How to Formulate Non-Equilibrium Local States in QFT?
– General Characterization and Extension to Curved Spacetime–

Dedicated to Professor Hiroshi Ezawa
on the occasion of his seventieth birthday

Izumi OJIMA
Research Institute for Mathematical Sciences,
Kyoto University, Kyoto 606-8502

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Abstract

The essence of a general formulation to accommodate non-equilibrium local states in relativistic quantum field theory is explained from the viewpoint of comparison at a spacetime point between unknown generic states to be characterized as such states and the known family of probabilistic mixtures of equilibrium states. Taking advantage of the local nature of the problem, we extend the formalism to the general-relativistic context with curved spacetimes.

1 Introduction

It is a great honour for me to make a contribution to this volume to commemorate Professor Ezawa’s 70th anniversary, especially because I have benefited very much from him and from what he wrote and said on physics in general and on quantum field theory in particular, at various stages of my research career. I have been impressed by his wide perspectives ranging from mathematical physics to any kind of physical aspects of nature, among which non-equilibrium statistical physics to be discussed in the following, is an important common subject between him and myself.
“Non-equilibrium” seems to be one of the characteristic features of domains or phenomena in which nature exhibits its most vivid essence. However, theoretical attempts of systematic approaches to it starting from the first principles of microscopic quantum theory seem to have been rather rare (aside from some attractive phenomenological theories in thermodynamic frameworks), in sharp contrast with equilibrium cases. For the latter, we know the existence of variety of achievements successfully attained in the clear-cut formulation based upon the notion of Gibbs ensembles or Kubo-Martin-Schwinger (KMS) states (as generalized version of the former applicable to infinitely extended systems in thermodynamic limit), ranging from detailed analyses of concrete models to abstract sophisticated mathematical treatments of general infinite systems. The reason for such a difference seems to be evident: pursuits for concise and universal characterization of non-equilibrium have been given up, for such reasons as

i) strong negative influence of poor and ambiguous images originating from negative ideas and pictures: in the word “non-equilibrium (states)” one sees only simple negation of equilibrium, missing positive contents.

ii) On the positive side, the experiences of being confronted with the huge variety exhibited by non-equilibrium domains can easily mislead one to a superstition that emphasis on ample individual features at macroscopic levels is equivalent to negating connections with their universal microscopic bases, which ends up with pessimism against ab initio discussions starting from the “first principles” of microscopic quantum theory.

We need to recall, however, that the great achievements in equilibrium statistical mechanics and solid state physics should be found in their unified understanding of macroscopic variety on the universal basis of microscopic quantum theory. At this point, we recall also many fruitful positive examples in the history of transitions to such domains with “non-”, as ⟨⟨from Euclidean to non-Euclidean geometries⟩⟩, ⟨⟨from commutative classical world to non-commutative quantum one⟩⟩, or ⟨⟨from standard to non-standard logic⟩⟩, and so on.

Taking analogy to the basic idea of manifolds exhibiting the process ⟨⟨from Euclidean to non-Euclidean geometries⟩⟩, I try here to re-view the general conceptual essence of our recent work [11][12] towards a general framework for treating nonequilibrium in relativistic QFT, where nonequilibrium local states are specified by a concise selection criterion and their thermal
interpretations are canonically fixed. (The emphasis here is on the conceptual aspects with technical details omitted.)

When we try to understand non-Euclidean geometry as the geometry of curved spaces $M$, e.g., surface of the earth, in a precise way, the aim is never attained with such insistence that what is curved should be treated as it stands. According to the common wisdom, we start from a small neighbourhood $U_i$ in $M$ so that effects of curvature are negligible and try to draw a precise map of $U_i$ on a flat Euclidean space, which is nothing but a usual local map in the case of surface of the earth. While the whole sphere cannot correctly be drawn on one sheet, a (geometrically) "precise" description of such a curved space as the earth sphere can be attained by an atlas as the totality of many local charts $\varphi_i : U_i \rightarrow \mathbb{R}^d$ covering $M = \bigcup_i U_i$.

This familiar discussion found at the beginning of any textbooks on manifolds tells us the following points: In our scientific attempts to describe something in nature, e.g., “curved space” $M$, as

i) our unknown target object to be described,

we inevitably need to relate it with

ii) something familiar to serve as a standard reference frame,

(such as a flat Euclidean space $\mathbb{R}^d$ in the example), which is implemented by

iii) the processes of measuring unknown target objects so that i) is mapped to ii) [: as the case of $\varphi_i$ above],

and then,

iv) the data obtained in iii) need be collected and organized into a coherent interpretation (through which a description is realized) [: the atlas in the example].

These are just the minimum ingredients for our purpose. What corresponds to these in our discussion of non-equilibrium local states can be identified as follows:

i') [unknown target object] = unknown quantum state $\omega$ to be identified as our non-equilibrium local state,
ii') standard reference frame = family \( K \) of thermal reference states consisting of convex combinations of global equilibrium states \( \omega_\beta \) at all the possible temperatures,

iii') processes of measuring to map i') to ii') = local thermal observables \( T \) which detect local thermal properties and whose measured values in an unknown state \( \omega \) in i') are to be compared with the corresponding values in known states belonging to \( K \),

iv') to organize data obtained in iii') into a coherent interpretation = criterion to select non-equilibrium local states + thermal interpretations of selected states in terms of measured values of thermal quantities obtained in iii').

In the following sections, the actual contents of ii')-iv') will be explained.

2 Thermal reference states

In relativistic QFT we identify global thermal equilibria with relativistic KMS states given as follows. The KMS condition \([3, 4]\) is a mathematical characterization of a KMS state \( \omega_\beta \) which generalizes familiar Gibbs states into a form applicable to infinitely extended systems by extracting characteristic relation

\[
\text{Tr}(e^{-\beta H} AB(t)) = \text{Tr}(e^{-\beta H} Ae^{iHt} Be^{-iHt}) = \text{Tr}(e^{-\beta H} B(t - i\beta)A). \tag{1}
\]

In a relativistic version, a state \( \omega_\beta \) as an expectation functional on the algebra \( \mathcal{A} \) of observables \( \omega_\beta : \mathcal{A} \ni A \mapsto \omega_\beta(A) \in \mathbb{C} \) is called a relativistic KMS state with an inverse temperature 4-vector \( \beta = (\beta^\mu) \in V_+ := \{x \in \mathbb{R}^4; x^2 \equiv (x^0)^2 - (\vec{x})^2 > 0, x^0 > 0\} \), if it satisfies the following relativistic KMS condition \([5]\): for any pair \( A, B \in \mathcal{A} \) there is a function \( h = h_{A,B} \), analytic in \( D_\beta := \mathbb{R}^4 + i(V_+ \cap (\beta - V_+)) \), and continuous on \( \overline{D_\beta} \) with the boundary conditions

\[
h(a) = \omega_\beta(A\alpha_a(B)), \quad h(a + i\beta) = \omega_\beta(\alpha_a(B)A), \tag{2}
\]

where \( \mathbb{R}^4 \ni a \mapsto \alpha_a \in Aut(\mathcal{A}) \) \( [\text{*-automorphism group of } \mathcal{A}] \) is a spacetime translation acting on \( \mathcal{A} \). Then, \( \omega_\beta \) can be seen to describe a global thermal equilibrium at a temperature \( T = (k_B\sqrt{\beta^2})^{-1} \) in a rest frame determined by a timelike unit vector \( e = \beta/\sqrt{\beta^2} \in V_+ \).

The totality \( K_\beta \) of relativistic KMS state with \( \beta \in V_+ \) is known \([4]\) to be a simplex admitting for each state \( \in K_\beta \) a unique decomposition into a convex
combination of extremal points, which can be identified with *thermodynamic pure phases* and can be parametrized uniquely by such thermodynamic parameters as $\beta$ (in combination with some such additional ones as chemical potentials $\mu$, if necessary).

A non-trivial Poincaré transformation $\lambda = (a, \Lambda) \in P_+ \times L_+^4 := \mathbb{R}^4 \times L_+^4$ transforms $\omega_{\beta} \in K_\beta$ into another one $\omega_{\beta} \circ \alpha_{\lambda}^{-1} \in K_{\Lambda \beta}$ with inverse temperature $\Lambda \beta$, through which a temperature defined by $1/\sqrt{\beta^2} = 1/\sqrt{(\Lambda \beta)^2}$ is unchanged but the state $\omega_{\beta} \circ \alpha_{\lambda}^{-1} \neq \omega_{\beta}$ can be different from the original one $\omega_{\beta}$, because of the change of reference frame $e = \beta \mu / \sqrt{\beta^2} \rightarrow \Lambda e \neq e$: this is the spontaneous breakdown of Lorentz invariance due to temperature [6]. When convenient for simplification in the following, we introduce the assumption of the *absence of phase transitions* formulated as the uniqueness of KMS state at each temperature $\beta \in V_+$, which implies the relation $\omega_{\beta} \circ \alpha_{\lambda}^{-1} = \omega_{\Lambda \beta}$, and hence, the invariance of $\omega_{\beta}$ under spacetime translations as well as its isotropy in the rest frame.

As ii') *family $K$ of thermal reference states* for local thermal description of an unknown state $\omega$, we take all the possible statistical mixtures $\omega = \int_B d\rho(\beta) \omega_{\beta} =: \omega_{\rho}$ of KMS states $\omega_{\beta}$ in which temperature $\beta$ is fluctuating over some compact subsets $B$ in $V_+$ with such a probability distribution $d\rho(\beta)$ that $\text{supp}(\rho) \subset B$. Namely, we adopt the definition

$$K := \bigcup_{B: \text{cpt} \subset V_+} K_B$$

with

$$K_B := \{ \omega_{\rho} = \int_B d\rho(\beta) \omega_{\beta}; \rho: \text{probability measure on } V_+ \text{ with } \text{supp}(\rho) \subset B \}.$$  

(4)

In more general situations, the requirement of compact supports of $\rho$ may have to be removed and, when the assumption of no phase transition is invalidated, we also add other order-parameters like chemical potential $\mu$, etc., so as for all the relevant thermodynamic pure phases to be discriminated. Then we denote generically the spaces of all the relevant thermodynamic parameters $(\beta, \mu)$ and of (a suitable class of) probability measures $d\rho(\beta, \mu)$, respectively, by $B_K$ and by $Th (= M_1(B_K) = \text{the space of probability measures on } B_K$, for instance): $K \ni \omega_{\rho} := \int_{B_K} d\rho(\beta, \mu) \omega_{\beta,\mu}, (\beta, \mu) \in B_K, \rho \in Th$. 

5
3 “Coordinatization” by local thermal observables

Next, we need “coordinatization map” iii’) connecting i’) to ii’). The basic idea for this is first to measure some thermal observables \( \{ \Phi_i \} \) in an unknown state \( \omega \) under consideration and then to plot on \( \{ \Phi_i \} \)-space the measured values \( \{ \omega(\Phi_i) = \Phi_i(\omega) \} \) regarding them as \( \{ \Phi_i \} \)-coordinates of \( \omega \). If we find a data set \( \{ \Phi_i(\omega_\beta) \} \) for a known equilibrium state \( \omega_\beta \in K_\beta \) s.t. \( \Phi_i(\omega) = \Phi_i(\omega_\beta) \), then our unknown \( \omega \) can be identified with this known \( \omega_\beta \in K \) as far as thermal properties determined by quantities \( \{ \Phi_i \} \) is concerned: \( \omega \equiv \{ \Phi_i \} \omega_\beta \). (The inclusion of mixture \( \omega_\rho = \int_B d\rho(\beta) \omega_\beta \) is just for the sake of wider range of data search to include temperature fluctuations.)

Now the problem is how to find physical quantities \( \{ \Phi_i \} \) suitable for describing local thermal properties of non-equilibrium states in the framework of relativistic QFT?

The aim of this section is to give an answer to this. While the most desirable form of the answer would be such that thermal properties of unknown states in a small spacetime region \( \mathcal{O} \) are determined by local observables measurable within \( \mathcal{O} \). In contrast to our motivating example of manifold, however, it is almost impossible to attain directly this goal starting from a finitely extended region.

Our strategy here is first to concentrate on a spacetime point \( x \) and then to extend the obtained results to a finitely extended region. However, we immediately encounter the well-known difficulty of ultraviolet (UV) divergences invalidating a quantum field at a point, which seems to make our desire hopeless! (Perhaps, this may be one of the reasons for which the programme to construct general framework of non-equilibrium starting from microscopic quantum theory has been discouraged for a long time.) It is too early, however, to give up here! There is an escape through which quantum field \( \hat{\phi}(x) \) at a point can be made meaningful. Since the cause to invalidate \( \hat{\phi}(x) \) is just the UV divergences due to high-frequency modes in quantum fields, \( \hat{\phi}(x) \) makes sense in states to which high energy components make no significant contributions.

This idea can be formulated in a mathematically meaningful form as follows. In many model examples in constructive field theory, the validity of energy-bound inequality has been checked \[ 7 \]: for \( \forall \lambda > 0 \) there exist \( m > 0 \) and a constant \( c > 0 \) s.t.

\[
\|(1 + H)^{-m} \hat{\phi}(f)(1 + H)^{-m}\| \leq c \int dx |(1 - \Delta)^{-\lambda}f(x)|, \quad (5)
\]

holds for \( \forall f \in \mathcal{S}(\mathbb{R}^4) \). Here \( H \) is a Hamiltonian defined in the vacuum
representation where operator norm \(|\cdot|\) is defined and \(\Delta\) is the Laplacian in \(\mathbb{R}^4\). Taking a sequence \(\delta_i\) of test functions s.t. \(\delta_i \to \delta_x\) (: Dirac measure on \(x\)), we have, for sufficiently large \(m > 0\),

\[
\lim_{i \to \infty} (1 + H)^{-m} \hat{\phi}(\delta_i) (1 + H)^{-m} =: (1 + H)^{-m} \hat{\phi}(x) (1 + H)^{-m}
\]

which justifies \(\hat{\phi}(x)\) mathematically. Then, \(\omega(\hat{\phi}(x))\) is meaningful for any state \(\omega\) s.t. \(\omega((1 + H)^{2m}) < \infty\).

By replacing \(H\) meaningful only in the vacuum representation with a local Hamiltonian \(H_O\) playing the role of \(H\) in a local region \(O\) independently of representations, we arrive at the condition

\[
\omega((1 + H_O)^{2m}) < \infty,
\]

to be imposed on states \(\omega\) in question. Actually this is automatically satisfied by any states admitting local thermal interpretation which should have finite energy locally. We denote \(E_O\) the totally of states \(\omega\) satisfying Eq.(7) with a suitable \(m > 0\),

\[
E_O := \{\omega; \omega: \text{state of } A \text{ and } \exists m > 0 \text{ s.t. } \omega((1 + H_O)^{2m}) < \infty\} \supset K,
\]

whose pointlike limit (projective limit)

\[
E_x := \lim_{\delta \to x} E_O \leftrightarrow K
\]

is given by the set of equivalence classes in \(\cup_O E_O\) with respect to the equivalence relation \(\sim\) defined by

\[
\omega_1 \sim \omega_2 \iff \exists \delta: \text{neighbourhood of } x \text{ s.t. } \omega_1 \mid_{\delta} = \omega_2 \mid_{\delta}.
\]

(The family \(O \mapsto E_O\) constitutes a presheaf of state germs whose stalk at \(x\) is given by \(E_x\).)

While the product structure of quantum fields is lost through this procedure, it can effectively be recovered by the notion of normal products in the operator-product expansion (OPE) reformulated recently by in a mathematically rigorous form. Namely, linear spaces \(\mathcal{N}(\hat{\phi}^2)_{q,x}\) consisting of normal products appearing in the expansion of \(\hat{\phi}(x + \zeta)\hat{\phi}(x - \zeta)\) around \(\zeta = 0\) (valid for sufficiently large \(n \in \mathbb{N}\)),

\[
|| (1 + H_O)^{-n} \left[ \hat{\phi}(x + \zeta)\hat{\phi}(x - \zeta) - \sum_{j=1}^{J(q)} c_j(\zeta) \hat{\Phi}_j(x) \right] (1 + H_O)^{-n} || \leq c' |\zeta|^q,
\]

(11)
as coefficients $\hat{\Phi}_j(x)$ of $c$-number singular functions $c_j(\zeta)$ in $\zeta$ are seen to serve as substitutes for the ill-defined $\hat{\phi}(x)^2$, and similarly $\mathcal{N}(\hat{\phi}^p)_{q,x}$ for higher power $\hat{\phi}(x)^p$.

Through the similar expansion of $\partial_\zeta \hat{\phi}(x + \zeta) \hat{\phi}(x - \zeta)$, the derivatives in the relative coordinates $\zeta$ (called “balanced derivatives” here),

$$|| (1 + H_\mathcal{O})^{-n} \left[ \partial_\zeta \hat{\phi}(x + \zeta) \hat{\phi}(x - \zeta) - \sum_{j=1}^{J(q)} \partial_\zeta c_j(\zeta) \hat{\Phi}_j(x) \right] (1 + H_\mathcal{O})^{-n} || \leq c'' |\zeta|^r,$$

(12)
can be similarly made meaningful (for sufficiently large $n, q \in \mathbb{N}$), which describe internal structures of composite operators at the same spacetime point $x$. The expectation values of these normal products determine $p$-point correlation functions around $x$. While derivatives $\partial_x$ in the centre of mass coordinates are sensitive to the spacetime inhomogeneity of an unknown state $\omega$, the corresponding quantities to $\omega(\partial_x(\cdots))$ in thermal reference states are all vanishing $\omega_\beta(\partial_x(\cdots)) = 0$, owing to the translational invariance of $\omega_\beta$. Since the comparison iii’) between $\omega$ and $\omega_\beta$ is for the sake of clarifying thermal properties of $\omega$ instead of spacetime ones, this discrepancy indicates that local observables involving $\partial_x$ should not be counted as local thermal observables suitable for detecting local thermal properties. With all such irrelevant observables excluded, a suitable choice of local thermal observables as “coordinatization map” in iii’) amounts to the linear space $\mathcal{T}_x$ of point-like fields,

$$\mathcal{T}_x := \sum_{p,q} \mathcal{N}(\hat{\phi}_0^p)_{q,x},$$

(13)
consisting of basic fields $\hat{\phi}_0(x)$ at $x$ together with their normal products $\mathcal{N}(\hat{\phi}_0^p)_{q,x}$.

What is remarkable about $\mathcal{T}_x$ is its natural hierarchical nesting structure ordered by indices $m, p, q$ related to energy bound and OPE, according to their increasing orders starting from scalar multiples of identity with basic fields $\hat{\phi}_0(x)$ coming next, and so on. Since $p$-point functions with larger $p$ govern those with smaller $p$, this hierarchy has an operationally intrinsic meaning in such a form as “the larger $p$, the finer resolution of thermal properties is provided by $\mathcal{N}(\hat{\phi}_0^p)_{q,x}, q > 0$”. In this context, macroscopic properties of thermal states are expected to be described by subspaces $\mathcal{N}(\hat{\phi}_0^p)_{q,x}$ with smaller $p,q$.

—Macroscopic interpretations of $\mathcal{T}_x$—
We now examine how these local thermal observables in $T_x$ provide information about macroscopic thermal properties of states in $K$. This is materialized by *thermal functions as macroscopic observables* as follows. In thermodynamics, the physical contents of relevant thermodynamic quantities like internal energy, entropy, etc., are specified by their dependence on temperature (together with other necessary thermodynamic parameters like pressure, chemical potentials, etc.). In parallel with this, all intensive thermal parameters associated with states in $K$ can be represented here by functions $B_K \ni (\beta, \mu) \mapsto F(\beta, \mu)$, which we call *thermal functions*.

The relation between quantum local thermal observables and classical macroscopic observables is described by a map $C$ associating a thermal function $C(A) := \{ (\beta, \mu) \mapsto \omega_{\beta,\mu}(A) \} \in C(B_K)$. (14)

In the case where all the thermal reference states $\omega_\beta$ are translation invariant, the thermal function $C(\Phi(x)) = \Phi_x$ corresponding to $\Phi(x) \in T_x$ is $x$-independent, which is invalidated, for instance, by the crystalline structures to break the spatial homogeneity, though. In the special case of no phase transitions where we have $\omega_\beta \circ \alpha_{(\Lambda,a)}^{-1} = \omega_{\Lambda\beta}$, the thermal function $C(\Phi(x)) = \Phi$ even becomes an $x$-independent Lorentz tensor in $\beta$.

We see now that thermal interpretation of each $\Phi(x) \in T_x$ is given by thermal function $(\beta, \mu) \mapsto \Phi_{\beta,\mu}(A) = C(\Phi(x))(\beta, \mu) = \omega_{\beta,\mu}(\Phi(x))$ (which amounts to recording the mean values of a local thermal observable $\Phi(x)$ in all equilibrium states $\omega_{\beta,\mu}$).

Since the map $C$ is normalized and positive linear, $C(1) = 1, C(A^*A) \geq 0$ taking values in a commutative algebra $C(B_K)$, it is a *completely positive* (CP) map characterized by the condition $\sum_{ij=1}^n f_i C(A_i^*A_j) f_j \geq 0$ for $\forall n \in \mathbb{N}, \forall f_1, \cdots, \forall f_n \in C(B_K)$ and $\forall A_1, \cdots, \forall A_n \in A$. The dual map $C^*$ of CP map $C$ defined on states by

$$C^*(\rho)(A) = \rho(C(A)) = \int_{B_K} d\rho(\beta, \mu) C(A)(\beta, \mu) = \int_{B_K} d\rho(\beta, \mu) \omega_{\beta,\mu}(A),$$

$$\implies C^*(\rho) = \int_{B_K} d\rho(\beta, \mu) \omega_{\beta,\mu} = \omega_{\rho} \in K,$$

becomes a *classical-quantum (c→q) channel* $C^* : Th \ni \rho \mapsto C^*(\rho) \in K$, mapping classical probabilities $\rho$ into quantum states $C^*(\rho) \in K$. (Recall that $Th = M_1(B_K)$ is the space of classical thermal states identified with
probability measures $\rho$ on $B_K$ describing the mean values of thermodynamic parameters $(\beta, \mu)$ together with their fluctuations.) Measuring a local thermal observable $\hat{\Phi}(x) \in T_x$ in this thermal reference state $C^*(\rho)$, we obtain

$$C^*(\rho)(\hat{\Phi}(x)) = \int_{B_K} d\rho(\beta, \mu) \omega_{\beta, \mu}(\hat{\Phi}(x)) = \int_{B_K} d\rho(\beta, \mu)[C(\hat{\Phi}(x))](\beta, \mu) = \rho(\Phi_x).$$

Thus the thermal interpretation of a quantum observable $\hat{\Phi}(x)$ in all thermal reference states of the form $C^*(\rho) = \omega_\rho \in K$ is given by the corresponding macroscopic thermal function $C(\hat{\Phi}(x))$ evaluated with the classical probability $d\rho(\beta, \mu)$ which describes the fluctuations of thermodynamic configurations $(\beta, \mu)$ in $\omega_\rho$.

This applies to the case where $\rho$ is already known. What we need in the actual situations is how to determine the unknown $\rho$ from the given data list $\Phi \mapsto \omega_\rho(\hat{\Phi}(x)) = \rho(\Phi_x)$ of expectation values of thermal functions $\Phi = C(\hat{\Phi})$ [e.g., internal energy, entropy density, etc.]: this problem can be solved if $T_x$ has sufficiently many local thermal observables so that the image $C(T_x)$ of $T_x$ is dense in $C(B_K)$ so as to approximate arbitrary continuous functions of $(\beta, \mu)$ (which need be checked in each concrete model). In this case $\rho$ is given as the unique solution to a (generalized) “moment problem”.

Thus we see:

★ If the set $T_x$ of local thermal observables is large enough to discriminate all the thermal reference states in $K$, any reference state $\in K$ can be written as $C^*(\rho)$ in terms of a uniquely determined probability measure $\rho$ on $B_K$ describing the statistical fluctuations of thermal parameters in the state in question. Then local thermal observables $\hat{\Phi}(x) \in T_x$ provide the same information on the thermal properties of states in $K$ as that provided by the corresponding classical macroscopic thermal functions $\Phi = C(\hat{\Phi})$ [e.g., internal energy, entropy density, etc.]: $\omega_\rho(\hat{\Phi}) = \rho(\Phi)$.

In this situation, any continuous function $F$ on compact $B \subset V_+$ can be approximated by thermal functions $\Phi_x = C(\hat{\Phi}(x))$ with arbitrary precision, even if $F$ itself is not an image of $C$. In spite of the absence of quantum $\hat{s}(x) \in T_x$ s.t. $\omega_\beta(\hat{s}(x)) = s(\beta)$: entropy density, $s(\beta)$ can be treated as an approximate thermal function.

The above (★) ensures the existence of inverse of $c\mapsto q$ channel $C^*$ on $K$:

$$K \ni \omega_\rho = C^*(\rho) \mapsto (C^*)^{-1}(\omega_\rho) = \rho \in Th,$$

(17)
and the thermal interpretation of thermal reference states \( \omega \in K \) is just given by this \( q \to c \) channel \( (C^*)^{-1} : K \ni \omega \mapsto \rho \in Th \) s.t. \( \omega = C^*(\rho) \), which can be regarded as a simple adaptation and extension of the notions of classifying spaces and classifying maps to the context involving (quantum) probability theory. We express formally the essence of the above situation (\( \blacklozenge \)) by

\[
K(\omega, C^*(\rho))/T_h \xrightarrow{q\mapsto c} Th((C^*)^{-1}(\omega), \rho)/C(T_h),
\]

with a quantum state \( \omega \in E_x \) and a probability measure \( \rho \in Th \). (The precise meaning of this can be understood as a categorical adjunction between two functors given by \( c \to q (C^*) \) and \( q \to c ((C^*)^{-1}) \) channels which connect \( K \) and \( Th \) both regarded as groupoids\(^1\) corresponding to the equivalence relations \( \omega_1 \equiv \omega_2 \) and \( \rho_1 \equiv \rho_2 \) defined, respectively, by \((\omega_1 - \omega_2)(T_h) = \{0\}\) and \((\rho_1 - \rho_2)(C(T_h)) = \{0\}\); in the form \((\blacklozenge)\), the essence of (\( \blacklozenge \)) can be generalized to wider contexts as selection criteria to choose states of relevance.\(^2\) From the conceptual viewpoint, what is important here is that two different levels, quantum statistical mechanics with family \( K \) of mixtures of KMS states and macroscopic thermodynamics described by \( Th \) of probability measures of fluctuating thermal parameters on the parameter space \( B_K \), are so interrelated by the two channels, \( c \to q (C^*) \) and \( q \to c ((C^*)^{-1}) \), that the following two points are simultaneously attained:

\[ a) \text{ characterization of thermal reference states } K \text{ as image of } C^*, \omega_\rho = C^*(\rho): \text{ selection criterion for } K, \]

\[ b) \text{ thermal interpretation of selected states in } K \text{ in terms of classical data, } \Phi_x = C(\Phi(x)) \text{ and } \rho = (C^*)^{-1}(\omega_\rho). \]

Then the problem is now boiled down into how to select suitable classes of non-equilibrium states \( \omega \notin K \) in such a way that some thermal interpretations are still guaranteed. This is what to be answered in the next section.

\(^1\) A groupoid \( \Gamma \) is, roughly speaking, a generalization of a group so that there are many unit elements constituting a set \( \Gamma_0 \). Each element \( \gamma \in \Gamma \) has its source \( s(\gamma) \) and target \( r(\gamma) \) in \( \Gamma_0 \) and these points are thought to be connected by \( \gamma, s(\gamma) \mapsto r(\gamma) \), in an invertible way: \( r(\gamma) \xrightarrow{r^{-1}} s(\gamma) \). Two elements \( \gamma_1, \gamma_2 \in \Gamma \) are not always composable but \( \gamma_1 \gamma_2 \) is meaningful only when \( r(\gamma_2) = s(\gamma_1) \). There is a one-to-one and onto correspondence between a groupoid \( \Gamma \) and an equivalence relation \( \sim \) on a set \( \Gamma_0 \) through \( [a \sim b \text{ for } a, b \in \Gamma_0] \iff [\exists \gamma \in \Gamma \text{ s.t. } a = r(\gamma) \text{ and } b = s(\gamma)] \). As a category, \( \Gamma \) is one with \( \Gamma_0 \) as the set of objects and with all its morphisms being invertible. In our case, they are defined by \( \Gamma_0 := K \) or \( Th \) together with the equivalence relation \( \equiv \) or \( \equiv \), respectively.
4 Characterization of non-equilibrium local states by hierarchized zeroth law of local thermodynamics and their thermal interpretations

Hierarchized zeroth law of local thermodynamics \cite{2}: to meet simultaneously the two requirements of characterizing an unknown state $\omega$ as a non-equilibrium local state and of establishing its thermal interpretation in a similar way to the above a) and b), we compare $\omega$ with thermal reference states $\in K = C^*(Th)$ by means of local thermal observables $\in T_x$ at $x$ whose physical meanings are exhibited by the associated thermal functions $\in C(T_x)$.

In view of the above conclusion \cite{3} and also of the hierarchy in $T_x$, we relax the requirement for $\omega$ to agree with $\exists \omega \rho_x := C^*(\rho_x) \in K$ up to some suitable sub-space $S_x$ of $T_x$. Then, we characterize $\omega$ as a non-equilibrium local state by the equalities

$$\omega(\hat{\Phi}(x)) = \omega_{\rho_x}(\hat{\Phi}(x)) = C^*(\rho_x)(\hat{\Phi}(x))$$  (19)

valid for $\forall \hat{\Phi}(x) \in S_x$. Namely, the unknown $\omega$ should look like a thermal reference state $\omega_{\rho_x}$ as far as the thermal properties described by $\hat{\Phi}(x) \in S_x$ are concerned. We denote this selection criterion by

$$\omega \equiv_{S_x} C^*(\rho_x),$$  (20)

and call such $\omega$ an $S_x$-thermal state. In terms of thermal functions $\Phi_x := C(\hat{\Phi}(x)) \in C(S_x)$, this can be rewritten as

$$\omega(\Phi)(x) := \omega(\hat{\Phi}(x)) = \rho_x(\Phi_x).$$  (21)

So, $\omega$: $S_x$-thermal implies that the selection criterion $\omega \equiv_{S_x} C^*(\rho_x)$ can be “solved” conditionally in favour of $\rho_x$ as “$(C^*)^{-1}((\omega) \equiv_{c(S_x)} \rho_x$, which provides the local thermal interpretation of $\omega$ \cite{2}. Physically this means the state $\omega$ looks like a thermal equilibrium $C^*(\rho_x)$ locally at $x$ to within a level controlled by a subset $S_x$ of thermal observables.

To be precise mathematically, we need here to be careful about the meaning of such a heuristic expression as “$(C^*)^{-1}((\omega)$ for $\omega \notin K$ in relation to our observation above: $\omega \notin K = C^*(Th)$. As we shall see below, “$(C^*)^{-1}$ outside of $K$ is certainly not a $q \rightarrow c$ channel preserving the positivity, whereas it can be seen to be still definable on the states $\omega$ selected out by the above criterion Eq. (20), by means of its equivalent reformulation given by:
**Criterion 1** For a subspace $S_x$ of $T_x$ containing 1, a state $\omega \in E_x$ is $S_x$-thermal iff there is a compact set $B \subset V_+$ s.t.

\[
|\omega(\hat{\Phi}(x))| \leq \tau_B(\hat{\Phi}(x)) := \sup_{(\beta,\mu)\in B_K, \beta \in B} |\omega_{\beta,\mu}(\hat{\Phi}(x))| \\
= \left|C(\hat{\Phi}(x))\right|_B, \text{ for } \hat{\Phi}(x) \in S_x.
\]  

(The above semi-norm is well-defined under the condition that $B_K \ni (\beta, \mu) \mapsto \omega_{\beta,\mu} \in K$ is (weakly) continuous, which requires singularities of critical points to be excluded from our considerations.)

While the requirement for \((C^*)^{-1}(\omega)\) to be a probability measure forces \(\omega\) to be among the reference states belonging to \(K\), the above inequality \((22)\) combined with the Hahn-Banach extension theorem (under the assumption for \(\tau_B\) to be a norm) allows us to extend \(C(S_x) \ni C(\hat{\Phi}(x)) \mapsto \omega(\hat{\Phi}(x))\) as a linear functional defined on \(C(S_x)\) to one \(\nu\) defined on \(C(T_x) = C(B_K)\), which should not be a positive-definite measure but is a signed measure: \(\nu = \nu_+ - \nu_-\), \(0 \leq \nu_\pm \in C(B_K)_+\), \(\nu_- \neq 0\), \(\nu_-|_{C(S_x)} = 0\), \(C^*(\nu_+) \big|_{S_x} = \omega \big|_{S_x}\).

The similar argument for this has already been used in \([1]\) to ensure the existence of a genuine non-equilibrium local state \(\omega\) which is \(S_x\)-thermal with finite-dimensional subspace \(S_x\) at a lower level of hierarchy in \(T_x\), but which shows deviations from \(K\) for observables outside of \(S_x\). (See this discussion also for the case with \(\tau_B\) being a semi-norm.) Thus, understanding the meaning of \((C^*)^{-1}(\omega)\) as the set of inverse images of \(\omega\) under \(C^*\) in the space \(C(B_K)^*\) of linear functionals,

\[
(C^*)^{-1}(\omega) := \{\nu \in C(B_K)^*; \nu = \nu_+ - \nu_-\}, \nu_\pm \geq 0, \nu_-|_{C(S_x)} = 0, C^*(\nu_+) \big|_{S_x} = \omega \big|_{S_x}\};
\]  

we can put Eq. \((20)\) into the similar form to Eq. \((18)\) as

\[
E_x(\omega, C^*(\rho_x))/S_x \overset{q_{\infty}}{=} Th((C^*)^{-1}(\omega), [\rho_x])/C(S_x),
\]  

where \([\rho_x] := \{\sigma \in Th; \sigma|_{C(S_x)} = \rho_x |_{C(S_x)}\}\) enters here owing to the non-uniqueness of \(\rho_x \in Th\) in Eq. \((20)\). This relation can be viewed as a form of “hierarchized zeroth law of local thermodynamics”; the reason for mentioning the “zeroth law” here is due to the implicit relevance of measuring processes of local thermal observables validating the above equalities, which require the contacts of two bodies, measured object(s) and measuring device(s), in a local thermal equilibrium, conditional on the chosen \(S_x\). (The transitivity of this contact relation just corresponds to the localized and hierarchized version of the standard zeroth law of thermodynamics.)
It is interesting to note that, in view of the relation
\[ \exists \nu = \nu_+ - \nu_- \in (C^*)^{-1}(\omega) \quad \text{with} \quad \nu_- = 0 \iff (C^*)^{-1}(\omega) = \{\nu\} \subset Th \]
\[ \iff \omega \in K \iff [\text{maximal choice of } S'_x \text{ s.t. } C^*(\nu_+) |_{S'_x} = \omega |_{S'_x}] = T_x, \] (25)
we can specify the extent to which a non-equilibrium \( S_x \)-thermal \( \omega \) deviates from equilibria belonging to \( K \) by the failure of state positivity (\( \nu_- \neq 0 \)) and can also measure it by the maximal size of \( S'_x \) in \( T_x \) such that \( S'_x \supset S_x, \nu_- |_{C(S'_x)} = 0 \) with all the possible choices of \( \nu \in (C^*)^{-1}(\omega) \): owing to the presence of \( \nu_- \), \( \omega \) ceases to be \( S'_x \)-thermal when \( S'_x \) is so enlarged that \( \nu_- |_{C(S'_x)} = 0 \) is invalidated, which shows that \( \omega \) shares with reference states in \( K \) only gross thermal properties described by smaller \( S'_x \). In this sense, the hierarchy of \( S'_x \) in \( T_x \) should have a close relationship with the thermodynamic hierarchy at various scales appearing in the transitions between non-equilibrium and equilibrium controlled by certain family of coarse graining procedures. Thus, we see that our selection criterion can give a characterization of states identifiable as non-equilibrium ones and, at the same time, provide associated relevant physical interpretations of the selected states in a systematic way.

—Fluctuations of thermal quantities; temperature as a physical quantity—

The present framework allows one also to judge whether a thermal function \( \Phi \) has locally a sharply specified value in a state \( \omega \) or is statistically fluctuating, which can be implemented if \( S_x \) is large enough for the mean value of \( \Phi_x \) together with its fluctuations to be determined within it. For instance, if \( S_x \) contains local observables \( \hat{\Phi}_1(x) \) and \( \hat{\Phi}_2(x) \) corresponding respectively to \( \Phi_1 = C(\hat{\Phi}_1(x)) \) and \( \Phi_2 = C(\hat{\Phi}_2(x)) \), we have a thermal function \( (\Phi_x - \kappa 1)^2 = C(\delta \hat{\Phi}_x(x)) \) with
\[ \delta \hat{\Phi}_x(x) := \hat{\Phi}_2(x) - 2\kappa \hat{\Phi}_1(x) + \kappa^2 1, \quad \kappa \in \mathbb{R}. \] (26)
Since this is non-negative in all thermal reference states \( \in K \) and vanishes only in those states with \( \Phi_x \) having a sharp value \( \kappa \), we can conclude that \( \Phi_x \) at \( x \) has the sharp value \( \kappa \) in such an \( S_x \)-thermal state \( \omega \) that \( \omega(\delta \hat{\Phi}_x(x)) = 0 \).

In virtue of this scheme it is meaningful to treat the (inverse) temperature \( \beta \) as a real physical quantity to be determined a posteriori through its measurements, which is in sharp contrast to the standard idea in statistical mechanics of treating it as an a priori given parameter. Choosing suitable spaces \( S_x \) (which is finite dimensional in generic cases \( \mathbb{I} \)), we can select a state \( \omega \) having locally a sharp temperature vector \( \beta_x \), i.e., \( \omega \equiv S_x \omega_{\beta_x} \). In
this case, all thermal functions $\Phi_x$ corresponding to $\hat{\Phi}(x) \in S_x$ have locally definite values. Concerning the possible objections against the introduction of a temperature $\beta_x$ (as well as any kind of thermal objects) at a point $x$ (without any extension), it is important to recall here that any state $\omega \in E_x$ relevant to our present context is already extended in spacetime effectively, owing to the regularity condition imposed on it. In this sense, the point $x$ in $\beta_x$ should not literally be understood to refer to a strictly microscopic spacetime point but to a macroscopic one with certain fuzzy extensions, which is taken into account on the side of chosen states.

—Space-time evolution of thermal properties—

Extending our formalism from a point $x$ to a (finitely extended) subregion $\mathcal{O} \subset \mathbb{R}^4$, we can now incorporate local states with thermal interpretation in $\mathcal{O}$. For simplicity, we keep the set of thermal functions fixed in each region, by identifying the spaces $S_x, x \in \mathcal{O}$ through translations:

$$S_x := \alpha_x(S_0), \quad x \in \mathcal{O}. \quad (27)$$

With this convention understood, we say that a state $\omega \in E_\mathcal{O}$ is $S_\mathcal{O}$-thermal in $\mathcal{O}$, if there exists $\omega_{\rho(x)} \in K$ for each $x \in \mathcal{O}$, s.t. $\omega \equiv \omega_{\rho(x)}$. The resulting functions $\mathcal{O} \ni x \mapsto \omega(\Phi)(x) := \omega(\hat{\Phi}(x))$ describe the space-time behaviour of mean values of thermal functions $\Phi$. Hence they provide the link between microscopic dynamics $\alpha_x$ and the evolution $x \mapsto \omega(\Phi)(x)$ of macroscopic thermal properties, i.e. thermo-dynamics of states. We have reached the same level as the familiar local formulation of manifolds at the beginning.

On this setting, thermal functions in a state near equilibrium are generally shown to satisfy a linear evolution equations, which can be viewed as a generalization of low energy theorems to thermal situations. This is consistent with interpretation of perturbations to equilibrium in terms of quasi-particles.

The two goals of identifying non-equilibrium local states admitting local thermal interpretation and of describing their specific thermodynamic properties are solved simultaneously by the above selection criterion based upon a localized and hierarchized form of the zeroth law of thermodynamics. In this framework, we have identified at least three different kinds of sources of derivations of an $S_x$-thermal non-equilibrium local state $\omega \in E_x$ from the genuine equilibrium states $\omega_\beta$ as

a) spacetime dependence of thermal parameters such as temperature distributions $x \mapsto \beta(x)$,
b) statistical fluctuations of thermal parameters at $x$ described by probability distributions $dp_x(\beta) \in Th$,

and

c) essential deviations of local states $\omega \in E_x$ from states in $K$ expressed by the positivity-violating term $\nu_+ - \nu_- \neq 0$ in $\nu = \nu_+ - \nu_- \in (C^*)^{-1}(\omega) \subset C(B_K)^*$ with $\nu_- |_{C(S_x)} = 0$, $C^*(\nu_+) |_{S_x} = \omega |_{S_x}$.

For concrete examples to exhibit the basic features, see [1]. Here discussions have been focused on the conceptual aspects developed in [2].

5 General-relativistic extension: global vs. local and flat vs. curved

–Global vs. local–

Looking back over what is done so far, we notice here some room for further improvements and generalizations in view of such restricted choices of global KMS states [12] on the side of thermal reference states. When compared with our motivating discussion of manifolds, it also looks strange that the whole theory is restricted only to within the flat Minkowski spacetime [13] in spite of the emphasis on the local aspects of states to be examined. Actually, in the comparison of an unknown state $\omega$ with a known reference state $\omega_\rho \in K$, the latter serves only to provide a reference data set $\omega_\rho(A)$ involving local thermal observables $A \in T_x$ or $S_x$ near the focus point $x$, which requires only the local restrictions of states $\omega_\rho \in K$ onto small neighbourhoods of $x$ (i.e., local state germs in $K \hookrightarrow E_x$). Therefore, once the reference states $\omega_\rho$ can properly be specified within small neighbourhoods of spacetime, we expect the freedom to go across the barriers separating the flat and curved spacetimes, existing at the global level but irrelevant locally. Such a possibility can naturally be read off in our selection criterion formulated as a relation of comparison (more appropriately, a categorical adjunction), Eq.(24), which is not necessarily required to be a strict equality between $\omega$ and $C^*(\rho)$ but should be a well-defined and suitably controllable relation, as is common in many cases of reference to standard objects constituting a model space, such as local charts referring to $\mathbb{R}^n$ in manifolds. On the basis of this observation, a more flexible setting up is envisaged to emerge through such a possibility that unknown $\omega$ to be examined can be generalized to those states living in curved background spacetimes: the mathematical basis for this physical ideas can already be found in the notions of local definiteness and/or local normality (see [14] [15]), which allow
one to treat generic localized states of quantum fields in curved spacetime backgrounds in the same Hilbert space of the vacuum representation in the Minkowski spacetime.

–Flat vs. curved spacetimes–

From the above point of view, we try now to extend the previous scheme to the situation with quantum fields in a curved spacetime by restricting the original thermal reference states to local small regions in the flat Minkowski spacetime. Note here that, in sharp contrast to the examined unknown $\omega$ being allowed to be a state in a curved spacetime, the reference states $\omega_\rho$ are understood as the local restrictions of mixtures of global KMS states still living in the flat Minkowski spacetime; this is not only in harmony with the line of thought found in our starting discussion of manifolds taking the flat $\mathbb{R}^n$ as the model space, but also is a very important and inevitable choice necessitated by the possible absence of appropriate vacua and/or KMS states in generic curved spacetimes.

In spite of the inherent slight delocalization of our selected states $\omega$ due to the condition (7), we can here benefit from the expressions referring to one spacetime point $x$ as follows. To a small neighbourhood of a point $x$ in a curved spacetime $M$ we can apply Einstein’s basic idea of equivalence principle based upon the free-falling frame at $x$ whose mathematical expression can be found in the notion of normal coordinates [16], the coordinates along geodesic flows starting from $x$ which are always definable in some neighbourhood $O_0$ of the origin 0 of the tangent space $T_x(M)$ at $x$ even for incomplete geodesic flows, $\text{Exp}_x : (T_x(M) \supset) O_0 \rightarrow \text{Exp}_x(O_0) = O_x(\subset) M$. Corresponding to this local diffeomorphism $\text{Exp}_x$, we can define a mapping $\Phi_x$ to transform locally a QFT defined in a flat $O_0(\hookrightarrow \mathbb{R}^4)$ into the local restriction of a QFT in curved $M$ on its small neighbourhood $O_x$ of $x$ (owing to the functoriality in the definition of quantum fields on curved spacetimes [17, 18]): $\Phi_x : \mathcal{A}_0(O_0) \rightarrow \mathcal{A}_M(O_x)$, where $O \mapsto \mathcal{A}_0(O)$ and $O \mapsto \mathcal{A}_M(O)$ denote the corresponding local nets, respectively, on the flat Minkowski spacetime and on a curved spacetime $M$. Then what we need is simply to modify our selection criterion Eq.(24) into $E_{M,x} (\omega, \mathcal{C}_x^\ast(\rho))/\Phi_x(S_0) := E_0(\omega \circ \Phi_x, \mathcal{C}_x^\ast(\rho))/S_0 \xrightarrow{\text{c}} T h((\mathcal{C}_x^\ast)^{-1}(\omega), [\rho])/\mathcal{C}(S_0)$, where $E_{M,x}$ and $\Phi_x(S_0)$ are the sets of local thermal states and of local thermal observables, respectively, at $x$ in the curved spacetime $M$ and $\mathcal{C}_x = \mathcal{C} \circ \Phi_x^{-1}$. In this way, our formulation of non-equilibrium local states can safely be extended to the general-relativistic context by simple restriction of reference states onto small neighbourhoods. (While the set $K_{M,x}$ of reference states at $x$ in a
curved spacetime $M$ can simply be defined here as the image $(\Phi^*_x)^{-1}(K)$ of the corresponding set $K$ on the flat spacetime through the normal coordinates $Exp_x$ in the $C^\infty$-context, the intrinsic characterization of the notions in $M$ related to the KMS condition will certainly require the analytic structure on $M$, as is the case in the discussion of analytic wavefront sets in [20].

–Interacting vs. free–

In view of our focus on small neighbourhoods of a spacetime point, the local normality allows us to treat the effects of interactions as a perturbation to the free dynamics, without complications related to the thermodynamic limit such as the Haag theorem, at least, at the abstract levels. Therefore, it will be very convenient if we can choose free field models for the reference system [12]: this will not only make the reference states more accessible to the practical computations, but also conceptually appealing in relation to the physical origin of temperature referring to the ideal gas in the equation of states as well as Boltzmann’s kinetic definition of it. To implement this idea, however, we should solve the difficulty taking the familiar form of ultraviolet divergences. While the combined use of the regularity condition (7) imposed on the states of relevance and the normal products in OPE can remove divergences order by order systematically in the perturbation, the available methods are not powerful enough to remove the full-order divergences at once, in spite of all the up-dated attractive tools for regularizing and renormalizing these divergences (e.g., the use of energy bounds, OPE [9], local perturbation scheme [19] of Epstein-Glaser type and Connes-Kreimer method [21] of renormalization). If we succeed in finding a satisfactory reason for terminating the perturbative expansions at some finite orders, then the algebraically formulated local perturbation scheme [19] will become physically relevant. Aside from this long-standing problem, what is also important in the present context is to attain the effective separation between order parameters to describe non-trivial structures in phase diagrams due to interactions and small fluctuations within fixed phases which are expected to be described by particle-like modes (22). In any case, it seems still premature to expect a practical and satisfactory solution to our desire in this direction.

Extrapolating the above logical lines, we can formulate a unified scheme for generalized sectors (discrete and/or continuous) based upon selection criteria, which provides new physical operational interpretations of superselection theory, extends it to spontaneously broken symmetries, and exhibits close relationship of basic notions in quantum measurement the-
ory with those in control theory [23], such as the notions of measurement scheme [24] and state preparation processes in connection with realizability and reachability, respectively, constituting the core of the latter. It would be important to note that applicability domain of a given theory is, in principle, encoded in this scheme in the matching relation between a chosen selection criterion for relevant states and the available observables.

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