in the indicated way. □

A.4 Asymptotics of Laplace-type integrals

Lemma A.3. *Let $\Omega : \mathbb{R} \to [1/m, \infty[$, $m > 0$, $z \in H_r := \{z \in \mathbb{C} \mid \mathrm{Re}\,(z) > 0\}$ and the asymptotic behaviour of Ω for $p \to \infty$ be given by:*

$$\Omega(p) = \sum_{k=-d}^{N} \frac{a_k}{p^k} + \mathcal{O}\left(\frac{1}{p^{N+1}}\right) \tag{A.4.1}$$

Then for $L > 0$, $z \in H_r$, $\int_0^\infty e^{-pz}\Omega(t)\mathrm{d}p$ can be written as

$$\int_0^\infty e^{-pz}\Omega(p)\,\mathrm{d}p = \sum_{k=0}^{d} \frac{k! a_{-k}}{z^{k+1}} - E_{N-1}(z)\ln\left(\frac{z}{L}\right) + \tilde{R}^{(N-1)}_{\Omega,L}(z)$$
$$E_{N-1}(z) = \sum_{k=0}^{N-1} \frac{(-z)^k a_{k+1}}{k!}$$

Here, $\tilde{R}^{(N-1)}_{\Omega,L}$ is an analytic functions on H_r, such that the limit $\epsilon \to 0$ of the function $R^{(N-1)}_{\Omega,L,\epsilon} : \mathbb{R} \ni r \mapsto \tilde{R}^{(N-1)}_{\Omega,L}(\epsilon + ir)$ in the sense of distributions is given by a C^{N-1}-function $R^{(N-1)}_{\Omega,L}$ with asymptotic expansion

$$R^{(N-1)}_{\Omega,L}(r) = \sum_{l=0}^{N-1} R_l \frac{(-ir)^l}{l!} + o(r^{N-1})$$
$$R_l = \lim_{M\to\infty}\left(\left(\int_0^M p^l\left(\Omega(p) - \sum_{j=0}^{d} a_{-j}p^j\right)\mathrm{d}p - \sum_{j=1}^{l}\frac{a_{l+1-j}}{j} M^j - a_{l+1}\log(ML)\right)\right.$$
$$\left. + a_{l+1}\left(-\gamma + \sum_{n=1}^{l}\frac{1}{n}\right)\right).$$

Proof. Using first that for $k \in \mathbb{N}_0$

$$\int_0^\infty p^k e^{-pz} = \frac{k!}{z^{k+1}}$$

the integral $\int_0^\infty e^{-pz}\Omega(p)\mathrm{d}p$ can be written for $z \neq 0$ as

$$\int_0^\infty e^{-pz}\Omega(p)\mathrm{d}p = \sum_{k=0}^{d}\frac{k! a_{-k}}{z^{k+1}} + \int_0^\infty e^{-pz}\tilde{\Omega}(p)\mathrm{d}p \tag{A.4.2}$$

where by (A.4.1) the function $\tilde{\Omega}(p) = \Omega(p) - \sum_{k=0}^{d} a_{-k}p^k$ has the asymptotic expansion

$$\tilde{\Omega}(p) = \sum_{k=1}^{N}\frac{a_k}{p^k} + \mathcal{O}\left(\frac{1}{p^{N+1}}\right)$$

To obtain the claimed splitting of the remaining integral $\int_0^\infty e^{-pz}\tilde{\Omega}(p)\mathrm{d}p$ consider the term

$$I(z) = \sum_{k=0}^{N-1}\frac{a_{k+1}}{k!}(-z)^k\left(\int_0^{1/L}\frac{e^{-pz}-1}{p}\,\mathrm{d}p + \int_{1/L}^\infty e^{-pz}\frac{\mathrm{d}p}{p}\right)$$

On the one hand, using the analyticity of $p \mapsto \frac{e^{-pz}-1}{p}$, $p \mapsto \frac{1}{p}$ and $p \mapsto \frac{e^{-pz}}{p}$ for p such that $\mathrm{Re}\,(p) > 0$, we have for z with $\mathrm{Re}\,(z) > 0 \Rightarrow \mathrm{Re}\,(\frac{1}{z}) > 0$:

$$\begin{aligned}
\int_0^{1/L} \frac{e^{-pz}-1}{p}\,\mathrm{d}p + \int_{1/L}^{\infty} e^{-pz}\frac{\mathrm{d}p}{p} &= \int_0^{1/z} \frac{e^{-pz}-1}{p}\,\mathrm{d}p + \int_{1/z}^{1/L} e^{-pz}\frac{\mathrm{d}p}{p} - \int_{1/z}^{1/L}\frac{\mathrm{d}p}{p} \\
&\quad - \int_{1/z}^{\infty} e^{-pz}\,\frac{\mathrm{d}p}{p} + \int_{1/L}^{1/z} e^{-pz}\,\frac{\mathrm{d}p}{p} \\
&= \int_0^{1/z} \frac{e^{-pz}-1}{p}\,\mathrm{d}p + \int_{1/z}^{\infty} e^{-pz}\,\frac{\mathrm{d}p}{p} - \log\left(\tfrac{z}{L}\right) \\
&= \int_0^{1} \frac{e^{-p}-1}{p}\,\mathrm{d}p + \int_{1}^{\infty} e^{-p}\,\frac{\mathrm{d}p}{p} - \log\left(\tfrac{z}{L}\right) \\
&= -\,\gamma - \log\left(\tfrac{z}{L}\right)
\end{aligned}$$

(this is true as long as the branch-cut of the logarithm is chosen to lie in the left half-plane; in the following it will be taken to lie on the negative real axis). Defining $E_{N-1}(z)$ by

$$E_{N-1}(z) = \sum_{k=0}^{N-1} \frac{a_{k+1}}{k!}(-z)^k$$

we have

$$I(z) = -E_{N-1}\left(\gamma + \log\left(\tfrac{z}{L}\right)\right)$$

On the other hand by induction one proves for $k \in \mathbb{N}$

$$\begin{aligned}
\frac{(-z)^k}{k!}\left(\int_0^{1/L} \frac{e^{-pz}-1}{p}\,\mathrm{d}p + \int_{1/L}^{\infty} e^{-pz}\,\frac{\mathrm{d}p}{p}\right) &= \int_0^{1/L} \frac{e^{-pz} - \sum_{j=0}^{k}\frac{(-pz)^j}{j!}}{p^{k+1}}\mathrm{d}p \\
&\quad + \int_{1/L}^{\infty} \frac{e^{-pz}}{p^{k+1}}\,\mathrm{d}p - L\,\frac{(-z)^{k-1}}{k!}\sum_{j=0}^{k-1}\sum_{l=0}^{j+1}\frac{j!}{l!}\left(-\frac{z}{L}\right)^{l-j} \qquad \text{(A.4.3)}
\end{aligned}$$

Using furthermore

$$\frac{1}{k!}\sum_{j=0}^{l}\frac{(j+k-1-l)!}{j!} = \frac{1}{k-l}\,\frac{1}{l!}$$

for $k, s \in \mathbb{N}$, $s \leq k-1$, the last term of (A.4.3) can be written as

$$\begin{aligned}
L\frac{(-z)^{k-1}}{k!}\sum_{j=0}^{k-1}\sum_{l=0}^{j+1}\frac{j!}{l!}\left(-\frac{z}{L}\right)^{l-j} &= \sum_{l=0}^{k-1}\frac{L^{k-l}}{k!}(-z)^l\sum_{j=0}^{l}\frac{(j+k-1-l)!}{j!} + \frac{(-z)^k}{k!}\sum_{j=0}^{k-1}\frac{1}{j+1} \\
&= \sum_{l=0}^{k-1}\frac{L^{k-l}(-z)^l}{(k-l)l!} + \frac{(-z)^k}{k!}\sum_{j=0}^{k-1}\frac{1}{j+1}
\end{aligned}$$

so $I(z)$ can alternatively be expressed as

$$I(z) = \sum_{k=0}^{N-1} a_{k+1}\Bigg(\int_0^{1/L} \frac{e^{-pz} - \sum_{j=0}^{k} \frac{(-pz)^j}{j!}}{p^{k+1}} \mathrm{d}p + \int_{1/L}^{\infty} \frac{e^{-pz}}{p^{k+1}} \mathrm{d}p - \sum_{l=0}^{k-1} \frac{L^{k-l}(-z)^l}{(k-l)l!} \\ - \frac{(-z)^k}{k!} \sum_{j=0}^{k-1} \frac{1}{j+1} \Bigg)$$

Using the above, $\int_0^\infty e^{-pz}\tilde{\Omega}(p)\mathrm{d}p$ can be written as

$$\begin{aligned}\int_0^\infty e^{-pz}\tilde{\Omega}(p)\mathrm{d}p &= \int_0^\infty e^{-pz}\tilde{\Omega}(p)\mathrm{d}p - I(z) + I(z) \\ &= \underbrace{\int_{1/L}^\infty \left(\tilde{\Omega}(p) - \sum_{k=0}^{N-1} \frac{a_{k+1}}{p^{k+1}}\right) e^{-pz}\mathrm{d}p}_{I_2(z)} + \sum_{k=0}^{N-1} a_{k+1} \sum_{l=0}^{k-1} \frac{L^{k-l}(-z)^l}{(k-l)l!} \\ &\quad + \underbrace{\int_0^{1/L} \tilde{\Omega}(p)e^{-pz} - \sum_{k=0}^{N-1} a_{k+1} \frac{e^{-pz} - \sum_{j=0}^{k} \frac{(-pz)^j}{j!}}{p^{k+1}} \mathrm{d}p}_{I_3(z)} \\ &\quad + \sum_{k=0}^{N-1} \frac{(-z)^k}{k!} a_{k+1} \sum_{j=1}^{k} \frac{1}{j} - E_{N-1}(z)\left(\log\left(\tfrac{z}{L}\right) + \gamma\right)\end{aligned}$$

We can now identify $\tilde{R}_{L,\Omega}^{(N-1)}(z)$ as

$$\tilde{R}_{L,\Omega}^{(N-1)}(z) = I_2(z) + I_3(z) + \sum_{k=0}^{N-1} a_{k+1} \sum_{l=0}^{k-1} \frac{L^{k-l}(-z)^l}{(k-l)l!} + \sum_{k=0}^{N-1} \frac{(-z)^k}{k!} a_{k+1} \sum_{j=1}^{k} \frac{1}{j} - \gamma E_{N-1}(z)$$

Setting $z = ir + \epsilon$ and integrating against an $h \in C_0^\infty(\mathbb{R})$, the last three sums, which are just polynomials in z, will go to the integrals obtained by setting $z = ir$ in the integrand, so only the integrals I_2 and I_3 have to be discussed. For these we have

$$\begin{aligned}\int_{\mathbb{R}} I_2(\epsilon + ir)h(r)\mathrm{d}r &= \int_{\mathbb{R}} \int_{1/L}^\infty \left(\tilde{\Omega}(p) - \sum_{k=0}^{N-1} \frac{a_{k+1}}{p^{k+1}}\right) e^{-p\epsilon - ipr}\mathrm{d}p\, h(r)\mathrm{d}r \\ \int_{\mathbb{R}} I_3(\epsilon + ir)h(r)\mathrm{d}r &= \int_{\mathbb{R}} \int_0^{1/L} \tilde{\Omega}(p)e^{-p\epsilon - ipr} - \sum_{k=0}^{N-1} a_{k+1} \frac{e^{-p\epsilon - ipr} - \sum_{j=0}^{k} \frac{(-p\epsilon - ipr)^j}{j!}}{p^{k+1}} \mathrm{d}p \\ &\quad \ldots \times h(r)\mathrm{d}r\,.\end{aligned}$$

Since, by assumption, $\tilde{\Omega}(p) - \sum_{k=0}^{N-1} \frac{a_{k+1}}{p^{k+1}}$ is in $\mathcal{O}\left(p^{-(N+1)}\right)$, the limit can be performed under the integral in I_2 by majorized convergence; since $w \mapsto \frac{e^{-w} - \sum_{j=0}^{k} \frac{(-w)^j}{j!}}{w^{k+1}} =: e_{k+1}(w)$ is an analytic function of w and thus bounded on any bounded set and in I_3 the p-integral extends only over the interval $[0, 1/L]$, while the r-integral is only over the compact support of h, also there we can perform the limit under the integral by majorized convergence and obtain

$$R^{(N-1)}_{L,\Omega}(r) = \tilde{R}^{(N-1)}_{L,\Omega}(ir)$$

Looking at the expressions for $I_2(ir)$ and $I_3(ir)$, using $\tilde{\Omega}(p) - \sum_{k=0}^{N-1} \frac{a_{k+1}}{p^{k+1}} \in \mathcal{O}\left(p^{-(N+1)}\right)$ and the analyticity of the e_{k+1} once more, we see that we can even differentiate $N-1$-times wrt. r under the integral and still obtain r-independent, convergent majorants, so by the criterion for differentiable dependence of integrals on parameters, we get that $R^{(N-1)}_{L,\Omega}$ is in fact C^{N-1}. Concerning the original $\tilde{R}^{(N-1)}_{L,\Omega}$ for arguments in H_r, using the same majorants and the fact that the integrands are analytic functions of z we get the analyticity statement on H_r.

To calculate the asymptotics for small r, one writes the z-dependent exponentials in $I_2(ir)$ and $I_3(ir)$ as

$$e^{-ipr} = \sum_{l=0}^{N-1} \frac{(-ipr)^l}{l!} + \underbrace{e^{-ipr} - \sum_{l=0}^{N-1} \frac{(-ipr)^l}{l!}}_{=(ipr)^N e_N(ipr)}$$

For r, p such that $0 < p < 1/L$ and $|r| < M$ for some $M \in \mathbb{R}$, $p \mapsto p^N e_N(ipr)$ is bounded, so

$$\begin{aligned} I_3(ir) = &\sum_{l=0}^{N-1} \frac{(-ir)^l}{l!} \int_0^{1/L} p^l \tilde{\Omega}(p) \mathrm{d}p - \sum_{k=0}^{N-1} a_{k+1} \sum_{l=k+1}^{N-1} \frac{(-ir)^l}{l!} \int_0^{1/L} p^{l-k-1} \mathrm{d}p \\ &+ (ir)^N \int_0^{1/L} p^N e_N(ipr) \mathrm{d}p - (ir)^N \sum_{k=0}^{N-1} a_{k+1} \int_0^{1/L} p^{N-k-1} e_N(p) \mathrm{d}p \,, \end{aligned}$$

which shows

$$I_3(ir) = \sum_{l=0}^{N-1} \frac{(-ir)^l}{l!} \int_0^{1/L} p^l \Omega(p) \mathrm{d}p - \sum_{k=0}^{N-1} a_{k+1} \sum_{l=k+1}^{N-1} \frac{(-ir)^l}{l!} \int_0^{1/L} p^{l-k-1} \mathrm{d}p + \mathcal{O}(r^N) \,. \tag{A.4.4}$$

For $w \in \mathbb{R}$ with $|w| > 1$ we have

$$|w\, e_N(w)| \leq 1 + \sum_{l=0}^{N-1} \frac{1}{l!} \,.$$

Together with the boundedness of $w \mapsto e_N(w)$ for $|w| < 1$ this implies that $p \mapsto irpe_N(irp)$ is bounded for $r \in \mathbb{R}$, $p \geq 1/L$ and goes to zero for $r \to 0$ and fixed p. For I_2 this implies

$$\begin{aligned} I_2(ir) = &\sum_{l=0}^{N-1} \frac{(-ir)^l}{l!} \int_{1/L}^{\infty} p^l \left(\tilde{\Omega}(p) - \sum_{k=0}^{N-1} \frac{a_{k+1}}{p^{k+1}} \right) \mathrm{d}p \\ &+ (ir)^{N-1} \int_{1/L}^{\infty} p^{N-1} e_N(pir) \left(\tilde{\Omega}(p) - \sum_{k=0}^{N-1} \frac{a_{k+1}}{p^{k+1}} \right) \mathrm{d}p \end{aligned}$$

and by dominated convergence the last integral goes to zero for $r \to 0$ which establishes

$$I_2(ir) = \sum_{l=0}^{N-1} \frac{(-ir)^l}{l!} \int_{1/L}^{\infty} p^l \left(\tilde{\Omega}(p) - \sum_{k=0}^{N-1} \frac{a_{k+1}}{p^{k+1}} \right) \mathrm{d}p + o(r^{N-1})$$

Together this yields

$$\begin{aligned}
R_{\Omega,L}^{(N-1)}(r) = &\sum_{l=0}^{N-1} \frac{(-ir)^l}{l!} \int_{1/L}^{\infty} p^l \tilde{\Omega}(p) - \sum_{k=0}^{N-1} a_{k+1} p^{l-k-1} \mathrm{d}p \\
&+ \sum_{k=0}^{N-1} a_{k+1} \sum_{l=0}^{k-1} \frac{L^{k-l}(-ir)^l}{(k-l)l!} \\
&+ \sum_{l=0}^{N-1} \frac{(-ir)^l}{l!} \int_0^{1/L} \tilde{\Omega}(p) p^l \mathrm{d}p - \sum_{k=0}^{N-1} a_{k+1} \sum_{l=k+1}^{N-1} \frac{(-ir)^l}{l!} \int_0^{1/L} p^{l-k-1} \,\mathrm{d}p \\
&+ \sum_{k=0}^{N-1} \frac{(-ir)^k}{k!} a_{k+1} \sum_{j=1}^{k} \frac{1}{j} + o(r^{N-1})
\end{aligned} \tag{A.4.5}$$

The first summand can be split as

$$\begin{aligned}
&\sum_{l=0}^{N-1} \frac{(-ir)^l}{l!} \int_{1/L}^{\infty} p^l \tilde{\Omega}(p) - \sum_{k=0}^{N-1} a_{k+1} p^{l-k-1} \mathrm{d}p \\
&\quad = \lim_{M\to\infty} \left[\sum_{l=0}^{N-1} \frac{(-ir)^l}{l!} \int_{1/L}^{M} p^l \tilde{\Omega}(p) \mathrm{d}p + \sum_{k=0}^{N-1} a_{k+1} \sum_{l=0}^{k-1} \frac{L^{k-l}(-ir)^l}{(l-k)l!} \right. \\
&\qquad \left. - \sum_{l=0}^{N-1} \frac{a_{l+1}}{l!} (-ir)^l \log(ML) - \sum_{k=0}^{N-1} a_{k+1} \sum_{l=k+1}^{N-1} \frac{\left(M^{l-k} - L^{k-l}\right)(-ir)^l}{(l-k)l!} \right]
\end{aligned}$$

Inserting this into (A.4.5) we get

$$\begin{aligned}
R_{\Omega,L}^{(N-1)}(r) &= \lim_{M\to\infty} \left[\sum_{l=0}^{N-1} \frac{(-ir)^l}{l!} \int_0^{M} p^l \tilde{\Omega}(p) \mathrm{d}p - \sum_{l=0}^{N-1} \frac{a_{l+1}}{l!} (-ir)^l \log(ML) \right. \\
&\qquad \left. - \sum_{k=0}^{N-1} a_{k+1} \sum_{l=k+1}^{N-1} \frac{M^{l-k}(-ir)^l}{(l-k)l!} \right] \\
&\quad + \sum_{l=0}^{N_1} \frac{a_{l+1}}{l!} (-ir)^l \sum_{j=1}^{l} \frac{1}{j} \\
&= \lim_{M\to\infty} \left[\sum_{l=0}^{N-1} \frac{(-ir)^l}{l!} \left(\int_0^{M} p^l \tilde{\Omega}(p) \mathrm{d}p - \sum_{k=0}^{l-1} \frac{a_{k+1} M^{l-k}}{l-k} \right. \right. \\
&\qquad \left. \left. - a_{l+1} \log(ML) \right) \right] + \sum_{l=0}^{N_1} \frac{a_{l+1}}{l!} (-ir)^l \sum_{j=1}^{l} \frac{1}{j}
\end{aligned}$$

so defining

$$R_l = \lim_{M\to\infty}\left(\int_0^M p^l\tilde{\Omega}(p)\mathrm{d}p - \sum_{k=1}^{l}\frac{a_{l+1-k}}{k}\,M^k - a_{l+1}\log(ML)\right) + a_{l+1}\left(-\gamma + \sum_{j=1}^{l}\frac{1}{j}\right)$$

we have the claimed asymptotic expansion for $R^{(k-1)}_{\Omega,L}$.

□

B Table of symbols

Symbol	Description	Page
$:\phi_1 \dots \phi_n:_{\text{SHP}}$	SHP Wick product (normal order wrt. $\mathcal{G}_k^{\text{SHP}}$)	17
$\Box_g$	Wave operator $g^{ab}\nabla_a\nabla_b$	12
$\overset{o}{\Box}$	Pseudo Minkowski wave operator $\partial_{\eta\eta} - \partial_{xx} - \partial_{yy} - \partial_{zz}$	79
∇	Levi-Civita connection associated to g	12
$\mathcal{A}(M, g)$	Algebra of the Klein-Gordon field on (M, g)	12
$\alpha_t^{e_0}$	Time translation automorphism for inertial observer on Minkowski spacetime	37
$\beta, \boldsymbol{\beta} = \beta e_0$	Inverse temperature $\frac{1}{k_B T}$; four-vector encoding inverse temperature and rest-frame.	38
c_k	Coefficients in the concrete construction of $\Omega^{()}$, $\Omega^{(\eta)}$ and $\Omega^{(\eta\eta')}$ as a sum of terms $(A + p^2)^{-(k+1/2)}$	102
C_{ab}	Renormalization ambiguity of T_{ab}^{ren}	56
$c_{0,m}$, $c_{2,m}$	Constants giving the difference between ordinary and SHP Wick products on Minkowski spacetime	49
$C^k(M)$, $C^\infty(M)$, $C_0^\infty(M)$	k-times differentiable, smooth and compactly supported, smooth functions on M	11
C	Squared scale factor, expressed in conformal time	21
$\eth$	Balanced derivative	43
$\mathcal{D}$, $\mathcal{D}'$	Modified derivatives wrt η respectively η'; $\mathcal{D} = \partial_\eta + \frac{C'(\eta)}{2C(\eta)}$	34
$D_{\eta\eta'}$	Conformal factor $\sqrt{C(\eta)}\sqrt{C(\eta')}$	34
$\Delta^{1/2}$, v_j	Functions defining the Hadamard parametrix	15
$\overset{o}{\Delta}{}^{1/2}$, $\overset{o}{v}_j$	Corresponding functions, calculated as in flat spacetime but with “time-dependent mass”	79
$E(3)$	Symmetry group of euclidean space	21
$\varepsilon_{ab}^\omega(x)$	Thermal stress tensor of LTE-state ω at $x \in M$	51
$\mathrm{E}^\pm$	Retarded and advanced Greens operators	12
$\mathscr{E}$	Commutator distribution	12
$\exp_x$	Exponential map at $x \in M$	14
$\phi(f)$	Klein-Gordon field	12
$\Phi[M, g]$	Locally covariant quantum field on (M, g)	17
$\mathcal{G}_k$, $\mathcal{G}_k^s$	Hadamard parametrix, its symmetric part	15
$H_\nu^{(1)}$	Hankel functions (of the first kind)	98

Symbol	Description	Page
$\hat{I} =]\eta_i, \eta_f[$	Range of the global, conformal time	20
$J^{\pm}(\cdot)$	Past/future set	12
$K^{()}(p)$, $K^{(\eta)}(p)$, $K^{(\eta\eta')}(p)$	Integral kernels of the state-dependent part of the covariant expectation values	94
$\mathcal{L}_{\beta'}(x), \mathcal{L}_{\beta'}(N)$	Set of $S_x^{(2)}$ resp. $S_N^{(2)}$-thermal states with inverse local temp. bounded below by β'	59
$\tilde{\mathrm{lo}}.$	Restriction of $[\log(\tilde{\sigma}_+)]^s - \log(\tilde{q})$ to $\eta = \eta'$	29
$\mathcal{M}^k[f]$	k-th moment of function $h \in \mathscr{S}$	42
(M, g)	Spacetime manifold with Lorentzian metric tensor g	11
$M_{\mathrm{RW}}(\hat{I}, C)$	Robertson Walker spacetime with range $\hat{I}$ of the conformal time and squared scale-factor C	21
μ_g	Measure on (M, g) induced by g	11
N_{τ^2}, ρ_{μ_2,μ_4}	Rapidly decreading functions appearing in the construction of LTE-states	109
$P_\omega(\epsilon)$, $P_\omega^{\mathrm{ren}}(\epsilon)$	Transition probability of detector, renormalized transition probability	41
$\mathcal{P}_\omega^k$	k-th moment of (ren.) transition probability as fct. of energy difference	43
$\mathrm{P}_{m,\xi}$	Klein-Gordon operator $\Box_g + m^2 + \xi R$	12
$\overset{o}{\mathrm{P}}_{m,\xi}$	Corresponding operator on functions with conformal factor	81
$Q_{m,\xi}$	"Time dependent mass" $(m^2 + (\xi - 1/6)R)C$ appearing in the differential equation for V_p	31
$P_0^{()}$, $P_{-1}^{(\eta\eta')}$, $P_0^{(-1)}$	Prefactors of the $\frac{1}{r_+^2}$ and $\frac{1}{r_+^4}$-terms in $[\mathcal{G}_k^s]_{\eta=\eta'}$ and $[\mathcal{D}\mathcal{D}'\mathcal{G}_k^s]_{\eta=\eta'}$	86
$Q_j^{()}$, $Q_j^{(\eta)}$, $Q_j^{(\eta\eta')}$	Prefactors of the logarithmic terms in $[\mathcal{G}_k^s]_{\eta=\eta'}$, $[\mathcal{D}\mathcal{G}_k^s]_{\eta=\eta'}$ and $[\mathcal{D}\mathcal{D}'\mathcal{G}_k^s]_{\eta=\eta'}$	86
q	Deviation of σ from ρ	23
$q(x, v; \beta')$, $q_{0/1}(\gamma, \eta, \beta')$	Lower bounds in the QWEIs	60
R_{ab}	Ricci tensor corresponding to ∇	12
R	Curvature scalar R_a^a	12
R_Δ	Part of $\Delta^{1/2}$ that contributes to expectation values on Robertson Walker spacetimes	79
R_v	Term appearing in the construction of $v^{(k)}$ on Robertson Walker spacetimes, disappears in coincidence limits	79
$\frac{1}{r_+^2}$, $\frac{1}{r_+^4}$	Restrictions of $\left[\frac{\tilde{q}}{\tilde{\sigma}_+}\right]^s$ respectively $\partial_\eta \partial_{\eta'} \left[\frac{\tilde{q}}{\tilde{\sigma}_+}\right]^s$ to $\eta = \eta'$.	26

Symbol	Description	Page
$R^{()}_{\mathcal{G}_k}$, $R^{(\eta)}_{\mathcal{G}_k}$, $R^{(\eta\eta')}_{\mathcal{G}_k}$	Finite remainder of Hadamard-parametrix when restricted to $\eta = \eta'$	86
$R^{()}$, $R^{(\eta)}$, $R^{(\eta\eta')}$	Difference between restricted Hadamard parametrix and its corresponding integral representations	92
ρ,	Pseudo Minkowski distance $\rho = \mathbf{x}^2 - (\eta - \eta')^2$	22
S_x	Space of local, thermal observables at point x	39
$S_x^{(n)}$	Space generated by first n balanced derivatives	50
σ, σ_ϵ	Signed squared geodesic separation; regularized	14
$\left[\frac{1}{\sigma_+}\right]^s$, $[\log(\sigma_+)]^s$	Symmetric part of regularized term $\frac{1}{\sigma}$ and $\log(\sigma)$	25
$T^{\mathrm{ren}}_{ab}(x)$	Renormalized stress-energy tensor	57
$T_x M$	Tangent space at $x \in M$	14
T	Time-function	12
$\vartheta^\omega(x)$	(Function of) the local temperature in LTE-state ω at point x	51
V_p	Mode function	31
$V_p^{(k)}$	Adiabatic vacua-like mode function	96
v_p	Modulus of mode function	117
ψ	Digamma function	103
ω	(General) state on $\mathcal{A}(M, g)$	13
$\omega^{\boldsymbol{\beta}}$	KMS-state at inverse temperature $\boldsymbol{\beta}^a\boldsymbol{\beta}_a$; rest-frame $\frac{\boldsymbol{\beta}^a}{\boldsymbol{\beta}^a\boldsymbol{\beta}_a}$	38
ω_{ini}	Initial state used in the construction of LTE-states	109
$\mathcal{W}(M, g)$	Enlarged algebra of the Klein-Gordon field containing e.g. Wick products	16
$\mathscr{W}_n^\omega$	n-point function of the state ω	13
$\mathscr{W}_2^{\omega,\mathrm{s}}$	Symmetric part of the two-point function	13
$\tilde{W}_{\Omega,+}$, $W_{\Omega,\epsilon}$	(Symmetry reduced) distributions corresponding to $[\mathcal{G}_k^s]_{\eta=\eta'}$, etc.	89
$\hat{w}^{()}$, $\hat{w}^{(\eta)}$, $\hat{w}^{(\eta\eta')}$	Fourier-transform of the symmetry reduced restrictions of $\mathscr{W}_2^{\omega,\mathrm{s}}$, $\mathcal{D}\mathscr{W}_2^{\omega,\mathrm{s}}$ and $\mathcal{D}\mathcal{D}'\mathscr{W}_2^{\omega,\mathrm{s}}$ to $\eta = \eta'$	35
Ξ	Function encoding the deviation of a state from a pure state	34

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