

ON CONSISTENCY OF QUANTUM THEORY AND MACROSCOPIC OBJECTIVITY

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We argue that the consistency problem between quantum theory and macroscopic objectivity must be placed inside a quantum description of macroscopic non-equilibrium systems. Resorting to thermodynamic concepts inside quantum field theory seems to be necessary.

1 The problem of measurement, where does it lead?

Discussions on the measurement problem in quantum mechanics are often tied with preconceptions about what physics should be, thus influencing what one appreciates to be or not to be a problem. Let us therefore first declare the preconceptions inherent in this contribution. Physics deals primarily with experiments that are reproducible in a laboratory and with the outcomes of these experiments. Often these experiments have an essentially statistical character: i.e., only frequencies of outcomes in many runs are reproducible. If a physical theory is proposed, its job is to adequately represent these reproducible experiences, thus obviously also delivering an insight but not necessarily a full representation of any piece of reality.

Quantum theory applies first of all to experiments with microsystems. In such experiments one has a source preparing something which undergoes interactions with suitable devices (targets, interferometers and so on) and is detected by at least one, or more generally by a suitable sequence of events inside devices called measuring apparatus. Frequencies of these events, if the number of experimental runs of one statistical experiment are large enough, are given to an astonishing accuracy by a probabilistic theory called quantum mechanics. We will sketch the modern formulation of this theory (MQT) and compare it with the initial formulation (QT) by Dirac and von Neumann: measurement is now no longer added by postulates about measurement, but is already inside the mathematical structure. Different ways led to MQT. One way is Ludwig's construction of axiomatic quantum mechanics through investigation and formalization of what measuring means inside physics[1]; in this approach an effort was also made to derive the underlying Hilbert space structure and the problem of a still lacking theory of macrosystems was clearly stated. Another independent way was taken by Holevo investigating in the quantum case typical aspects of general probability theory[2]. Fundamental contributions already appeared in the classical book by Davies[3]. Concrete motivation also come from representation of new experimental situations especially in quantum optics[4].

In MQT the reproducible statistical preparation of a microsystem by a source and afterward by a controlled evolution during which certain events can arise is represented up to time t by a statistical operator ρ_t in \mathcal{H} . Let $\mathcal{K}(\mathcal{H})$ be the set of statistical operators in \mathcal{H} , i.e., the set of positive operators in \mathcal{H} with trace one. Consider now the Banach space $\mathcal{T}(\mathcal{H})$ of trace class operators in \mathcal{H} , each $A = A^\dagger \in \mathcal{T}(\mathcal{H})$ can be written as $A = \lambda_1 \rho_1 - \lambda_2 \rho_2$ with $\rho_1, \rho_2 \in \mathcal{K}(\mathcal{H})$, $\lambda_1, \lambda_2 \in \mathbb{R}^+$, and taking the infimum of $\lambda_1 + \lambda_2$ on these representations one gets the trace norm $\|A\|_1 = \text{Tr}|A| = \inf(\lambda_1 + \lambda_2)$, so that $\mathcal{K}(\mathcal{H})$ generates $\mathcal{T}(\mathcal{H})$. Here one can already note the main evolution in the use of mathematical tools comparing textbook QT with MQT: in QT the set of states is given by $\{\psi \in \mathcal{H} : \|\psi\| = 1\}$, in MQT it is given by $\mathcal{K}(\mathcal{H}) = \{W \in \mathcal{T}(\mathcal{H}) : W \geq 0, \text{Tr} W = 1\}$. Obviously also QT allows for preparations given by statistical operators as mixtures of pure states but this appears there only as a mean to take into account practical deficiency in the control of the experimental setting. The most relevant consequence of this difference lies in the representation of transformations of states in QT and of preparations in MQT, e.g., by time evolution, by insertion of additional devices, by changing the environment, by symmetry transformations: unitary operators on \mathcal{H} in QT, affine maps on $\mathcal{K}(\mathcal{H})$ in MQT. This difference opens in the mathematical context a new world, as can be appreciated comparing von Neumann's book *Die Mathematischen Grundlagen der Quantenmechanik*[5] with the recent *Statistical Structure of Quantum Theory* by Holevo[6]. A map from $\mathcal{K}(\mathcal{H})$ to $\mathcal{K}(\mathcal{H})$ having a physical meaning must be affine and can therefore be extended over $\mathcal{T}(\mathcal{H})$ as a positive, trace preserving endomorphisms; if in addition it has an inverse, i.e., if it represents a reversible transformation, it has a unitary (or anti-unitary) structure related to \mathcal{H} : $\mathcal{U}\rho = X\rho X^\dagger$ ($XX^\dagger = 1$) and provides an isomorphism on $\mathcal{T}(\mathcal{H})$.

The experimental setup inside which the system evolves might allow events to be produced and registered, by which physical insight is achieved and a decomposition of ρ_t into subcollections can be concretely performed. These events can be associated to fixed time intervals or sequences of them, by switching apparatus on and off at different time points. If a small time interval $[t_1, t_1 + \Delta t_1]$ is considered the event can be associated practically to time t_1 : let us describe a little more this particular case also in order to obtain QT as a very particular case of the more general description. Let us assume that the event possibly registered in a time interval $[t_1, t_1 + \Delta t_1]$ can be labeled by a k -uple of real numbers (e.g., an apparatus is effected, which displays k scale indexes). Let us represent these events, as it is standard in probability theory, by the elements B of a σ -algebra $\Sigma_{t_1}^{t_1 + \Delta t_1}$ over a space $\mathcal{Y}_{t_1}^{t_1 + \Delta t_1}$ of outcomes, which can be taken in this simplest case in \mathbb{R}^k , with its Borel σ -algebra $\mathcal{B}(\mathbb{R}^k)$. The theoretical description of this measurement is contained in a measure on $\Sigma_{t_1}^{t_1 + \Delta t_1}$, whose values are positive contractive affine maps $\mathcal{M}_{t_1}^{t_1 + \Delta t_1}(B)$ on $\mathcal{K}(\mathcal{H})$, normalized in the sense that

$$\mathcal{M}_{t_1}^{t_1 + \Delta t_1}(\mathbb{R}^k)\rho_{t_1} = \rho_{t_1 + \Delta t_1}.$$

$\mathcal{M}_{t_1}^{t_1 + \Delta t_1}(B)\rho_{t_1}$ represents the subcollection related to the event B and

$$p(B) = \text{Tr} \mathcal{M}_{t_1}^{t_1 + \Delta t_1}(B)\rho_{t_1} \quad B \in \mathcal{B}(\mathbb{R}^k)$$

is the related probability, which can also be written

$$p(B) = \text{Tr} F(B)\rho_{t_1}, \quad F(B) = \mathcal{M}_{t_1}^{t_1 + \Delta t_1'}(B)I, \quad (1)$$

$\mathcal{M}_{t_1}^{t_1+\Delta t_1}(B)$ being the adjoint map on the space of bounded operators $\mathcal{B}(\mathcal{H})$. $F(B)$ is a p.o.v. measure on $\Sigma_{t_1}^{t_1+\Delta t_1}$ such that $\text{Tr } F(\mathbb{R}^k)\rho_{t_1} = \text{Tr } \rho_{t_1+\Delta t_1} = 1$. The expectations $\langle \mathbf{x} \rangle_{t_1} = \int_{\mathbb{R}^k} \mathbf{x} \text{Tr}(\rho_{t_1} dF)$ define a set of symmetric operators \mathbf{A} in \mathcal{H} by which one has the very simple representation:

$$\langle \mathbf{x} \rangle_{t_1} = \text{Tr } \mathbf{A} \rho_{t_1} = \int_{\mathbb{R}^k} \mathbf{x} \text{Tr}(\rho_{t_1} dF). \tag{2}$$

In general these operators, while useful for expectations of stochastic variables $\mathbf{x} \in \mathbb{R}^k$, are not so useful for the expectations of functions $g(\mathbf{x})$ of them.

There is however a particular situation in which the underlying Hilbert space is put in major evidence: let us assume that $F(B)$ is projection valued

$$F(B)^2 = F(B) \quad \forall B \in \mathcal{B}(\mathbb{R}^k), \tag{3}$$

then \mathbf{A} defined by (2) is a set of k commuting self-adjoint operators, $F(B)$ is their spectral measure and for any real-valued measurable function $g(\mathbf{x})$ the expectation of the stochastic variable $g(\mathbf{x})$

$$\langle g(\mathbf{x}) \rangle_{t_1} = \int_{\mathbb{R}^k} g(\mathbf{x}) \text{Tr}(\rho_{t_1} dF)$$

is written in terms of the self-adjoint operator $g(\mathbf{A}) = \int_{\mathbb{R}^k} g(\mathbf{x}) dF$ as

$$\langle g(\mathbf{x}) \rangle_{t_1} = \text{Tr } g(\mathbf{A}) \rho_{t_1}.$$

If $F(B)$ is a projection operator the subspace $F(B)\mathcal{H}$ of the Hilbert space \mathcal{H} is associated with the event B and for any element $\psi \in F(B)\mathcal{H}$ a preparation ρ_{t_1} can be envisaged of the form $\rho_{t_1} = |\psi\rangle\langle\psi|$. Then $p(B) = 1$ and the preparation $|\psi\rangle$ can be described claiming that the observables $g(\mathbf{A})$ of the system have some value $g(\mathbf{x})$ with $\mathbf{x} \in B$. Let us finally describe the particular situation $F(B) \neq 0$ for B reducing to points $\mathbf{x} \in \mathbb{R}^k$. This can happen, if \mathcal{H} is separable, for a countable set of points giving the support of the p.o.v. measure $F(B) = \sum_{\mathbf{x}_n \in B} F(\mathbf{x}_n)$. Then \mathbf{x}_n are called the possible values of the observables \mathbf{A} , self-adjoint commuting operators with a point spectrum, \mathbf{x}_n being the eigenvalues, $F(\mathbf{x}_n)$ the related projections. A very simple way of constructing a map $\mathcal{M}(B)$ which produces $F(B)$ by (1) is $\mathcal{M}(B)\rho = \sum_{\mathbf{x}_n \in B} F(\mathbf{x}_n)\rho F(\mathbf{x}_n)$, giving the simplest representation of the measuring process of observables \mathbf{A} . We have recalled all these consequences of (3), to show how the core of QT is immediately reobtained.

Let us assume that in between two measurements the microsystem is isolated. In fact experiments consist both in looking for events produced inside detectors, and in shielding and protecting the microsystem from the environment on its way from the source to the detector. The situation of isolated evolution is represented by a family of maps $\mathcal{U}_{t_1}^{t_2}$

$$\mathcal{U}_{t_1}^{t_2} \rho_{t_1} = U(t_2, t_1) \rho_{t_1} U^\dagger(t_2, t_1), \quad U(t_2, t_1) = T e^{-\frac{i}{\hbar} \int_{t_1}^{t_2} dt' H_{t'}} \tag{4}$$

which are isomorphisms of $\mathcal{K}(\mathcal{H})$: $\rho_{t_2} = \mathcal{U}_{t_1}^{t_2} \rho_{t_1}$. These families of maps on $\mathcal{T}(\mathcal{H})$ or of operators on \mathcal{H} obey the composition law:

$$\mathcal{U}_{t_1}^{t_3} = \mathcal{U}_{t_2}^{t_3} \mathcal{U}_{t_1}^{t_2}, \quad U(t_3, t_1) = U(t_3, t_2) U(t_2, t_1).$$

Skipping for brevity precise discussion of differentiability with respect to time, the following time evolution equation holds:

$$\frac{d\rho_t}{dt} = -\frac{i}{\hbar}[H_t, \rho_t].$$

Here a fundamental element of the theory appears, i.e., the Hamiltonian H_t of the microsystem: a self-adjoint operator in \mathcal{H} generating the time evolution on \mathcal{H} through $U(t_2, t_1)$ and on $\mathcal{K}(\mathcal{H})$ through $\mathcal{U}_{t_1}^{t_2}$. The isolation of the system should be just the condition under which the re-preparations $\rho_{t_1} \rightarrow \rho_{t_2}$ due to passing time are spontaneous processes determined only by ρ_{t_1} itself. Then an affine map on $\mathcal{K}(\mathcal{H})$ is introduced and, if also reversibility is asked for, the map has the structure (4) and the self-adjoint operator H_t is met, associated with the energy of the microsystem. This is the important link between reversibility of $\mathcal{U}_{t_1}^{t_2}$ and the phenomenologically consolidated law of energy conservation. Let us stress that consistently with the concept of isolation no decomposition of the map $\mathcal{U}_{t_1}^{t_2}$ in terms of events produced by the microsystem in the time interval $[t_1, t_2]$ is possible.

Instead sequences can be considered of practically point-like time intervals $[t_\alpha, t_\alpha + \Delta t_\alpha]$, during which isolation is broken to allow detecting devices to be triggered. By composition of the previous maps, e.g.,

$$\mathcal{U}_{t_{\alpha_2} + \Delta t_{\alpha_2}}^{t_2} \mathcal{M}_{t_{\alpha_2}}^{t_{\alpha_2} + \Delta t_{\alpha_2}}(\mathbb{R}^k) \mathcal{U}_{t_{\alpha_1} + \Delta t_{\alpha_1}}^{t_{\alpha_2}} \mathcal{M}_{t_{\alpha_1}}^{t_{\alpha_1} + \Delta t_{\alpha_1}}(\mathbb{R}^k) \mathcal{U}_{t_1}^{t_{\alpha_1}}, \quad (5)$$

an evolution map allowing for repeated measurements can be considered, by which ρ_{t_2} is decomposed into subcollections

$$\mathcal{U}_{t_{\alpha_2} + \Delta t_{\alpha_2}}^{t_2} \mathcal{M}_{t_{\alpha_2}}^{t_{\alpha_2} + \Delta t_{\alpha_2}}(B_{t_{\alpha_2}}) \mathcal{U}_{t_{\alpha_1} + \Delta t_{\alpha_1}}^{t_{\alpha_2}} \mathcal{M}_{t_{\alpha_1}}^{t_{\alpha_1} + \Delta t_{\alpha_1}}(B_{t_{\alpha_1}}) \mathcal{U}_{t_1}^{t_{\alpha_1}} \rho_{t_1},$$

according to the results $\mathbf{x}_{t_{\alpha_2}} \in B_{t_{\alpha_2}}$, $\mathbf{x}_{t_{\alpha_1}} \in B_{t_{\alpha_1}}$. The event $\mathbf{x}_{t_{\alpha_2}} \in B_{t_{\alpha_2}}$, $\mathbf{x}_{t_{\alpha_1}} \in B_{t_{\alpha_1}}$ has probability $\text{Tr } F(B_{t_{\alpha_2}} \times B_{t_{\alpha_1}}) \rho_{t_1}$ with

$$F(B_{t_{\alpha_2}} \times B_{t_{\alpha_1}}) = \mathcal{U}_{t_1}^{t_{\alpha_1}'} \mathcal{M}_{t_{\alpha_1}}^{t_{\alpha_1} + \Delta t_{\alpha_1}'}(B_{t_{\alpha_1}}) \mathcal{U}_{t_{\alpha_1} + \Delta t_{\alpha_1}}^{t_{\alpha_2}} \mathcal{M}_{t_{\alpha_2}}^{t_{\alpha_2} + \Delta t_{\alpha_2}'}(B_{t_{\alpha_2}}) I.$$

Notice that one cannot expect (3) to hold for this operator even if it holds for $\mathcal{M}_{t_{\alpha_1}}^{t_{\alpha_1} + \Delta t_{\alpha_1}'}(B_{t_{\alpha_1}}) I$ and $\mathcal{M}_{t_{\alpha_2}}^{t_{\alpha_2} + \Delta t_{\alpha_2}'}(B_{t_{\alpha_2}}) I$, thus excluding the naive way in which \mathcal{H} is used in QT for these slightly more complicated experiments. In a more general and realistic description of measurement the time location of the events has a statistical character and it is rather intuitive that this situation can be represented by composition of subsequent evolution maps in the limit of an infinite number of factors showing infinitesimal difference with respect to the evolution map \mathcal{U}_t^{t+dt} : this is the description of continuous measurement (see [7] for references and Holevo's book [6] for a review). The outcome space becomes the trajectory space for a set of classical stochastic processes replacing the too rigid structure we have just indicated in example (5). In this way a microsystem is monitored by the events it produces separated by time intervals during which it is isolated. In these time intervals its Hamiltonian drives the spontaneous evolution.

Any kind of explicit macroscopic description of these events is completely lacking, apart from their time specifications. However symmetry transformations as space roto-translations and inertial frame transformations can be done in a reversible way leading to isomorphisms of

$\mathcal{T}(\mathcal{H})$ and therefore to unitary transformations on \mathcal{H} : this Hilbert space in case of an isolated system must carry a unitary projective representation of the Galilei group. Then the most natural characterization of \mathcal{H} for an elementary microsystem is one carrying an irreducible unitary projective representation of the Galilei group: this leads to spin, mass and internal energy of the microsystem and provides a very satisfactory understanding of such systems based on first principles[8]. Extension of this point of view to composite systems is based on tensor product of Hilbert spaces, symmetrized or antisymmetrized in case of identical components, thus leading also to the mathematical structure of Fock-space as the Hilbert space where to describe structures of any number of one given elementary microsystem. In this framework great achievements were obtained in low energy physics, also including an understanding of equilibrium and near to equilibrium behavior of simple macroscopic isolated systems, described as structures of N interacting microsystems, with very large N . It is clear that such an understanding is good enough to allow designing, construction and setting up of sources of microsystems and of detectors in which microsystems start processes which are registered as events. However this way of using quantum theory is essentially based on skillful guessing and on phenomenological intuition. The very concept of a macroscopic state of a system, which is preliminary to the notion of event, by which such state could be changed, is not contained in any neat way in QT. On the contrary the idea that such a state should be linked to an element ψ , representing the system in its Hilbert space, an idea which is very natural in QT, although less compelling in MQT, was recently shown[9] to be incompatible with use of a macrosystem as measuring apparatus of a microsystem. Actually this theoretical building has such solid foundations, allowing for such a compact construction, that no space appears left for the concept of macrostate that was a prerequisite for the logical construction itself and is a practical notion driving phenomenological handling with the theory. Also from this standpoint the strong unsatisfaction expressed by Bell[10], claiming for *beables* inside QT, appears well-founded.

Until now we recalled this history forgetting however a basic shock to all this: relativity is there and quantum field theory is now the basic theoretical framework. This means having removed microsystems from their place of building factors in the Fock-space structure to components of asymptotic states in an S-matrix formalism. Maybe it is not appreciated enough how this removal has left the whole building of modern physics, which still remains strongly anchored in the non-relativistic limit, as only asymptotically supported in reality. Since the previously criticized excessive compactness of the non-relativistic building is dissolved in reality, we are now going to reconsider the problem of consistency of measuring processes from a new point of view, which sets quantum field theory in the foreground. This obviously means that the whole question becomes much more involved and we are only able to indicate a possible program and make some first steps. If first the problem of measurement was forced in a too tight framework, now it glides over a huge landscape.

2 Introduction to macrostates in quantum theory

The Hilbert space structure of quantum theory of microsystem suggests itself as representation space of quantum Schödinger fields $\hat{\psi}_\alpha(\mathbf{x}, \omega)$ ($\omega = 1, \dots, 2s_\alpha + 1$) for the different components α of the system, associated to different microsystems with mass m_α , electric charge q_α , magnetic moment $\mu_\alpha \mathbf{S}$ and spin s_α , taken as confined inside a region $\Omega \subset \mathbb{R}^3$, which

represents the first state specification pertaining to the system. Even if this description arises in a standard way taking the microsystems as confined inside Ω , it is worthwhile to stress that it can be obtained without any reference to microsystems, starting instead with classical wave theory: electromagnetism for massless matter, Klein Gordon and Dirac fields, whose non-relativistic limit results in classical Schödinger fields, for massive and charged matter interacting with the electromagnetic field. This provides a theoretical basis for modern optics of massive charged and neutral beams. Restricting for simplicity to a single component, normal modes are stationary waves $\phi_n(\mathbf{x}, \omega, t) = e^{-\frac{i}{\hbar} E_n t} u_n(\mathbf{x}, \omega)$, solutions of the classical Schödinger field equation with the boundary condition $\phi_n(\mathbf{x}, \omega, t) = 0$ for $\mathbf{x} \in \partial\Omega$, representing reflecting walls. The Hamiltonian contains both external electromagnetic potentials and other fields, external or effective, acting on the system. By rather general mathematical conditions on the external fields and on the region Ω the Hamiltonian can be suitably extended to define a self-adjoint operator and the normal modes provide a complete orthonormal set of elements in $L^2(\Omega) \otimes \mathbb{C}^{2s+1}$. Quantum Schödinger fields are defined as $\hat{\psi}(\mathbf{x}, \omega) = \sum_n \hat{a}_n u_n(\mathbf{x}, \omega)$ for $\mathbf{x} \in \Omega$, where \hat{a}_n are annihilation operators $\hat{a}_n \Phi_0 = 0$, Φ_0 being the vacuum and quantization being given by the c.c.r. which have an irreducible representation in the Fock-space $\mathcal{H}_F(\Omega)$, generated applying products of creation operators to the vacuum.

We take over the structure of MQT sketched in Sec. 1 for microsystems, *assuming it as the basic general theory*: then preparations of the system are statistical operators belonging to $\mathcal{K}(\mathcal{H}_F(\Omega))$ and physics of the isolated system, i.e., its spontaneous reparations due to passing time, is given by the Hamiltonian describing the interactions between the component fields. Indicating by $H^{(1)}$ the single particle Hamiltonian we write \hat{H} , for a one component system, i.e., one field $\hat{\psi}(\mathbf{x}, \omega)$

$$\begin{aligned} \hat{H} = & \sum_{\omega} \int_{\Omega} d^3\mathbf{x} \hat{\psi}^{\dagger}(\mathbf{x}, \omega) \widehat{(H^{(1)}\psi)}(\mathbf{x}, \omega) \\ & + \frac{1}{2} \sum_{\omega_1 \omega_2} \int_{\Omega} d^3\mathbf{x} \int_{\Omega} d^3\mathbf{y} \hat{\psi}^{\dagger}(\mathbf{x}, \omega_1) \hat{\psi}^{\dagger}(\mathbf{y}, \omega_2) U(|\mathbf{x} - \mathbf{y}|) \hat{\psi}(\mathbf{y}, \omega_2) \hat{\psi}(\mathbf{x}, \omega_1). \end{aligned} \quad (6)$$

The short range behavior of the potential, taken as strongly repulsive or hard-core, introduces on the one side local stability of the model, on the other side makes it clear that we are relying only on an effective description, which becomes insufficient if detailed structure of this short range behavior should emerge: then a more basic model (e.g., electrodynamics) must be considered. Preparations $\hat{\rho}_t$ of an isolated system are linked together by the map $\mathcal{U}_{t_1}^{t_2}$. Then systems, invariant under time evolution, immediately emerge, described by statistical operators of the form

$$\hat{\rho}_{\beta, \mu} = \frac{e^{-\beta(\hat{H} - \mu \hat{N})}}{\text{Tr} e^{-\beta(\hat{H} - \mu \hat{N})}}, \quad (7)$$

which displays the state parameters β, μ , real numbers such that the exponent in (7) is essentially self-adjoint and defines a trace class operator, \hat{N} being the number operator. This situation can arise since the Hamiltonian has a point spectrum with a lower bound, due to confinement inside Ω and to the hard core behavior of the interaction potentials.

Let us stress that explanation of equilibrium thermodynamics, based on structure (7) for the statistical operator is a great achievement and appears as completely satisfactory in a

vast experimental context, including the recent highlight of Bose-Einstein condensation. Let us observe that the concept of microsystems is not explicit in this description, nor the idea of a system as a structure of microsystems has a precise meaning. On the other side, just introduction of confinement in the region Ω , thus breaking translation symmetry and blurring the concept of particle which was recalled at the end of Sec. 1, makes it possible to introduce the trace class operators (7) carrying the state parameters β, μ .

We shall now pursue this description, further enlarging the set of state parameters and aiming at a whole geometry of macrostates indicated by physical operations and suggested by mathematical structures. In order to represent concrete preparations one has to start from equilibrium states by modifications related to concrete ways of producing non-equilibrium systems, most naively putting together parts being in local equilibrium. These additional terms of the exponent in (7) are taken from a countable set M of linearly independent symmetric operator-valued fields $\hat{A}_j(\mathbf{x})$, chosen as will be discussed later on. Let us consider sets of real-valued fields $\zeta_j(\mathbf{x})$ in correspondence with $\hat{A}_j(\mathbf{x})$ such that

$$\hat{\Phi}(\beta, \mu, \zeta) \equiv \beta(\hat{H} - \mu\hat{N}) + \sum_j \int_{\Omega} d^3\mathbf{x} \zeta_j(\mathbf{x}) \hat{A}_j(\mathbf{x}) \quad (8)$$

is essentially self-adjoint and $\exp(-\hat{\Phi}(\beta, \mu, \zeta))$ is trace class. The variations, belonging to the linear span \mathcal{LM} of M and specified by the state parameters ζ , allow to exploit the trace class property of the equilibrium state (7): β, μ, ζ will be called a macrostate, the element of $\mathcal{K}(\mathcal{H}_F(\Omega))$ given by

$$\hat{w} \equiv \hat{w}_{\beta, \mu, \zeta} = \frac{e^{-\hat{\Phi}(\beta, \mu, \zeta)}}{\text{Tr} e^{-\hat{\Phi}(\beta, \mu, \zeta)}} \quad (9)$$

is called a Gibbs state related to the macrostate and the expression $-k \text{Tr} \hat{w} \log \hat{w} = S(\beta, \mu, \zeta)$, if it exists, is called entropy of the macrostate. Differently from previous treatments by ourselves[11] and from information thermodynamics[12], this concept of macrostate is introduced as a purely geometric structure induced on $\mathcal{K}(\mathcal{H}_F(\Omega))$ by: the region Ω , \hat{H} and \hat{N} , the choice of M . Here the macrostates β, μ with additional specifications of the sets of classical fields $\zeta_j(\mathbf{x})$ (depending on β, μ) will have a role analogous to partitions of *energy shells*, being a phase-space lacking. Only in the case of a deterministic macroscopic dynamics, we shall associate a family of macrostates β_t, μ_t, ζ_t with a system, and shall assume that a measurement of the relevant variables \hat{H} , \hat{N} and $\hat{A}_j(\mathbf{x})$ provides expectations of these variables as given by the Gibbs states \hat{w}_t . These expectations can be expressed by derivations of the partition function $Z(\beta, \mu, \zeta) = \text{Tr} e^{-\hat{\Phi}(\beta, \mu, \zeta)}$. Given a macrostate, the Gibbs state is the least biased choice of a statistical operator having these expectations for the relevant variables. The concept of macrostates must be given independently of the expectations of relevant variables when a system has a non deterministic macroscopic dynamics. In fact let us take a statistical mixture of two macrostates β_1, μ_1, ζ_1 and β_2, μ_2, ζ_2 with probabilities p_1 and $p_2 = 1 - p_1$: for this mixture the expectations of the relevant variables are given by

$$E = p_1 E_1 + p_2 E_2, \quad N = p_1 N_1 + p_2 N_2, \quad A_j(\mathbf{x}) = p_1 A_{j1}(\mathbf{x}) + p_2 A_{j2}(\mathbf{x}). \quad (10)$$

Even if the expectations (10) are related in a statistical ensemble to the variables that are relevant in characterizing macrostates, one cannot expect that they belong to the range of

values of some other macrostate corresponding to physically meaningful state parameters. A geometrical structure on $\mathcal{B}(\mathcal{H}_F(\Omega))$ induced by each macrostate is useful,

$$\langle \hat{C}, \hat{B} \rangle_{\hat{w}} = \text{Tr} \hat{C}^\dagger \int_0^1 du e^{-u\hat{\Phi}(\beta, \mu, \zeta)} \hat{B} e^{+u\hat{\Phi}(\beta, \mu, \zeta)} \hat{w}, \quad (11)$$

defined on $\mathcal{B}(\mathcal{H}_F(\Omega)) \times \mathcal{B}(\mathcal{H}_F(\Omega))$, sesquilinear and positive definite if the kernel of $\hat{w}_{\beta, \mu, \zeta}$ is trivial. It is known as Bogoliubov scalar product and allows to express derivatives of expectations of relevant variables with respect to the state parameters of a macrostate, i.e., generalized susceptibilities. Several authors contributed recently to these mathematical aspects[13, 14]. Let us come now to the choice of M , which has a basic role in our treatment: by it not only macrostates enter in the description, but also microsystems will acquire a role by events, which characterize stochastic changes of macrostates. The choice must be done shaping the theory in accordance with the phenomenology one tries to describe: M typically includes densities of fundamental mechanical quantities such as mass density, momentum density and kinetic energy density. Typical features of these relevant variables are: i) bilinear expressions in terms of the field operators; ii) a quasi-local character, e.g., $\hat{A}_j(\mathbf{x})$ only depends on the field operators and their first derivatives. Feature i) eliminates correlation between fields inside the relevant variables and is related with the fact that these correlations are hardly under control in concrete preparations and represents a very important simplification, also immediately causing the linear span of M not to be invariant under the map $\mathcal{U}_{t_1}^{t_2}$ when the second line of the Hamiltonian (6) is not neglected. It makes therefore impossible to interpret Gibbs states \hat{w} with time dependent parameters as preparations $\hat{\rho}_t$ of the system. However if interactions between fields allow bound states, time persistent correlations arise corresponding to dynamical composed structures. In this sense one must learn from dynamics what are the additional variables multi-linear in the fields to be included in M . Finally relevant variables should be slow enough, contributions from normal modes with too high energy should not arise: this can be obtained very simply replacing $\hat{\psi}(\mathbf{x}, \omega)$ in the expression of relevant variables by $\sum_{n, E_n \leq \bar{E}} \hat{a}_n u_n(\mathbf{x}, \omega)$. We observe that the geometric structure of macrostates has been introduced without direct reference to microphysical components, which are involved only at the level of expectations of relevant variables. We claim that these macrostates should assume the role of beables, not at all hidden properties but empirically evident ones like velocity and temperature fields for a fluid. Let us stress, mainly for the sake of clarity, that there is in our approach a kind of upset about microsystems: while we are obviously aware of their phenomenological evidence and take MQT as recalled in Sec. 1 as the theory of microsystems, we do not consider the subject of physics of general systems and in particular the question of interaction of a microsystem with a target as conceptually subordinated to a more fundamental theory of interacting microsystems, as it is instead usually done. All this would sound cumbersome or even nonsensical if one had a fundamental field theory available: talking about systems is then only an application of a structure already elucidated at a microphysical level. If instead such lucid description is not so manifest the cumbersome way can become a reasonable and challenging program, especially in a relativistic context, aiming to a theory describing both microsystem and macrostates.

3 Introduction to dynamics of macrostates

The basic problem is now to relate the statistical operators $\hat{\rho}_t = \mathcal{U}_{t_1}^t \hat{\rho}_{t_1}$ during the time evolution of the isolated system with trajectories in the space of macrostates β_t, μ_t, ζ_t . From the standpoint that both microsystems and macrostates are indeed important and coexistent, one is led to the idea that deterministic dynamics of macrostates represents just a basic and simple but not at all exhaustive situation. The general dynamics of a macrosystem should rather be of the kind of a piecewise deterministic process. The importance of this type of dynamics has been recently pointed out for an open system[4]. Also for an isolated system, as in our framework, the subset of relevant variables appears as an open system in the presence of the irrelevant variables $\mathcal{U}_{t_1}^{t_2} \mathcal{L}M$ that have an unavoidable role due to the fact that $\mathcal{L}M$ is not invariant under time evolution. Our first concern is therefore to characterize particular situations to be associated with the deterministic evolution of a macrostate. We assume for $\hat{\rho}_t$ the following structure

$$\hat{\rho}_t = Z_t^{-1} e^{-(\hat{\Phi}(t) + \hat{S}(t))} \quad Z_t = \text{Tr} e^{-(\hat{\Phi}(t) + \hat{S}(t))}, \quad (12)$$

where $\hat{\Phi}(t)$ is the exponent of the Gibbs state (9) associated to the macrostate β_t, μ_t, ζ_t as in (8) and $\hat{S}(t)$ is a correction built in terms of irrelevant variables $\mathcal{U}_{t'}^t \hat{A}_j(\mathbf{x}) = \hat{A}_j(\mathbf{x}, -(t' - t))$ with $t' \leq t$, which can be viewed as back evolved of relevant variables in Heisenberg picture. That such a correction is indeed necessary was most clearly pointed out by Zubarev[15]. In fact the expectations of observables of the form $\hat{A}_j(\mathbf{x}) = \frac{i}{\hbar} [\hat{H}, \hat{A}_j(\mathbf{x})]$ generally do not belong to M so one cannot expect their formal expectations related to $\hat{w}_t \equiv \hat{w}_{\beta_t, \mu_t, \zeta_t}$ to be physically meaningful. Physically most important contributions to equations for $\frac{d}{dt} \text{Tr} \hat{A}_j \hat{\rho}_t = \text{Tr} \dot{\hat{A}}_j \hat{\rho}_t$ are related to the first order correction $\hat{S}(t)$ as shown by Zubarev. He first stressed the role of a quantum field theoretical approach in dynamics of a macrosystem and suggested a general structure of non-equilibrium statistical operator. Our approach endorses this kind of analysis for the deterministic piece of dynamics and provides an alternative foundation of non-equilibrium statistical operator. We show now that the hypothesis that for t in a given interval the statistical operator (12) is associated with a family of macrostates leads to a very natural condition on the structure of the irrelevant part $\hat{S}(t)$: if this condition is satisfied such family of macrostates obeys an integrodifferential evolution equation. By the unitary structure of $\mathcal{U}_{t_0}^t$ one has

$$\hat{\rho}_t = \mathcal{U}_{t_0}^t \hat{\rho}_{t_0} = Z_t^{-1} e^{-(\mathcal{U}_{t_0}^t \hat{\Phi}(t_0) + \mathcal{U}_{t_0}^t \hat{S}(t_0))}.$$

In a formal way one can trivially rewrite $\mathcal{U}_{t_0}^t \hat{\Phi}(t_0)$ in terms of $\hat{\Phi}(t)$ by[12]

$$\mathcal{U}_{t_0}^t \hat{\Phi}(t_0) = \hat{\Phi}(t) - \int_{t_0}^t dt' \frac{d}{dt'} (\mathcal{U}_{t'}^t \hat{\Phi}(t')) = \hat{\Phi}(t) - \int_{t_0}^t dt' \mathcal{U}_{t'}^t \left[\dot{\hat{\Phi}}(t') + \frac{d}{dt'} \hat{\Phi}(t') \right]$$

$$\dot{\hat{\Phi}}(t) = \frac{i}{\hbar} [\hat{H}, \hat{\Phi}(t)]$$

so that comparing with (12) one has

$$\hat{S}(t) = - \int_{t_0}^t dt' \mathcal{U}_{t'}^t \left[\dot{\hat{\Phi}}(t') + \frac{d}{dt'} \hat{\Phi}(t') \right] + \mathcal{U}_{t_0}^t \hat{S}(t_0), \quad (13)$$

showing the general composition property

$$\hat{S}(t) = - \int_{t_1}^t dt' \mathcal{U}_{t'}^t \left[\dot{\hat{\Phi}}(t') + \frac{d}{dt'} \hat{\Phi}(t') \right] + \mathcal{U}_{t_1}^t \hat{S}(t_1) \quad t_0 \leq t_1 \leq t.$$

Using the formula $e^{-\frac{1}{2}(\hat{A}+\hat{B})} = (1 - \int_0^{\frac{1}{2}} du e^{-u(\hat{A}+\hat{B})} \hat{B} e^{u\hat{A}}) e^{-\frac{1}{2}\hat{A}}$ and its adjoint, setting $\frac{1}{2}\hat{\mathcal{S}}(t) \equiv \int_0^{\frac{1}{2}} du e^{-u(\hat{\Phi}(t)+\hat{S}(t))} \hat{S}(t) e^{+u\hat{\Phi}(t)}$ one can write (12) as:

$$\hat{\rho}_t = Z_t^{-1} \left[\hat{w}_t - \frac{1}{2}(\hat{\mathcal{S}}(t)\hat{w}_t + \hat{w}_t\hat{\mathcal{S}}^\dagger(t)) + \frac{1}{4}\hat{\mathcal{S}}(t)\hat{w}_t\hat{\mathcal{S}}^\dagger(t) \right]. \quad (14)$$

At first sight the long time behavior of $\hat{\rho}_t$ seems to be at variance with a statistical collection in which the Gibbs state \hat{w}_t has an important role: in fact by (13) $\hat{S}(t)$ formally involves a large set of irrelevant variables and one could have the impression of an increasing importance of the positive contribution $\hat{\mathcal{S}}(t)\hat{w}_t\hat{\mathcal{S}}^\dagger(t)$ for growing t . Actually the physical evidence of deterministic evolution toward equilibrium states indicates that a general mechanism should be brought in, reassessing the role of the Gibbs state. As we shall see at the end of this section the following approximation is at hand

$$\text{Tr}[\hat{O}(\mathbf{x})\hat{\mathcal{S}}(t)\hat{w}_t\hat{\mathcal{S}}^\dagger(t)] \approx \text{Tr}(\hat{O}(\mathbf{x})\hat{w}_t) \text{Tr}(\hat{\mathcal{S}}(t)\hat{w}_t\hat{\mathcal{S}}^\dagger(t)), \quad (15)$$

when $\hat{O}(\mathbf{x})$ is a quasi-local field observable. By (15), with reference to observables $\hat{O}(\mathbf{x})$ for which such representation holds one can claim that the statistical operator given by (14) is equivalent to

$$\hat{\rho}_t \approx Z_t^{-1} \left[\hat{w}_t - \frac{1}{2}(\hat{\mathcal{S}}(t)\hat{w}_t + \hat{w}_t\hat{\mathcal{S}}^\dagger(t)) + \frac{1}{4}\hat{w}_t \text{Tr}(\hat{\mathcal{S}}(t)\hat{w}_t\hat{\mathcal{S}}^\dagger(t)) \right]. \quad (16)$$

By (16) the fact that \hat{w}_t is the macrostate associated to $\hat{\rho}_t$, i.e.,

$$\text{Tr} \hat{A}_j(\mathbf{x}) \hat{\rho}_t = \text{Tr} \hat{A}_j(\mathbf{x}) \hat{w}_t \quad (17)$$

is equivalent to

$$\text{Tr}[\hat{A}_j(\mathbf{x})(\hat{\mathcal{S}}(t)\hat{w}_t + \hat{w}_t\hat{\mathcal{S}}^\dagger(t))] = \text{Tr}[\hat{A}_j(\mathbf{x})\hat{w}_t] \text{Tr}[\hat{\mathcal{S}}(t)\hat{w}_t + \hat{w}_t\hat{\mathcal{S}}^\dagger(t)] \quad (18)$$

which is an important clustering property of $\hat{\mathcal{S}}(t)$ as a consequence of its structure in terms of the state parameters. This property holds only for local variables belonging to M according to the fact that both (15) and (17) have been used, for variables such as $\hat{A}_j(\mathbf{x})$ such a clustering property does not hold. Setting

$$2Z_t \langle \hat{A}_j(\mathbf{x}) \rangle_t^{\text{irr}} \equiv \text{Tr}[\hat{A}_j(\mathbf{x})\hat{w}_t] \text{Tr}[\hat{\mathcal{S}}(t)\hat{w}_t + \hat{w}_t\hat{\mathcal{S}}^\dagger(t)] - \text{Tr}[\hat{A}_j(\mathbf{x})(\hat{\mathcal{S}}(t)\hat{w}_t + \hat{w}_t\hat{\mathcal{S}}^\dagger(t))]$$

the expectation of $\hat{A}_j(\mathbf{x})$ by (16) takes the form

$$\text{Tr} \hat{A}_j(\mathbf{x}) \hat{\rho}_t = \text{Tr} \hat{A}_j(\mathbf{x}) \hat{w}_t + \langle \hat{A}_j(\mathbf{x}) \rangle_t^{\text{irr}}$$

so that by $\frac{d}{dt} \text{Tr} \hat{A}_j(\mathbf{x}) \hat{w}_t = \frac{d}{dt} \text{Tr} \hat{A}_j(\mathbf{x}) \hat{\rho}_t = \text{Tr} \dot{\hat{A}}_j(\mathbf{x}) \hat{\rho}_t$ the final evolution equations for the macrostate is found

$$\frac{d}{dt} \text{Tr} \hat{A}_j(\mathbf{x}) \hat{w}_t = \text{Tr} \dot{\hat{A}}_j(\mathbf{x}) \hat{w}_t + \langle \dot{\hat{A}}_j(\mathbf{x}) \rangle_t^{\text{irr}}.$$

This equation together with the conservation laws links in principle the time derivatives of the parameters β_t, μ_t, ζ_t to $\hat{S}(t_0)$ and to the parameters themselves in the time interval $[t_0, t]$: these are integrodifferential equations for the deterministic evolution of the state parameters, in strong analogy with Zubarev's equations. All this relies on (15). In brief the statistical operators given by (12) are determined by the macrostate β_t, μ_t, ζ_t , depending on relevant variables, and have a part $\hat{S}(t)$ depending on irrelevant variables and representing the preparation of the system for $t' < t$. The general form (13) suggests an analogous structure for $\hat{S}(t_0)$. Indeed the experimental preparation procedure not only controls the initial macrostate but also the initial time derivatives of the expectations of the relevant variables. One can expect that it must have a finite, possibly short duration: it must be extended over a preparation time interval $[t_0 - \tau, t_0]$ and (13) suggests a structure containing time derivatives of both relevant variables and duly assigned preparation parameters. Note that the preparation part consists therefore of $\hat{\Phi}(t_0)$ at time t_0 and of $\hat{S}(t_0)$ referring to the time interval $[t_0 - \tau, t_0]$ so that a time arrow is introduced and irreversibility comes in. In this picture one concretely claims that history of the system can be forgotten after a time τ , small on the time scale of the description we are considering. The part $\hat{S}(t_0)$ of $\hat{\rho}_{t_0}$ should be a small correction to $\hat{\Phi}(t_0)$, since τ is small. The idea of a decay of previous history can be consistently assumed also for $t > t_0$. Then (15) can be understood since $\hat{S}(t) \hat{w}_t \hat{S}^\dagger(t)$ contains the short memory part quadratically, and this contribution is negligible by smallness of τ , like it is at $t = 0$. For the remaining part, due to the action of $U_t^{t'}$ with $t - t' > \tau$, non-local contributions arise, so that generally clustering occurs when the trace with a local field observable $\hat{O}(\mathbf{x})$ is taken. Furthermore since $\hat{S}(t_0)$ is small, taking $\hat{S}(t_0)$ to first order in $\hat{S}(t_0)$, (18) at initial time t_0 can be written, as one can show, in a more geometrical way exploiting (11): $\langle \hat{A}_j(\mathbf{x}), \hat{S}(t_0) \rangle_{\hat{w}_{t_0}} - \text{Tr}(\hat{A}_j(\mathbf{x}) \hat{w}_{t_0}) \text{Tr}(\hat{S}(t_0) \hat{w}_{t_0}) = 0$.

4 Outlook

The clustering condition (15) has a strategical role in the equivalence of representation (14) of $\hat{\rho}_t$ given by dynamics with (16) which allowed deterministic evolution. Eq. (14) can also be written as

$$\hat{\rho}_t = \lambda_t \frac{\hat{w}_t - \frac{1}{2} \hat{S}(t) \hat{w}_t + \hat{w}_t \hat{S}^\dagger(t)}{1 - \frac{1}{2} \text{Tr}(\hat{S}(t) \hat{w}_t + \hat{w}_t \hat{S}^\dagger(t))} + (1 - \lambda_t) \frac{\hat{S}(t) \hat{w}_t \hat{S}^\dagger(t)}{\text{Tr}(\hat{S}(t) \hat{w}_t \hat{S}^\dagger(t))} \quad (19)$$

$$\lambda_t = \frac{1 - \frac{1}{2} \text{Tr}(\hat{S}(t) \hat{w}_t + \hat{w}_t \hat{S}^\dagger(t))}{1 - \frac{1}{2} \text{Tr}(\hat{S}(t) \hat{w}_t + \hat{w}_t \hat{S}^\dagger(t)) + \frac{1}{4} \text{Tr}(\hat{S}(t) \hat{w}_t \hat{S}^\dagger(t))}.$$

By condition (18) the operator in the first term at r.h.s. of (19) is equivalent to \hat{w}_t relatively to variables $A_j(\mathbf{x})$ belonging to M . Then one can look at (19) as a dynamical demixture of

$\hat{\rho}_t$ into a component equivalent to \hat{w}_t , with weight λ_t , and another component given by the second term at r.h.s. of (19), still equivalent to \hat{w}_t if clustering (15) holds. If at a certain time \bar{t} (15) does not hold, a new dynamical behavior arises, already prepared at time $\bar{t} - \tau$. Then the explicit structure of $\hat{S}(\bar{t} - \tau)$ arising in (19) taken at time $t = \bar{t} - \tau$ must be considered in terms of field operators. We take it as a polynomial structure, commuting with \hat{N} . Generally all fields $\hat{\psi}^\dagger(\mathbf{y}, \omega)$, $\hat{\psi}(\mathbf{y}, \omega)$ with $\mathbf{y} \in \Omega$ contribute and the parts with \mathbf{y} in a neighborhood of \mathbf{x} remain correlated with $\hat{O}(\mathbf{x})$. A simple example of expressions that are met is:

$$\sum_{\omega_1 \omega_2} \int_{\Omega} d^3 \mathbf{y}_1 \int_{\Omega} d^3 \mathbf{y}_2 \text{Tr} \hat{O}(\mathbf{x}) \mathcal{U}_{\bar{t}-\tau}^t (\hat{\psi}^\dagger(\mathbf{y}_1, \omega_1) \hat{w}_{\bar{t}-\tau} \hat{\psi}(\mathbf{y}_2, \omega_2)) \langle \mathbf{y}_1, \omega_1 | \rho_{\bar{t}-\tau}^{(1)} | \mathbf{y}_2, \omega_2 \rangle$$

with $\langle \mathbf{y}_1, \omega_1 | \rho_{\bar{t}-\tau}^{(1)} | \mathbf{y}_2, \omega_2 \rangle$ a positive kernel. Expressions of this form were already pointed out describing macrosystems perturbed by a microsystem[16], and macrosystems decomposable into a source part and a detecting part correlated via a microsystem[17]. There $\langle \mathbf{y}_1, \omega_1 | \rho_{\bar{t}-\tau}^{(1)} | \mathbf{y}_2, \omega_2 \rangle$ was interpreted as linked to matrix element of a one-particle statistical operator and deterministic macroscopic dynamics was referred to as *simple dynamics* of a macrosystem. Expression $\mathcal{U}_{\bar{t}-\tau}^t (\hat{\psi}^\dagger(\mathbf{y}_1) \hat{w}_{\bar{t}-\tau} \hat{\psi}(\mathbf{y}_2))$ introduces the problem of dynamics of a macrosystem perturbed by a microsystem. To represent this evolution the parametrization in terms of the sole state parameters related to the second component of (19) is not sufficient, also the stochastic evolution of the microsystem interacting with the macrosystem must be taken into account: this is still an open problem. In the case in which the approximation that the macrosystem remains in an equilibrium state holds the problem of the dynamics of the microsystem received great attention since long time, see for example[18] for some recent results, also in connection with current experiments.

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