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Towards Local Temperature States in QFT*

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1 Simple example of local temperature state

Aiming at a general formulation of non-equilibrium states in the framework of QFT, we start from a simple model-example of local temperature state: Let $\varphi(x)$ be a massless free scalar field (in four dimensions) characterized by

$$\Box\varphi = 0, \tag{1}$$

$$[\varphi(x), \varphi(y)] = iD(x-y) = \int \frac{d^4p}{(2\pi)^3} e^{-ip(x-y)}\epsilon(p_0)\delta(p^2). \tag{2}$$

Given a two-point function $\omega^{(2)}(\varphi(x)\varphi(y))$, we can define a *quasi-free* state ω of φ through the Wick formula:

$$\omega(\varphi(x_1)\varphi(x_2)\cdots\varphi(x_r)) := \begin{cases} \sum_{pairings} \omega^{(2)}(\varphi(x_{i_1})\varphi(x_{i_2}))\cdots\omega^{(2)}(\varphi(x_{i_{r-1}})\varphi(x_{i_r})) & (\text{if } r \text{ :even}) \\ 0 & (\text{if } r\text{: odd}). \end{cases} \tag{3}$$

When a two-point function $\omega^{(2)}$ is chosen consistently with Eqs.(1, 2) as

$$\omega_\beta^{(2)}(\varphi(x)\varphi(y)) = \int \frac{d^4p}{(2\pi)^3} e^{-ip(x-y)}\epsilon(p_0)\delta(p^2)\frac{1}{1-e^{-\beta p_0}}, \tag{4}$$

the corresponding quasi-free state $\omega = \omega_\beta$ describes a global thermal equilibrium satisfying the KMS condition for any pair of polynomial fields $A = \varphi(x_1)\cdots\varphi(x_r)$ and $B = \varphi(y_1)\cdots\varphi(y_s)$,

$$\omega_\beta(A\alpha_{(i\beta,\mathbf{0})}(B)) = \omega_\beta(BA), \tag{5}$$

*Talk based on a joint work of D.Buchholz, H.Roos and I.O. in progress where $\alpha_{(i\beta,\mathbf{0})}(B) := \varphi(y_1 + (i\beta, \mathbf{0})) \cdots \varphi(y_s + (i\beta, \mathbf{0}))$ (symbolically). In place of $\omega_\beta^{(2)}$, such a choice of two-point function as

$$\omega^{(2)}(\varphi(x)\varphi(y)) = \int \frac{d^4p}{(2\pi)^3} e^{-ip(x-y)} \epsilon(p_0)\delta(p^2) \frac{1}{1 - e^{-\beta^\mu(\frac{x+y}{2})p_\mu}}, \tag{6}$$

is also allowed consistently with Eqs.(1, 2) if a spacetime-dependent inverse-temperature four-vector is given by $\beta^\mu(x) = \beta^\mu + \gamma^\mu_\nu\, x^\nu$[1]. In this case we can verify

$$\omega^{(2)}(\varphi(x)\varphi(y + i\beta(\frac{x+y}{2})) = \omega^{(2)}(\varphi(y)\varphi(x)), \tag{7}$$

which can be interpreted as a *localized* version of KMS condition. Contrary to the case of the global equilibrium ω_β, however, it is *not* possible to generalize this relation to n-point functions with $n \geq 3$ in the similar form to Eq.(5): e.g.,

$$\begin{aligned} &\omega(\varphi(x_1)\varphi(x_2)\cdots\varphi(x_r)\varphi(y_1 + i\beta(\frac{x_1+y_1}{2}))\varphi(y_2 + i\beta(\frac{x_2+y_2}{2}))\cdots \\ &\qquad \cdots\varphi(y_r + i\beta(\frac{x_r+y_r}{2}))) \\ \neq\ &\omega(\varphi(y_1)\varphi(y_2)\cdots\varphi(y_r)\varphi(x_1)\varphi(x_2)\cdots\varphi(x_r)), \end{aligned} \tag{8}$$

just because of the spacetime dependence of $\beta^\mu(x)$. Namely, the similarity of the state ω given by Eqs.(6, 3) to a global thermal equilibrium ω_β holds only up to two-point function $\omega^{(2)}$. In this way, ω can be taken as a model example of a local temperature state such that it is only locally in equilibrium in the sense of Eq.(7).

Remark: The breakdown of KMS condition for n-point functions with $n \geq 3$ is natural as a signal of non-equilibrium, in view of the zeroth law of thermodynamics which claims the validity of transitive law in the thermal equilibrium contact relations of two bodies: To inspect for the breakdown of transitivity due to non-equilibrium, we need to examine the relation among three bodies.

Generalized Stefan-Boltzmann law and "Local Thermometers"
Now, a remarkable property of this state ω is found in the following formula:

[1]Because of the positivity condition to be satisfied by $\omega^{(2)}$, the region allowed for x and y may not cover all the spacetime $\mathbb{R}^4$.

$$
\begin{aligned}
\lim_{\xi\to 0} \quad & \omega(\partial^{\xi}_{\mu_1}\partial^{\xi}_{\mu_2}\cdots\partial^{\xi}_{\mu_r} : \varphi(X-\frac{\xi}{2})\varphi(X+\frac{\xi}{2}) :) \\
= \quad & \lim_{\xi\to 0} [\omega(\partial^{\xi}_{\mu_1}\partial^{\xi}_{\mu_2}\cdots\partial^{\xi}_{\mu_r}\varphi(X-\frac{\xi}{2})\varphi(X+\frac{\xi}{2})) \\
& \qquad -\omega_{\mathrm{vac}}(\partial^{\xi}_{\mu_1}\partial^{\xi}_{\mu_2}\cdots\partial^{\xi}_{\mu_r}\varphi(X-\frac{\xi}{2})\varphi(X+\frac{\xi}{2}))] \\
= \quad & T(X)^{r+2}C_{\mu_1\mu_2\cdots\mu_r},
\end{aligned} \tag{9}
$$

where ω_{vac} is a vacuum state corresponding to $\beta = \infty$ and $C_{\mu_1\mu_2\cdots\mu_r}$ is a constant tensor vanishing for r =odd. $T(X)$ defined by

$$T(X) := 1/\sqrt{\beta^{\mu}(X)\beta_{\mu}(X)} \tag{10}$$

is a local temperature. In the case of $r = 2$ the left-hand side of this formula can easily be related to the energy density with a suitable tensorial combination, in view of which it gives a generalization of the well-known Stefan-Bolzmann law, $e = \sigma T^4$, for the radiation energy e. In the sense of Eq.(9), the operator $\partial^{\xi}_{\mu_1}\partial^{\xi}_{\mu_2}\cdots\partial^{\xi}_{\mu_r} : \varphi(X-\frac{\xi}{2})\varphi(X+\frac{\xi}{2}) :$ works as a "local thermometer" to measure a local temperature $T(X)$ at the centre-of-mass point $X = \frac{x+y}{2}$ of very close two points $x = X - \frac{\xi}{2}$ and $y = X + \frac{\xi}{2}$ in the limit $\xi \to 0$. Further the totality of operators of this sort are seen to give rise on the right-hand side to all the even powers of local temperature $T(X)$ (times some Lorentz tensors of even degree) which generate an algebra of functions of non-negative temperatures $T(X) \geq 0$.

2 Definitions of generalized and local thermal states

Motivated by this example, we explore the possible framework for accommodating some class of states describing local thermal situations: Basic idea is to compare a given state in a small neighbourhood of a spacetime point with all the KMS states at possible temperatures by means of certain set of point-like local observables playing the role of "thermometers". For this purpose, we need the following definitions.

Definitions:

(i) *Set of thermal states* K is defined by the closed convex hull of all the KMS states, $K := \overline{\mathrm{conv}(\bigcup_{\beta\in\mathbb{R}_+} K_\beta)}$, where K_β is the set of KMS states at inverse temperature β.

NB: The relativistic version can be obtained by replacing $\beta \in \mathbb{R}_+$ with $\beta^\mu \in V_+ :=$ forward lightcone, where $\beta = \sqrt{\beta^\mu \beta_\mu}$. Depending on the situations, we freely move from one version to another.

(ii) A set $\mathcal{T} = \{A_n;\ n \in \mathbb{N}\}$ of (point-like) local observables A_n is called a *thermometer set* or a *discriminating set* if $\omega(A_n) = \omega'(A_n)$ $(\forall n \in \mathbb{N})$ for $\omega, \omega' \in K$ implies $\omega = \omega'$. The linear hull of $\mathcal{T}$ is denoted by $\mathcal{L}$: $\mathcal{L} := \mathrm{Lin}\mathcal{T}$. Although the identity operator $\mathbf{1}$ is irrelevant to the purpose of discriminating different states, we understand by convention that it belongs to $\mathcal{T}$: $\mathbf{1} \in \mathcal{T}$.

(iii) *K-norm* $\|A\|_K$ of a local observable A is defined by $\|A\|_K := \sup_{\omega \in K} |\omega(A)|$. For the sake of simplicity, we assume the absence of phase transition, i.e., $K_\beta = \{\omega_\beta\}$ for $\forall \beta \in V_+$, in which case $\|A\|_K = \sup_{\beta \in V_+} |\omega_\beta(A)|$.

(iv) A local observable A satisfying $\omega(A) \geq 0$ for $\forall \omega \in K$ is called a *K-positive* element, the totality of which constitute a *K-positive cone* denoted by $\mathcal{P}_K := \{A;\ \omega(A) \geq 0\ \forall \omega \in K\} = \{A;\ \omega_\beta(A) \geq 0\ \forall \beta \in V_+\}$. We also denote $\mathcal{P}_\mathcal{L} := \mathcal{P}_K \cap \mathcal{L}$, the set of *K-positive* thermometers.

(v) The set of *thermal functions* is defined by $\mathcal{F}_0 := \mathrm{Lin}\{f_n;\ f_n(\beta) := \omega_\beta(A_n), A_n \in \mathcal{T},\ n \in \mathbb{N}\}$, $\mathcal{F} := \overline{\mathcal{F}_0}^{\|\cdot\|_\infty}$ with $\|\cdot\|_\infty$ being the supremum norm.

Further, we impose the following two restrictions on the thermometer set $\mathcal{T}$:

– $\{f_n\}$ is linearly independent,

– $\mathcal{F}_0$ is dense in $C_0(V_+)$.

From these it immediately follows that

– $A_n \in \mathcal{T}$ implies $\alpha_x(A_n) \notin \mathcal{T}$ for any spacetime translations α_x because of the relation $\omega_\beta \circ \alpha_x = \omega_\beta$,

– $\Phi:\ A_n \in \mathcal{T} \longmapsto f_n \in \mathcal{F}_0$ defines an isometric 1-1 map of $\mathcal{L}$ onto $\mathcal{F}_0$, where $\mathcal{F}_0$ is equipped with the supremum norm, and $\mathcal{L}$ with the K-norm $\|\cdot\|_K$.[2]

Criteria for *generalized thermal states*:

A state ω is called a *generalized thermal state* w.r.t. a thermometer set $\mathcal{T}$ ("$\mathcal{T} - GTstate$" or "$GTstate$", in short) if it is K-bounded and K-positive on $\mathcal{L}$ in the following sense:

$$|\omega(\sum c_n A_n)| \leq C\ \|\sum c_n A_n\|_K\ ; \qquad \omega\restriction_{\mathcal{P}_\mathcal{L}} \geq 0\ .$$

[2]Of course, the K-norm does not define a Hausdorff topology on $\mathcal{L}$.

The physical meaning of this criterion is seen in the following result:
Lemma: A generalized thermal state ω defines a positive linear functional $\varphi_\omega \in \mathcal{F}^*$ by $\varphi_\omega := \omega \circ \Phi^{-1}$ on $\mathcal{F}_0$, i.e., $\varphi_\omega(\sum c_n f_n) = \omega(\sum c_n A_n)$, and extension by continuity. Therefore, φ_ω is represented by a probability measure μ_ω on $\mathbb{R}_+$ in such a form as

$$\omega(\sum c_n A_n) = \varphi_\omega(\sum c_n f_n) = \int d\mu_\omega(\beta) \sum c_n f_n(\beta) = \int d\mu_\omega(\beta)\ \omega_\beta(\sum c_n A_n);$$

in short: $\omega \restriction_{\mathcal{L}} = \int d\mu_\omega\ \omega_\beta \restriction_{\mathcal{L}}$.

Namely, a generalized thermal state is a state which can be approximated around a spacetime point by a statistical average over thermal equilibrium states. More strongly, a GT state ω is called a *local temperature state* (or LT state, in short) if μ_ω is concentrated on a single point $\beta \in \mathbb{R}_+$.

Remarks:

i) It is due to our convention of $\mathbf{1} \in \mathcal{T}$ that the measure μ_ω is normalized as a probability measure: $1 = \omega(\mathbf{1}) = \int d\mu_\omega(\beta)\ \omega_\beta(\mathbf{1}) = \int d\mu_\omega(\beta)$.

ii) Any state $\omega \in K$ (given as convex combination of KMS states) is a generalized thermal state w.r.t. any $\mathcal{T}$, since $\omega(B) > 0\ \forall B \in \mathcal{P}_K \supset \mathcal{P}_{\mathcal{L}}$. Therefore, the notion of GT states defined above actually give a generalization of thermal equilibrium states in a three-fold way, in their being i) relativistic, ii) mixtures of different temperatures, and iii) localized in small neighbourhoods of spacetime points.

iii) "Point-like local observables" belonging to $\mathcal{T}$ can be formulated in the context of local nets as the objects dual to state germs (in the sense of [1] and [2]).

iii) When a K-bounded state ω is allowed to be non-K-positive, then φ_ω becomes a signed measure.

iv) $\omega^{(\mu)} := \int d\mu\ \omega_\beta$ may be a $\mathcal{T}$-GT state even if μ is not positive.

Desired localization properties of $\mathcal{T}$: For any spacetime point x, there is a thermometer set $\mathcal{T}$ consisting of local observables belonging (more appropriately, affiliated) to $\mathcal{A}(\mathcal{O})$ where $\mathcal{O}$ is an arbitrary small neighbourhood $\mathcal{O}$ of x ("*$\mathcal{T}$ concentrated at x*").
Existence of local thermometer sets: Assume (i) weak additivity, (ii) norm continuity of $\beta \mapsto \omega_\beta \restriction_{\mathcal{A}(\mathcal{O})}$ for bounded regions $\mathcal{O}$, then there is a thermometer set $\mathcal{T} \subset \mathcal{A}(\mathcal{O}_0)$ (or $\mathcal{T} \subset \{A;\ A\ \eta\ \mathcal{A}(\mathcal{O}_0)\}$) for an arbitrary

small $\mathcal{O}_0$.

Lemma: Let $\mathcal{T}$ be concentrated at $0 \in \mathbb{R}^4$; furthermore, let $\omega \circ \alpha_{-x}$ be a $\mathcal{T}$-GT state for x in a neighbourhood $\mathcal{N}$ of 0, i.e., ω is locally a generalized thermal state at the point x, defining a corresponding measure μ_x. Then μ_x is weakly continuous, i.e., $\int d\mu_x(\beta)F(\beta)$ depends continuously on $x \in \mathcal{N}$ for all $F \in \mathcal{C}_0(\mathbb{R}_+)$.

Especially, if the *mean temperature at* x is defined by $\overline{T}(x) := \int d\mu_x(\beta)\beta^{-1}$, then $x \mapsto \overline{T}(x)$ is continuous in $\mathcal{N}$.

2.1 Choice of thermometers: Equivalence classes of $A \in \mathcal{T}$

We define an equivalence relation $A \sim B$ between $A, B \in \mathcal{T}$ by $\omega(A) = \omega(B)$ for $\forall \omega \in K$ and denote the equivalence class of A by $[A]$. It is clear that the K-norm and the K-positivity are independent of the choice of the representatives in $[A_n]$, $n \in \mathbb{N}$. However, the validity of the above criteria for GT-states will in general depend on the choice of specific representatives from $[A_n]$. Although this point need be further elaborated, the best choice seems to be given by considering "derivatives conserving the center of mass": e. g. $\partial_\mu^\xi(\Phi(\xi/2)\Phi(-\xi/2)) \restriction_{\xi=0}$. To justify it as a reasonable choice, we recall here that the requirement of linear independence of $\mathcal{T}$ forbids the operation of translations α_x on elements of $\mathcal{T}$: i.e., $A_n \in \mathcal{T}$ implies $\alpha_x(A_n) \notin \mathcal{T}$, because $\omega_\beta \circ \alpha_x = \omega_\beta$. In view of the relation for two-point product operators $\varphi(x)\varphi(y)$

$$\frac{d}{dt}\alpha_{te_\mu}(\varphi(X-\frac{\xi}{2})\varphi(X+\frac{\xi}{2}))|_{t=0} = \partial_\mu^X(\varphi(X-\frac{\xi}{2})\varphi(X+\frac{\xi}{2})),$$

this amounts in its infinitesimal version to excluding derivatives ∂_μ^X w.r.t. the centre-of-mass coordinates $X = \frac{x+y}{2}$. In fact, the derivative ∂_ξ w.r.t. the relative coordinates $\xi = y - x$ is sufficient to generate the whole thermometer set in our previous discussion of local temperature states in the massless free scalar field. In general, we will be led to the choice of operators in such a form as

$$\partial_\mu^\xi(\Phi_1(X+\gamma_1\xi)\Phi_2(X+\gamma_2\xi)\dots\Phi_n(X+\gamma_n\xi)) \restriction_{\xi=0} \text{ with} \sum \gamma_i = 0\,.$$

Concerning this choice we can see its deeper meanings in more general contexts such as the classification of states from the viewpoint of singularity and also as the extension of the locally thermal notions to curved spacetime situations:

i) The data for classifying different spieces of states, such as vacuum, temperature states, and so on, can be provided by quantities defined on the *cotangent spaces* of spacetime which are closely related with the separation into centre-of-mass coordinates X^μ and relative ones ξ^μ in the case of two-point functions. For instance, in the discussion of massless free scalar field model of local temperature states, we have seen that the "normal product" relative to a vacuum, $\rho(X,\xi) \equiv \omega(: \varphi(X-\frac{\xi}{2})\varphi(X+\frac{\xi}{2}) :) = \omega(\varphi(X-\frac{\xi}{2})\varphi(X+\frac{\xi}{2})) - \omega_{\text{vac}}(\varphi(X-\frac{\xi}{2})\varphi(X+\frac{\xi}{2}))$, plays an important role. This takes care of the separation of the most singular and less singular terms at $\xi \to 0$: Namely, rewriting Eq.(9) as

$$\omega(\varphi(X-\frac{\xi}{2})\varphi(X+\frac{\xi}{2})) = \omega_{\text{vac}}(\varphi(X-\frac{\xi}{2})\varphi(X+\frac{\xi}{2})) + \rho(X,\xi), \quad (11)$$

we note that the vacuum term on the RHS gives the most singular contribution in the limit $\xi \to 0$. In this sense, thermal aspects can be taken as those concerning the next-to-leading contributions at a point X with $\xi = 0$.

ii) This can be seen more clearly in the microlocal spectrum condition characterizing the vacuum states in curved spacettime (see e.g., [3]). Here, the condition for vacuum states is formulated in terms of *wave front set* which specifies the locations of singularities of distibutions in the cotangent bundle (more precisely, sphere bundle) of spacetime manifold. While we do not need the details of the microlocal spectrum condition here, its essence lies in the condition imposed upon the wave front sets of n-point functions from the viewpoint of parallel transportability of momenta between vertices and it is interesting to note that this condition gives a close relationship between the characterization of states and the singularities of Wightman functions in *cotangent spaces.*

Remark: The wave front set, WF(ϕ), of a distribution $\phi \in \mathcal{D}'(V)$ ($V \subseteq \mathbb{R}^d$) is defined in $V \times (\mathbb{R}^d \setminus \{0\})$ as the complement of the set of points (ξ', p') satisfying the property that there exist some neighbourhood U of ξ' and some conic neighbourhood Σ of p' such that, for $\forall f \in C_0^\infty(U), \forall N \in \mathbb{N} \cup \{0\}, \forall p \in \mathbb{R}^d \setminus \{0\}$

$$p \in \Sigma \Longrightarrow |< \phi, e^{-i<\cdot,p>} f >| \leq C_{f,N}(1+|p|)^{-N}$$

holds with some constant $C_{f,N}$. Here, Σ: conic, means that $p \in \Sigma$ implies $tp \in \Sigma$ for all $t > 0$. If ϕ does not contain any singularity, the validity of the above inequality can easily be understood by the

Paley-Wiener theorem. This *growth condition* in the limit of $p \to \infty$ in momentum space just corresponds in coordinate space to the limit of $\xi \to \xi'$ because of the arbitrariness of smooth functions $f \in C_0^\infty(U)$ in the neighbourhood of ξ'.

iii) If we apply this notion to our distribution $\omega(\varphi(X - \frac{\xi}{2})\varphi(X + \frac{\xi}{2}))$ with ξ as its argument, the most singular term at $\xi \to 0$ corresponds to the vacuum term $\omega_{\text{vac}}(\varphi(X - \frac{\xi}{2})\varphi(X + \frac{\xi}{2}))$ on RHS of Eq.(11). Once we remove it, $\rho(X, \xi)$ remaining as the less singular term is smooth (or more suitably, *analytic* according to the result of [4]) in ξ. In the massless free scalar field model of local temperature states, we have seen that the function $\xi \mapsto \rho(X, \xi)$ together with its ξ-derivatives are sufficient for identifying a local temperature $T(X)$. The Fourier transform of this function, $p \mapsto \int d\xi\ e^{ip\xi}\rho(X, \xi) \doteq \tilde{\rho}(X, p)$, (in $p \to \infty$) can be viewed as a function defined on the cotangent space at $\xi = 0$ in relative coordinates.

iv) Applying the derivative ∂_μ^ξ w.r.t. relative coordinates ξ (acting in the fiber-direction of the cotangent bundle) corresponds to multiplication by p_μ in momentum space. If the relevant functions in the above iii) are always ensured to be analytic, then $(X, p) \mapsto \tilde{\rho}(X, p)$ and its ξ-derivatives will exhaust all the necessary information as (the expectation value of) the discriminating set $\mathcal{T}$.

v) The above formulation based upon quantities in cotangent bundles can become crucial in the attempt of extending basic ingredients in locally thermal situations to *curved spacetimes.* While the reference system K of thermodynamic equilibria is treated in our formulation as *global* KMS states, the roles of these equilibrium states lie in assigning a temperature or temperature distribution to each *spacetime point* in reference to the thermometer set $\mathcal{T}$ prepared in its small neighbourhood. Thus, with the aid of normal coordinates and the exponential map (which maps flat tangent spaces onto curved spacetime), it should be possible to reformulate K as an object living in the tangent bundle of spacetime, if we restrict our spacetime manifold to the one admitting *complexification* (which is crucial for the formulation of KMS condition or its relativistic generalization due to [4]). In the context of this generalization, the 4-vector nature of inverse temperature $\beta_\mu(X)$ will be very interesting in relation with its role to specify the rest frame at each spacetime point and also its close relationship with the 4-vector nature of entropy density current $s_\mu(X)$. Before discussing the thermodynamic behaviours of generalized thermal states in terms of these local densities, we need first to examine more closely the *thermostatics* in the set K of all the KMS states in order to extend the mutual relations of these thermal quantities from equilibrium regions to those of our generalized thermal states.

3 Thermostatics in K

3.1 Definition of local rest frame and equivalence principle

From the relativistic viewpoint, inverse temperature β and entropy density s need be understood as Lorentz four-vectors, β^μ and s^μ, respectively: In a reference frame $\mathcal{S}$, let $\vec{v}$ denote the relative velocity of rest frame of our thermal system in thermal equilibrium (at temperature T), and u^μ the corresponding 4-vector defined by $u^\mu = (\frac{1}{\sqrt{1-|\vec{v}|^2}}, \frac{\vec{v}}{\sqrt{1-|\vec{v}|^2}})$, $u^\mu u_\mu = 1$). Then inverse temperature has to be treated as a four-vector $\beta^\mu = \tau^{-1}u^\mu$ [5] with $\tau := k_B T$ (formally this is understood as the generalization of the Boltzmann factor $\exp(-\beta E)$ to the invariant expression $\exp(-\beta^\mu p_\mu)$). The same holds true of the entropy density: it is to be considered as the four-vector $s^\mu = s_{\mathrm{eq}} u^\mu$ where s_{eq} is the density of equilibrium entropy. (This allows to generalize the expression $\tau^{-1}s_{\mathrm{eq}}$ to $\beta^\mu s_\mu$.)

If one can find the *local rest frame* of the system at each spacetime point in the present context of *generalized* thermal states, the essence of equilibrium thermodynamics should be reproduced there locally and the descriptions in general frames can be derived kinematically through the Lorentz transformations parametrized by the relative velocity u^μ which relate the former to the latter. This is just Einstein's equivalence principle applied to thermodynamics.

3.2 Thermodynamic relations in equilibrium

To develop machinery for analyzing the general thermal states, we aim here at extracting the useful essence from thermodynamic relations valid for *equilibrium states in the rest frame* in order to extend it to their *arbitrary mixtures* (belonging to the set K) and to *arbitrary Lorentz frames.*

In general Lorentz frame, an equilibrium state ω_β is characterized by the relativistic KMS condition w.r.t. a fixed $\beta \in V_+$ [4], and hence, our set K of all the KMS states viewd from such a frame can be expressed by

$K := \overline{\text{conv}\,\{\omega_\beta;\, \beta \in V_+\}}$. We try to extend the notions of entropy density, energy density, free energy density, and possibly temperature to all states belonging to K starting from a rest frame characterized by the relations $u^\mu = (1, \mathbf{0})$, $\beta^\mu = \beta u^\mu = (\beta, \mathbf{0})$, $s^\mu = s u^\mu = (s, \mathbf{0})$.

For a system in equilibrium in the rest frame, let $s(\omega_\beta) \equiv s_{\text{eq}}(e, \cdots)$ be the equilibrium entropy density; it is a *concave* function of the energy density e and of other conserved quantities, indicated by the dots, such as baryon number density n_B, lepton number density n_L, electric charge density q, etc. In the sequel, we shall mostly disregard all other variables than e; our considerations can easily be extendend to the general case. The quantities s_{eq} and e refer to the rest frame of the system under consideration. The corresponding temperature $\tau (:= k_B T)$ is given as usual by $\tau^{-1} = \partial s_{\text{eq}} / \partial e$.

For an equilibrium state ω_β we have

$$u^\mu_{\text{th}}(\beta) s_\mu(\omega_\beta) = s_{\text{eq}}(e_\beta), \quad \sqrt{\beta^2} = \tau^{-1} = \frac{\partial s_{\text{eq}}}{\partial u}(e_\beta), \tag{12}$$

with

$$e_\beta = u^\mu_{\text{th}}(\beta) u^\nu_{\text{th}}(\beta)\, T_{\mu\nu}(\omega_\beta), \tag{13}$$

where $T_{\mu\nu}(\omega_\beta) := \omega_\beta(T_{\mu\nu})$ is the energy momentum tensor evaluated in the equilibrium state ω_β. (Contrary to some treatments of relativistic thermodynamics, the rest mass is included in the ("inner") energy density defined above). Relations (12) and (13) follow from the invariance of the expressions by evaluation in the rest system ($u_{\text{th}} = (1, 0, 0, 0)$).

A general state $\omega \in K$ is of the form $\omega = \int_{V_+} d\rho(\beta)\ \omega_\beta$ with a probability measure ρ on V_+. Denoting the average of a function $g(\beta)$ on K w.r.t. this probability measure ρ by $\langle g \rangle_\omega := \int d\rho(\beta)\ g(\beta)$, we see that the energy density in $\omega \in K$ is given by

$$e(\omega) = \langle e_\beta \rangle_\omega \equiv \langle e(\omega_\beta) \rangle_\omega.$$

We define the entropy of ω by

$$s^\mu(\omega) = \int_{V+} d\rho(\beta)\ s^\mu(\beta). \tag{14}$$

This is a natural definition in view of the fact that two KMS states ω_β and $\omega_{\beta'}$ in infinite systems are disjoint for $\beta \neq \beta'$ [Bratteli -Robinson II], which implies that the entropy is additive: $s(\lambda_1 \omega_\beta + \lambda_2 \omega_{\beta'}) = \lambda_1 s(\omega_\beta) + \lambda_2 s(\omega_{\beta'})$.

Concerning the question as to how the mean temperature of the state $\omega = \int_{V+} d\rho(\beta)\, \omega_\beta$ should be defined, there are a few possibilities such as

$$\beta(\omega) := \langle \beta \rangle_\omega\,, \qquad \text{or} \qquad \beta(\omega)^{-1} = T(\omega) := \langle \beta^{-1} \rangle_\omega .$$

A better, and more natural definition is given by

$$\beta(\omega) := \frac{\partial s}{\partial e}(e(\omega), \dots). \tag{15}$$

From covariance consideration we can determine the form of $T^{\mu\nu}(\omega_\beta)$: The equilibrium state ω_β may depend on other conserved quantities as well, but we assume that they are only scalar ones, such that β resp. u_{th} are the only four-vectors available.
Hence $T^{\mu\nu}$ is of the form

$$T^{\mu\nu}(\omega_\beta) = A(\beta^2, \dots)\, g^{\mu\nu} + B(\beta^2, \dots)\, u^\mu_{\mathrm{th}} u^\nu_{\mathrm{th}}\,, \tag{16}$$

A and B are scalar functions which depend on the system under consideration.

Combination of equations (13) and (16) yields

$$e_\beta = A(\beta^2) + B(\beta^2)\,, \tag{17}$$

i. e. e_β is a function of β^2 only. The same holds true of $s_{\mathrm{eq}}(e_\beta)$, we can write

$$s^\mu(\omega_\beta) = \sigma v^\mu_{\mathrm{th}}; \quad \sigma = s_{\mathrm{eq}}(e_\beta)\,. \tag{18}$$

As a consequence of equation (17) we can express $\sigma(\beta^2)$ in terms of A and B:

$$\sqrt{\beta^2} = \frac{\partial s_{\mathrm{eq}}}{\partial u}(e_\beta) = \frac{\partial \sigma}{\partial \beta^2}\left(\frac{\partial u_\beta}{\partial \beta^2}\right)^{-1} = \frac{\sigma'}{A' + B'}\,; \tag{19}$$

$$\sigma = \int^{\beta^2} dx\, \sqrt{x}(A'(x) + B'(x)) = -\int_{\beta^2}^{\infty} dx\, \sqrt{x}(A'(x) + B'(x)). \tag{20}$$

(The prime denotes the derivative w.r.t. $x \equiv \beta^2$; the integration constant is chosen so that the entropy vanishes for $\tau = 0$.)

s_{eq} is a concave function, and, as a consequence we note that

$$A' + B' < 0\,. \tag{21}$$

With the help of (19) the proof is easy (differentiability assumed, again we put $x = \beta^2$ and make use of (17)):

$$\begin{aligned} 0 > \frac{\partial^2 s_{eq}}{\partial u^2} &= \frac{\partial}{\partial u}\frac{\partial s_{eq}}{\partial u}(e_\beta) = \frac{\partial}{\partial x}\left(\frac{\partial s_{eq}}{\partial u}(e_\beta)\right)\left(\frac{\partial(e_\beta)}{\partial x}\right)^{-1} \\ &= \left(\frac{\sigma''}{e'_\beta} - \frac{\sigma'}{{e'_\beta}^2}e''_\beta\right)(e'_\beta)^{-1} = \frac{1}{{e'_\beta}^2}\left(\sigma'' - \sigma'\frac{e''_\beta}{e'_\beta}\right) . \end{aligned}$$

Since $\sigma' = \sqrt{x}\, e'_\beta$, the expression in brackets, which has to be negative, equals $\sigma'' - \sqrt{x}e''_\beta < 0$; differentiating σ' once more, we get $\sigma'' = \frac{1}{2\sqrt{x}}e'_\beta + \sqrt{x}e''_\beta$ and thus

$$0 > \sigma'' - \sqrt{x}e''_\beta = \frac{1}{2x}\sigma' = A' + B'.$$

3.3 Second Law of Thermodynamics

The next task is to give a generalized formulation of the second law of thermodynamics. For systems at rest w.r.t. the given frame of reference, for which the energy density is fixed, $e(\omega) = e_0$, the entropy density is maximal for ω_β with $\sqrt{\beta^2} = \frac{\partial s_{eq}}{\partial u}(e_0)$. Now consider an arbitrary frame of reference, characterized by a four-velocity vector u^μ, $u \cdot u = 1$, defining the time axis of the frame. For the sake of brevity we shall denote it by "the frame u". Let $\omega = \int_{V+} d\rho(\beta)\, \omega_\beta$ be an arbitrary state in K. Clearly, the energy density of ω in the frame u is given by

$$e(\omega; u) = u^\mu u^\nu \omega(T_{\mu\nu}) = u^\mu u^\nu \int_{V+} d\rho(\beta)\, T_{\mu\nu}(\omega_\beta) . \tag{22}$$

Let us keep this quantity fixed, $e(\omega; u) = e_0$, and ask for the state in K which maximizes the entropy density. The best guess seems to be the following:
Generalized Second Law: *The supremum*

$$\sup \{u^\mu s_\mu(\omega);\ \omega \in K,\ e(\omega; u) = e_0\}$$

is attained for the KMS state ω_β with

$$\beta^\mu = \tau^{-1}u^\mu, \quad \tau^{-1} = \frac{\partial s_{eq}}{\partial u}(e_0) . \tag{23}$$

Due to equations (12) and (18), the supremum is given by

$$u^\mu s_\mu(\omega_\beta) = s_{eq}(e_0) = \sigma(\beta^2) . \tag{24}$$

Although this cannot be directly verified, it can be shown under the assumption that the following holds:

Restricted Second Law: *Given* e_0, *then* $u^\mu s_\mu(\omega_\beta)$ *is maximal if* $\beta^\mu = \sqrt{\beta^2}\, u^\mu$.

Together with the Second Law in the rest system, this then implies the full Generalized Second Law:

Lemma: Since $s_{\text{eq}}(e)$ is a concave function, and $s_{\text{eq}}(e) = \sigma(\beta^2)$ with $\sqrt{\beta^2} = \partial_e s_{\text{eq}}(e)$, the Restricted Second Law implies the Generalized Second Law.

In the model of a massless free field, the validity of the Restricted Second Law can be checked: The energy momentum tensor is is given by

$$T_{\mu\nu} =: \partial_\mu \Phi\, \partial_\nu \Phi : -\frac{1}{2} g_{\mu\nu} : \partial_\rho \Phi\, \partial^\rho \Phi :,$$

its expectation value in the equilibrium state ω_β being

$$\omega_\beta(T_{\mu\nu}) = T_{\mu\nu}(\omega_\beta) = \text{const} \int \frac{d^3p}{2|\vec{p}|} \frac{e^{-\beta\bar{p}}}{1 - e^{-\beta\bar{p}}}\, \bar{p}_\mu \bar{p}_\nu \ ,$$

where $\bar{p} = (|\vec{p}|, \vec{p})$ is the four-momentum on the mass shell $m = 0$. Calculation of $u^\mu_{\text{th}}(\beta) u^\nu_{\text{th}}(\beta)\, T_{\mu\nu}(\omega_\beta) = A(\beta^2) + B(\beta^2)$, see equations (13) and (17), with the help of the above integral, and insertion into (16) yields

$$T_{\mu\nu}(\omega_\beta) = \text{const}(\beta^2)^{-1} \left(-g_{\mu\nu} + 4 v^{\text{th}}_\mu(\beta) u^{\text{th}}_\nu(\beta) \right) . \tag{25}$$

Let us denote the constant by c, which is positive. Evidently, we have

$$A(x) = -cx^{-2} \ , \quad B(x) = 4cx^{-2} \, .$$

(The relation $B(x) = -4A(x)$ holds due to (16) whenever $T^\mu_{\ \mu} = 0$.) From (20) it then follows that

$$\sigma(x) = \int_x^\infty y^{1/2}\, 6cx^{-3}\, dy = 4cx^{-3/2} \ ,$$

and therefore, for $\Sigma(x)$ defined by $\Sigma(x) := \sigma(x)\sqrt{\frac{e_0 - A(x)}{B(x)}} = \sigma(x)\xi = u^\mu s_\mu(\omega_\beta)$, we have

$$\Sigma'(x) = -cx^{-5/2} \left(\frac{e_0}{c} x^2 + 1 \right)^{-1/2} \left(\frac{e_0}{c} x^2 + 3 \right) .$$

Since $\Sigma' < 0$, the maximum is reached at the upper limit of the range of x, i. e. at $\xi = 1$, as assumed above.

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