DESCRIPTION OF ISOLATED MACROSCOPIC SYSTEMS INSIDE QUANTUM MECHANICS

L. LANZ¹, O. MELSHEIMER² AND B. VACCHINI¹,²†

¹Dipartimento di Fisica dell'Università di Milano and INFN, Sezione di Milano, Via Celoria 16, I-20133, Milan, Italy
²Fachbereich Physik, Philipps-Universität, Renthof 7, D-35032, Marburg, Germany
(e-mail: lanz@mi.infn.it; melsheim@mail.uni-marburg.de; vacchini@mi.infn.it)

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For an isolated macroscopic system classical state parameters $\zeta(t)$ are introduced inside a quantum mechanical treatment. By a suitable mathematical representation of the actual preparation procedure in the time interval $[T, t_0]$ a statistical operator is constructed as a solution of the Liouville-von Neumann equation, exhibiting at time $t$ the state parameters $\zeta(t')$, $t_0 \leq t' \leq t$, and preparation parameters related to times $T \leq t' < t_0$. Relation with Zubarev's nonequilibrium statistical operator is discussed. A mechanism for memory loss is investigated and time evolution by a semigroup is obtained for a restricted set of relevant observables, slowly varying on a suitable time scale.

1. Introduction

Quantum mechanical nonseparability is considered as an obstacle for an objective description of physical systems. Such obstacle can be partly overcome if one consistently takes quantum mechanics as a description of preparation and measuring procedures, rather than of the intrinsic structure of things. The assignment of a suitable statistical operator to represent an objectively given preparation procedure is therefore the turning point: that this is not a simple task is immediately clear if one realizes that this must be done inside a framework in which at least isolated macrosystems can be described: this already requires a field description inside a Fock-space. Actually the typical parameters one takes into account when determining a concrete experimental realization have no direct connection with properties related to microphysical structure of the system one is dealing with. Well-known examples of such parameters are velocity, temperature and chemical potential fields, by which a large variety of preparations can be described: these

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preparations contribute however only a very small part of those performed using what nature already has prepared. Usually the duration of the previously indicated preparations referring to rather simple systems is very small, while for complex systems it can be extremely long. It seems reasonable to expect that the use of any given quantum field theory is effective only if preparations are considered of not exceedingly high complexity. We stress that these preparation parameters characterize the subset of relevant statistical operators, therefore they can be associated with each element of the prepared statistical collection. In this way one recovers nonstatistical features of experimental settings and then objectivity appears. Obviously statistics plays its role when measurements are done on the prepared system (then it is no longer isolated). Let us remark that also the set of meaningful measurements is restricted and related to the preparation procedure, e.g., the dynamics of the relevant variables must be slow enough; otherwise the isolation carried out during the preparation would no longer be sufficient to avoid influence from the environment. Isolation of the system has a decisive role, subsets of statistical operators must be chosen and too fast observables must be avoided, all this amounts to the fact that the mathematical framework must be less rigid than it usually is inside quantum field theory in the thermodynamic limit.

2. Classical state parameters for a macroscopic system

According to the general point of view described in Section 1, we have to choose a suitable set of relevant observables. Let the microphysical structure underlying the system be described in terms of nonrelativistic interacting particles, associated with Schrödinger fields $\hat{\psi}_\alpha(x,\omega)$

$$\left[\hat{\psi}_\alpha(x,\omega), \hat{\psi}_{\alpha'}^*(x',\omega')\right] = \delta_{\alpha,\alpha'} \delta_{\omega,\omega'} \delta^3(x - x'), \quad \omega = 1, 2, \ldots, 2s_\alpha + 1,$$

$\alpha$ denoting different types of particles and $s_\alpha$ the corresponding spin. If the system is confined inside a space region $\Omega$, with boundary $\partial \Omega$, one represents the fields in terms of a complete orthonormal set of functions (normal modes) $u_n(x,\omega)$, such that

$$-\frac{\hbar^2}{2m_\alpha} \Delta u_n(x,\omega) = E_n u_n(x,\omega), \quad x \in \Omega, \quad u_n(x,\omega) = 0, \quad x \in \partial \Omega,$$

so that $\hat{\psi}_\alpha(x,\omega) = \sum_n \hat{u}_\alpha n u_n(x,\omega)$, with $[\hat{u}_\alpha n, \hat{u}_{\alpha'} n']^\pm = \delta_{\alpha,\alpha'} \delta_{n,n'}$, $[\hat{u}_\alpha n, \hat{u}_{\alpha'} n']^\pm = 0$. The relevant variables are functions of the fields, typically densities of conserved quantities in suitable configuration spaces, for example:

$$\hat{\rho}_\alpha(x,\omega) = m_\alpha \hat{\psi}_\alpha^*(x,\omega) \hat{\psi}_\alpha(x,\omega), \quad \hat{\rho}_\alpha(x,\omega) = \frac{1}{2} \left\{ [i\hbar \nabla \hat{\psi}_\alpha^*(x,\omega)] \hat{\psi}_\alpha(x,\omega) + \text{h.c.} \right\},$$

$$\hat{f}_\alpha(r, p) = \sum_{\omega} \int_\Omega dx \int_\Omega dx' \hat{\psi}_\alpha^*(x,\omega) \langle x, \omega | \hat{f}(r, p) | x', \omega \rangle \hat{\psi}_\alpha(x',\omega),$$

for each kind of particle being respectively the mass density, the momentum density, the one-particle distribution function ($\hat{f}(r, p)$ is a suitable one-particle phase space density $[1]$). Also an energy density $\hat{e}(x)$ can be introduced by slightly more complicated
expressions, related to the Hamiltonian $\hat{H}$ by $\hat{H} = \int d^3x \hat{e}(x)$. Indicating generally these densities by $\hat{A}_j(\xi)$, conservation equations hold taking the form $\hat{A}_j(\xi, t) = -\text{div} \hat{J}_j(\xi, t)$, where time dependence is given in Heisenberg picture $\hat{A}_j(\xi, t) = e^{+\frac{i}{\hbar} \hat{H} t} \hat{A}_j(\xi)e^{-\frac{i}{\hbar} \hat{H} t}$. The relevance of densities of conserved quantities has been stressed in nonequilibrium statistical mechanics, e.g., by Zubarev [2]. They provide in most natural way slow enough quantities, if smeared with sufficiently homogeneous probe functions. A central role has the determination of a statistical operator once the expectation values of the set $\mathcal{M}$ of relevant observables are given: in general $\mathcal{M}$ is not a separating set, i.e., it is not large enough to uniquely determine a statistical operator at any time $t$; any set $\{\langle \hat{A}_j(\xi) \rangle_t \}$ of expectations of the relevant, linearly independent observables determines a set of statistical operators $\mathcal{M}_t(\{\langle \hat{A}_j(\xi) \rangle_t \})$ that we shall call macrostate [3]. Inside a macrostate the criterion of maximal von Neumann entropy (assumed finite for each macrostate) allows, under very general conditions on $\mathcal{M}$, to determine a unique trace class operator having the typical structure of Gibbs state. Let us indicate by $\hat{w}_{\xi(t)}$ such (generalized) Gibbs state

$$\hat{w}_{\xi(t)} = \frac{\exp \left\{ -\sum_j \int d\xi \zeta_j(\xi, t) \hat{A}_j(\xi) \right\}}{Z[\zeta_j(t)]} \equiv \exp \left\{ -\zeta_0(t) \hat{1} - \sum \int d\xi \zeta_j(\xi, t) \hat{A}_j(\xi) \right\},$$

with $\zeta_0(t) = \log Z[\zeta_j(t)], Z[\zeta_j(t)] = \text{Tr} \exp \left\{ -\sum_j \int d\xi \zeta_j(\xi, t) \hat{A}_j(\xi) \right\}$ being the partition function of the system at time $t$, while $\zeta_j(\xi, t)$ are the Lagrange parameters related to the maximization procedure. $\hat{w}_{\xi(t)}$ represents the least biased choice and $-k\text{Tr} \hat{w}_{\xi(t)} \log \hat{w}_{\xi(t)} = S(\zeta(t))$ is taken as the entropy of the macrostate. The fact that we intend to describe isolated systems is taken into account by $(\hat{H} - \langle \hat{H} \rangle)^2 \in \mathcal{M}$ and assuming that: $\langle (\hat{H} - \langle \hat{H} \rangle)^2 \rangle^\frac{1}{2} \ll \langle |\hat{H}| \rangle$. From the physical point of view it is important that the set $\mathcal{M}$ is small enough: in fact if for example the linear span of $\mathcal{M}$ were invariant under time evolution, or if $\mathcal{M}$ were a separating set, $S(\zeta(t))$ would be constant [4], contrary, for a nonequilibrium system, to the second principle of thermodynamics. Due to the fact that the relevant observables are a relatively small subset of all observables one can safely assume that invariance of $\mathcal{M}$ under time evolution does not occur for realistic Hamiltonians; on the other hand just by this fact, the naive identification of the statistical operator $\hat{\varrho}_t = e^{-\frac{i}{\hbar} \hat{H}(t-t_0)} \hat{\varrho}_{t_0} e^{+\frac{i}{\hbar} \hat{H}(t-t_0)}$ with $\hat{w}_{\xi(t)}$ for all $t$ becomes impossible. The next section treats the intriguing problem of the relationship between $\hat{\varrho}_t$ and $\hat{w}_{\xi(t)}$.

At any time $t$, at least as far as the expectations of the relevant observables are concerned, the statistical collection is characterized in a natural way by the parameters $\zeta(t)$: therefore one is induced to take $\zeta(t)$ as an objective property of each member of the statistical collection. This is indeed the case in the typical applications of nonequilibrium statistical mechanics. This is most typically seen in the case of the velocity field for a continuum, related to the expectations of relevant observables by: $v(x, t) = \langle p(x) \rangle_t / \langle \rho(x) \rangle_t$. However, $v(x, t)$ has also an objective meaning for each individual system, as seen in the phenomenological description of macroscopic systems inside mechanics of continua. Similar considerations can be made also for other macroscopic (classical) fields, e.g., the temperature field. The very fact that the expectation values of relevant observables are
linked to the *objective* parameters $\zeta(t)$ implies that the perturbation of the macrosystem produced by the measurement of relevant observables does not affect too much the expectation values themselves: in fact physics points out that measurements not disturbing the parameters $\zeta(t)$ of the system are indeed feasible. On the contrary one cannot expect that the same situation occurs for the probability distribution of the relevant observables (in case of fluctuating variables). Just this different status of average values in comparison to probability distributions is the key point to make objectivity of macrosystem compatible with the typical issue arising due to quantum mechanical measurement. A check of this statement can be done inside the theory of continuous measurement: the perturbation of the no longer isolated macrosystem due to the measuring apparatus can be represented by a non-Hamiltonian contribution $L_{int}$ to the generator of time evolution. Then a continuous measurement can be described of suitable observables already specified inside $L_{int}$, obtaining the whole statistics for these observables. It is seen that expectation values depend in a regular way on $L_{int}$, so that in the limit $L_{int} \to 0$ the isolated system dynamics is recovered. On the contrary already the second momenta of probability distributions diverge in this limit \cite{5}. We intend to treat this problem in more general way in future papers.

3. Preparation procedure for a macroscopic system

The first problem which is now to be faced in order to construct the dynamics of a macrosystem, isolated for times $t > t_0$, is to give its statistical operator $\hat{\sigma}$ and to elucidate the relationship between $\hat{\sigma}$ and the representative $\hat{\omega}_{\zeta(t)}$ of the macrostate $M_t$. The basic ingredient to start with is the unitary evolution $\hat{\sigma} = e^{-\frac{i}{\hbar} \hat{H}(t-t_0)} \hat{\sigma}_{t_0} e^{\frac{i}{\hbar} \hat{H}(t-t_0)}$, $\hat{H} = \hat{H}^t$ being the Hamiltonian for the isolated system. If $t_0$ is taken as initial time the most straightforward approach would be to take $\hat{\sigma} = \hat{\sigma}_{t_0}$; however, such an assumption is not satisfactory since the initial time $t_0$ would have a privileged role, being in general $\hat{\sigma} \neq \hat{\omega}_{\zeta(t)}$. Let us stress that this is not appreciated as a problem, typically inside information thermodynamics, if the statistical operator is considered as representative of the information about the system: then at time $t_0$ the only available information is just $M_{t_0}$, while at time $t$ information increases since $M_t$, $t' \in [t_0, t]$, is in principle known. Our standpoint about $\hat{\sigma}$ is different: it represents the concrete preparation procedure of the statistical collection for all times $t' \leq t$. Then choice (1) should be motivated on the basis of the way the system was prepared at times $t' < t_0$. The meaning of choice (1) is that all the history $\{M_{t'}, t' < t_0\}$ is irrelevant for the subsequent dynamical evolution: the fact that $\hat{\sigma} \neq \hat{\omega}_{\zeta(t)}$ for $t > t_0$ indicates in principle that this is no longer true for $t > t_0$; then (1) becomes the key problem. One could check condition (1) measuring the expectation values ($\hat{A}_j(\xi)$) of the variables $\hat{A}_j(\xi) = \frac{i}{\hbar}[\hat{H}, \hat{A}_j(\xi)]$ and comparing with $\text{Tr} (\hat{A}_j(\xi) \hat{\omega}_{\zeta(t_0)})$. Physics indicates a profound difference between $\hat{\sigma}$ and $\hat{\omega}_{\zeta(t)}$: as far as the von Neumann entropy is concerned $-k \text{Tr} \hat{\sigma} \log \hat{\sigma} = -k \text{Tr} \hat{\sigma}_{t_0} \log \hat{\sigma}_{t_0}$, while $-k \text{Tr} \hat{\omega}_{\zeta(t)} \log \hat{\omega}_{\zeta(t)}$ can in general increase. As
a general assumption (1) would be acceptable if \( t_0 \) were a very special time (big bang time!), when no previous history exists, or has been erased. Actually an experimental preparation implies a separation of a physical system from the environment: one must start with isolated systems (open macroscopic systems remain of course an open physical problem) and this preparation is operatively associated to a finite time interval: \([T, t_0]\). Then \( \hat{\rho}_{t_0} \) represents what has been done with the system in a laboratory during the time interval \([T, t_0]\). Let us observe that \( \hat{\rho}_t, t > t_0 \) still represents a family of preparations arising for the isolated system, due to spontaneous time evolution: our goal is to give a prescription to build the set \( \hat{\rho}_t, t > t_0 \), compatible with respect to the unitary evolution.

We formalize the preparation procedure \([T, t_0]\) by sharp measurements of \( M_t \) at time points \( T \) and \( t_0 \), isolation of the system being achieved at time \( t_0 \), and by control measurements of variables \( \int_{t_0}^{t_0} dt' \hat{A}_j(\xi, t')h_{\alpha}(t') \), \( h_{\alpha}(t') \) being suitable test functions (e.g., \( h_{\alpha}(t) = \cos \omega_{\alpha} t \)). One expects that not only the densities \( \hat{A}_j(\xi, t) \) should be controlled but also the corresponding currents \( \hat{J}_j(\xi) \). To express the fact that the system is only biased by these measurements and controls, we use the principle of maximal entropy to determine \( \hat{\rho}_{t_0} \). Then \( \hat{\rho}_{t_0} \) has the following structure:

\[
\hat{\rho}_{t_0} = \exp \left\{ -\sum_j \int d\xi \gamma_j(\xi, t_0) \hat{A}_j(\xi) + \sum_{j_0} \int d\xi \gamma_{j_0}(\xi) \int_{t_0}^{t_0} dt' \hat{A}_j(\xi, -(t_0 - t')) h_{j_0}(t') \right. \\
+ \sum_{j_0} \int d\xi \gamma_{j_0}(\xi) \int_{t_0}^{t_0} dt' \hat{J}_j(\xi, -(t_0 - t')) h_{j_0}(t') - \sum_j \int d\xi \gamma_j(\xi, T) \hat{A}_j(\xi, -(t_0 - T)) \right\}.
\]

(2)

Let us express the decisive role of the measurement of the relevant observables \( \hat{A}_j(\xi) \) at time \( t_0 \), assuming that

\[
\gamma_j(\xi, t_0) = \zeta_j(\xi, t_0),
\]

(3)

where \( \{\zeta(t_0)\} \) is the macroscopic state of the system. We call a preparation procedure a suitable preparation procedure if (3) is satisfied. Let us observe that due to the asymmetry between \( \gamma_j(\xi, t) \) and \( \gamma_j(\xi, T) \) introduced by (3) a time arrow is introduced in a very clear way. Among the constants of motion \( \hat{C}_t \) a particular role has the identity operator: its contribution to the exponential (2) accounts for normalization as it was indicated in Section 1. The time evolution of \( \hat{\rho}_{t_0} \) is straightforward:

\[
\hat{\rho}_t = e^{-\frac{i}{\hbar} \hat{H}(t-t_0)} \hat{\rho}_{t_0} e^{+\frac{i}{\hbar} \hat{H}(t-t_0)} = \exp \left\{ -\zeta_0(t) \hat{1} - \sum_j \int d\xi \zeta_j(\xi, t_0) \hat{A}_j(\xi, -(t - t_0)) \right. \\
+ \sum_{j_0} \int d\xi \gamma_{j_0}(\xi) \int_{t_0}^{t_0} dt' \hat{A}_j(\xi, -(t - t')) h_{j_0}(t') \\
+ \sum_{j_0} \int d\xi \gamma_{j_0}(\xi) \int_{t_0}^{t_0} dt' \hat{J}_j(\xi, -(t - t')) h_{j_0}(t') - \sum_j \int d\xi \gamma_j(\xi, T) \hat{A}_j(\xi, -(t - T)) \right\}.
\]

(4)
then one can determine the macrostate at time $t$, using the expectations $C_{lt} = C_{lt_0}$, 
$\langle \hat{A}_j(\xi) \rangle_t = \text{Tr} (\hat{A}_j(\xi) \hat{\omega}_t)$, and solving the equations

$$
\text{Tr} \left( \hat{C}_t \hat{\omega}_{\xi(t)} \right) - C_{lt_0}, \quad \text{Tr} \left( \hat{A}_j(\xi) \hat{\omega}_{\xi(t)} \right) - \langle \hat{A}_j(\xi) \rangle_t,
$$

according to the definition given in Section 1. Let us now rewrite $\zeta_j(\xi, t_0) \hat{A}_j(\xi, -(t - t_0))$ using the $\zeta_j(\xi, t)$ determined in this way,

$$
\zeta_j(\xi, t_0) \hat{A}_j(\xi, -(t - t_0)) = \zeta_j(\xi, t) \hat{A}_j(\xi) - \int_{t_0}^{t} dt' \frac{d}{dt'} \left[ \zeta_j(\xi, t') \hat{A}_j(\xi, -(t - t')) \right]
$$

$$
= \zeta_j(\xi, t) \hat{A}_j(\xi) - \int_{t_0}^{t} dt' \zeta_j(\xi, t') \hat{A}_j(\xi, -(t - t')) + \int_{t_0}^{t} dt' \zeta_j(\xi, t') \text{div} \hat{J}_j(\xi, -(t - t')).
$$

Replacing (5) inside (4) one has:

$$
\hat{\omega}_t = \exp \left\{ - \zeta_0(t) \mathbf{1} - \sum_j \int d\xi \zeta_j(\xi, t) \hat{A}_j(\xi) + \sum_j \int_{t_0}^{t} dt' \int d\xi \zeta_j(\xi, t') \hat{A}_j(\xi, -(t - t')) \right. 
$$

$$
+ \sum_{j} \int_{T}^{t_0} dt' \int d\xi \gamma_{j\alpha}(\xi) \hat{A}_j(\xi, -(t - t')) \hat{h}_{j\alpha}(t') - \sum_{j} \int_{t_0}^{t} dt' \int d\xi \zeta_j(\xi, t') \text{div} \hat{J}_j(\xi, -(t - t'))
$$

$$
+ \sum_{j} \int_{T}^{t_0} dt' \int d\xi \gamma_{j\alpha}(\xi) \cdot \hat{J}_j(\xi, -(t - t')) \hat{h}_{j\alpha}(t') - \sum_{j} \int d\xi \gamma_{j\alpha}(\xi, T) \hat{A}_j(\xi, -(t - T)) \right\}.
$$

Comparing $\hat{\omega}_t$ given by (6) with $\hat{\omega}_{t_0}$ given by (2) one observes that the basic structure is preserved: $\hat{\omega}_t$ represents a new preparation composed of the initial preparation procedure and the subsequent spontaneous evolution up to time $t$, which replaces $t_0$, the initial macrostate parameters $\zeta_j(\xi, t_0)$ being replaced by $\zeta_j(\xi, t)$. The contribution representing the past history now extends from $T$ to $t$ and a new part is displayed, related to the time interval $[t_0, t]$. In place of the parameters $\sum_{\alpha} \gamma_{j\alpha}(\xi) h_{j\alpha}(t')$ which described the preparation procedure in the time interval $[T, t_0]$, now the parameters $\hat{J}_j(\xi, t)$ appear, in place of the term $\sum_{j} \gamma_{j\alpha}(\xi, -(t - t')) \hat{h}_{j\alpha}(T)$ one deals with $- \sum_{j} \zeta_j(\xi, t') \text{div} \hat{J}_j(\xi, -(t - t'))$. In this way a solution is given to the problem of justifying assumption $\hat{\omega}_{t_0}$ for the description of a preparation procedure of a macrosystem. Furthermore the structure (4) of $\hat{\omega}_t$ also suggests a practical solution method, that will be discussed in Section 3. Not only $\hat{\omega}_t$ provides by construction the expectation values of the relevant observables through the expressions $\text{Tr} (\hat{A}_j(\xi) \hat{\omega}_t)$ which are linked to the objective state parameter, but also provides probability distributions for measurements which can be performed on the system by the usual tools of quantum mechanics (in the most refined case instruments or operation valued measures). The result (4) is very close to the "nonequilibrium statistical operator" proposed by Zubarev [2] though in his...
approach no clear distinction is introduced between the preparation of the system and its spontaneous time evolution, so that he always takes the limit $T \to -\infty$, which would be meaningless for a real preparation procedure. Moreover the limit $T \to -\infty$ presupposes a thermodynamic limit and introduces big difficulties for a nonequilibrium system. The practical difference between the two approaches vanishes if memory effects are not relevant [3].

4. Evolution equation for the classical state parameters $\{\zeta(t)\}$

The structure (6) strongly suggests that the first terms in the argument of the exponential are more important than the remaining ones, since they alone already determine the expectations of the relevant observables. Then a perturbation theory becomes very natural in which the last part of the exponential is treated as a perturbation, the typical cumulant expansion. The first contributions are:

$$\frac{\text{Tr} \hat{C} e^{\hat{A} + \hat{B}}}{\text{Tr} e^{\hat{A} + \hat{B}}} = \frac{\text{Tr} \hat{C} e^{\hat{A}}}{\text{Tr} e^{\hat{A}}} + \frac{\text{Tr} \hat{C} \int_0^1 du e^{u\hat{A}} \hat{B} e^{(1-u)\hat{A}}}{\text{Tr} e^{\hat{A}}} - \frac{\text{Tr} \hat{C} e^{\hat{A}}}{\text{Tr} e^{\hat{A}}} \frac{\text{Tr} \hat{B} e^{\hat{A}}}{\text{Tr} e^{\hat{A}}} + \cdots.$$  

The typical equation yielding the time evolution of the macrostate is given in terms of $\hat{\omega}_t[\zeta]$, by the condition, arising from the definition of macrostate:

$$\frac{d}{dt} \text{Tr} (\hat{A}_j(\zeta(t)) \hat{\omega}_t[\zeta]) = \frac{d}{dt} \text{Tr} (\hat{A}_j(\zeta(t)) \hat{\omega}_t[\zeta]) = -\sum_l \int d\xi' \langle \hat{A}_j(\xi'), \hat{A}_l(\xi') \rangle \hat{\omega}_t[\zeta, t].$$

where the Kubo correlation function has been introduced

$$\langle \hat{A}, \hat{B} \rangle \hat{\omega}_t[\zeta] \equiv \text{Tr} \hat{A} \int_0^1 du e^{u\hat{C}(t)} \hat{B} e^{(1-u)\hat{C}(t)} - \text{Tr} \hat{A} \hat{\omega}_t[\zeta] \text{Tr} \hat{B} \hat{\omega}_t[\zeta].$$

with $\hat{C}(t) = -[\zeta_0(t) \hat{1} - \sum_j \int d\xi \zeta_j(\xi, t) \hat{A}_j(\xi)]$. Since $d\hat{\omega}_t/dt = -\frac{i}{\hbar} [\hat{H}, \hat{\omega}_t]$, the first term of (8) becomes $\text{Tr} (\frac{i}{\hbar} [\hat{H}, \hat{A}_j(\zeta, t)] \hat{\omega}_t[\zeta, t])$. Let us represent $\hat{\omega}_t$ in the form (7), then the following evolution equation for the state parameters arises:

$$\langle \hat{A}_j(\xi'), \hat{A}_l(\xi') \rangle \hat{\omega}_t[\zeta, t]$$

$$= \text{Tr} \left( \frac{i}{\hbar} [\hat{H}, \hat{A}_j(\xi)] \hat{\omega}_t[\zeta, t] + \int_T^t dt' \langle \frac{i}{\hbar} [\hat{H}, \hat{A}_j(\xi)], \hat{S}(t') \rangle \hat{\omega}_t[\zeta, t], \right.$$

$$\left. - \sum_l \int d\xi' \langle \frac{i}{\hbar} [\hat{H}, \hat{A}_j(\xi)], \hat{A}_l(\xi', -(t - T)) \rangle \hat{\omega}_t[\zeta, t], \hat{S}(t') \rangle \hat{\omega}_t[\zeta, t], \right.$$  

In these equations the whole history of the system arises represented by the term $\hat{S}(t')$ and by $\gamma_l(\zeta', T)$, where $\hat{S}(t')$ is given by

$$\left\{ \begin{array}{ll}
\sum_{j, \alpha} \int d\xi' [\gamma_{j, \alpha}(\zeta', t) \hat{A}_j(\xi, -(t - t')) + \gamma_{j, \alpha}(\zeta', -(t - t')) \hat{J}_j(\xi, -(t - t'))] \hat{h}_{j, \alpha}(t'), & T \leq t' \leq t_0, \\
\sum_j \int d\xi' \left[ \zeta_j(\xi', t') \hat{A}_j(\xi, -(t - t')) - \zeta_j(\xi', t') \text{div} \hat{J}_j(\xi, -(t - t')) \right], & t_0 \leq t' \leq t. \end{array} \right.$$  

(10)
It is seen that time evolution provides an additional preparation represented by the parameters \( \zeta_j(\xi', t') \) and \( \zeta_j(\xi', t') \); thus (9) are integrodifferential evolution equations for \( \zeta_j(\xi, t) \). Formally the whole memory of the macrostate for \( T \leq t' \leq t \) appears inside the expression of \( \zeta_j(\xi', t') \) through the correlation functions:

\[
\left( \frac{i}{\hbar} [\hat{H}, \hat{A}_j(\xi)], \hat{A}_i(\xi', -(t-t')) \right)_{\zeta(t)} = \left( \frac{i}{\hbar} [\hat{H}, \hat{A}_j(\xi)], \hat{J}_i(\xi', -(t-t')) \right)_{\zeta(t)}, \quad T \leq t' \leq t.
\]

By the first order approximation inside (7) the whole dynamics of the macrostate is controlled through two point Kubo correlation functions for relevant observable and their time derivatives (currents). Higher order correlation functions are introduced in the higher approximations. Actually most applications of nonequilibrium thermodynamics already fit inside the first order approximation scheme. Now one can take advantage from a general feature of correlation functions: they have a decaying behaviour in time. The basic assumption about the preparation procedure, that was assumed to be restricted inside the finite time interval \( [T, t_0] \), could be consistently assumed also at later times. Indicating qualitatively \( \tau \) as typical decay time of the correlation functions, the structure of \( \hat{\varrho}_t \) appears justified if \( t_0 - T > \tau \); furthermore one expects that the r.h.s. of (9) can be simplified for \( t - t_0 > \tau \), dropping the last term and replacing the integration interval \( [T, t] \) with \( [t - \tau, t] \), in this way providing a universal character to the time evolution equations by elimination of the preparation parameters. Decaying behaviour of correlation functions is a central issue in statistical mechanics often achieved making use of the thermodynamic limit, while in our case a less schematic and more sophisticated attitude must be taken; in fact we are considering a confined system, separated and isolated from the environment: then the Hamiltonian has a point spectrum and correlation functions have a quasiperiodical time behaviour. Loss of memory arises through an interplay between choice of observables and characterization of suitable preparation procedures. Let us observe that correlation functions always appear inside time integrals: by these integrations the quasiperiodical behaviour of correlation functions can very well produce a decaying behaviour, provided other factors inside the time integrals are smooth enough. Looking at (9) and (10) these factors are seen to be the functions \( h_{j\alpha}(t') \) and the state parameters \( \zeta_j(\xi', t') \), which are linked to the expectation values \( \langle \hat{A}_j(\xi) \rangle \). Also the integration on \( \xi \) will have a smoothing effect, provided the state parameters are homogeneous enough, which in turn depends on suitable choice of space-time variation scale of the relevant observables. Let us note that neglecting in (9) history in the time interval \( [T, t-\tau], \tau \) being the previously introduced typical decay time, amounts to taking at time \( t-\tau \) an initial state \( \hat{\varrho}_{t-\tau} = \hat{w}_{\xi(t-\tau)} \), so that \( \hat{\varrho}_t = e^{-\frac{i}{\hbar}\hat{H}\tau \hat{w}_{\xi(t-\tau)}} e^{\frac{i}{\hbar}\hat{H}\tau} \), leading in a straightforward way to the iterated inequality: \( S_t \geq S_{t-\tau} \geq S_{t-2\tau} \geq \ldots \geq S_{t-n\tau} \), loosely a mean stepwise increase of entropy. As long as \( \hat{\varrho}_t \) is not a Gibbs state one has the strict inequality \( S_t > S_{t-\tau} \): this is indeed the case, due to the history contribution. Since by the constants of motion \( A_j = \int d\xi \langle \hat{A}_j(\xi) \rangle_t \) the finite bound \( S(\{ \hat{A}_j(\xi) = \hat{A}_j/V \}) \geq S(\{ \hat{A}_j(\xi) \}) \) is put on the entropy, one can in this way conclude that the system approaches for \( t \to +\infty \) the Gibbs state, determined by the constants of motion: i.e., its equilibrium state. To take further into account the particular role of the constants of motion, let us replace the relevant
density field $\hat{A}_j(\xi)$ with a suitable set of transformed variables $\hat{a}_{jn} = \int d\xi u^n_\alpha(\xi)\hat{A}_j(\xi)$, 
where $u^n_\alpha(\xi)$ is some suitable complete orthonormal set of functions (e.g., Fourier functions) defined in the phase space region on which the fields are defined. Let us assume that $u_0(\xi)$ is constant so that the variables $\hat{a}_{j0}$ we have related to densities of conserved quantities, coincide with the conserved observables; then (9) becomes:

$$- \sum_{j' n'} \langle \hat{a}_{j0}, \hat{a}_{j'n'} \rangle \dot{\xi}_{j'n'}(t) = 0. \quad (11)$$

$$- \sum_{j' n'} \langle \hat{a}_{jn}, \hat{a}_{j'n'} \rangle \dot{\xi}_{j'n'}(t) = \text{Tr} \left( \frac{i}{\hbar} [\hat{H}, \hat{a}_{jn}] \hat{w}(\xi(t)) \right) + \int^t_T dt' \langle \frac{i}{\hbar} [\hat{H}, \hat{a}_{jn}], \hat{S}(t') \rangle \hat{w}_{\xi(t)},$$

$$- \sum_{j' n'} \langle \frac{i}{\hbar} [\hat{H}, \hat{a}_{jn}], \hat{a}_{j'n'}(-(t - T)) \rangle \hat{w}_{\xi(t)}, \quad n > 0,$$

where $\hat{S}(t')$ can be easily rewritten in terms of the new variables. The general problem of extracting a system of integrodifferential equations for $\xi_{jn}(t)$ can be solved restricting to a finite subset of variables $\{\hat{a}_{jn}\}_{n \leq N}$, and taking the inverse of the matrix $\langle \hat{a}_{jn}, \hat{a}_{j'n'} \rangle \hat{w}_{\xi(t)}$.

5. Dynamical semigroup description

A separate role is now given to the constants of motion $\hat{a}_{j0}$, having constant expectations and in this way influencing the state variables through the first line of (11), as compared to the other observables, which drive the dynamics through the second line of (11). It will turn out to be useful to formalize in the following way these different roles: by means of the Gibbs state $\hat{w}_{\xi(t)}$ a sesquilinear form on the space of operators [6] can be defined by $\langle \hat{A}, \hat{B} \rangle_{\hat{w}_{\xi(t)}}$, by which a time-dependent Hilbert space structure on the space of operators can be introduced, linked to the macrostate at time $t$. Let us consider the subspace spanned by the constants of motion $\hat{a}_{j0}$ and decompose the observables $\hat{a}_{jn}$, $n \geq 1$, in a parallel and orthogonal component with respect to this subspace. Obviously we can restrict the study of time evolution to these orthogonal components $\hat{a}_{jn+}$, $n \geq 1$. One can expect that if the state parameters depend solely on time during the relevant part of history, differential equations for time evolution instead of the integrodifferential equations discussed in Section 3 should arise. Let us treat (6) rewritten in terms of the variables $\hat{a}_{jn}$ in a slightly different way:

$$\dot{\hat{w}}_t = \exp \left\{ - \sum_{jn} \xi_{jn}(t)\hat{a}_{jn} + \sum_{jn \geq 1} \int_{t_0}^t dt' \xi_{jn}(t')\hat{a}_{jn}(-(t - t')) \right. \right.$$

$$\left. + \sum_{jn \geq 1} \int_{t_0}^t dt' \gamma_{jn}(t')\hat{a}_{jn}(-(t - t'))h_{jn}(t') + \sum_{jn \geq 1} \int_{t_0}^t dt' \xi_{jn}(t')\hat{a}_{jn}(-(t - t')) \right.$$

$$\left. + \sum_{jn \geq 1} \int_{t_0}^t dt' \gamma_{jn}(t')\hat{J}_{jn}(-(t - t'))h_{jn}(t') - \sum_{jn \geq 1} \gamma_{jn}(T)\hat{a}_{jn}(-(t - T)) \right\}. \right.$$
The state parameters are given by the equations: \( \text{Tr} \, \hat{\alpha}_{jn} \hat{\omega}_{\zeta(t)} = \text{Tr} \, \hat{\alpha}_{jn} \hat{\epsilon}; \) let us now look whether a differential equation for \( \zeta(t) \) can be derived from these

\[
\text{Tr} \, \hat{\alpha}_{jn} \hat{\omega}_{\zeta(t)} = \text{Tr} \, \hat{\alpha}_{jn} \hat{\omega}_{\zeta(t)} = E_{jn} ,
\]

(12)

\[
\text{Tr} \, \hat{\alpha}_{jn} \hat{\omega}_{\zeta(t)} = \text{Tr} \, \hat{\alpha}_{jn} \hat{\omega}_{\zeta(t)} + \sum_{j'/n' \geq 1} \int_{t_0}^{t} dt' \left\{ \langle \hat{\alpha}_{jn}, \hat{\alpha}_{jn'}(-(t-t')) \rangle \hat{\omega}_{\zeta(t)} \hat{\zeta}_{jn'}(t') \right. \\
\left. + \langle \hat{\alpha}_{jn}, \hat{\alpha}_{jn'}(-(t-t')) \rangle \hat{\omega}_{\zeta(t)} \hat{\zeta}_{jn'}(t') \right\}
\]

In (12) we have taken into account that the contribution of \( n' = 0 \) can be dropped due to orthogonality with \( \hat{\alpha}_{jn} \) \( (n \geq 1) \). As we already did in Section 3, let us use the time decay of the history of the macrosystem, characterized by the typical time \( \tau \); if \( t - t_0 > \tau \), we can neglect the preparation part represented by the last three terms of (12) and we can rewrite the second part of (12) in the form

\[
\sum_{j'/n' \geq 1} \frac{1}{\tau} \int_{0}^{\tau} dt' \left\{ \langle \hat{\alpha}_{jn}, \hat{\alpha}_{jn'}(-(t-t')) \rangle \hat{\omega}_{\zeta(t)} \hat{\zeta}_{jn'}(t-t') + \langle \hat{\alpha}_{jn}, \hat{\alpha}_{jn'}(-(t-t')) \rangle \hat{\omega}_{\zeta(t)} \hat{\zeta}_{jn'}(t-t') \right\} = 0.
\]

(13)

The main point is now to assume that the relevant observables have a time evolution that is slow enough; more precisely one has for the state parameters:

\[
\zeta_{jn'}(t-t') \approx \zeta_{jn'}(t); \quad \zeta_{jn'}(t-t') \approx \zeta_{jn'}(t); \quad \tau' \leq \tau.
\]

(14)

A similar property is exhibited by the expectations and we can expect it also for correlation functions \( \langle \hat{\alpha}_{jn}, \hat{\alpha}_{jn'}(-(t-t')) \rangle \hat{\omega}_{\zeta(t)} \). We represent the first term of (13) using (14),

\[
- \sum_{j'/n' > 1} \langle \hat{\alpha}_{jn}, \hat{\alpha}_{jn'} \rangle \hat{\omega}_{\zeta(t)} \hat{\zeta}_{jn'}(t) = \frac{1}{\tau} \int_{0}^{\tau} dt' \langle \hat{\alpha}_{jn}, \hat{\alpha}_{jn'}(-(t-t')) \rangle \hat{\omega}_{\zeta(t)} \hat{\zeta}_{jn'}(t) = \frac{d}{dt} \frac{\text{Tr} \, \hat{\alpha}_{jn} \exp \left\{ -\sum_{lm} \zeta_{lm}(t) \hat{\alpha}_{lm} \right\}}{\text{Tr} \exp \left\{ -\sum_{lm} \zeta_{lm}(t) \hat{\alpha}_{lm} \right\}} = \frac{1}{\tau} \int_{0}^{\tau} dt' \sum_{j'/n' \geq 1} \langle \hat{\alpha}_{jn}, \hat{\alpha}_{jn'}(-(t-t')) \rangle \hat{\omega}_{\zeta(t)} \hat{\zeta}_{jn'}(t) = \frac{d}{dt} \frac{\text{Tr} \, \hat{\alpha}_{jn} \exp \left\{ -\sum_{lm} \zeta_{lm}(t) \hat{\alpha}_{lm} \right\}}{\text{Tr} \exp \left\{ -\sum_{lm} \zeta_{lm}(t) \hat{\alpha}_{lm} \right\}}.
\]

The structure of the second term of (13) is as follows:

\[
\frac{1}{\tau} \int_{0}^{\tau} dt' \left[ \frac{\text{Tr} \hat{A} \int_{0}^{1} du e^{-u \hat{C}_{t}} \hat{H} \hat{C}_{t} e^{-(1-u) \hat{C}_{t}}}{\text{Tr} e^{-\hat{C}_{t}}} - \frac{\text{Tr} \hat{A} e^{-\hat{C}_{t}}}{\text{Tr} e^{-\hat{C}_{t}}} \frac{1}{\hat{h}} \left[ \hat{H}, \hat{C}_{t} \right] e^{(1-u) \hat{C}_{t}} \right],
\]

(15)
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where $\dot{C}_t = \sum_{lm} \zeta_{lm}(t) \dot{a}_{lm}$, $\dot{A} = \dot{a}_{jn \perp}$. We replace now inside (15) expressions like $\exp\{-\alpha \dot{C}_t\}$ by $\exp\{-\alpha \dot{C}_t(-\tau) - \alpha(\dot{C}_t(-\tau) - \dot{C}_t)\}$ and expand with respect to $\dot{C}_t(-\tau) - \dot{C}_t$ by a perturbative expansion retaining the first terms, so that (15) becomes

$$-rac{1}{\tau} \int_0^\tau d\tau' \left[ \frac{\text{Tr} \frac{1}{\hbar} [\dot{H}, e^{-\dot{C}_t(-\tau')}] + \text{Tr} \frac{1}{\hbar} [\dot{H}, \dot{C}_t(-\tau')] e^{-\dot{C}_t(-\tau')}}{\text{Tr} e^{-\dot{C}_t}} \right].$$

Due to the cyclicity of the trace operation the last term vanishes and the first one becomes

$$\frac{1}{\tau} \int_0^\tau d\tau' \frac{\text{Tr} \dot{A}(\tau') e^{-\dot{C}_t}}{\text{Tr} e^{-\dot{C}_t}} = \frac{1}{\tau} \frac{\text{Tr} \left( \dot{A}(\tau) - \dot{A}(0) \right) e^{-\dot{C}_t}}{\text{Tr} e^{-\dot{C}_t}}.$$

The first order result is

$$\frac{d}{dt} \text{Tr} \dot{a}_{jn \perp} \exp \left\{ -\sum_{lm} \zeta_{lm}(t) \dot{a}_{lm} \right\} = \frac{\text{Tr} \left( \frac{\dot{a}_{jn \perp}(\tau) - \dot{a}_{jn \perp}(0)}{\tau} \right) \exp \left\{ -\sum_{lm} \zeta_{lm}(t) \dot{a}_{lm} \right\}}{\text{Tr} \exp \left\{ -\sum_{lm} \zeta_{lm}(t) \dot{a}_{lm} \right\}}.$$

(16)

where the contribution of higher order correlation functions, e.g., the second term on the r.h.s. of (14), have been neglected. Equation (16) must be considered together with (12), which refers to the constants of motion $\dot{a}_{j0}$. The parameter $\tau$ has been introduced by the following criteria: it is long enough to make the dynamics of expectations $\langle \dot{a}_{jn \perp} \rangle_t$ be independent of the history referring to times $t' < t - \tau$; short enough to allow macroscopic state parameters to be considered practically constant in a time interval $\tau$ and furthermore higher order correlation functions have been neglected to obtain (16). If all this turns out to be true, and one can safely expect that this is a rather general situation, e.g., when the system is close enough to the equilibrium state, then the r.h.s. of (16) should be independent on $\tau$, so that one can write $[\dot{a}_{jn \perp}(\tau) - \dot{a}_{jn \perp}(0)]/\tau = \mathcal{L}' \dot{a}_{jn \perp}$, $n \geq 1$, with $\mathcal{L}'$ a suitable map defined on the linear span of macroscopic observables $\dot{a}_{jn \perp}$. By this map the whole dynamics can be expressed by differential equations generated by $\mathcal{L}'$

$$(\dot{a}_{jn \perp})_\zeta(t) = E_{jn \perp}; \quad \frac{d}{dt}(\dot{a}_{jn \perp})_\zeta(t) = \text{Tr} \left( (\mathcal{L}' \dot{a}_{jn \perp})_\zeta(t) \right).$$

Then one has a reduced dynamics on a time scale $\tau$, restricted to the variables $\dot{a}_{jn \perp}$, for which the Gibbs states $\dot{w}_\zeta(t)$ have the role of states. In this way contact is established with the well-known master equation approach to statistical mechanics [7]: in a sense a justification for it has been given, but with a main difference. One does not obtain a semigroup evolution for the statistical operator $\dot{a}_t$, which at this stage does no longer appear in the formalism, but instead one has a dynamical map [8] $\mathcal{L}'$ defined on the relevant observables, which are not constants of motion; we shall not discuss now the problem that naturally arises from studying expressions $e^{+\hbar t}$ $\dot{a}_{jn \perp} e^{-\hbar t}$ for asymptotic times, averaged on suitable statistical operators, depending on the state parameters, in order to determine the actual structure of $\mathcal{L}'$. While the Hamilton operator plays the central role for the dynamics described in Section 3, in this reduced dynamics description the map $\mathcal{L}'$ arises, which no longer has a Hamiltonian character [9].
6. Conclusions and outlook

Our approach points toward following developments: state parameters $\zeta(t)$ in more general situations than already well established hydrodynamics [2], should be considered: e.g., a generalized chemical potential $\mu(\xi)$ related to a kinetic description (as already pointed out in reference [10]); also the relevance of the state parameters related to the energy dispersion, first pointed out in other context [11] by Ingarden, should be further investigated. The way in which the parameters $\zeta(t)$ and the additional preparation parameters determine the statistical operator is the main point in this paper: one has the indication that the concrete feature of the preparation procedure can be represented inside the formalism; so we expect that the concept of suitable preparation procedure should be amenable to experimental text. The result described in Section 5 points to a dynamical semigroup description for a restricted set of slow enough variables [12]. This leads to the conjecture that some classical insight into the microphysical dynamical behaviour of the system can be gained by means of a decomposition of the evolution map on a suitable trajectory space. Such insight would be desirable, since so far the classical objective dynamics of $\zeta(t)$ arises from quantum physics for normal modes in field theory, quite far away from classical intuition.

REFERENCES