Thermodynamic Properties of Non-Equilibrium States in Quantum Field Theory

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Abstract

Within the framework of relativistic quantum field theory, a novel method is established which allows to distinguish non-equilibrium states admitting locally a thermodynamic interpretation. The basic idea is to compare these states with global equilibrium states (KMS states) by means of local thermal observables. With the help of such observables, the states can be ordered into classes of increasing local thermal stability. Moreover, it is possible to identify states exhibiting certain specific thermal properties of interest, such as a definite local temperature or entropy density. The method is illustrated in a simple model describing the spatio-temporal evolution of a “big heat bang”.

1 Introduction

States of macroscopic systems which are in global thermal equilibrium can be distinguished in a clearcut manner within the setting of quantum statistical mechanics by the Kubo-Martin-Schwinger (KMS) condition \cite{KMS}. This condition, which comprises the pertinent features of the Gibbs ensemble in the case of finite and infinite quantum systems \cite{Gibbs}, has proved to be a powerful ingredient, both, in the construction of equilibrium states in concrete models and in their general structural analysis.

However, there does not exist a similarly general and powerful characterization of states complying with the heuristic idea of being only locally in thermal equilibrium, \textit{e.g.} having only locally a definite temperature which varies from point to point. The physical origin of this conceptual difficulty is obvious: if one deviates from a global equilibrium situation, there appear a variety of possibilities, ranging
from mild perturbations of equilibrium states through steady states, whose properties are governed by external heat baths, or hydrodynamic flows up to systems which no longer admit a description in terms of thermodynamic notions. Thus, what is required are concepts allowing to distinguish between these different situations and describing the respective local thermal properties of the corresponding classes of states.

There exists an extensive literature on this subject, cf. the comprehensive treatment in [3] and references quoted there. Most approaches are based on a maximal entropy principle, suggesting a modified Gibbs ansatz in a suitable (large time) limit of the theory. Other methods proceed by some procedure of “coarse graining” directly to an effective macroscopic description. The conceptual basis of these approaches, however, does not always seem clear. In any case, the question of identifying the states of interest in the microscopic theory is left aside.

In the present article we analyse systematically this problem in the setting of relativistic quantum field theory. This framework is particularly well suited for such an investigation since it provides an assignment of observables to space-time regions, yielding a description of the local properties of physical states. In particular, it allows a local comparison of different states, which has proved to be an important element of structural analysis [4]. Within the present thermodynamic context, it was used as an ingredient in discussions of local thermal aspects of physical states in [5, 6, 7] and we will also make use of it here.

Before going into technical details, let us outline the heuristic ideas underlying our approach. The basic ingredients are suitable “local thermal observables”, assigned to the space-time points \( x \), by which any given state can be compared with the members of the family of global equilibrium states. If a state happens to coincide at \( x \) with a global equilibrium state to some degree of accuracy, i.e. if the expectation values of a sufficiently large number of thermal observables at \( x \) coincide in the two states, it is meaningful to say that the given state is approximately in equilibrium at \( x \). The larger the number of observables for which the two expectation values agree, the better the state complies with the idea of local equilibrium.

The use of local observables for the description of thermal properties requires some justification since thermodynamic notions are usually regarded as being of a macroscopic nature. Let us discuss this for the case of temperature. What one needs to measure temperature is a suitable thermometer, i.e. a device which allows discrimination of equilibrium states of different temperatures. In dealing with very large systems in global equilibrium it does not matter where and when this measurement takes place. The thermometer may be coupled to any part of the system under consideration at any time. If one increases its sensitivity, its spatial extension can be taken to be arbitrarily small. Moreover, as the system is in a stationary state, time averages can be replaced by the mean value of sufficiently many measurements at arbitrarily short time intervals. Therefore, for a system in global equilibrium, it is possible to determine the temperature by observables in
arbitrarily small space-time cells, provided the corresponding measurements are repeated sufficiently often. The smaller the cell the larger are the fluctuations of the results of the individual measurements; but the collection of these data provides the desired information.

This simple observation suggests the following definition of local temperature in a given space-time cell of a non-equilibrium system (provided a whole ensemble, *i.e.*, a large number of copies of the system, can be prepared): take sufficiently many readings of a suitable observable in that particular cell and compare them with those in global equilibrium states of arbitrary temperature. If the two sets of data happen to coincide for some value of the temperature, it is meaningful to ascribe that temperature value to the chosen cell of the non-equilibrium system under consideration. Thus the local temperature is to be regarded as a property of the ensemble, not of an individual member of it. But as quantum theory is a statistical theory, this point of view fits naturally into its mathematical framework.

It is conceptually convenient to proceed from the measurements in finite space-time cells to the idealization of temperature measurements performed at a space-time point. Such measurements can, however, no longer be described by observables (operators); one has to use quadratic forms. But since this causes no major mathematical difficulties, it seems natural to perform this additional step.

The idea of using local observables (or quadratic forms) for the description of the thermal properties of non-equilibrium states can be extended to other intensive thermal parameters of interest such as the energy density and the charge density. Again one has to exhibit suitable local observables which are sufficiently sensitive to these properties and to calibrate them by using the global equilibrium states as reference systems. The measured data taken in a non-equilibrium state have to be compared with those recorded in global equilibrium and if these data agree for a particular reference state one can attribute the values of the corresponding thermal parameters to the state describing the non-equilibrium situation. If, in particular, a state admits locally an interpretation in this manner in terms of a unique global equilibrium state, then all its local thermal parameters are fixed, including fundamental quantities such as the entropy density.

Transforming this idea into action, we have to cope with a difficulty which we have ignored so far: the notion of equilibrium in general refers to the state of a system at rest with respect to the observer. Dealing with an arbitrary state (*e.g.*, a hydrodynamic flow) we have to take into account that these rest systems may vary from point to point. Consequently, the set of thermal observables should be sufficiently rich to determine these local rest systems and the set of thermal reference states should include all Lorentz-transformed equilibrium states, too. Moreover, in order to cover also situations, where the thermal parameters do not have sharp values, we have also to admit mixtures of global equilibrium states as thermal reference states.

Thus, to summarize, a properly chosen set of local thermal observables together with the set of thermal reference states, fixed by the theory, will be our tool for
the analysis and interpretation of the local thermal properties of non-equilibrium states.

After this exposition of the heuristic ideas underlying our approach, let us turn now to its mathematical formulation. In the next section we recall some basic elements of thermal quantum field theory and introduce the thermal reference states. Section 3 contains the characterization of the local thermal observables. In Sec. 4 we identify with their help a hierarchy of physical states which may be regarded as being locally close to thermal equilibrium with increasing degree of accuracy. An instructive model, illustrating various points of our general analysis, is discussed in Sec. 5 and the article concludes with remarks on some conceptual aspects of our approach. In the appendix we establish a theory of thermostatics for the set of thermal reference states used in the main text.

2 Thermal reference states

As we are dealing here with a conceptual problem, the present investigation is carried out in the general setting of thermal quantum field theory. We begin by recalling some relevant notions and results, primarily in order to fix our notation.

The basic objects in our analysis are local observable fields, such as conserved currents, the stress energy tensor, etc., denoted generically by $\phi(x)$ (with tensor indices omitted). Quantum fields at a point are known to be quite singular objects which are only defined in the sense of quadratic forms on a suitable domain, cf. the subsequent section. It is therefore common to proceed from the point fields $\phi(x)$ to averages with suitable test functions $f$ having compact support in Minkowski space $\mathbb{R}^4$,

$$\phi(f) \doteq \int dx \, f(x) \phi(x).$$

These are defined as operator-valued distributions on some common dense and stable domain $\mathcal{D}$ in the underlying Hilbert space $\mathcal{H}$, where the theory has been constructed (usually the vacuum sector). The finite sums and products of the averaged field operators generate a *-algebra $A$, called the algebra of observables, consisting of all polynomials $A$ of the form

$$A = \sum \phi(f_1)\phi(f_2)\cdots\phi(f_n).$$

We assume that also all multiples of the unit operator 1 are elements of $A$. As the fields $\phi$ are real (being observable), the *-operation (Hermitian conjugation) on $A$ is defined by

$$A^* \doteq \sum \phi(\overline{f_1})\cdots\phi(\overline{f_2})\phi(\overline{f_n}),$$

where $\overline{f}$ denotes the complex conjugate of $f$. The Poincaré transformations $\lambda \in \mathcal{P}^\uparrow$ act on $A$ by automorphisms $\alpha_\lambda$,

$$\alpha_\lambda(A) \doteq \sum \phi(f_{1,\lambda})\phi(f_{2,\lambda})\cdots\phi(f_{n,\lambda}),$$
where $f_\lambda$ is defined by $f_\lambda(x) \equiv D(\lambda) f(\lambda^{-1} x)$ and $D$ is a matrix representation of $P_+^\dagger$, corresponding to the tensor character of the respective field $\phi$. If $\lambda$ is a pure translation, $\lambda = (1, a)$, $a \in \mathbb{R}^4$, we denote the corresponding automorphism by $\alpha_a$. Note that the action of these automorphisms on $\mathcal{A}$ is well-defined; there is no need to assume that they are unitarily implemented.

As we restrict attention here to observable fields, there is one further important ingredient in this general setting, namely locality (Einstein causality). It is the requirement that fields localized at spacelike separated points commute. We will make use of this property at some technical points in the subsequent analysis.

The states of the physical systems are described by positive normalized expectation functionals on the algebra $\mathcal{A}$, generically denoted by $\omega$. We recall that these functionals have the defining properties $\omega(c_1 A_1 + c_2 A_2) = c_1 \omega(A_1) + c_2 \omega(A_2)$, $c_1, c_2 \in \mathbb{C}$ (linearity), $\omega(A^* A) \geq 0$ (positivity), and $\omega(1) = 1$ (normalization).

Basic examples are states of the form

$$\omega(A) = \text{Tr} \rho A, \quad A \in \mathcal{A},$$

where $\rho$ is a density matrix in the underlying Hilbert space $\mathcal{H}$ and $\text{Tr}$ denotes the corresponding trace. It is, however, important to note that not all states of interest here can be represented in this way. For, if $\mathcal{H}$ is the vacuum Hilbert space, all states of the form (2.3) describe mixtures of local excitations of the vacuum; thus global thermal states are not among them. An explicit formula for the thermal states, analogous to (2.3), would require a change of the Hilbert space representation of the algebra of observables $\mathcal{A}$. Since we deal here with states describing very different physical ensembles, it is, however, more convenient to rely on the abstract characterization of states given above. We mention as an aside that one can recover from any such state an explicit representation in terms of density matrices on some Hilbert space by the Gelfand-Naimark-Segal reconstruction theorem [4]. But we make no use of this fact here.

As has been outlined in the introduction, an important ingredient in the present investigation are the global equilibrium states which are characterized by the KMS condition [2]. Given a Lorentz frame, fixed by some positive time-like vector $e \in V_+$ of unit length, this condition can be stated as follows.

**KMS condition:** A state $\omega_\beta$ satisfies the KMS condition at inverse temperature $\beta > 0$ in the given Lorentz frame if for each pair of operators $A, A' \in \mathcal{A}$ there is some function $h$ which is analytic in the strip $S_\beta \equiv \{ z \in \mathbb{C} : 0 < \text{Im} z < \beta \}$ and continuous at the boundaries such that

$$h(t) = \omega_\beta(A' \alpha_{te}(A)), \quad h(t + i \beta) = \omega_\beta(\alpha_{te}(A)A'), \quad t \in \mathbb{R}.$$  \hspace{1cm} (2.6)

In this situation $\omega_\beta$ is called a KMS state.

We will have occasion to make also use of a slightly stronger version of the KMS condition, proposed in [8]. It can be established under quite natural constraints on the number of local degrees of freedom of the underlying theory and is a remnant
of the relativistic spectrum condition in the vacuum sector. It was therefore called relativistic KMS condition in [3].

**Relativistic KMS condition:** A state $\omega_\beta$ is said to satisfy the relativistic KMS condition at inverse temperature $\beta > 0$ in the given Lorentz frame if for each pair of operators $A, A' \in \mathcal{A}$ there is some function $h$ which is analytic in the tube $\mathbb{R}^4 + i \left( V_+ \cap (\beta e - V_+) \right)$ such that in the sense of continuous boundary values [8]

$$h(a) = \omega_\beta(A' \alpha_a(A)), \quad h(a + i\beta e) = \omega_\beta(\alpha_a(A)A'), \quad a \in \mathbb{R}^4.$$  \hfill (2.7)

It is a well established fact that any KMS state $\omega_\beta$ describes an ensemble which is in thermal equilibrium in the distinguished Lorentz frame, describing the rest system of the state. As we have to keep track of both, temperatures and rest systems, it is convenient to combine this information into a four vector $\beta e \in V_+$, which will again be denoted by $\beta$. The temperature and the rest system can be recovered from any such temperature vector $\beta \in V_+$ in an obvious manner.

For given $\beta \in V_+$, the corresponding convex set $C_\beta$ of all KMS states $\omega_\beta$ is known to form a simplex under quite general conditions [2]. This implies in particular that all states in $C_\beta$ can be distinguished with the help of “classical” (central) observables. Familiar examples of such observables are the chemical potential in theories with a conserved charge or the mean density differentiating different phases. In order to simplify the subsequent discussion, we assume here that each family $C_\beta$ is non-degenerate, i.e. for any given $\beta$ there is a unique KMS state $\omega_\beta$. The case of more complex families $C_\beta$ can be treated similarly but requires some heavier notation.

Let us briefly discuss the consequences of this uniqueness assumption for the transformation properties of the KMS states under Poincaré transformations. For any given KMS state $\omega_\beta$ and transformation $\lambda = (\Lambda, a)$, the corresponding Poincaré-transformed state is given by $\omega_\beta \circ \alpha^{-1}_\lambda$, where the circle denotes the composition of maps. It follows from the definition of KMS states that $\omega_\beta \circ \alpha^{-1}_\lambda$ is again a KMS state belonging to the family $C_\Lambda \beta$. In view of our uniqueness assumption we thus obtain the simple transformation formula

$$\omega_\beta \circ \alpha^{-1}_\lambda = \omega_\Lambda \beta.$$ \hfill (2.8)

Thus the KMS states considered here are in particular isotropic in their rest system and invariant under space-time translations. On the other hand, velocity transformations in general change these states, in accordance with the well known fact that the Lorentz group is spontaneously broken in thermal equilibrium states [9]. Note, however, that the temperature, fixed by the length of $\beta$, remains unaffected by Poincaré transformations.

So far we have considered only KMS states, where the temperature vector $\beta$ is sharply defined. Yet thinking of macroscopic ensembles in thermal equilibrium where $\beta$ is not precisely known or statistically fluctuating, it is natural to consider also mixtures of KMS states. We therefore define for any compact subset $B \subset V_+$
corresponding families $\mathcal{C}_B$ of states consisting of all mixtures of KMS states $\omega_\beta$ with $\beta \in B$.

In order to obtain a more explicit description of the states in $\mathcal{C}_B$ and to avoid mathematical subtleties, we assume that the KMS states $\omega_\beta$ are weakly continuous in $\beta$, i.e. all functions

$$\beta \mapsto \omega_\beta(A), \quad A \in \mathcal{A},$$

(2.9)

are continuous. Apart from phase transition points (which are excluded here by our uniqueness assumption on $\mathcal{C}_\beta$), this property is expected to hold quite generally. With this input, the states $\omega_B \in \mathcal{C}_B$ can be represented in the form

$$\omega_B(A) = \int d\rho(\beta) \omega_\beta(A), \quad A \in \mathcal{A},$$

(2.10)

where $\rho$ is a positive normalized measure which has support in $B$. Note that in the case of degenerate families $\mathcal{C}_\beta$ the measure would also have support on the spectrum of all other classical observables parameterizing the KMS states.

The elements of $\mathcal{C} = \bigcup \mathcal{C}_B$, where the union extends over all compact subsets $B \subset V_+$, will be our reference states for the characterization of the local thermal observables and the interpretation of the local thermal properties of non-equilibrium systems. This choice turns out to be particularly convenient in the present investigation; yet without problems one could also admit reference states $\omega_B$ corresponding to non-compact sets $B \subset V_+$.

### 3 Local thermal observables

Although the algebra $\mathcal{A}$ contains all local observables of the underlying theory, it is not well suited for the description of the local thermal properties of physical states. For, all elements of $\mathcal{A}$ have quite fuzzy localization properties due to the integration of the point fields with test functions. So they do not have an interpretation in terms of physical properties which can be assigned to spacetime points. Furthermore, $\mathcal{A}$ contains an abundance of elements which are of no relevance to the thermodynamic interpretation of physical states.

For this reason we will proceed first from the algebra $\mathcal{A}$ to linear spaces $\mathcal{Q}_x$ of quadratic forms which can be interpreted as observables localized at the spacetime points $x \in \mathbb{R}^4$. In a second step we will then select from each $\mathcal{Q}_x$ suitable subspaces $\mathcal{T}_x$. The elements of $\mathcal{T}_x$ will be regarded as thermal observables at $x$ whose thermal interpretation is fixed by the thermal reference states in $\mathcal{C}$.

#### 3.1 Point fields as idealized local observables

For the step from smeared field operators to point fields, let us assume that in the vacuum sector $\mathcal{H}$ there hold energy bounds of the form

$$\pm \phi(f) \leq \nu(f) (1 + H)^k,$$

(3.1)
where $f$ is any real test function with compact support, $\nu(\cdot)$ is some Schwartz norm on the space of test functions, $H$ is the (positive) Hamiltonian, and $k > 0$ depends only on the field $\phi$. This condition has a clearcut physical interpretation: it says that the observed values of $\phi(f)$ can become large only in states of large energy. Such energy bounds have been established in many models \[10\].

As has been shown in \[11\], one can proceed from (3.1) to an improved estimate (for arbitrary $l > 0$ and corresponding sufficiently large $m > 0$)

$$
|| (1 + H)^{-m} \phi(f) (1 + H)^{-m} || \leq c \int dx |(1 - \Delta)^{-l} f(x)|,
$$

(3.2)

where $|| \cdot ||$ denotes the operator norm in $H$ and $\Delta$ is the Laplacian on $\mathbb{R}^4$. It follows from this bound that for sufficiently large $m$ and suitable sequences of test functions $\delta_i$, $i \in \mathbb{N}$, converging to the Dirac $\delta$-function at the space-time point $x$, there exists the (norm) limit

$$
(1 + H)^{-m} \phi(x) (1 + H)^{-m} \xrightarrow{i \to \infty} \lim (1 + H)^{-m} \phi(\delta_i) (1 + H)^{-m}.
$$

(3.3)

Thus the field $\phi(x)$ at $x$ is well defined in the form sense in those states $\omega$ in the vacuum sector, cf. (2.5), which satisfy $\omega((1 + H)^{2m}) < \infty$. We denote the linear spaces of point fields $\phi(x)$, $x \in \mathbb{R}^4$, for which $|| (1 + H)^{-m} \phi(x) (1 + H)^{-m} || < \infty$ by $Q_{m,x}$, $m > 0$. These spaces are generically finite dimensional and invariant under the automorphic action of the stability group of $x$ in $P_+^\uparrow$. Evidently, $Q_{m,x} \subset Q_{m',x}$ if $m \leq m'$.

The symmetric elements of $Q_{m,x}$ may be regarded as (idealized) observables at $x$ whose expectation values are well-defined in the states characterized above. Since the product of fields at a point is meaningless, their higher moments are ill-defined, however. We therefore propose to take as a substitute the normal products of these fields which can be defined with the help of the Wilson-Zimmermann operator-product expansion \[12\].

A novel approach to these notions has recently been established by Bostelmann \[13\]. Within this general setting one finds that for each $\phi(x) \in Q_{m,x}$ and spacelike $\zeta \in \mathbb{R}^4$ the product $\phi(x + \zeta)\phi(x - \zeta)$ is well-defined in the form sense. Moreover, for any given $q > 0$, there exist a finite number of distinguished fields $\phi_j(x) \in Q_{n,x}$, $n$ sufficiently large, and analytic functions $\zeta \mapsto c_j(\zeta)$, $j = 1, \ldots J(q)$, such that

$$
||(1 + H)^{-n} \left( \phi(x + \zeta)\phi(x - \zeta) - \sum_{j=1}^{J(q)} c_j(\zeta) \phi_j(x) \right) (1 + H)^{-n} || \leq c |\zeta|^q
$$

(3.4)

for $\zeta$ tending to 0 in any proper spacelike cone. Thus a meaningful substitute for the ill-defined square of $\phi(x)$ are the subspaces $\mathcal{N}(\phi^2)_{q,x} \subset Q_{n,x}$ generated by the fields $\phi_j(x)$, $j = 1, \ldots J(q)$. In a similar manner one obtains spaces $\mathcal{N}(\phi^p)_{q,x}$ corresponding to higher powers $p$ of $\phi(x)$ \[13\]. Given $r > 0$ and choosing $q$ and $n$ sufficiently large, the convergence in (3.4) can be made sufficiently rapid such that
also

\[ \|(1 + H)^{-n} \left( \partial_\zeta \phi(x + \zeta) \phi(x - \zeta) - \sum_{j=1}^{J(q)} \partial_\zeta c_j(\zeta) \phi_j(x) \right) (1 + H)^{-n} \| \leq c |\zeta|^r, \quad (3.5) \]

where \( \partial_\zeta \) is any monomial in the partial derivatives with respect to the components of \( \zeta \). Thus the spaces \( N(\phi^2)_{q,x} \) contain, for large \( q \), also fields approximating the “balanced” derivatives \( \partial_\zeta \phi(x + \zeta) \phi(x - \zeta) \) for small \( \zeta \).

So far, we have restricted our attention to point fields in the vacuum sector. Since we are interested here primarily in thermal states, let us discuss next the circumstances under which these fields can be defined in such states as well. Here we rely on the fact that there exist also local versions of the preceding statements in generic cases. More precisely, in the above estimates the Hamiltonian \( H \) can be replaced by a suitable local Hamiltonian \( H_0 \) with the help of e.g. the universal localizing maps considered in [14]. The operators \( H_0 \) induce the time translations of the observables in each region \( O \subset \mathbb{R}^4 \) in the sense that the commutators of \( H_0 \) and of \( H \) with these observables coincide. Roughly speaking, the local Hamiltonians \( H_0 \) may be thought of as the energy density integrated with suitable smoothed-out characteristic functions of compact support; so these operators can also be used to determine the local energy content of the states [14]. Thus if a state \( \omega \) has locally finite energy in the sense that \( \omega((1 + H_0)^{2n}) < \infty \), we conclude that the expectation values of all point fields \( \phi(x) \in Q_{n,x}, x \in O \), are well-defined in this state.

It is evident that states allowing locally a thermal interpretation must have locally finite energy. So the upshot of this discussion is the insight that the states of interest can be extended to the spaces \( Q_{n,x} \), \( n > 0 \), for \( x \) varying in some region \( O \). For our thermal reference states \( \omega_B \in \mathcal{C} \), this can also be seen more directly by noticing that, due to the invariance of these states under space-time translations, one has

\[ \omega_B(\phi(x)) = \omega_B(\phi(f)) \quad (3.6) \]

for any test function \( f \) with \( \int dx f(x) = 1 \). Relation (3.6) may be regarded as a formal expression of the statement, made in the introduction, that in thermal equilibrium states the expectation values of intensive observables can be determined in arbitrarily small space-time cells.

### 3.2 Selection of local thermal observables

As has been indicated above, the algebra \( \mathcal{A} \), and consequently the spaces \( Q_{n,x} \), contain many elements which are of no relevance to the thermal interpretation of states at the space-time point \( x \). Examples are the derivatives \( \partial_\zeta \phi(x) \) of point fields which are sensitive to the spatio-temporal variations of states and therefore vanish in all thermal reference states. So we have to select from the spaces \( Q_{n,x} \) suitable subspaces, cf. also the concluding remarks. This is accomplished as follows.

For small \( n \), the spaces \( Q_{n,x} \) contain only multiples of the identity. With increasing \( n \), there will appear, at a certain value \( n_0 > 0 \) in the corresponding space
Let us explain next how the elements of $\mathcal{T}_x$ provide information about the macroscopic thermal properties of the states in $\mathcal{C}$. In order to simplify this discussion, we consider only the generic case where $\mathcal{T}_x$ separates these states. As we are assuming uniqueness of the KMS states, all intensive thermal parameters attached to these states can be represented by functions $\beta \mapsto F(\beta)$ of

$\mathcal{Q}_{n_0,x}$, also some point field $\phi_0(x)$ which we regard as a basic thermal observable. Next, as has been explained above, a meaningful substitute for the square of $\phi_0(x)$ are the normal product spaces $\mathcal{N}(\phi_0^2)_{q,x}, q > 0$. Similarly, to its higher powers $p \in \mathbb{N}$ there correspond the spaces $\mathcal{N}(\phi_0^p)_{q,x}, q > 0$. Thus the elements of all these spaces are to be regarded as thermal observables as well. They form a proper subspace $\mathcal{T}_x$ of the space of all point fields,

$$\mathcal{T}_x \doteq \sum_{p,q} \mathcal{N}(\phi_0^p)_{q,x},$$

where we put $\mathcal{N}(\phi_0^0)_{q,x} \doteq \mathbb{C} 1$ and $\mathcal{N}(\phi_0^1)_{q,x} \doteq \mathbb{C} \phi_0(x), q > 0$. Assuming for simplicity that the algebra $\mathcal{A}$ is generated by the averages (2.1) of the basic observable $\phi_0$ and its normal products, we are thus led to take $\mathcal{T}_x$ as the space of thermal observables at $x$. Such spaces can also be defined in more general situations in a systematic manner, but we refrain from giving details here.

The above procedure introduces a natural hierarchy amongst the thermal observables in $\mathcal{T}_x$. In order to reveal this fact, let us consider any thermal reference state $\omega_B \in \mathcal{C}$. Assuming that the KMS states satisfy the relativistic KMS condition, given in Sec. 2, it follows that the two-point functions $\zeta \mapsto \omega_B(\phi_0(x \mp \zeta) \phi_0(x \pm \zeta))$ are the boundary values of analytic functions in the tips of the forward and backward tubes $\mathbb{R}^4 \pm i V_+$, respectively. Furthermore, they coincide for spacelike $\zeta$ because of locality. Thus, by the Edge-of-the-Wedge Theorem, they are analytic for spacelike $\zeta$. In view of the operator-product expansion (3.4) and of the invariance of $\omega_B \in \mathcal{C}$ under space-time translations, these two-point functions are therefore already determined by the expectation values of the observables $\phi_j(x) \in \mathcal{N}(\phi_0^0)_{q,x}, q > 0$, in the state $\omega_B \in \mathcal{C}$. In a similar manner, the spaces $\mathcal{N}(\phi_0^p)_{q,x}, q > 0$, fix the $p$-point functions for any $p \in \mathbb{N}$, unless these functions exhibit essential singularities at coinciding points.

As the $p$-point functions for large $p$ govern the properties of those for smaller $p$ (for the KMS states this is an immediate consequence of the cluster property which is, in turn, a consequence of their uniqueness), we conclude that the spaces $\mathcal{N}(\phi_0^p)_{q,x}, q > 0$, allow, for increasing $p$, an increasingly finer resolution of the properties of the thermal states. As a matter of fact, the above argument provides evidence to the effect that the set $\mathcal{T}_x$ of all thermal observables at $x$ in general separates the states in $\mathcal{C}$ and is sufficiently big in order to determine all properties of the thermal states with arbitrary precision. In other words, if one is only interested in the gross (macroscopic) properties of these states, it suffices to analyze them with the help of some subset of thermal observables taken from the spaces $\mathcal{N}(\phi_0^p)_{q,x} \subset \mathcal{T}_x$ for small $p$ and $q$.

### 3.3 Macroscopic interpretation of local thermal observables

Let us explain next how the elements of $\mathcal{T}_x$ provide information about the macroscopic thermal properties of the states in $\mathcal{C}$. In order to simplify this discussion, we consider only the generic case where $\mathcal{T}_x$ separates these states.

As we are assuming uniqueness of the KMS states, all intensive thermal parameters attached to these states can be represented by functions $\beta \mapsto F(\beta)$ of
the temperature vector, called thermal functions in what follows. Hence for mixed thermal states \( \omega_B \in \mathcal{C} \), the mean values of the thermal functions \( F \) are given by

\[
\omega_B(F) = \int d\rho(\beta) F(\beta),
\]

(3.8)

where \( \rho \) is the measure appearing in the decomposition (2.10) of \( \omega_B \). The notation in (3.8) indicates that the thermal functions \( F \) are to be regarded as (macroscopic) observables which can be evaluated in all states in \( \mathcal{C} \); more precisely, the states can uniquely be extended to these functions which appear as limits of suitable central sequences of local observables.

It is crucial for our approach that the local observables in \( \mathcal{T}_x \) provide the same information about the thermal properties of the states in \( \mathcal{C} \) as the macroscopic observables. Namely, one can reconstruct with their help all relevant thermal functions, in particular the entropy density, as is shown in the appendix. Moreover, since the thermal observables \( \mathcal{T}_x \) separate the thermal states, they can be used to determine the measures \( \rho \) in the decomposition (2.10), which are needed for the evaluation of mean values.

Let us exhibit this fact more explicitly. Given any \( \phi(x) \in \mathcal{T}_x \), it follows from the transformation formula (2.8) that the function

\[
\beta \mapsto \Phi(\beta) = \omega_\beta(\phi(x))
\]

(3.9)

(which is continuous according to (2.9) and (3.6)) does not depend on \( x \) and is a Lorentz tensor (corresponding to the tensorial character of \( \phi \)) built out of the temperature vector \( \beta \). It may thus be regarded as some thermal function. We use the fact that for each \( \phi(x) \) the corresponding function \( \Phi \), fixing the thermal interpretation of \( \phi(x) \), is known (by (3.9)). As was outlined in the introduction, this amounts in practice to recording the mean values of the local thermal observables in all equilibrium states. In the following we will consistently make use of the above notation: lower case Greek letters, such as \( \phi, \xi, \epsilon \), denote the microscopic thermal observables whereas the respective upper case letters \( \Phi, \Xi, E \) denote the corresponding macroscopic thermal functions.

Evaluating \( \phi(x) \in \mathcal{T}_x \) in an arbitrary state \( \omega_B \in \mathcal{C} \) one obtains

\[
\omega_B(\phi(x)) = \int d\rho(\beta) \omega_\beta(\phi(x)) = \int d\rho(\beta) \Phi(\beta) = \omega_B(\Phi),
\]

(3.10)

which fixes some (generalized) moment of the \textit{a priori} unknown measure \( \rho \). By letting \( \phi(x) \) run through all of \( \mathcal{T}_x \), the corresponding thermal functions \( \Phi \) run through a dense set of continuous functions on \( B \subset V_+ \) (since \( \mathcal{T}_x \) separates the states in \( \mathcal{C} \)). Then all moments of the measure are known, hence one can reconstruct the measure itself from these data, \textit{cf.} the subsequent section. At the same time this density property also implies that the space spanned by the thermal functions \( \Phi \) can be used to approximate any continuous function \( F \) on compact subsets \( B \subset V_+ \) with arbitrary precision even if \( F \) is not a member of this space.
This is of significance for quantities such as the entropy density, which may not be expected to correspond to any local thermal observable in $\mathcal{T}_x$. In order to determine locally the exact mean values of such thermal functions in the states $\mathcal{C}$, one needs information on the expectation values of an infinite number of suitable local thermal observables.

On the other hand, one may expect that basic thermal functions, such as the thermal energy density $E$, can in general be determined by some element $\epsilon(x) \in \mathcal{T}_x$. Note, however, that the observable $\epsilon(x)$ need not coincide with the full stress energy density $\theta(x)$ of the underlying theory even though both observables have the same expectation values in thermal states,

$$\omega_\beta(\epsilon(x)) = E(\beta) = \omega_\beta(\theta(x)), \quad \beta \in \mathbb{V}^+.$$  \hspace{1cm} (3.11)

This peculiarity may be understood if one notices that $\theta(x)$ determines not only the local thermal energy of states but also other forms of energy contained, e.g., in the internal stress of the system. As the energy density of the states $\omega_\beta$ in their rest systems is entirely of thermal nature, the observable $\epsilon(x)$ has to be sensitive only to this type of energy. This point will be exemplified in the model discussed in Sec. 5.

## 4 Thermal properties of non-equilibrium states

Having specified the thermal reference states and the local thermal observables of the theory, we have now at our disposal the necessary tools for the analysis of the local thermal properties of non-equilibrium states. Throughout this section we assume without further mentioning that the states $\omega$ we are interested in can be extended to the local thermal observables.

### 4.1 Characterization of locally thermal states

As has been explained in the introduction, we shall determine the thermal properties of arbitrary states by comparing them with states in $\mathcal{C}$ with the help of the local thermal observables. Given $x \in \mathbb{R}^4$ and any subspace $\mathcal{S}_x \subset \mathcal{T}_x$, we say that a state $\omega$ is $\mathcal{S}_x$-compatible with a thermal interpretation at $x$ ($\mathcal{S}_x$-thermal, for short) if there exists some $\omega_B \in \mathcal{C}$ such that

$$\omega(\phi(x)) = \omega_B(\phi(x)), \quad \phi(x) \in \mathcal{S}_x.$$  \hspace{1cm} (4.1)

Thus $\omega$ looks like a thermal state with respect to all observables in $\mathcal{S}_x$. Under these circumstances one can consistently define mean values of the corresponding thermal functions in the state $\omega$ at the space-time point $x$, setting

$$\omega(\Phi)(x) = \omega(\phi(x)), \quad \phi(x) \in \mathcal{S}_x,$$  \hspace{1cm} (4.2)

where $\Phi$ corresponds to $\phi(x)$, cf. (3.9). For if two observables $\phi_1(x), \phi_2(x) \in \mathcal{T}_x$ give rise to the same $\Phi$, it follows that $\omega_B(\phi_1(x)) = \omega_B(\Phi) = \omega_B(\phi_2(x))$ for all $\omega_B \in \mathcal{C}$. So, for the given $x$, the basic relation (4.2) provides a lift of $\omega$ to the
subspace of thermal functions $\Phi$ fixed by $S_x$. It thereby leads to a local thermal interpretation of this state.

The preceding characterization of states admitting locally a thermal interpretation is physically meaningful but difficult to use in practice because of the apparent need to compare these states with all members of the family $C$. It is therefore gratifying that there exists an equivalent characterization which relies entirely on the space of thermal observables $T_x$. To see this we introduce on this space a family of seminorms $\tau_B$ for all compact subsets $B \subset V_+$, setting

$$
\tau_B(\phi(x)) = \sup_{\beta \in B} |\Phi(\beta)|.
$$

(4.3)

Bearing in mind that the functions $\Phi$ are continuous, it is clear that the supremum exists. The following criterion makes use of this notion.

**Criterion:** Let $S_x$ be any subspace of $T_x$ containing the identity and let $\omega$ be any state on $A$. The state is $S_x$-thermal if and only if there is some compact subset $B \subset V_+$ such that

$$
|\omega(\phi(x))| \leq \tau_B(\phi(x)), \quad \phi(x) \in S_x.
$$

(4.4)

The latter condition has a simple physical interpretation: the mean values of the local thermal observables should not exceed their maximal possible values in the thermal states. This constraint can be checked more easily in applications.

The mathematical justification of the criterion relies on standard measure theoretic arguments: let $\omega$ be $S_x$-thermal. Then there exists some positive, normalized measure $\rho$ with support in $B$, cf. (2.10), such that

$$
\omega(\phi(x)) = \omega_B(\phi(x)) = \int d\rho(\beta) \omega(\phi(x)) = \int d\rho(\beta) \Phi(\beta), \quad \phi(x) \in S_x.
$$

(4.5)

Relation (4.4) then follows by a straightforward estimate. Conversely, if relation (4.4) holds for $\omega$ and some $B$, the linear functional $\omega(\Phi)(x) = \omega(\phi(x))$ on the space of thermal functions $\Phi$ corresponding to $\phi(x) \in S_x$ is well-defined. For $\Phi = 0$ implies $\tau_B(\phi(x)) = \sup_{\beta \in B} |\Phi(\beta)| = 0$ and consequently $\omega(\Phi)(x) = 0$. Moreover, as $|\omega(\Phi)(x)| \leq \tau_B(\phi(x)) = \sup_{\beta \in B} |\Phi(\beta)|$, this functional can be extended in $\Phi$ by the Hahn-Banach Theorem to the space of all continuous functions $F$ on $B$ such that

$$
|\omega(F)(x)| \leq \sup_{\beta \in B} |F(\beta)| = ||F||_B.
$$

(4.6)

As the functions $F$ with norm $|| \cdot ||_B$ form a $C^*$-algebra with unit and as $\omega(1)(x) = 1$, it follows that $\omega(\cdot)(x)$ defines a positive, normalized functional on this algebra [13]. But any such functional can be represented in the form [16]

$$
\omega(F)(x) = \int d\rho(\beta) F(\beta),
$$

(4.7)
where $\rho$ is some positive, normalized measure with support in $B$. Setting
\[
\omega_B(A) \doteq \int d\rho(\beta) \omega_\beta(A), \quad A \in \mathcal{A},
\] (4.8)
we have thus found a state $\omega_B \in \mathcal{C}$ which coincides with $\omega$ in the sense of condition (4.1). Hence $\omega$ is $S_x$-thermal.

The thermal states $\omega_B$ describing the local thermal properties of $\omega$ are not fixed by condition (4.1) if the set of thermal observables $S_x$ is too small. If $\omega$ admits, however, a thermal interpretation in the sense of (4.1) with respect to all thermal observables $T_x$, then the corresponding state $\omega_B \in \mathcal{C}$ (and hence the corresponding measure $\rho$) is in general unique by the arguments given in the preceding section.

### 4.2 Existence of locally thermal non-equilibrium states

For any given finite dimensional subspace $S_x$ of local thermal observables and any compact subset $B \subset V_+$, there exists an abundance of states $\omega$ on $\mathcal{A}$ which coincide on $S_x$ with some thermal state $\omega_B \in \mathcal{C}_B$ but are not $T_x$-compatible with a thermal interpretation. So they correspond to a non-equilibrium situation at $x$ which admits, however, an interpretation in terms of the subset of thermal functions corresponding to $S_x$.

To establish this fact, let us first assume that $\tau_B$ defines a norm on $S_x$, i.e. $\tau_B(\phi(x)) = 0$ for $\phi(x) \in S_x$ implies $\phi(x) = 0$. Picking any state $\omega_0$ on $\mathcal{A}$ and taking into account that on a finite dimensional space all linear functionals are continuous and all norms are equivalent, we get
\[
|\omega_0(\phi(x))| \leq c \tau_B(\phi(x)), \quad \phi(x) \in S_x
\] (4.9)
for some suitable constant. Thus we can lift $\omega_0$ to the space of thermal functions, setting $\omega_0(\Phi)(x) \doteq \omega_0(\phi(x)), \phi(x) \in S_x$. Moreover, by the Hahn-Banach Theorem, the latter functional can be extended to the space of all continuous functions $F$ on $B$ such that
\[
|\omega_0(F)(x)| \leq c \sup_{\beta \in B} |F(\beta)|.
\] (4.10)
We may assume that this extension is hermitian, replacing $\omega_0(F)(x)$ by the expression $2^{-1}(\omega_0(F)(x) + \overline{\omega_0(F^*)(x)})$, if necessary. As any linear, hermitian and continuous functional on the $C^*$-algebra of continuous functions on $B$ can be represented by a signed measure $\sigma$ with support in $B$ [16], we conclude that
\[
\omega_0(F)(x) = \int d\sigma(\beta) F(\beta).
\] (4.11)
Decomposing $\sigma$ into its positive and negative parts $\sigma_\pm, \sigma = \sigma_+ - \sigma_-$, and setting
\[
\omega(A) \doteq (1 + \sigma_-(B))^{-1} (\omega_0(A) + \int d\sigma_-(\beta) \omega_\beta(A)), \quad A \in \mathcal{A},
\] (4.12)
we have thus exhibited a state $\omega$ on $A$ such that

$$\omega(\phi(x)) = \omega_B(\phi(x)) = \sigma_+(B)^{-1} \int d\sigma_+(\beta) \omega_\beta(\phi(x)), \quad \phi(x) \in S_x,$$

i.e. $\omega$ is $S_x$-thermal. But in general it is not $T_x$-thermal since $\omega_0$ was completely arbitrary. As is seen from relation (4.12), the state $\omega$ so constructed may be interpreted as a perturbation of a thermal background state in $C_B$.

Let us turn now to the case where there is some non-trivial subspace $S_{x,0} \subset S_x$ which is annihilated by $\tau_B$. If, as expected in the absence of phase transitions, the thermal functions $\Phi$ are analytic on $V_+$, the relation $\tau_B(\phi(x)) = 0$ implies $\Phi = 0$ if $B$ has an open interior, i.e. there exist non-trivial relations between the thermal functions $\Phi, \phi(x) \in S_x$. The existence of such relations has a simple physical interpretation: it amounts to the existence of equations of state (such as the relation between energy density and pressure, for example).

For the construction of non-equilibrium states which are $S_x$-thermal, we pick now any state $\omega_0$ on $A$ which complies with these equations, i.e. which annihilates the subspace $S_{x,0}$. Such states which are not $T_x$-thermal also ought to exist in abundance; for the local validity of some equation of state does in general not imply that the system is locally in perfect thermal equilibrium in the sense that all correlations described by the elements of $T_x$ are of a thermal nature. We will exemplify this fact in the model discussed in the subsequent section.

In view of its proper kernel, the functional $\omega_0$ can be projected to the (finite dimensional) quotient space $S_x/S_{x,0}$ on which $\tau_B$ induces a norm. Hence, as before, $\omega_0$ satisfies the bound (4.9) and the subsequent construction can be carried out. So we conclude that there exist non-equilibrium states admitting a thermal interpretation for any given finite dimensional subspace of thermal observables.

4.3 The degree of thermal stability

Let us discuss next how the states admitting locally a thermal interpretation can be ordered into classes of increasing thermal stability (thermalization). Here enters the hierarchical structure of the thermal observables $T_x$, exhibited in the preceding section. Starting with the trivial subspace $S_x = C1$, all states are $S_x$-thermal since only their normalization is tested. By adding to $S_x$ the basic thermal observable $\phi_0(x)$ one imposes already some non-trivial constraint. For $\phi_0(x)$ is an unbounded quadratic form, hence arbitrary states generically violate condition (4.4) for given $B$. Next, one adds to $S_x$ the elements of the normal product spaces $N(\phi_0^q)_{q,x}$ for increasing $q$ which provide information about the correlations of the basic observable $\phi_0(x)$ at neighboring points. Using these enlarged spaces $S_x$ in the compatibility condition (4.1) one selects subsets of states where these correlations are of a thermal nature. Note that these constraints resemble the conditions imposed on states in the derivation of transport equations.

Proceeding in this manner, one arrives at spaces $S_x$ containing also elements of $N(\phi_0^p)_{q,x}$ for higher powers $p$. As has been explained in the preceding section, the resulting compatibility conditions distinguish states which exhibit increasingly more refined features of thermal equilibrium states and, in this sense, come closer
to the idea of a genuine equilibrium situation. Thus, for states which are \( S_x \)-thermal, the size of \( S_x \) may be taken as a measure for their degree of thermal stability.

### 4.4 Determination of specific thermal properties

To judge whether in a given state \( \omega \) some thermal function \( \Phi \) has locally a definite value, one has to make sure that the state is compatible with a thermal interpretation on some sufficiently large space \( S_x \). For one has to determine not only the mean value of \( \Phi \) but also its statistical fluctuations. If, for example, \( S_x \) contains observables \( \phi_1(x) \) and \( \phi_2(x) \) corresponding to \( \Phi \) and \( \Phi^2 \), respectively, then the observable

\[
\delta \phi_\kappa(x) = \phi_2(x) - 2 \kappa \phi_1(x) + \kappa^2 1, \quad \kappa \in \mathbb{R},
\]

(4.14)

corresponds to the thermal function \((\Phi - \kappa 1)^2\). It is therefore non-negative in all thermal reference states \( \mathcal{C} \) and vanishes only in those states in which \( \Phi \) has the sharp value \( \kappa \). Thus if \( \omega \) is \( S_x \)-thermal and \( \omega(\delta \phi_\kappa(x)) = 0 \) for some \( \kappa \), we may conclude that \( \Phi \) has the sharp value \( \kappa \) at \( x \) in this state. It is apparent that this conclusion can also be drawn under more general conditions.

For suitable spaces \( S_x \) one can also distinguish in this manner states which locally have a sharp temperature vector \( \beta \), i.e. which coincide on \( S_x \) with the KMS state \( \omega_\beta \). The minimal spaces admitting such an analysis are finite dimensional in generic cases, cf. the discussion in the subsequent section.

If a state \( \omega \) coincides on \( S_x \) with some KMS state \( \omega_\beta \), all thermal functions \( \Phi \) corresponding to \( \phi(x) \in S_x \) have locally definite values in this state. However, by enlarging \( S_x \), \( \omega \) may cease to have a thermal interpretation. Phrased differently, \( \omega \) may share only certain gross thermal properties with the KMS state \( \omega_\beta \) and a more refined analysis would reveal its non-equilibrium nature. Thus the method of analyzing the local thermal properties of states with the help of suitable subsets of thermal observables amounts to some procedure of coarse graining. It leads to the identification of an abundance of states having locally certain definite thermal properties. Such an approach seems natural if one deals with non-equilibrium systems.

### 4.5 Space-time evolution of thermal properties

The formalism established so far can easily be extended to states admitting a thermal interpretation in subregions \( \mathcal{O} \subset \mathbb{R}^4 \). Yet in order to obtain a sufficiently simple description, one has to keep the thermal functions fixed in the respective regions. This is accomplished by identifying the spaces \( S_x, x \in \mathcal{O} \), with the help of the automorphic action of the translations, setting

\[
S_x = \alpha_x(S_0), \quad x \in \mathcal{O}.
\]

(4.15)

With this convention understood, we say a state \( \omega \) is \( S_\mathcal{O} \)-compatible with a thermal interpretation in \( \mathcal{O} \) if for each \( x \in \mathcal{O} \) there is some \( \omega_B \in \mathcal{C} \) (in general depending on \( x \)) such that relation (4.1) holds for the respective \( S_x \). The resulting functions

\[
x \mapsto \omega(\Phi)(x) = \omega(\phi(x)), \quad x \in \mathcal{O},
\]

(4.16)
then describe the space-time behavior of the mean values of the thermal functions \( \Phi \). Hence they provide the link between the microscopic dynamics and the evolution of the macroscopic thermal properties, \( i.e. \) the thermodynamics of the states. It is an intriguing question under which circumstances this evolution can also be described in terms of transport equations.

We have thus solved the conceptual problem of identifying non-equilibrium states admitting locally a thermal interpretation, and of describing their specific thermodynamic properties. This formalism can now be applied to the analysis of non-equilibrium states in concrete models, as will be exemplified in Sec. 5. Furthermore, it is a suitable starting point for a general structural analysis of these states.

### 4.6 Field equations and quasiparticles

As a first illustration of the latter point, let us show how the microscopic dynamics leads to linear differential equations for the evolution of mean values of thermal functions in states which are sufficiently close to thermal equilibrium. We start from the assumption that our basic observable \( \phi_0(x) \) satisfies a field equation of the form

\[
\Box_x \phi_0(x) = \xi_0(x),
\]

where \( \xi_0(x) \) is some linear combination of elements in the normal product spaces \( \mathcal{N}(\phi_0^{p_0})_{q_0,x} \) for certain \( p_0 \) and \( q_0 \) (hence it is a thermal observable). As \( \omega_\beta(\xi_0(x)) = \omega_\beta(\Box_x \phi_0(x)) = \Box_x \omega_\beta(\phi_0(x)) = 0 \) because of the invariance of the KMS-states under space-time translations, we conclude that the thermal function \( \Xi_0 \) corresponding to \( \xi_0(x) \) vanishes.

Now let \( \mathcal{S}_x \) be any space of thermal observables containing the above normal product spaces \( \mathcal{N}(\phi_0^{p_0})_{q_0,x} \), hence in particular \( \phi_0(x) \) and \( \xi_0(x) \), and let \( \omega \) be any state which is \( \mathcal{S}_O \)-compatible with a thermal interpretation in \( O \). Then the local mean values of the thermal function \( \Phi_0 \) in this state necessarily satisfy the wave equation in \( O \), as is seen from the chain of equalities

\[
\Box_x \omega(\Phi_0)(x) = \Box_x \omega(\phi_0(x)) = \omega(\Box_x \phi_0(x)) = \omega(\xi_0(x)) = \omega(\Xi_0)(x) = 0.
\]  (4.17)

There exist many other thermal observables for which such behavior of the mean values in suitable states can be established. To reveal the underlying simple mechanism, we proceed from the elementary relation

\[
\Box_x \phi_0(x + \zeta) \phi_0(x - \zeta) = -\Box_\zeta \phi_0(x + \zeta) \phi_0(x - \zeta) + 2\xi_0(x + \zeta) \phi_0(x - \zeta) + 2\phi_0(x + \zeta) \xi_0(x - \zeta),
\]  (4.18)

which holds in the form sense for spacelike \( \zeta \). Taking into account the remark after relation (3.5) about balanced derivatives, it is clear that the expressions on the right hand side of this equality can be approximated in the limit of small spacelike \( \zeta \) by elements of the normal product spaces \( \mathcal{N}(\phi_0^{p_0})_{q_0,x} \) for suitable \( p \) and \( q \). Similarly, the expression \( \phi_0(x + \zeta) \phi_0(x - \zeta) \) can be approximated by elements of \( \mathcal{N}(\phi_0^{p_0})_{q_0,x} \). Comparing both sides of relation (4.18), one thus finds thermal observables \( \phi(x) \) in \( \mathcal{N}(\phi_0^{p_0})_{q_0,x} \) for which \( \Box_x \phi(x) = \xi(x) \) is also a thermal observable. As before one can then show that the local mean values of the thermal function \( \Phi \) corresponding
to $\phi(x)$ are solutions of the wave equation in states which are compatible with a thermal interpretation on sufficiently large subspaces of thermal observables.

So the space-time evolution of these thermal functions exhibits patterns of a massless particle propagating through the state $\omega$, provided $\omega$ is locally sufficiently close to thermal equilibrium. Note that this thermal compatibility condition imposes quite stringent constraints on the state in the case of interaction, since the spaces $S_x$ then have to contain thermal observables in $\mathcal{N}(\phi^p_0)_{q,x}$ for $p > 2$. For states slightly violating this condition in the sense that $\omega(\xi(x))$ is different from 0 but small, the above equations are, however, still valid in an approximate sense. This result is in accordance with the familiar quasi-particle interpretation of perturbations of equilibrium states. It emerges here as a by-product of our approach to the characterization of the local thermal properties of non-equilibrium states.

5 An instructive example

In this section we illustrate the preceding abstract notions and results in the theory of a free massless scalar field. We have chosen this particularly simple example since it allows the elementary computation of many quantities of interest by scaling arguments. After a brief outline of the model we will determine the structure and physical significance of its local thermal observables. We then exhibit interesting examples of non-equilibrium states, describing a “big heat bang”, for which a definite temperature, thermal energy and entropy density can be defined at every space-time point in the future cone of some given initial point.

5.1 The model

The free massless scalar field $\phi_0(x)$ on $\mathbb{R}^4$, playing the role of a basic thermal observable in the present model, is characterized by the field equation and commutation relation

$$\square_x \phi_0(x) = 0, \quad [\phi_0(x_1), \phi_0(x_2)] = (2\pi)^{-3} \int dp e^{-i(x_1-x_2)p} \varepsilon(p_0) \delta(p^2) \cdot 1. \quad (5.1)$$

It generates a polynomial *-algebra $\mathcal{A}$, describing the local observables of the theory. This algebra is stable under the actions of the Poincaré group $\mathcal{P}^+_+$, given by $\alpha_{\Lambda,a}(\phi_0(x)) = \phi_0(\Lambda x + a)$, the dilations $\mathbb{R}_+$, given by $\delta_s(\phi_0(x)) = s \phi_0(sx)$, and the gauge group $\mathbb{Z}^2$, given by $\gamma(\phi_0(x)) = -\phi_0(x)$.

We restrict attention here to states $\omega$ on $\mathcal{A}$ which are gauge invariant, i.e. $\omega \circ \gamma = \omega$, so the respective $n$-point functions of $\phi_0$ vanish if $n$ is odd. The simplest examples of this type are quasifree states. They are completely determined by their two-point functions through the formula

$$\omega(\phi_0(x_1)\phi_0(x_2)\ldots\phi_0(x_n))$$

$$\doteq \begin{cases} \sum_{\text{pairings}} \omega(\phi_0(x_{i_1})\phi_0(x_{i_2})\ldots\phi_0(x_{i_{n-1}})\phi_0(x_{i_n})) & n \text{ even}, \\ 0 & n \text{ odd}. \end{cases} \quad (5.2)$$
Whenever a (generalized) function \( \omega(\phi_0(x_1)\phi_0(x_2)) \) is consistent with the constraints imposed by (5.1) and the positivity condition \( \omega(\phi_0(f)\phi_0(f)) \geq 0 \) for all test functions \( f \); the functional \( \omega \) obtained by linear extension from (5.2) defines a state on \( \mathcal{A} \). Thus there is a large supply of simple states from which we will also draw the non-equilibrium states considered below.

5.2 Thermal reference states

It is a well known fact that the algebra \( \mathcal{A} \) has a unique gauge invariant KMS state \( \omega_\beta \) for each temperature vector \( \beta \in V_+ \). This state is quasifree, so it is determined by its two-point function given by

\[
\omega_\beta(\phi_0(x_1)\phi_0(x_2)) = (2\pi)^{-3} \int dp \frac{e^{-i(x_1-x_2)p}}{1 - e^{-\beta p}}. \tag{5.3}
\]

We mention as an aside that these states satisfy the relativistic KMS condition and comply with our continuity assumption (2.9). In fact, the respective functions are analytic on \( V_+ \), as is easily verified.

As outlined in Sec. 2, the KMS states \( \omega_\beta, \beta \in V_+ \), fix the convex set \( \mathcal{C} \) of thermal reference states which enters into our analysis of the thermal properties of (gauge invariant) non-equilibrium states.

5.3 Local thermal observables

Let us turn now to the analysis of the local thermal observables in this model. We will consider primarily the spaces \( \mathcal{N}(\phi^2_0)_{q,x} \), \( q > 0 \), which are generated by the Wick square of \( \phi_0 \), its balanced derivatives and the unit operator 1. Introducing the multi-index notation \( \mu = (\mu_1, \mu_2, \ldots, \mu_m) \) and setting \( \partial_\mu \zeta = \partial \zeta^{\mu_1} \cdots \partial \zeta^{\mu_m} \), these balanced derivatives are defined by

\[
\partial_\mu : \phi^2_0 : (x) = \lim_{\zeta \to 0} \partial_\mu \zeta (\phi_0(x + \zeta)\phi_0(x - \zeta) - \omega_\infty(\phi_0(x + \zeta)\phi_0(x - \zeta)) 1), \tag{5.4}
\]

where \( \omega_\infty \) denotes the vacuum state (which can be recovered from (5.3) in the limit of large time-like \( \beta \)). Note that for odd \( m \) the balanced derivatives vanish, since \( \phi_0(x + \zeta)\phi_0(x - \zeta) \) is even in \( \zeta \) as a consequence of locality.

For the determination of the thermal functions corresponding to these observables one proceeds from the relation

\[
\omega_\beta(\phi_0(x + \zeta)\phi_0(x - \zeta)) - \omega_\infty(\phi_0(x + \zeta)\phi_0(x - \zeta)) = (2\pi)^{-3} \int \frac{dp}{|p|} \cos(2\zeta p) (e^{\beta p} - 1)^{-1} = (2\pi)^{-3} \sum_{n=1}^{\infty} \int \frac{dp}{|p|} \cos(2\zeta p) e^{-n\beta p}, \tag{5.5}
\]

where \( p \equiv (|p|, p) \). The even derivatives with respect to \( \zeta \), when applied to the latter integral, can be replaced by \( \partial_\beta^\mu \), multiplied with appropriate constants. We omit the remaining simple computations and only state the final result:

\[
\beta \mapsto \omega_\beta(\partial_\mu : \phi^2_0 : (x)) = c_m \partial_\beta^\mu (\beta^2)^{-1}, \tag{5.6}
\]

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where \( c_m = 0 \) if \( m \) is odd and \( c_m = (-1)^{m/2}(4\pi)^m (m + 2)!^{-1} B_{m+2} \) if \( m \) is even, \( B_n \) being the Bernoulli numbers. It is instructive to have a closer look at these functions for small \( m \).

(a) The thermal function attached to the density \( \phi_0^2 (x) \) is \( \beta \mapsto (12 \beta^2)^{-1} \), i.e. the square of the temperature (apart from a constant).

(b) The balanced derivatives \( \epsilon^{\mu \nu} (x) \hat{=} (1/4) \bar{\partial}^{\mu \nu} : \phi_0^2 (x) \) give rise to the thermal functions

\[
\beta \mapsto E^{\mu \nu} (\beta) \hat{=} (\pi^2/90) (4 \beta \mu \beta \nu - \beta^2 g^{\mu \nu}) (\beta^2)^{-3}. \tag{5.7}
\]

So they coincide with the expectation values of the components of the standard (symmetric and traceless) stress energy tensor \( \theta^{\mu \nu} (x) \) in the states \( \omega_\beta \). This fact can be understood if one notices that this tensor can be represented in the form

\[
\theta^{\mu \nu} (x) = \epsilon^{\mu \nu} (x) + (1/12) (\bar{\partial}^{\mu} \bar{\partial}^{\nu} - g^{\mu \nu} \Box_x) : \phi_0^2 (x), \tag{5.8}
\]

where the second tensor on the right hand side vanishes in all equilibrium states because of the derivatives with respect to \( x \). Since this tensor is the coboundary of the vector-valued two-form \( (1/12) (\bar{\partial}^{\mu} g^{\nu \rho} - \bar{\partial}^{\rho} g^{\mu \nu}) : \phi_0^2 (x) \), it follows from Gauss’ law that it also does not contribute to the total energy of states which deviate only locally from an equilibrium situation. On the other hand, it is of relevance in non-equilibrium states, where it describes the transport of energy driven by sources which are localized at the boundary of the system.

We call \( \epsilon^{\mu \nu} (x) \) the thermal energy tensor. It is conserved and symmetric, but its trace \( \epsilon^{\mu}_\mu (x) = (1/4) \Box_x : \phi_0^2 (x) \) does not vanish identically. According to the discussion at the end of the preceding section, it is, however, zero in all states which are sufficiently close to equilibrium.

The thermal energy tensor and the Wick square can be used to distinguish KMS states in \( C \) corresponding to a given temperature vector. To establish this fact we consider, for fixed \( \varkappa \in V_+ \), the thermal observable

\[
\delta_\varkappa \epsilon (x) \hat{=} (30/\pi^2) \varkappa_\mu \varkappa_\nu \epsilon^{\mu \nu} (x) - 24 : \phi_0^2 (x) + (\varkappa^2)^{-1} 1 \tag{5.9}
\]

with corresponding thermal function

\[
\beta \mapsto (1/3) (4 (\beta \varkappa)^2 - \beta^2 \varkappa^2) (\beta^2)^{-3} - 2 (\beta^2)^{-1} + (\varkappa^2)^{-1}. \tag{5.10}
\]

As \( (\beta \varkappa)^2 \geq \beta^2 \varkappa^2 \), where equality holds if and only if \( \beta, \varkappa \in V_+ \) are parallel, this function is evidently positive on \( V_+ \) apart from the point \( \beta = \varkappa \), where it vanishes. Hence if \( \omega_B (\delta_\varkappa \epsilon (x)) = 0 \) for some state \( \omega_B \in C \) one can conclude that it must be the KMS state \( \omega_\varkappa \) corresponding to the temperature vector \( \varkappa \). Thus in this model a finite number of thermal observables are sufficient to decide whether a state has locally a definite temperature and a well-defined rest system.

(c) Turning to the higher balanced derivatives, it follows from (5.6) that all corresponding thermal functions are solutions of the wave equation since \( \Box_\beta (\beta^2)^{-1} = 0 \)
on $V_+$. So the subspace generated by these functions does not separate the states in $\mathcal{C}$. Yet it is sufficiently large in order to approximate the entropy current $S^\mu$,

$$\beta \mapsto S^\mu(\beta) = (2\pi^2/45) \beta^\mu (\beta^2)^{-2},$$

(5.11)
on any compact subset $B \subset V_+$. (The determination of the entropy current from the microscopic data is outlined in the appendix.)

For the proof of this assertion we pick any lightlike vector $l$ and contract the balanced derivative $\partial^\mu : \phi^2_0 : (x)$ with the tensor $l_\mu$. The corresponding thermal function is, cf. relation (5.6),

$$\beta \mapsto c_m (l\partial_\beta)^m (\beta^2)^{-1} = c_m m! 2^m (l\beta)^m (\beta^2)^{-m-1}$$

(5.12)

if $m$ is even; for odd $m$ it is identically zero. As $(l\beta)(\beta^2)^{-1}$ is positive and bounded on any compact subset $B \subset V_+$ and the (positive) square root is holomorphic on the right complex half plane, it follows that $\beta \mapsto (l\beta)(\beta^2)^{-1} = (l\beta)^2 (\beta^2)^{-2})^{1/2}$ can be represented on $B$ as a convergent power series involving only even powers $(l\beta)^m (\beta^2)^{-m}, m \in 2\mathbb{N}_0$. This proves that $\beta \mapsto lS(\beta)$ can be approximated on $B$ by linear combinations of the thermal functions $\beta \mapsto (l\beta)^m (\beta^2)^{-m-1}, m \in 2\mathbb{N}_0$. Since $l$ was arbitrary and the lightlike vectors generate a basis of $\mathbb{R}^4$, we conclude that also the entropy current can be approximated on any $B$ with arbitrary precision by the thermal functions corresponding to the balanced derivatives. Thus any state which admits a thermal interpretation on the space generated by these derivatives has a well-defined mean entropy density at the space-time point $x$.

5.4 Examples of non-equilibrium states

We have already seen in the abstract analysis that there exist non-equilibrium states admitting a thermal interpretation on finite dimensional subspaces of thermal observables. Here we consider non-equilibrium states which are substantially closer to a thermal equilibrium situation, namely, these states admit a thermal interpretation on the infinite dimensional spaces $S_x$ of thermal observables generated by $\mathcal{N}(\phi^p_0)_{q,x}, p = 0, \ldots, 3, q > 0$, for all $x$ in some future light cone. Moreover, they have a definite temperature, thermal energy and entropy density at all of these space-time points.

We are taking here the simplest states of this type in order to illustrate our general method. Yet these examples are also of some physical interest. They describe the spatio-temporal evolution of systems which have infinite temperature at some space-time point (corresponding to a “big heat bang”). Although we are dealing with a massless free field theory, our results provide some idea of the dynamical effects of such singularities in more realistic theories. For the masses of particles and their interaction should play a secondary role in the neighborhood of such singular points.

The non-equilibrium states considered here are quasi-free with two-point functions of the form, $\gamma > 0$ being fixed and $x_1, x_2 \in V_+$,

$$\omega_{bab}(\phi_0(x_1)\phi_0(x_2)) = (2\pi)^{-3} \int dp e^{-i(x_1-x_2)p} \varepsilon(p_0) \delta(p^2) \frac{1}{1 - e^{-\gamma(x_1+x_2)p}}.$$
These functions are consistent with the field equation and commutation relation in (5.1). They are also invariant under Lorentz transformations and dilations but not under translations. Moreover,

\[
\omega_{bhb}(\phi_0(x_1)\phi_0(x_2)) = \omega_\infty(\phi_0(x_1)\phi_0(x_2)) + (2\pi)^{-3} \sum_{n=1}^\infty \int \frac{dp}{|p|} \cos \left((x_1 - x_2)p\right) e^{-n\gamma(x_1 + x_2)\mathcal{L}},
\]

(5.14)
hence, decomposing the cosine according to Euler’s formula, it follows at once that each functional \(\omega_{bhb}\) satisfies the positivity condition \(\omega_{bhb}(\phi_0(f)) \geq 0\) if \(\text{supp} f \subset V_+\). By standard arguments it can therefore be extended to all of \(\mathcal{A}\) to a (singular) state. Since we are not interested here in this extension we do not dwell upon this point any further.

The computation of the expectation values of the balanced derivatives yields for even \(m\) and \(x \in V_+\)

\[
\omega_{bhb}(\partial^\mu: \phi_0^2: (x)) = (2\pi)^{-3} \sum_{n=1}^\infty \int \frac{dp}{|p|} \left(-1\right)^{m/2} \frac{m\mu}{\gamma^2 \mathcal{L}} e^{-n\gamma x \mathcal{L}} = \omega_{\beta(x)}(\partial^\mu: \phi_0^2: (x)),
\]

(5.15)
where \(\omega_{\beta(x)}\) is the KMS state corresponding to the temperature vector \(\beta(x) = 2\gamma x\). Thus \(\omega_{bhb}\) is \(S_{V_+}\)-thermal, \(S_x\) being the subspaces of thermal observables generated by \(\mathcal{N}(\phi_0^q)_{q,x}\), \(p = 0, \ldots, 3\), \(q > 0\). Note that \(\omega_{bhb}\) is compatible with a thermal interpretation on the spaces \(\mathcal{N}(\phi_0^q)_{q,x}\) for odd \(p\) and \(q > 0\) since it is, like the KMS states, gauge invariant. It has, however, no longer a thermal interpretation on the spaces \(\mathcal{N}(\phi_0^q)_{q,x}\), \(q > 0\), as one verifies by direct computation. So the higher correlations of the field \(\phi_0\) in this state are of a non-thermal nature. But the state approaches equilibrium for large time-like translations \(a\) in the sense that for all local observables \(A \in \mathcal{A}\)

\[
\lim_a \omega_{bhb} \circ \alpha_a(A) = \omega_\infty(A),
\]

(5.16)
i.e. \(\omega_{bhb}\) looks asymptotically like the vacuum \(\omega_\infty\).

Let us turn now to the local thermal interpretation of this state. As \(\delta_{\varepsilon}(x) \in S_x\), cf. relation (5.9), and \(\omega_{bhb}(\delta_{\varepsilon}(x)) = 0\) for \(\varepsilon = \beta(x)\), we conclude that \(\omega_{bhb}\) coincides on \(S_x\) with the KMS state \(\omega_{\beta(x)}, x \in V_+\) (which is also apparent from relation (5.13)). Its local temperature \(T(x) = (\beta(x)^2)^{-1/2} = (4\gamma^2 x^2)^{-1/2}\) decreases monotonically in time-like directions and all Lorentz observers moving along some world line \(\mathbb{R}_+\) record the same temperature at a given time after the big heat bang at 0.

The thermal energy density in the state \(\omega_{bhb}\) at the space-time points \(x \in V_+\) can be read off from the tensor

\[
\omega_{bhb}(E^\mu\nu)(x) = \omega_{bhb}(\epsilon^\mu\nu(x)) = \frac{\pi^2}{90} \left(4\beta^\mu(x)\beta^\nu(x) - g^\mu\nu \beta(x)^2\right) (\beta(x)^2)^{-3} = \frac{\pi^2}{1440\gamma^4} \left(4x^\mu x^\nu - g^\mu\nu x^2\right) (x^2)^{-3},
\]

(5.17)
describing a flow of massless particles in $V_+$ which is isotropic for the above Lorentz observers. They also find that the relation between the thermal energy density and temperature is in accordance with Stefan-Boltzmann’s law for scalar massless particles.

Since $\epsilon^\mu_\mu(x) = (1/4) \Box_x : \phi_0^2 : (x)$ and because $\omega_{hbb}(E^\mu_\mu)(x) = 0$, it follows that $\Box_x \omega_{hbb}(\phi_0^2 : (x)) = 0$, so the density $\phi_0^2 : (x)$ propagates through the state like a massless particle, in accordance with the general results in Sec. 4. As a matter of fact, relation (5.15) implies that $\Box_x \omega_{hbb}(\bar{\phi} : (x)) = 0$ for all balanced derivatives.

It is an interesting fact that the full energy density of the state $\omega_{hbb}$ is larger than its thermal energy density. Making use of relation (5.8) one obtains

$$\omega_{hbb}(\theta^{\mu\nu}(x)) = \left(\frac{\pi^2}{1440 \gamma^4} + \frac{1}{288 \gamma^2}\right)(4x^\mu x^\nu - g^{\mu\nu}x^2)(x^2)^{-3}. \quad (5.18)$$

Thus the coboundary term in relation (5.8) leads to an additional contribution due to the transport of energy from the hot boundary of the light cone into its interior. Note that for $\gamma = 1$ this term is of the same order of magnitude as the thermal energy, but it is not visible in the local thermal properties of the state. In other words, if one would try to determine the energy density of the state from its temperature by using Stefan-Boltzmann’s law, one would underestimate its value. This feature of an apparently “missing energy” may be of significance in cosmological models.

As $\omega_{hbb}$ is compatible with a thermal interpretation on all spaces $N(\phi_0^2)_{q,x}$, $q > 0$, one can consistently attribute to it the mean entropy current

$$\omega_{hbb}(S^\mu)(x) = \left(\frac{2\pi^2}{45}\right) \beta^\mu(x)(\beta(x^2))^{-2} = \left(\frac{\pi^2}{180 \gamma^3}\right) x^\mu(x^2)^{-2} \quad (5.19)$$

for $x \in V_+$, cf. the discussion in the preceding subsection. Since the model does not describe dissipative effects due to the lack of interaction, it does not come unexpectedly that this current is conserved,

$$\partial_\mu \omega_{hbb}(S^\mu)(x) = 0, \quad (5.20)$$

so there is no entropy production. The entropy current decreases monotonically in time-like directions. But the total entropy within spacelike sections of $V_+$ of the form $|x| < v|x_0|$ for fixed $v < 1$ stays constant for $x_0 > 0$. Thus, from a macroscopic point of view, the state $\omega_{hbb}$ describes an equilibrium situation at all points in $V_+$ in spite of the fact that it is microscopically out of equilibrium.

We conclude our discussion of the state $\omega_{hbb}$ with the remark that one can generate from it other states which are still $S_{V_+}$-thermal. Namely, for any given translation $a \in V_+$ the state $\omega_{hbb} \circ \alpha_a$ has this property, too, since $\alpha_a(S_{V_+}) \subset S_{V_+}$ and the thermal reference states in $C$ are invariant under translations. Moreover, since $C$ is stable under convex combinations, the states $\int d\nu(a) \omega_{hbb} \circ \alpha_a$, where $\nu$ is any positive normalized measure with compact support in $V_+$, are also $S_{V_+}$-thermal. If $\nu$ differs from the Dirac measure, these states have, however, locally no longer a definite temperature vector and the corresponding expectation values of the thermal functions exhibit a more complex space-time behavior.
6 Concluding remarks

We have established in the present article a novel method for the characterization and analysis of non-equilibrium states admitting locally a thermal interpretation. The basic idea in our approach is to compare these states with global equilibrium states by means of local observables. The inevitable step of “coarse graining” in the passage from a microscopic theory to a macroscopic description has been accomplished by restricting attention to distinguished subspaces of thermal observables, in accordance with the basic ideas of statistical mechanics having their origin with Boltzmann. As the selection of these observables is of vital importance in our approach, it seems appropriate to comment on this point in somewhat more detail.

At first sight it might seem natural to implement the idea of comparing states by defining a suitable distance between them. This can be accomplished by introducing a norm \( || \cdot || \) on the observables \( A \) (e.g. by fixing suitable Schwartz norms on the underlying spaces of test functions) and making use of the inherent net structure of the observables, providing to each space-time region \( O \subset \mathbb{R}^4 \) some subalgebra \( A(O) \subset A \) generated by observables \( A \) whose underlying test functions have support in \( O \), cf. relation (2.2). A physically meaningful local norm distance between any two states \( \omega_1, \omega_2 \) can then be defined, setting

\[
||\omega_1 - \omega_2||_{O} = \sup \{ |\omega_1(A) - \omega_2(A)| : A \in A(O), ||A|| \leq 1 \},
\]

which is just the maximal possible difference of the expectation values of normalized observables in \( A(O) \) in the two states.

Making use of this notion, one could try to distinguish non-equilibrium states \( \omega \) admitting a thermal interpretation at space-time point \( x \) by the condition that there is some state \( \omega_B \in C \) and some \( q > 0 \) such that for each sequence of regions \( O_\varepsilon \ni x \) with diameter \( \varepsilon \)

\[
||\omega - \omega_B||_{O_\varepsilon} \leq c \varepsilon^q \quad \text{for} \quad \varepsilon \to 0.
\]

For states \( \omega \) coming close to the idea of local equilibrium, the exponent \( q \) should be large. This condition turns out to be too stringent, however. Namely if \( \omega \) has locally finite energy, it follows from (6.2) that \( \omega \) and \( \omega_B \) coincide on some space of quadratic forms \( Q_{n(q),x} \), where \( n(q) \) is large for large \( q \). But for sufficiently large \( q \) the spaces \( Q_{n,x} \) contain, together with some observable \( \phi(x) \), also its derivatives \( \partial_x \phi(x) \) [13]. Hence \( \partial_x \omega(\phi(x)) = \omega(\partial_x \phi(x)) = \omega_B(\partial_x \phi(x)) = 0 \) if \( \omega \) is, in the above sense, sufficiently close to local thermal equilibrium. So, for states satisfying the above condition in some space-time region, the expectation values of these observables necessarily exhibit a trivial spatio-temporal behavior in that region. In other words, non-equilibrium states which are only locally close to equilibrium in general do not comply with this strong constraint.

It is noteworthy that one arrives at a similar conclusion in the C*-algebraic setting of local quantum physics, where the forms \( Q_{n,x} \) appear as dual spaces of the germs of states of (locally) finite energy [13, 17].
We have solved this conceptual problem by distinguishing certain subspaces $T_x$ of thermal observables, relying on the notion of normal product. Intuitively, these observables describe density-like quantities which can be attributed to space-time points, in contrast to their derivatives, which are sensitive to the spatio-temporal changes of states. The spaces $T_x$ have a natural hierarchical structure, ranging from observables which are sensitive to gross thermal properties up to quantities which allow to determine the subtle features of higher correlations.

Non-equilibrium states admitting a thermal interpretation can be distinguished by the condition that they coincide with thermal reference states on subspaces of the thermal observables $T_x$ and their degree of thermal stability can be read off from the size of the respective spaces. This characterization is the appropriate substitute for the apparently too restrictive condition (6.2).

As has been explained in Sec. 4, the spaces $T_x$ still contain certain derivatives of observables, but their appearance is of dynamical origin (it is a consequence of the field equations). Their existence leads, on the one hand, to relations between the thermal functions, corresponding to equations of state. On the other hand, they explain the quasi-particle-like propagation of densities in states which are sufficiently close to thermal equilibrium.

We have restricted our attention to the simplest class of theories, both, with regard to the structure of the observables and the family of thermal reference states. But our arguments can be extended to more complex situations with only little more effort. We therefore believe that our approach provides a natural setting for the analysis of the thermodynamic properties of non-equilibrium states in concrete models as well as in the general framework of quantum field theory. It should help to shed new light on the complex features of non-equilibrium systems.

A particularly interesting issue is the phenomenon of thermalization (approach to equilibrium) which is related to the problem of the arrow of time. As any local quantum field theory is PCT-symmetric and the spaces of thermal observables transform covariantly under this symmetry, there is no such arrow encoded in the algebraic structures used in the present approach to select the states admitting a thermal interpretation. Yet the states can break the PCT symmetry in the sense that they are compatible with a thermal interpretation either in some future or in some past light cone, but not in all of Minkowski space (unless they are in global equilibrium). The state $\omega_{bhb}$ considered in Sec. 5 nicely illustrates this point: it does not have a thermal interpretation extending beyond $V_+$, and similarly the state $\omega_{bhb} \circ \vartheta$, obtained from $\omega_{bhb}$ by the action of the anti-automorphism $\vartheta$ implementing the PCT symmetry, is thermal only in the past light cone $-V_+$. A proof establishing such a one-sidedness of thermalization in generic cases would be an important step towards the understanding of the microscopic origin of the arrow of time. We hope to return to this problem elsewhere.
A Thermostatics in $C$

In this appendix we determine the thermostatic properties of the thermal reference states. As in the main text, we assume that for each temperature vector $\beta \in V_+$ there is a unique KMS state $\omega_\beta$. By application of the fundamental laws of thermodynamics, the thermal functions can be determined if the corresponding expectation values of the stress energy tensor $\theta^{\mu\nu}(x)$ or of the thermal energy tensor $\epsilon^{\mu\nu}(x) \in T_x$, respectively, are known [18]. We will discuss in which sense these functions retain their interpretation in thermal reference states which are no proper equilibrium states.

In view of the tensor character of $\theta^{\mu\nu}(x)$ and relation (2.8), the corresponding thermal function $E^{\mu\nu}$ has the form

$$\beta \mapsto E^{\mu\nu}(\beta) = \omega_\beta(\theta^{\mu\nu}(x)) = Q(\beta^2) \, e^\mu e^\nu - P(\beta^2) \, g^{\mu\nu},$$  \hspace{1cm} (A.1)

where $e = (\beta^2)^{-1/2} \beta$ specifies the rest system of the state and $Q, P$ depend on the underlying theory. As we are dealing with an equilibrium situation, the function $P$ can be interpreted as pressure and $Q(\beta^2) = -2\beta^2 P'(\beta^2)$ [18, Ch. 4]. Because of relativistic covariance, the entropy current $S^\mu$ is of the form

$$\beta \mapsto S^\mu(\beta) = S(\beta^2) \, e^\mu,$$  \hspace{1cm} (A.2)

where $S$ is fixed by the Gibbs relation in the rest system [18, Ch. 4],

$$S(\beta^2) = (\beta^2)^{1/2} Q(\beta^2).$$  \hspace{1cm} (A.3)

The free energy density $F^{\mu\nu}$ is given by the tensor

$$\beta \mapsto F^{\mu\nu}(\beta) = E^{\mu\nu}(\beta) - (1/2)(\beta^2)^{-1/2}(e^\mu S^\nu(\beta) + e^\nu S^\mu(\beta)).$$  \hspace{1cm} (A.4)

Inserting the preceding expressions for the entropy and energy, one finds that it coincides in all Lorentz frames with the negative pressure,

$$F^{\mu\nu}(\beta) = -P(\beta^2) \, g^{\mu\nu}.$$  \hspace{1cm} (A.5)

Turning to the interpretation of these functions in the thermal reference states $\omega_B = \int d\rho(\beta) \, \omega_\beta$, there appears no problem with the energy density which can be determined by the local observable $\theta^{\mu\nu}(x)$. Hence its expectation values are

$$\omega_B(E^{\mu\nu}) = \int d\rho(\beta) \, E^{\mu\nu}(\beta).$$  \hspace{1cm} (A.6)

It is less obvious, however, that the expectation values of $S^\mu$,

$$\omega_B(S^\mu) = \int d\rho(\beta) \, S^\mu(\beta),$$  \hspace{1cm} (A.7)

can be interpreted as entropy currents of the non-equilibrium states $\omega_B$. In order to justify this interpretation, we make the following physically meaningful
assumptions: the entropy density \( S \) is a concave function of the energy density \( E = Q - P \), and the pressure \( P \) as well as \( E - P \) increase monotonically with the temperature \( T = (\beta^2)^{-1/2} \). The latter condition means that the negative free energy (the isothermal work which can be extracted from equilibrium states in their rest systems) increases with increasing temperature, yet less rapidly than the total energy.

We will show that these assumptions entail a version of the second law based on (A.7). To this end let us determine in any given Lorentz frame \( e' \in V_+ \), \( e'^2 = 1 \), the states \( \omega_B \in \mathcal{C} \) with fixed energy density \( e'_\mu e'_\nu \omega_B(E^{\mu\nu}) = E' \) which maximize the entropy functional \( \omega_B \mapsto e'_\mu \omega_B(S^\mu) \). Considering first the KMS states \( \omega_\beta \) and making the substitution \( \beta = (\beta^2)^{1/2} e \rightarrow (E, e) \), we have

\[
e'_\mu e'_\nu \omega_\beta(E^{\mu\nu}) = ((E + P(E)) (e'e)^2 - P(E)) = E' \tag{A.8}
\]
\[
e'_\mu \omega_\beta(S^\mu) = S(E) (e'e). \tag{A.9}
\]

Inserting \((e'e)\) from relation (A.8) into (A.9), we get

\[
e'_\mu \omega_\beta(S^\mu) = S(E)((E' + P(E))/(E + P(E)))^{1/2}. \tag{A.10}
\]

The logarithmic derivative of the right hand side of this equality with respect to \( E \) satisfies

\[
(dS/dE)/S + (dP/dE)/2(E' + P) - (1 + dP/dE)/2(E + P) \geq 1/ST - (1 + dP/dE)/2(E + P) = (1 - dP/dE)/2(E + P) \geq 0, \tag{A.11}
\]

where we made use of (A.3) and of the preceding assumptions, implying \( 0 \leq dP/dE \leq 1 \). Thus the expression (A.10) attains its maximum for the maximal possible energy \( E = E' \) (corresponding to \( e = e' \)) compatible with (A.8), i.e.

\[
e'_\mu \omega_\beta(S^\mu) = S(E) (e'e) \leq S(E'). \tag{A.12}
\]

Turning to the general case, let \( \omega_B = \int d\rho(\beta) \omega_\beta \) be any state with

\[
e'_\mu e'_\nu \omega_B(E^{\mu\nu}) = \int d\sigma(E, e) ((E + P(E)) (e'e)^2 - P(E)) = E', \tag{A.13}
\]

where \( \sigma \) is the normalized measure obtained from \( \rho \) by the substitution \( \beta \rightarrow (E, e) \). In view of the preceding results and the concavity of \( S \) we obtain

\[
e'_\mu \omega_B(S^\mu) = \int d\sigma(E, e) S(E) (e'e) \leq \int d\sigma(E, e) S((E + P(E)) (e'e)^2 - P(E)) \leq S\left( \int d\sigma(E, e) ((E + P(E)) (e'e)^2 - P(E)) \right) = S(E'), \tag{A.14}
\]

and equality holds in (A.14) if and only if the measure \( \sigma \) is concentrated at the point \( E', e' \). Thus \( \omega_{\beta'} \), where \( \beta' = (\beta'')^{1/2} e' \) and \( \beta'' \) is fixed by \( E' \), is the unique state in \( \mathcal{C} \) which maximizes the entropy functional \( \omega_B \mapsto e'_\mu \omega_B(S^\mu) \) under the
given conditions. As this functional is also additive, the interpretation of \((A.7)\) as entropy current is justified.

Similarly, one can define the mean free energy density of the states in \(C\),

\[
\omega_B(F^{\mu\nu}) = \int d\rho(\beta) F^{\mu\nu}(\beta) = -\int d\rho(\beta) P(\beta^2) g^{\mu\nu}. \tag{A.15}
\]

It thus coincides with the negative mean pressure in all Lorentz frames and has a sharp value for all states \(\omega_B\) with a definite temperature \(T\), corresponding to measures \(\rho\) which are concentrated on the manifold \(\beta^2 = T^{-2}\). Hence the set of states minimizing the free energy functional \(\omega_B \mapsto e'_\mu e'_\nu \omega_B(F^{\mu\nu})\) for given temperature is degenerate.

We conclude this appendix by illustrating the preceding notions for the case of a dilation invariant theory, where the stress energy tensor \(\theta^{\mu\nu}(x)\) is traceless, \(\theta^\mu_\mu(x) = 0\), and transforms canonically under the dilations according to \(\delta_s(\theta^{\mu\nu}(x)) = s^4 \theta^{\mu\nu}(sx)\), \(s \in \mathbb{R}_+\). A special example is the model discussed in Sec. 5. It follows from the definition of KMS states and their uniqueness that \(\omega_\beta \circ \delta_s = \omega_{s^{-1}\beta}\). Plugging these pieces of information into equation \((A.1)\), we obtain

\[
E^{\mu\nu}(\beta) = C (4\beta^\mu \beta^\nu - \beta^2 g^{\mu\nu})(\beta^2)^{-3}, \tag{A.16}
\]

where \(C\) is a constant depending on the underlying theory. Thus the temperature dependence of the energy density in the rest system is given by \(E(\beta) = 3C(\beta^2)^{-2}\), in accordance with Stefan-Boltzmann’s law, and the pressure satisfies

\[
P(\beta) = C (\beta^2)^{-2}. \tag{A.17}
\]

So \(E = 3P\), which also follows directly from the fact that the stress energy tensor is traceless. In particular, \(0 \leq dP/dE \leq 1\), as was anticipated in the preceding analysis. Finally, the entropy current is given by

\[
S^\mu(\beta) = 4 C \beta^\mu (\beta^2)^{-2}, \tag{A.18}
\]

so the pertinent thermal functions are completely fixed apart from the value of the constant \(C\).

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