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Generalized Gibbs ensembles for time dependent processes

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An information theory description of finite systems explicitly evolving in time is presented for classical as well as quantum mechanics. We impose a variational principle on the Shannon entropy at a given time while the constraints are set at a former time. The resulting density matrix deviates from the Boltzmann kernel and contains explicit time odd components which can be interpreted as collective flows. Applications include quantum brownian motion, linear response theory, out of equilibrium situations for which the relevant information is collected within different time scales before entropy saturation, and the dynamics of the expansion.

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I. INTRODUCTION

The microscopic foundations of thermodynamics are well established using the Gibbs hypothesis of statistical ensembles maximizing the Shannon entropy[1].When the thermodynamic limit can be taken, the various Gibbs ensembles for infinite systems converge to a unique thermodynamic equilibrium [28]. However, many systems studied in physics do not correspond to this mathematical limit of infinite systems[13] and, in fact, finite systems are now, per se, a subject of a very intense research activity, from metallic clusters[3, 4] to Bose condensates[5, 6], from nanoscopic systems[7] to atomic nuclei [8, 9] and elementary particles[10]. The question thus arises: can the equilibrium of a finite systems be defined.

A priori, the Gibbs concept of statistical ensembles of replicas which is applicable for an arbitrary number of particles, seems an ideal tool to define the thermodynamics of finite systems. However, in a finite system the various Gibbs ensembles are not equivalent[11] and lead to different equilibria which physical meaning and relevance has to be investigated. In the different physical cases, which in the following encompass both the case of isolated systems and of systems in contact with a finite or infinite reservoir[29], the identification of the relevant statistical ensemble is a key issue.

From a macroscopic point of view, a common interpretation of a statistical ensemble is an infinite collection of infinite subsystems of the studied infinite system in a specific thermodynamic situation. The required independence of the different subsystems is insured by the thermodynamic limit. Within this interpretation, a single system can be considered as a statistical ensemble and thus can be discussed in terms of equilibrium. This kind of equilibrium is not relevant for a finite system since i) the interface interactions between subsystem cannot be neglected, ii) the procedure of coarse-graining modifies the entropic properties of the system and iii) a finite system does not lead to an infinite ensemble of subsystems. In fact a single realization of a finite system cannot be discussed in statistical physics terms.

An alternative viewpoint is given by the Boltzmann ergodic assumption. In this interpretation the statistical ensemble represents the collection of successive snapshots of a physical system evolving in time. The equivalence between this time average and the Gibbs ensemble is then insured by the ergodic theorem [30]. This interpretation however suffers from important drawbacks. First, not only a proof of the ergodic hypothesis under fairly general conditions is lacking, but even for a truly ergodic Hamiltonian, a finite time experiment may very well achieve ergodicity only on a subspace of the total accessible phase space[14]. Moreover, ergodicity applies to confined systems and thus it requires the definition of boundary conditions when the thermodynamic limit does not apply. Then the statistical ensemble in general explicitly depends on the boundary conditions and we will discuss in this article that an exact knowledge of the boundary corresponds to an infinite information and is therefore hardly compatible with the very principles of statistical mechanics, as a reduction of the many body information to a (small) number of state variables.

Finally, in many physical situation the ergodicity ideas do not apply. Indeed, many physics experiments do not follow the time evolution of a single system, but rather concern averages over a great number of events, i.e. of physical replicas of systems experimentally prepared or sorted in similar way which are then observed at a given time. In such a context there is a priori no connection between the measuring time and the time it takes for an ergodic system to visit evenly the energy shell. Moreover, the systems experimentally accessible are often not confined but freely evolve in the vacuum, as it is notably the case for atomic and nuclear clusters and high energy heavy ion collisions. These open transient finite systems are isolated but never stationary. The concept of a well defined stationary equilibrium, uniquely defined by the variables conserved by the dynamics in an hypothetical constraining box, is certainly not useful for these finite systems.

However statistical approaches, expressing the reduction of the available information to a limited number of collective observables, can still be of some pertinence for such complex many body systems [15]. The physical meaning of such statistical ensembles is different from the case of an ergodic system or a macroscopic coarse graining. The standard assumption is that the dynamics is sufficiently complex (chaotic or mixing)[16, 17, 18] such that, repeating an experiment many times, the ensemble of events dynamically populates a phase space in a "democratic" enough way such that the gross features of the ensemble of events are dominated by few collective variables. In this case, the maximum entropy postulate cannot be justified from the ergodic theorem but has to be interpreted as a minimum information postulate which finds its justification in the complexity of the dynamics independent of any time scale[1, 15].

This information theory approach is a very powerful extension of the classical Gibbs equilibrium: any arbitrary observable including time odd quantities can act as a state variable, and all statistical quantities as equations of state and phase diagrams can be unambiguously defined for any number of particles[19]. The price to be paid for such a generalization is that the density matrix continuously evolve in time as soon as the constraining observables are not restricted to conserved quantities, meaning that we have to take into account the time dependence of the process.

A well known example of application of the information theory to a dynamical process is given by time dependent mean field theories, which can be viewed as the solution of a maximum entropy variational problem under the time dependent constraint of the knowledge of all one body observables [15].

In this article, we develop an information theory approach to the physics of finite systems evolving in time. We show that such an approach provides a description of the thermalization process. In presence of non linear dynamics it may lead to deviation from the Boltzmann-like exponential distributions and thus might provide an explanation for the appearance of non-extensive statistics[2]. In a mean-field context this dynamical extension envolves the RPA matrix leading to the introduction the collective degrees of freedom. For unconfined systems, we will show that their finite size at a finite time can be accounted for by introducing, in the Shannon information, additional constraints describing the system's compactness (size and shape). This provides a natural solution to the boundary condition problem. The same formalism describes incompletely known boundary conditions, confinement by a potential, and unconfined self bound or unbound systems. The time dependence of the process naturally leads to the appearance of new time-odd constraints or collective flows. In the case of an ideal gas of particles or clusters we will show that the extension and flow constraints forms a closed algebra together with the energy operator allowing an exact description of the free expansion of the system in vacuum.

II. STATISTICAL EQUILIBRIA

Let us first recall the standard formalism of statistical equilibria which we will then extend to the case of time dependent processes involving finite systems.

In order to describe a statistical ensemble, we introduce either the classical density $\hat{D}\left(\vec{Q},\vec{P}\right)$ in the many-body phase space associated with all the particle positions $\vec{Q}=\{q_i\}$ and momenta $\vec{P}=\{p_i\}$ or the quantum density matrix $\hat{D}=\sum_{(n)}\left|\Psi^{(n)}\right\rangle\ p^{(n)}\ \left\langle\Psi^{(n)}\right|$ where $\left|\Psi^{(n)}\right\rangle$ are the state of the different events (n) and $p^{(n)}$ the associated occurrence probability. According to the Gibbs hypothesis, equilibria are maxima of the Shannon entropy[1]

$$S=-\mathrm{Tr}\hat{D}\log\hat{D}, \tag{1}$$

where Tr means an integral over the coarse-grained classical phase space, $\left(\vec{Q},\vec{P}\right)$, or the trace over the quantum Fock or Hilbert space of states $|\Psi\rangle$. In this article we implicitly use units such that the Boltzmann constant $k=1$.

When the system is characterized by L observables, $\vec{\hat{A}}=\{\hat{A}_\ell\}$, known in average $<\hat{A}_\ell>=\mathrm{Tr}\hat{D}\hat{A}_\ell$, one should maximize the constrained entropy

$$S'=S-\sum_\ell\lambda_\ell<\hat{A}_\ell>$$

where the $\vec{\lambda}=\{\lambda_\ell\}$ are L Lagrange multipliers associated with the L constraints $<\hat{A}_\ell>$. The Gibbs equilibrium is then given by

$$\hat{D}_{\vec{\lambda}}=\frac{1}{Z_{\vec{\lambda}}}\exp-\vec{\lambda}.\vec{\hat{A}}, \tag{2}$$

where $\vec{\lambda}.\vec{\hat{A}}=\sum_{\ell=1}^{L}\lambda_\ell\hat{A}_\ell$ and where $Z_{\vec{\lambda}}$ is the associated partition sum insuring the normalization of $\hat{D}_{\vec{\lambda}}$.

To interpret the Gibbs ensemble as resulting from the contact with a reservoir or to guarantee the stationarity of the equilibrium eq.(2), it is often assumed that the observables $\hat{A}_\ell$ are conserved quantities such as the energy $\hat{H}$ or the particle (or charge) numbers $\hat{N}_i$. However, there is no formal reason to limit the state variables to constants of the motion and, in fact, the introduction of non conserved quantities is a way to take into account some non ergodic aspects. Indeed, an additional constraint reduces the entropy, limiting the phase space and modifying the event distribution. This point will be developed at length in the next sections.

It should be noticed that the formalism recalled above encompass microcanonical thermodynamics[8] which can be obtained from the variation of the Shannon entropy eq.(1) in a fixed energy subspace with no external constraints. In this case the maximum of the Shannon entropy can be identified with the Boltzmann entropy

$$max\left(S\right)=\log W\left(E\right),$$

where W is the total state density with the energy E.

The microcanonical case can also be seen as a particular Gibbs equilibrium (2) for which both the energy and its fluctuation are constrained. This so called Gaussian ensemble in fact interpolates between the canonical and microcanonical ensemble depending upon the constraint on the energy fluctuation[12]. The same procedure can be applied to any conservation law so that the Gibbs formulation (2) can be considered as the most general statistical ensemble.

III. MULTIPLE TIME STATISTICAL ENSEMBLES

Eq. (2) represents the standard statistical description of a physical system at a given time. Indeed, if some of the observables $\hat{A}_\ell$ are not constants of motion, then the statistical ensemble (2) is not stationary, but will evolve in time. This specific role played by time stresses that this information theory "equilibrium" cannot be justified using the usual ergodic arguments, but through the fact that the global features of the replicas of the considered system are characterized, at a given time, by few observables, i.e. that the information is concentrated in few degrees of freedom. In many physical cases one can clearly identify a specific time ("freeze out" time) at which the information concentrated in a given observable is frozen (i.e. the observable expectation value ceases to evolve or presents a trivial dynamics). However this freeze out time may be fluctuating or different for different observables. For example for the ultra-relativistic heavy ion reactions two freeze-out times are discussed, one for the chemistry and one for the thermal agitation. To solve these questions we need to introduce time as an explicit variable and define a statistical ensemble constrained by informations coming from different times.

A. Formulation of the issue

Let us assume that the evolution of an ensemble can be written as

$$\partial_t \hat{D} = \mathcal{F}[\hat{D}], \tag{3}$$

where $\mathcal{F}[\hat{D}]$ is a functional of the density matrix $\hat{D}$. This is a very general dynamical evolution since it includes classical and quantal Hamiltonian evolutions

$$\partial_t \hat{D} = \{\hat{H}, \hat{D}\}, \tag{4}$$

where $\hat{H}$ is the system Hamiltonian and $\{.,.\}$ are Poisson bracket in classical physics and commutators divided by $i\hbar$ in quantum physics. Eq. (3) also includes non-linear approaches such as mean-field approximations and more generally variational treatments for which $\hat{H}$ is replaced by an effective operator which depends upon the actual state $\hat{D} : \hat{H} \rightarrow \hat{H}[\hat{D}]$. Eq. (3) also includes the stochastic extensions of such approaches, $\hat{D}$ being the ensemble average of the stochastic evolutions.

Let us now suppose that the different informations on the system, $< \hat{A}_\ell >$, are known at different times, t_ℓ:

$$< \hat{A}_\ell >_{t_\ell} = \mathrm{Tr}\hat{D}\left(t_\ell\right)\hat{A}_\ell.$$

A generalization of the Gibbs idea would be that at a time t the least biased state of the system corresponds to the maximum of the Shannon entropy, considering all informations as constraints. Causality arguments imply that this time t should be larger or equal to all the t_ℓ. It should be noticed that in the case of a Hamiltonian evolution (4) because the entropy is a constant of motion this remark has no implications and the maximization can be performed at any time leading to the very same result. In the case of dissipative systems the entropy grows and eventually saturates. In this case the Maximum Entropy principle has to be applied at the time of entropy saturation (or the observation time if it occurs before).

The maximization of the entropy at time t with the various constraints $< \hat{A}_\ell >_{t_\ell}$ known at former times t_ℓ corresponds to the free maximization of

$$\begin{aligned} S' &= S\left(t\right) - \sum_{\ell=1}^{L} \lambda_\ell < \hat{A}_\ell >_{t_\ell} \\ S' &= -\mathrm{Tr}\left(\hat{D}\left(t\right)\log\hat{D}\left(t\right) + \sum_{\ell=1}^{L}\lambda_\ell \hat{A}_\ell \hat{D}\left(t_\ell\right)\right), \end{aligned} \tag{5}$$

where the λ_ℓ are the Lagrange parameters associated with all the constraints.

B. Minimum information under fluctuating-time constraints

Let us first assume that the various times only slightly differ by $\delta t_\ell = t - t_\ell$, thus we can use the equation of motion (3) to link the various times by

$$\hat{D}\left(t_\ell\right) = \hat{D}\left(t\right) - \delta t_\ell \mathcal{F}[\hat{D}\left(t\right)]$$

in order to explicitly write the constrained entropy as a function of a unique density $\hat{D} = \hat{D}\left(t\right)$

$$S' = -\mathrm{Tr}\left(\hat{D}\left(\log\hat{D} + \sum_{\ell=1}^{L}\lambda_\ell\hat{A}_\ell\right) - \sum_{\ell=1}^{L}\delta t_\ell\lambda_\ell\hat{A}_\ell\mathcal{F}[\hat{D}]\right) . \tag{6}$$

Computing the variation $\delta S'$ of S' induced by a modification of the density matrix $\hat{D} \to \hat{D} + \delta\hat{D}$ we get

$$\delta S' = -\mathrm{Tr}\delta\hat{D}\left(\log\hat{D} + 1 + \sum_{\ell=1}^{L}\lambda_\ell\hat{A}_\ell + \sum_{\ell=1}^{L}\lambda_\ell\delta t_\ell\hat{B}_\ell[\hat{D}].\right),$$

where the operator $\hat{B}_\ell$ are related to $\hat{A}_\ell$ and to the functional derivative $\mathcal{M}_{[1,2]}[\hat{D}] = \partial\mathcal{F}_{[1]}[\hat{D}]/\partial\hat{D}^T_{[2]}$ by

$$\hat{B}_{[1]}[\hat{D}] = -\mathrm{Tr}_{[2]}\hat{A}_{[2]}\mathcal{M}_{[2,1]}[\hat{D}], \tag{7}$$

where the indices $[i]$ indicate the space over which the operators are acting and where $\hat{D}^T_{[1]}$ is the transposed matrix when it applies, i.e. in quantum mechanics. In this case, if we introduce a base $\{|I\rangle\}$ to explicit the trace, eq. (7) reads:

$$\hat{B}_{IJ}[\hat{D}] = -\sum_{KL}\hat{A}_{KL}\frac{\partial\mathcal{F}_{LK}[\hat{D}]}{\partial\hat{D}_{JI}}. \tag{8}$$

The minimum biased density matrix (solution of $\delta S' = 0$) is given by

$$\hat{D}_{\vec{\lambda}}\left(t\right) = \frac{1}{Z_{\vec{\lambda}}\left(t\right)}\exp - \sum_{\ell=1}^{L}\lambda_\ell\hat{A}'_\ell[\hat{D}_{\vec{\lambda}}\left(t\right)], \tag{9}$$

where we have introduced a modified observable

$$\hat{A}'_\ell[\hat{D}_{\vec{\lambda}}\left(t\right)] = \left(\hat{A}_\ell + \delta t_\ell\hat{B}_\ell[\hat{D}_{\vec{\lambda}}\left(t\right)]\right) \tag{10}$$

which takes into account the time difference between the various observations. The associated Lagrange parameters are defined by the equations of states

$$< \hat{A}_\ell >_{t_\ell} = \mathrm{Tr}\left(\hat{D}_{\vec{\lambda}}\left(t\right) - \delta t_\ell\mathcal{F}[\hat{D}_{\vec{\lambda}}\left(t\right)]\right)\hat{A}_\ell, \tag{11}$$

The partition sum is defined as

$$Z_{\vec{\lambda}}\left(t\right) = \mathrm{Tr}\exp - \sum_{\ell=1}^{L}\lambda_\ell\hat{A}'_\ell[\hat{D}_{\vec{\lambda}}\left(t\right)]. \tag{12}$$

The equation $< \hat{A}'_\ell >_t = -\partial Log Z_{\vec{\lambda}}(t)/\partial\lambda_\ell$ always holds but a similar relation between the equation of state (11) and the partition sum (12) is valid only if $\mathcal{F}[\hat{D}]$ is a linear functional of $\hat{D}$. In such a case $< \hat{A}_\ell >_{t_\ell} = < \hat{A}'_\ell >_t = -\partial Log Z_{\vec{\lambda}}(t)/\partial\lambda_\ell$.

The minimum information density matrix eq.(9) looks like a standard Gibbs equilibrium but this formal analogy hides important differences. Indeed the constraining observables are modified according to (10) which contains new operators $\hat{B}_\ell$. If the original observables $\hat{A}_\ell$ were time even, the operators $\hat{B}_\ell$ are time odd, and therefore correspond to non stationary situations.

This can be more easily seen if we interpret eq. (9) as an extended Gibbs equilibrium under the set of constraints $\{\hat{A}_\ell, \hat{B}_\ell\}$

$$\hat{D}_{\vec{\lambda},\vec{\nu}}(t) = \frac{1}{Z_{\vec{\lambda},\vec{\nu}}(t)} \exp - \sum_{\ell=1}^{L} \lambda_\ell \hat{A}_\ell - \sum_{\ell=1}^{L} \nu_\ell \hat{B}_\ell [\hat{D}_{\vec{\lambda},\vec{\nu}}(t)], \tag{13}$$

where the parameters ν_ℓ contains the time information $\nu_\ell = \delta t_\ell \lambda_\ell$.

Because of the possible $\hat{D}$ dependence of the $\hat{B}_\ell$ operators, the distribution $\hat{D}_{\vec{\lambda}}(t)$ might deviate significantly from the usual exponential behavior. This opens an interesting possibility to encounter non Gibbsian statistics. In the literature[2], non Gibbsian information kernels are usually derived from a modification of the entropy as, for example, in the case of a Tsallis distribution. Here these anomalous statistics might be obtained from the time dependence of the studied system. In the following sections we will elaborate more on this subject.

C. Hamiltonian evolution

Let us illustrate the above results in the case of a Hamiltonian evolution (4). Then the entropy is a constant of the motion $\dot{S} = -\mathrm{Tr}\left(\{\hat{H}, \hat{D}(t)\}(\log \hat{D} + 1)\right) = \mathrm{Tr}\left(\hat{H}\{(\log \hat{D} + 1), \hat{D}(t)\}\right) = 0$ so that the minimum biased trajectory is independent of the time t at which the entropy is maximized. Introducing

$$\hat{D}(t_\ell) = \hat{D}(t) - \delta t_\ell \{\hat{H}, \hat{D}(t)\},$$

and using the cyclic invariance of the trace (or the by part integration in the phase space integral for the classical case), eq.(6) can be written as

$$S' = -\mathrm{Tr}\left(\hat{D}\left(\log \hat{D} + \sum_{\ell=1}^{L} \lambda_\ell \hat{A}_\ell + \sum_{\ell=1}^{L} \delta t_\ell \lambda_\ell \{\hat{H}, \hat{A}_\ell\}\right)\right) . \tag{14}$$

In Eq. (14) we can introduce

$$\hat{A}'_\ell = \hat{A}_\ell + \delta t_\ell \{\hat{H}, \hat{A}_\ell\}$$

in agreement with the Heisenberg picture, in which the observables would evolve from time t_ℓ up to a common time t. The generalized information theory result, i.e. the extremum of the variation S', is given by

$$\hat{D}_{\vec{\lambda}}(t) = \frac{1}{Z_{\vec{\lambda}}(t)} \exp - \vec{\lambda}.\vec{\hat{A}}'. \tag{15}$$

In this case the $\hat{A}'$ operators do not depend on $\hat{D}$ so that the distribution (15) is similar to a standard Gibbs equilibrium. The Lagrange parameter λ_ℓ are defined by the constraints

$$< \hat{A}_\ell >_{t_\ell} = \mathrm{Tr}\hat{D}_{\vec{\lambda}}(t_\ell)\, \hat{A}_\ell = \mathrm{Tr}\hat{D}_{\vec{\lambda}}(t)\, \hat{A}'_\ell = -\partial_{\lambda_\ell} \log Z_{\vec{\lambda}}(t)\,.$$

Eq. (15) can also be interpreted as the introduction of additional constraints

$$\hat{B}_\ell = \{\hat{H}, \hat{A}_\ell\}$$

and additional Lagrange parameter ν_ℓ associated with the out of equilibrium minimum biased density matrix

$$\hat{D}_{\vec{\lambda},\vec{\nu}} = \frac{1}{Z_{\vec{\lambda},\vec{\nu}}} \exp - \vec{\lambda}.\vec{\hat{A}} - \vec{\nu}.\vec{\hat{B}}. \tag{16}$$

The equations of state are given by $< \hat{A}_\ell >_t = -\partial_{\lambda_\ell} \log Z_{\vec{\lambda},\vec{\nu}}(t)$ and $< \hat{B}_\ell >_t = -\partial_{\nu_\ell} \log Z_{\vec{\lambda},\vec{\nu}}(t)$. Then the specific case (15) is obtained requiring $\nu_\ell = \lambda_\ell \delta t_\ell$, the λ's being defined by the constraints $< \hat{A}_\ell >_{t_\ell} = < \hat{A}_\ell >_t + \delta t_\ell < \hat{B}_\ell >_t$.

D. Minimum information under multiple-time constraints

This procedure can be easily extended to longer time intervals. To do that, we have to integrate the evolution from t_ℓ to t

$$\hat{D}\left(t_\ell\right)=\hat{D}\left(t\right)-\int_{t_\ell}^{t}dt'\mathcal{F}[\hat{D}\left(t'\right)].$$

The variations of the density matrix at various times are related by

$$\delta\hat{D}\left(t'\right)=\delta\hat{D}\left(t\right)-\int_{t'}^{t}dt"\mathcal{F}[\hat{D}\left(t"\right)+\delta\hat{D}\left(t"\right)]-\mathcal{F}[\hat{D}\left(t"\right)],$$

which leads to the relation

$$\delta\hat{D}_{[1]}\left(t'\right)=\delta\hat{D}_{[1]}\left(t\right)-\int_{t'}^{t}dt"\,\mathrm{Tr}_{[2]}\frac{\partial\mathcal{F}_{[1]}[\hat{D}\left(t"\right)]}{\partial\hat{D}_{[2]}^{T}}\delta\hat{D}_{[2]}\left(t"\right),\tag{17}$$

where the indices $[i]$ indicates the space over which the operators are acting (see equation (7)). This equation can be integrated giving

$$\delta\hat{D}_{[1]}\left(t'\right)=\delta\hat{D}_{[1]}\left(t\right)-\sum_{p=1}^{\infty}\frac{(t-t')^p}{p!}\mathrm{Tr}_{[2]}\mathcal{M}_{[1,2]}^{(p)}\left(t,t'\right)\delta\hat{D}_{[2]}\left(t\right),$$

where the matrices $\mathcal{M}_{[1,2]}^{(p)}$ are defined iteratively by

$$\mathcal{M}_{[1,2]}^{(p+1)}\left(t,t'\right)\;=\;-\frac{p+1}{(t-t')^{p+1}}\int_{t'}^{t}dt"\,\mathrm{Tr}_{[3]}\frac{\partial\mathcal{F}_{[1]}[\hat{D}\left(t"\right)]}{\partial\hat{D}_{[3]}^{T}}\mathcal{M}_{[3,2]}^{(p)}\left(t,t"\right)\left(t-t"\right)^p.$$

with $\mathcal{M}_{[1,2]}^{(0)}=1$. If we introduce this expression into the constrained entropy S' eq.(5) to compute the variation $\delta S'$,we get

$$\delta S'=-\mathrm{Tr}\delta\hat{D}\left(t\right)\left(\log\hat{D}\left(t\right)+1+\sum_{\ell=1}^{L}\lambda_\ell\left(\hat{A}_\ell+\sum_{p=1}^{\infty}\frac{(t-t_\ell)^p}{p!}\hat{B}_\ell^{(p)}\left(t,t_\ell\right)\right)\right),$$

where the operator $\hat{B}_\ell^{(p)}$ are related to $\hat{A}_\ell$ and to the matrices $\mathcal{M}_{[1,2]}^{(p)}$ through

$$\hat{B}_{\ell_{[1]}}^{(p)}\left(t,t_\ell\right)=-\mathrm{Tr}_{[2]}\hat{A}_{\ell_{[2]}}\mathcal{M}_{[2,1]}^{(p)}\left(t,t_\ell\right).\tag{18}$$

In the special case of a Hamiltonian evolution, the operators $\hat{B}_\ell^{(p)}$ are simply $p-$uple commutators $\hat{B}^{(p)}=\{\hat{H},\hat{B}^{(p-1)}\}$ with $\hat{B}^{(0)}=\hat{A}$. Therefore in this special case they do not depend neither on time nor on $\hat{D}$. Coming back to the general case, as in eq.(10) above, we can introduce the new observable

$$\hat{A}'_\ell\left(t,t_\ell\right)=\hat{A}_\ell+\sum_{p=1}^{\infty}\frac{(t-t_\ell)^p}{p!}\hat{B}_\ell^{(p)}\left(t,t_\ell\right)$$

The minimum biased density matrix is given by

$$\hat{D}_{\vec{\lambda}}\left(t\right)=\frac{1}{Z_{\vec{\lambda}}\left(t\right)}\exp-\vec{\lambda}.\vec{\hat{A}}'\left(t,t_\ell\right).\tag{19}$$

where the partition sum $Z_{\vec{\lambda}}\left(t\right)=\mathrm{Tr}\exp-\vec{\lambda}.\vec{\hat{A}}'\left(t,t_\ell\right)$ insures the normalization of $\hat{D}_{\vec{\lambda}}\left(t\right)$. The Lagrange parameter λ_ℓ are defined by the constraints

$$<\hat{A}_\ell>_{t_\ell}=\mathrm{Tr}\left(\hat{D}_{\vec{\lambda}}\left(t\right)-\int_{t_\ell}^{t}dt'\;\mathcal{F}[\hat{D}_{\vec{\lambda}}\left(t'\right)]\right)\hat{A}_\ell,\tag{20}$$

which only for a linear dependence of $\partial_t \hat{D}$ on $\hat{D}$ such as in the particular case of a Hamiltonian evolution give back the standard expression for the equations of state $< \hat{A}_\ell >_{t_\ell} = -\partial_{\lambda_\ell} \log Z_{\vec{\lambda}}(t)$ since in this case $< \hat{A}_\ell >_{t_\ell} = \mathrm{Tr}\hat{D}_{\vec{\lambda}}(t)\, \hat{A}'_\ell(t, t_\ell) =< \hat{A}'_\ell >_t$. It is interesting to note that if the evolution is Hamiltonian, the $\hat{A}'_\ell$ represent the time evolution of the constraining observables $\hat{A}_\ell$ in the Heisenberg representation $\hat{A}'_\ell(t, t_\ell) = \hat{A}'_\ell(\Delta t_\ell) = e^{-i\Delta t_\ell \hat{H}} \hat{A}_\ell e^{i\Delta t_\ell \hat{H}}$ where $\Delta t_\ell = t - t_\ell$.

Coming back to the general case, as for eq.(9) above, eq. (15) can also be interpreted as the introduction of additional constraints $\hat{B}^{(p)}_\ell$ and additional Lagrange parameters $\nu^{(p)}_\ell$ associated with the time evolution of the system

$$\hat{D}_{\vec{\lambda},\vec{\nu}} = \frac{1}{Z_{\vec{\lambda},\vec{\nu}}} \exp -\vec{\lambda}.\hat{A} - \sum_{p=1}^{\infty} \vec{\nu}^{(p)}.\vec{\hat{B}}^{(p)}, \tag{21}$$

where the Lagrange parameter $\nu^{(p)}_\ell$ are related to λ_ℓ by $\nu^{(p)}_\ell = \frac{(t-t_\ell)^p}{p!}\lambda_\ell$.

It is important to notice that Eqs. (19) or (21) provide exact solution of the complete many body evolution problem eq.(3) with a minimum information hypothesis on the final time t having made a set of observations $< \hat{A}_\ell >$ at previous times t_ℓ. We can see from eq.(21) that in general an infinite amount of information, i.e. an infinite number of Lagrange multipliers are needed if we want to follow the evolution of the density matrix for a long time, or if the time interval between each constraint is long. However, if we are only interested in short time scales the series will rapidly converge. Moreover in the next sections we will show that different interesting physical situations exist, for which the series can be analytically summed up. In this case, a limited information (the knowledge of a small number of average observables) will be sufficient to describe the whole density matrix at any time, under the unique hypothesis that the information was finite at a given time.

In the next sections we will illustrate this theory with two representative examples: a dissipative non-Hamiltonian dynamics and a self consistent case.

E. Application: Brownian motion

The description of the dynamics of quantum systems interacting with their environment is, in general, a very difficult task due to the system-reservoir interaction that usually involves a huge or even an infinite number of degrees of freedom. The Liouville-von Neumann equation for the total closed system is therefore useless for a reasonable description. The standard prescription is then to construct effective equations of motion for the reduced density matrix of the system by tracing over the environmental variables in the exact dynamics. The resulting quantum master equation includes dissipative and stochastic terms that take into account the irrelevant degrees of freedom in an approximate way.

One prototype of system-reservoir models is the Caldeira-Leggett model [20] for a Brownian particle of mass m, with coordinate $\hat{r}$ and momentum $\hat{p}$, in a bath consisting of a large number of harmonic oscillators. After performing a series of approximations[20], the density matrix of the Brownian particle is found to satisfy the following Liouvillian quantum master equation :

$$\partial_t \hat{D} = \mathcal{F}[\hat{D}] = \frac{1}{i\hbar}\left[\frac{\hat{p}^2}{2m}, \hat{D}\right] - \frac{i\gamma}{\hbar}\left[\hat{r}, \left[\hat{p}, \hat{D}\right]_+\right] - \frac{d}{\hbar^2}\left[\hat{r}, \left[\hat{r}, \hat{D}\right]\right] \tag{22}$$

The first term describes the free Hamiltonian dynamics. The second term, proportional to the friction coefficient γ, is a dissipative term associated to the mean coupling to the bath. The last term, with the diffusion coefficient d satisfying the Einstein relation $d = 2m\gamma/\beta$ where β^{-1} is the bath temperature, describes thermal fluctuations.

Let us apply the general formalism of section III D to a one dimensional Brownian particle prepared, at a time t_0 , with a mean kinetic energy $< \hat{K} >_{t_0} =< \frac{\hat{p}^2}{2m} >_{t_0}$, and which is observed at a later time t. Following the procedure of section III D, the information theory ansatz for the density matrix $\hat{D}(t)$ is a generalized statistical equilibrium with the constraining observables $\hat{B}^{(0)} = \hat{K}$ and $\hat{B}^{(p)}_{[1]} = -\mathrm{Tr}_{[2]}\hat{B}^{(p-1)}_{[2]}\partial\mathcal{F}_{[2]}/\partial\hat{D}^T_{[1]}$. With the irreversible dynamics (22), we easily show that

$$\hat{B}^{(1)} = 4\gamma\hat{K} - \frac{d}{m} \tag{23}$$

$$\hat{B}^{(p)} = 4\gamma\hat{B}^{(p-1)} = (4\gamma)^{p-1}\,\hat{B}^{(1)} \tag{24}$$

Using (19), the density matrix $\hat{D}(t)$ can be written as

$$\hat{D}_\lambda(t) = \frac{1}{Z'_\lambda(t)} \exp -\lambda \hat{K}'(t),$$

where $Z'_\lambda(t) = \mathrm{Tr} \exp -\lambda \hat{K}'(t)$ and where the modified constraining operator $\hat{K}'(t)$ can be actually resumed as

$$\hat{K}'(t) = \sum_{p=0}^{\infty} \frac{(t-t_0)^p}{p!} \hat{B}^{(p)} = e^{4\gamma(t-t_0)} \hat{K} - \frac{d}{4m\gamma} \left(e^{4\gamma(t-t_0)} - 1 \right). \tag{25}$$

The Lagrange parameter λ fulfills the equation of state $< \hat{K}' >_t = -\partial_\lambda \log Z'_\lambda(t)$ which gives after an explicit calculation of the partition sum

$$\frac{1}{2\lambda} = e^{4\gamma(t-t_0)} < \hat{K} >_t . \tag{26}$$

Since the evolution Kernel $\mathcal{F}[\hat{D}]$ is a linear functional of $\hat{D}$, the relation $< \hat{K}' >_t = < \hat{K} >_{t_0}$ holds (see eq.(20)). Taking advantage of the explicit expression (25) of the observable $\hat{K}'(t)$ we get

$$< \hat{K} >_t = < \hat{K} >_{t_0} e^{-4\gamma(t-t_0)} + \frac{d}{4m\gamma} \left(1 - e^{-4\gamma(t-t_0)} \right) \tag{27}$$

This expression corresponds to the exact mean value of the kinetic term at time t, as deduced from the equation of motion of $< \hat{K} >$ induced by the quantum master equation (22)

$$\frac{d < \hat{K} >}{dt} = -4\gamma < \hat{K} > + \frac{d}{m}$$

which clearly shows the damping role played by γ and the fluctuation ensure by d.

Let us now interpret the above results. Since $\hat{K}'(t)$ is a combination of the unit and kinetic operator, the density matrix can be recasted as

$$\hat{D}_{\lambda(t)}(t) = \frac{1}{Z_{\lambda(t)\nu(t)}} \exp -\lambda(t)\nu(t) \hat{K},$$

with $\nu(t) = exp(4\gamma(t-t_0))$. In the above equation we have make explicit the fact that the Lagrange multiplier λ is time dependent as can be seen solving Eq. (26) with the help of Eq. 27. This density matrix can be interpreted as a canonical equilibrium with a time dependent temperature defined by $T^{-1}(t) = \lambda(t)\nu(t)$. Indeed the equation of state defining $\lambda(t)$ implies $T(t) = 2 < \hat{K} >_t$ which is the standard result for an ideal 1D gas. Using eq.(27) we can work out the time dependence of the temperature

$$T(t) = 2 < \hat{K} >_{t_0} e^{-4\gamma(t-t_0)} + \beta^{-1} \left(1 - e^{-4\gamma(t-t_0)} \right)$$

$T(t)$ exponentially relaxes from the initial temperature $2 < \hat{K} >_{t_0}$ to the bath temperature β^{-1} with the correct characteristic time $1/4\gamma$, in agreement with the exact dynamics[20].

Thus applying the generalized Gibbs ensembles for time dependent processes to the problem of a quantum particle in contact with a reservoir we have been able to describe the general evolution as a succession of canonical statistical ensembles correctly relaxing toward the expected equilibrium. This exemple illustrates the potential of the developed formalism to statistically describe time dependent out-of-equilibrium phenomena.

F. Application: Mean-field and non-linear dynamics

As an illustration of a non-linear dynamics, let us study the case of self-consistent approaches which are of the mean-field type. To be more specific, we consider a quantum system characterized by its one body density $\hat{\rho}$, which can either be seen as the density matrix projected over all particles but one ($\hat{\rho}_{[1]} = \mathrm{Tr}_{[2,\ldots,N]} \hat{D}_{[1,2,\ldots,N]}$) or the expectation value of a generic one body operator $\hat{\rho}_{I,J} = < a_J^+ a_I >$ where $a_J^+(a_I)$ are creation(anihilation) operators of a particle in the orbital $J(I)$. Since we are studying a one-body approach we will restrict the discussion to one-body operators $\hat{A}_\ell$.

The time dependent mean-field dynamics is given by

$$\partial_t \hat{\rho} = \{\hat{W}[\hat{\rho}], \hat{\rho}\}, \tag{28}$$

where $\hat{W}[\hat{\rho}]$ is the self-consistent mean-field Hamiltonian. Using a variational approach[15] $\hat{W}[\hat{\rho}]$ can be related to the functional derivative of the energy $E =< \hat{H} >$: $\hat{W}[\hat{\rho}]_{[1]} = \partial E/\partial \hat{\rho}^T_{[1]}$ i.e. $\hat{W}[\hat{\rho}]_{IJ} = \partial E/\partial \hat{\rho}^T_{JI}$. If we consider a small deviation from an equilibrium solution, $\hat{\rho} = \hat{\rho}_0 + \delta\hat{\rho}$ the dynamics of $\delta\hat{\rho}$ follows the time dependent linear response (RPA) equation[21]

$$\partial_t \delta\hat{\rho}_{[1]} = \{\hat{W}[\hat{\rho}], \delta\hat{\rho}\}_{[1]} + \left\{ \sum_{[2]} \hat{V}_{[1,2]}[\hat{\rho}]\delta\hat{\rho}_{[2]}, \hat{\rho} \right\}_{[1]}, \tag{29}$$

where $\hat{V}_{[1,2]} = \partial \hat{W}[\hat{\rho}]_{[1]}/\partial \hat{\rho}^T_{[2]}$, i.e. $\hat{V}_{IL,JK}[\hat{\rho}] = \partial \hat{W}[\hat{\rho}]_{IJ}/\partial \hat{\rho}_{KL}$, is interpreted as the residual interaction. It is more convenient to introduce the Liouville space, considering the density matrices $\hat{\rho}$ as vectors $\parallel \rho \gg$ of components $\alpha = (i, j)$ and one body operators $\hat{A}$ as dual vectors $\ll A \parallel$ using the scalar product $\ll A \parallel \rho \gg = \mathrm{Tr}\hat{A}^+\hat{\rho}$ [31]. In this representation the dynamics of $\delta\hat{\rho}$ can be written[22]

$$i\partial_t \parallel \delta\rho \gg = \mathcal{H} \parallel \delta\rho \gg = (\mathcal{W} - \mathcal{N}\,\mathcal{V}) \parallel \delta\rho \gg \tag{30}$$

where the RPA matrix $\mathcal{H}$ has a commutator structure $\mathcal{W} \parallel \cdot \gg = \parallel [W, \cdot] \gg$, $\mathcal{N} \parallel \cdot \gg = \parallel [\rho, \cdot] \gg$ and $\mathcal{V} \parallel \cdot \gg = \parallel \frac{\partial W}{\partial \rho^T} \cdot \gg$.

It is easy to verify that the matrix $\mathcal{M}_{[1,2]} = \partial \mathcal{F}_{[1]}/\partial \hat{\rho}^T_{[2]}$ introduced in section III D is $-i$-times the RPA matrix $\mathcal{H}$

$$i\mathcal{M}_{IJ,KL} = \mathcal{H}_{IJ,KL} = \hat{W}_{IK}\delta_{LJ} - \delta_{IL}\hat{W}_{KJ} + \hat{V}_{IL,MK}\hat{\rho}_{MJ} - \hat{\rho}_{IM}\hat{V}_{ML,JK}$$

while the new operators $\hat{B}_\ell$ introduced to take into account the propagation of the information $< \hat{A}_\ell >$ over the time interval $\delta t_\ell = t - t_\ell$ are given by

$$\ll B_\ell \parallel = i \ll A_\ell \parallel \mathcal{H} = i \ll A_\ell \parallel (\mathcal{W} - \mathcal{N}\mathcal{V}) \tag{31}$$

To get a deeper insight into this relation, let us introduce the energies ω_ν and eigenstates $\delta\hat{\rho}_\nu$ of the RPA matrix [32]

$$\omega_\nu \parallel \delta\rho_\nu \gg \;=\; \mathcal{H} \parallel \delta\rho_\nu \gg \tag{32}$$

$$\ll C_\upsilon \parallel \mathcal{H} \;=\; \omega_\nu \ll C_\upsilon \parallel \tag{33}$$

where $\ll C_\upsilon \parallel$ represents the dual basis $\ll C_{\upsilon'} \parallel \delta\rho_\nu \gg = \delta_{\nu'\nu}$. The operators $\hat{B}_\ell$ can be expressed as

$$\ll B_\ell \parallel = i \sum_\nu \omega_\nu \ll A_\ell \parallel \delta\hat{\rho}_\nu \gg \ll C_\upsilon \parallel \tag{34}$$

Expanding the $\ll A_\ell \parallel$ over the same basis

$$\ll A_\ell \parallel = \sum_\nu \ll A_\ell \parallel \delta\hat{\rho}_\nu \gg \ll C_\upsilon \parallel \tag{35}$$

we observe that $\hat{A}_\ell$ and $\hat{B}_\ell$ are akin to conjugated operators. To make this relation more explicit let us assume that the operator $\hat{A}_\ell$ excites mainly one state ν_ℓ with a real frequency ω_ν with an excitation amplitude $\ll A_\ell \parallel \delta\hat{\rho}_{\nu_\ell} \gg = a_{\nu_\ell}$. Taking care of the fact that RPA eigenstates appears by pairs[21], $\hat{A}_\ell$ and $\hat{B}_\ell$ can be written as (see appendix C for details)

$$\hat{A}_\ell \;=\; a_{\upsilon_\ell}\hat{C}_{\upsilon_\ell} + a^*_{\upsilon_\ell}\hat{C}^+_{\upsilon_\ell} \tag{36}$$

$$\hat{B}_\ell \;=\; i\omega_{\nu_\ell} a_{\upsilon_\ell}\hat{C}_{\upsilon_\ell} - i\omega_{\nu_\ell} a^*_{\upsilon_\ell}\hat{C}^+_{\upsilon_\ell} \tag{37}$$

If $\hat{A}_\ell$ is interpreted as a collective coordinate associated with the creation of a collective mode through the $\hat{C}^+_{\upsilon_\ell}$ operator, then the extra constraint $\hat{B}_\ell$ taking care of the time dependence has the structure of the associated momentum.

It is interesting to notice that if the RPA matrix does not evolve in time, the above treatment can be iterated to propagations over a finite time t. In this case $\ll B_\ell^{(p+1)} \| = i \ll B_\ell^{(p)} \| \mathcal{H}$ so that if we consider a single mode

$$\hat{B}_\ell^{(2p)} = \left(-\omega_{\nu_\ell}^2\right)^p \hat{A}_\ell \tag{38}$$

$$\hat{B}_\ell^{(2p+1)} = \left(-\omega_{\nu_\ell}^2\right)^p \hat{B}_\ell \tag{39}$$

then the time dependence of the process can be accounted through a simple time dependence of the constraining operator

$$\hat{A}'_\ell(t) = \hat{A}_\ell \cos\omega_{\nu_\ell}(t - t_\ell) + \hat{B}_\ell \omega_{\nu_\ell}^{-1} \sin\omega_{\nu_\ell}(t - t_\ell).$$

which represents an oscillation in the RPA collective phase space $\hat{A}_\ell$ and $\hat{B}_\ell$.

Thus applying the proposed formalism to non-linear dynamics we have shown that the Gibbs ensembles description for time dependent processes can take into account new degrees of freedom. In the mean-field example, the RPA modes appear naturally and the generalized ensemble correctly describe their collective oscillation. This demonstrates how the developed formalism allows to go beyond the standard approaches to take into account dynamical aspects in a statistical manner.

IV. UNBOUND SYSTEMS AND THE DYNAMICS OF THE EXPANSION

An interesting application of the developed formalism is given by the case of finite systems in the presence of a continuum. For such physical systems the boundary condition problem is far from being trivial as we discuss below. We will show that the only consistent way to describe the boundary of unbound systems is to introduce in the Gibbs equilibrium at least one observable related to the system's extension (size and shape). Since these observables are not constants of the motion, such states are not stationary: in the absence of a confining force, the size of the system increases with time and collective flows are generated. An especially relevant physical case is given by nuclear collisions [9, 26] which produce a transient correlated high density state that subsequently freely expands in the vacuum. We will show that the out of equilibrium expansion can be accounted for at any time within a finite amount of information, with the natural emergence of time odd collective flow observables among the state variables.

A. Boundary condition problem

The information theory formalism is valid for any system size and thus can be, a priori, applied to finite systems. However, as soon as one $\hat{A}_\ell$ (e.g. $\hat{H}$) contains differential operators such as a kinetic energy, the standard Gibbs equilibrium eq. (2) is is a priori not defined, unless boundary conditions are specified. The same is true for microcanonical thermodynamics, since this latter can be seen as a special case of the more general Gibbs formalism. Boundary conditions are irrelevant at the thermodynamic limit (when it exists), or if the system is bound: in both cases the definition of a boundary corresponds to negligeable surface effects. However, in a finite system in the presence of a continuum this is never the case, and in this respect the statistical physics of small unbound systems is ill-defined.

1. *Systems in an external potential*

Physical situations occur in which an external potential is used to confine the system, as for recent studies of bosons or fermions in traps. In this case boundary conditions are not a problem since the confinement is directly insured by the external potential and the boundaries can be rejected to infinity as is the case of self bound systems.

However, the external potential directly appears in the system Hamiltonian and thus it is clear that the statistical properties of the system directly depend upon the considered potential. For example, systems are often trapped in a one body harmonic potential well $\hat{U} = \sum_n \hat{u}_n$ where the sum runs over all the particles n and where $\hat{u} = k\hat{r}^2/2$. The corresponding canonical ensemble reads

$$\hat{D}_{\beta,k} = \frac{1}{Z_{\beta,k}} \exp -\beta(\hat{H} + k\hat{R}^2/2), \tag{40}$$

where $\hat{R}^2 = \sum_n \hat{r}_n^2$ is the total radius squared.

We can see that the confinement via a potential is equivalent to an extra constraint defining the compactness of the system $\hat{R}^2$ through the introduction of a Lagrange multiplier given by the oscillator strength.[33]

2. Systems in a fictitious box

In the absence of a physical constraining potential, systems presenting states in the continuum are often confined through boundary conditions: a fictitious container is introduced in the theoretical description of unbound systems to limit the Hilbert space in order to be able to define a statistical ensemble [23]. The introduction of such an unphysical box not only directly affects the energy spectrum and thus the thermodynamics properties of the system, but also leads to an intrinsic inconsistency of the statistical theory, as we now show.

Let us write the eigenvalue problem for an Hamiltonian operator $\hat{H}$ containing a non-local term such as the kinetic energy. To be solved we must specify boundary conditions which directly modify the non-local operators. As an example, let us consider the standard case of the annulation of the wavefunction on the surface S of a containing box V. Introducing the projector, $\hat{P}_S$, over the surface S and its exterior, the boundary conditions reads $\hat{P}_S \left|\Psi\right\rangle = 0$ or, using $\hat{P}_S^2 = \hat{P}_S$, $\left\langle\Psi\right| \hat{P}_S \left|\Psi\right\rangle = 0$. The eigenvalue equation is then equivalent to a variational principle where the boundary and the normalization constraints have to be taken into account through the introduction of two Lagrange multipliers b_S and E

$$\delta\left(\left\langle\Psi\right| \hat{H} \left|\Psi\right\rangle - E(\left\langle\Psi\right. \left|\Psi\right\rangle - 1) - b_S \left\langle\Psi\right| \hat{P}_S \left|\Psi\right\rangle\right) = 0. \tag{41}$$

leading to a modified Schrödinger equation

$$\hat{H} \left|\Psi_{ES}\right\rangle - b_S \hat{P}_S \left|\Psi_{ES}\right\rangle = E \left|\Psi_{ES}\right\rangle \tag{42}$$

Equation (42) shows that the energy E and wavefunction $\left|\Psi_{ES}\right\rangle$ directly depend upon the boundary conditions.

Let us now extend this discussion to mixed states. The boundary condition $\hat{P}_S \left|\Psi^{(n)}\right\rangle = 0$ is exactly equivalent to the extra constraint $< \hat{P}_S >= \mathrm{Tr}\hat{D}\hat{P}_S = 0$. If we note again $\vec{\hat{A}}$ the observables characterizing a given equilibrium, the density matrix including the boundary condition reads

$$\hat{D}_{\vec{\lambda}S} = \frac{1}{Z_{\vec{\lambda}S}} \exp - \vec{\lambda}.\vec{\hat{A}} - b_S \hat{P}_S \tag{43}$$

which shows that the thermodynamics of the system does not only depend on the Lagrange multiplier b_S, but on the whole surface S.

For the very same global features such as the same average particle density or energy, we will have as many different thermodynamics as boundary conditions. More important, to specify the density matrix, the projector $\hat{P}_S$ has to be exactly known and this is in fact impossible. The nature of $\hat{P}_S$ is intrinsically different from the usual global observables $\hat{A}_\ell$. At variance with the $\hat{A}_\ell$, $\hat{P}_S$ is a many-body operator which does not correspond to any physical measurable observable. The knowledge of $\hat{P}_S$ requires the exact knowledge of each point of the boundary surface while no or few parameters are sufficient to define the $\hat{A}_\ell$. This infinity of points corresponds to an infinite amount of information to be known to define the density matrix (43). This requirement is in contradiction with the statistical mechanics principle of minimum information. Thus eq.(43) is unphysical.

This incoherence should be solved by a statistical treatment of our knowledge on the boundary condition. The density matrix should be an average over the boundary surfaces of $\hat{D}_{\vec{\lambda}S}$ weighted by the associated boundary probability derived applying information theory on our actual knowledge of the boundaries. A simple way to perform this task is presented in the next section.

3. Incomplete knowledge on the boundaries

One way to get around the difficulties encountered to take into account our incomplete knowledge on the boundaries is to introduce a hierarchy of observables describing the size and shape of the matter distribution.

If the system is unbound, the unconstrained equilibrium corresponds to an infinitely expanded system. However, the relevant physical problem in general concerns the state of the system before this asymptotic stage, when it has only expanded to a finite volume. This transient stage is constrained by a finite size, i.e. a finite average of an observable related to the system's size.

For example, if only the average system size $< \hat{R}^2 >$ is known, information theory requires the introduction of one additional Lagrange multiplier imposing this information, i.e. one of the $\hat{A}_\ell$ describing the system is $\hat{R}^2$. [34] If the additional information reduces to the energy, the Lagrange multipliers associated with the state variables $< \hat{H} >$ and $< \hat{R}^2 >$ are respectively $\lambda_H = \beta = 1/T$, the inverse of a temperature and λ_{R^2}, which has the dimension of a pressure

when divided by a typical scale R_0 and by the temperature, $\lambda_{R^2} = \beta P R_0$. The minimum information principle implies

$$\hat{D}_{\beta,P} = \frac{1}{Z_{\beta,P}} \exp -\beta \left(\hat{H} + P R_0 \hat{R}^2 \right), \tag{44}$$

which is akin to an isobar canonical ensemble. It is interesting to remark that the term proportional to $\hat{R}^2$ can be equivalently viewed as a mean square radius constraint or as an harmonic external potential modifying the effective Hamiltonian of the system as in the equilibrium (40). Similarly the expectation value $< \hat{H} + P R_0 \hat{R}^2 >$ can be interpreted as an enthalpy or as a constrained energy.

A typical application of eq.(44) is given by the freeze-out hypothesis proposed for the unconfined transient finite systems produced in atomic or nuclear collisions[9, 26]. At a given time the main evolution (i.e. the main creation of entropy) is assumed to stop. Before this freeze-out time the evolution is assumed to be complex enough such that all the partitions compatible with common gross features are freely (i.e. with no bias) explored. After the freeze-out time, partitions are supposed to be essentially frozen because of the lack of interactions. Typically thermal and chemical equilibrium is assumed, meaning that the information on the energetics and particle numbers is limited to the observables $< \hat{H} >$ and $< \hat{N}_f >$ for the different species f [9, 23].

The freeze-out occurs when the system has expanded to a finite size. Then at least one measure of the system's compactness should be included among the collective variables characterizing the statistical ensemble. The limited knowledge of the system extension leads to a minimum biased density matrix given by eq.(44). [35]

Such an ensemble does not suffer from the drawbacks of models introducing a constraining box: i.e. both the arbitrariness of such a fictitious box and the conceptual problems of the statistical treatment of boundary conditions.

To conclude this section, we have shown that all the different ways to describe boundary conditions in finite unbound systems lead to the introduction of additional constraints in the set of relevant observables $\hat{A}_\ell$ describing the statistical ensemble. The more information are known on the spatial extension of the system, the more complex are the additional observables. In other words, only Gibbs equilibria with compactness constraints are physically meaningful when discussing small systems in the presence of continuum states. Since outside the thermodynamic limit statistical ensemble are never equivalent, the thermodynamics of finite unbound systems always depends on the compactness conditions.

B. Unconfined finite ideal gas

Let us first consider the case of a finite ideal gas, i.e. the Hamiltonian is reduced to the one body kinetic term

$$\hat{H} = \hat{K} \equiv \sum_n \frac{\vec{\hat{p}}_n^2}{2m} \equiv \frac{\vec{\hat{P}}^2}{2m}. \tag{45}$$

Let us assume that the first constraining observable is $\hat{A}_1 = \hat{K}$ and so the associated Lagrange multiplier is the usual inverse temperature β. As discussed in subsection IV A, any statistical ensemble is ill-defined unless boundary conditions are specified. In the case of an unbound system, one is forced to introduce additional observables constraining the spatial extension of the system to a finite size. This is a situation often encountered experimentally: a finite system of loosely interacting particles or clusters with a finite extension after an expansion during a limited time in an open space. The minimal assumption needed to characterize statistically the ensemble of states, is given by one single observable related to the size, e.g. the knowledge at a given time of the mean square radius $< \vec{\hat{R}}^2 >$ (with $\vec{\hat{R}}^2 = \sum_n \vec{\hat{r}}_n^2$). Then we have to introduce the constraining observable $\hat{A}_2 = \vec{\hat{R}}^2$ associated with a Lagrange multiplier λ_0 in the statistical description. The maximum entropy solution is given by

$$\hat{D}_{\beta\lambda_0} = \frac{1}{Z_{\beta\lambda_0}} \exp -\beta \sum_n \left(\frac{\vec{\hat{p}}_n^2}{2m} + \frac{\lambda_0}{\beta} \vec{\hat{r}}_n^2 \right). \tag{46}$$

Eq.(46) is akin to a system of non-interacting particles trapped in an harmonic oscillator potential with a string constant $k = 2\lambda_0/\beta$. From the partition sum, the EOS are easily derived. For example, in the classical case using the equipartition and the virial theorem it is easy to derive the system EOS for each particle $n = 1, \ldots, N$

$$\frac{< \vec{\hat{p}}_n^2 >}{2m} = \frac{\lambda_0}{\beta} < \vec{\hat{r}}_n^2 > = \frac{3}{2\beta},$$

i.e.

$$< \vec{\hat{p}}_n^2 >= \frac{3m}{\beta} \quad ; \quad < \vec{\hat{r}}_n^2 >= \frac{3}{2\lambda_0}.$$

Since in the presented derivation, the $\lambda_0 \vec{\hat{R}}^2$ term is not an external confining potential but only a finite size constraint , the minimum biased distribution (46) is not stationary ($\{\hat{H}, \hat{D}_{\beta\lambda_0}\} \neq 0$). The system represented by eq.(46) at a time t_0 will evolve in time according to the Hamiltonian (45).

The physical situation we are describing can be explicitly realized experimentally by taking a system in equilibrium in an harmonic trapping potential $k\vec{\hat{r}}_n^2/2$ and by suddenly removing the confining potential at a time t_0. After that, the non-interacting particles freely expand ballistically (see section IV A 1). In this case the information theory ansatz (46) with $\lambda_0 = k\beta/2$ describes the standard static equilibrium just before the trapping potential is removed, and is therefore the exact initial state. This is akin to the actual experimental procedure used in Bose condensates studies[5, 6]. This physical situation is also the picture underlying the freeze-out hypothesis used to describe data in heavy ion collisions (see section IV A 3). At a given time the system is supposed to occupy a given volume and to behave thereafter like an ideal gas of fragments or particles. At variance with experiments in traps, for collision experiments the minimum biased distribution (46) at time t_0 is only an ansatz, implying that other observables might be needed to correctly describe the density matrix at the initial time t_0. This more complicated case is studied in the next section.

What is common to both these situations, is that the state (46) will evolve in time. So let us apply the formalism developed in section III D assuming that $< \vec{\hat{R}}^2 >$ is known at a time t_0 while the system is observed at a later time t. Since energy is a trivial constant of any Hamiltonian motion, $\{\hat{H}, \hat{H}\} = 0$, we do not have to introduce a specific time for the observation of the energy.

According to section (III D) to take into account the time evolution, we must introduce additional constraining observables

$$\begin{aligned} \hat{B}_R^{(1)} &= \{\hat{H}, \vec{\hat{R}}^2\} = -\sum_n \frac{1}{m}\left(\vec{\hat{p}}_n \cdot \vec{\hat{r}}_n + \vec{\hat{r}}_n \cdot \vec{\hat{p}}_n\right) \\ \hat{B}_R^{(2)} &= \{\hat{H}, \hat{B}_R^{(1)}\} = \sum_n \frac{2\vec{\hat{p}}_n^2}{m^2}. \end{aligned}$$

Since $\{\hat{H}, \hat{B}_R^{(2)}\} = 0$, all the other $\hat{B}_R^{(p)}$ with $p > 2$ are zero. The above relations are valid both in quantum and classical mechanics. Then the most general density matrix corresponding to the time-dependent Gibbs ensemble is given by

$$\hat{D}_{\beta,\lambda_0}(t) = \frac{1}{Z_{\beta,\lambda_0}} \exp \sum_n -\beta'(t)\frac{\vec{\hat{p}}_n^2}{2m} - \lambda_0 \vec{\hat{r}}_n^2 + \frac{\nu_0(t)}{2}\left(\vec{\hat{p}}_n \cdot \vec{\hat{r}}_n + \vec{\hat{r}}_n \cdot \vec{\hat{p}}_n\right), \tag{47}$$

with

$$\beta'(t) = \beta + 2\lambda_0 (t - t_0)^2 / m \tag{48}$$

and

$$\nu_0(t) = 2\lambda_0 (t - t_0)/m. \tag{49}$$

Let us explicitly show that the density matrix (47) can be interpreted as a radially expanding ideal gas. Indeed the distribution can be written as

$$\hat{D}_{\beta,\lambda_0}(t) = \frac{1}{Z_{\beta,\lambda_0}} \exp \sum_n -\beta'(t)\frac{\left(\vec{\hat{p}}_n - m h_0(t)\vec{\hat{r}}_n\right)^2}{2m} - \lambda_0'(t)\vec{\hat{r}}_n^2 \tag{50}$$

where the Hubblian factor reads

$$h_0 = \frac{\nu_0(t)}{\beta'(t)} = \frac{2\lambda_0 (t - t_0)}{\beta m + 2\lambda (t - t_0)^2} \tag{51}$$

while the confining Lagrange multiplier is transformed into

$$\lambda'(t) = \lambda_0 - \frac{m}{2}\frac{\nu_0^2(t)}{\beta'(t)} = \frac{\lambda_0 \beta m}{\beta m + 2\lambda_0 (t-t_0)^2} \tag{52}$$

In the density matrix (50) the term $mh_0(t)\vec{\hat{r}}_n$ correcting the momentum can be interpreted as a collective motion produced by a radial velocity $h_0(t)\vec{\hat{r}}_n$. This proportionality of the velocity with $\hat{r}_n$ shows that the motion is akin to a self-similar Hubble expansion. As a consequence, when this collective motion is subtracted from the particle momentum, the density matrix (50) corresponds at any time to a standard equilibrium (46) in the local rest frame.

Computing the time evolution of the distribution (50) under the action of the Hamiltonian (45), it is easy to verify that the information theory ansatz (50) is, at every time t, the exact solution of an ideal gas initially trapped in an harmonic oscillator potential up to the time t_0, and then freely expanding in the vacuum after the confining potential has been suppressed. In this case the infinite information which is a priori needed to follow the large-time evolution of the density matrix according to eq.(21), reduces to the three observables $\vec{\hat{r}}^2$, $\vec{\hat{p}}^2$, $\vec{\hat{r}}\cdot\vec{\hat{p}}+\vec{\hat{p}}\cdot\vec{\hat{r}}$. Indeed these operators form a closed Lie algebra containing the Hamiltonian operator, implying that the exact evolution of (50) preserves it algebraic structure.

An easy way to follow this time dependence is to compute the evolution of the 3 averages $<\vec{\hat{r}}_n^2>$, $<\vec{\hat{p}}_n\cdot\vec{\hat{r}}_n+\vec{\hat{r}}_n\cdot\vec{\hat{p}}_n>$ and $<\vec{\hat{p}}_n^2>$. Using $\partial_t <\hat{A}>= -\{\hat{H},\hat{A}\}$ we can easily show that

$$\partial_t <\vec{\hat{r}}_n^2> = \frac{1}{m} <\vec{\hat{p}}_n\cdot\vec{\hat{r}}_n+\vec{\hat{r}}_n\cdot\vec{\hat{p}}_n>$$
$$\partial_t <\vec{\hat{p}}_n\cdot\vec{\hat{r}}_n+\vec{\hat{r}}_n\cdot\vec{\hat{p}}_n> = \frac{2}{m} <\vec{\hat{p}}_n^2> .$$

The energy being constant, $<\vec{\hat{p}}_n^2>$ is also constant so that the radial momentum $<\vec{\hat{p}}_n\cdot\vec{\hat{r}}_n+\vec{\hat{r}}_n\cdot\vec{\hat{p}}_n>$ linearly depends upon time while the motion of $<\vec{\hat{r}}_n^2>$ is uniformly accelerated. This evolution of the constraints corresponds the dynamics of β', ν_0 and λ' deduced above.

The description of the time evolution when considering unconfined finite systems has introduced a new phenomenon: the expansion. One should then consider a more general equilibrium of a finite-size expanding finite-systems with β', h_0 and λ_0' as free parameters. Then, if the observed minimum biased distribution at time t is coming from a confined system at time t_0, the three parameters β', h_0 and λ_0' should be linked to the time t_0, the initial temperature β^{-1} and the initial λ_0 by equations (48), (51) and (52)[25].

The important consequence of that is that radial flow is a necessary ingredient of any statistical description of unconfined finite systems in the presence of a continuum: the static (canonical or microcanonical) Gibbs ansatz in a confining box which is often employed[23] misses this crucial point. On the other hand, if a radial flow is observed in the experimental data, the formalism we have developed allows to associate this flow observation to a distribution at a former time when flow was absent. This initial distribution corresponds to a standard static Gibbs equilibrium in a confining harmonic potential, i.e. to an isobar ensemble. We will see in the following that more complex non-Hubblian flows can be associated with additional constraints on the matter distribution.

C. Deformed unconfined systems

The systems formed in many experimental situations, ranging from asymmetric atomic traps[6] to non-central or incompletely damped nuclear collisions[26], present an explicit deformation. The simplest one is of quadrupolar nature, and corresponds to a non-zero $<\hat{Q}_{20}>$ where $\hat{Q}_{20}$ is the standard quadrupole moment $\hat{Q}_{20} = \sum_n \hat{q}_{20_n}$ where the single particle operator reads $\hat{q}_{20_n} = 2\hat{z}_n^2 - (\hat{x}_n^2 + \hat{y}_n^2)$. Therefore, the constraining observable $\hat{Q}_{20}$ associated with the Lagrange multiplier λ_2 should be introduced in the definition of the out of (spherical) equilibrium statistical ensemble. In addition, following the procedure explained above to take into account the influence of the time dependence, this observable should be complemented by its multiple commutators with $\hat{H}$

$$\hat{B}_Q^{(1)} = \{\hat{H},\hat{Q}_{20}\} = -\frac{1}{m}\sum_n 2\hat{p}_{z_n}\hat{z}_n - \hat{p}_{x_n}\hat{x}_n - \hat{p}_{y_n}\hat{y}_n + (\vec{p}\leftrightarrow\vec{r}) \tag{53}$$

which is nothing but an asymmetric flow, and

$$\hat{B}_Q^{(2)} = \{\hat{H},\hat{B}_Q^{(1)}\} = \frac{2}{m^2}\sum_n 2\hat{p}_{z_n}^2 - \hat{p}_{x_n}^2 - \hat{p}_{y_n}^2, \tag{54}$$

a deformation in p space. Again, since $\{\hat{H}, \hat{B}_Q^{(2)}\} = 0$, all the other $\hat{B}_Q^{(p)}$ with $p > 2$ are zero.

Then the minimum biased density matrix characterized at a time t_0 by the compactness $< \vec{\hat{R}}^2 >$ associated with a Lagrange multiplier λ_0, a quadrupole deformation $< \hat{Q}_{20} >$ at a time t_2 imposed by a second Lagrange multiplier λ_2, and by an average energy $< \vec{\hat{P}}^2/2m >$, is given by

$$\begin{aligned}\hat{D}_{\beta,\lambda_0,\lambda_2}\ (t) = & \frac{1}{Z_{\beta,\lambda_0,\lambda_2}} \exp \sum_n -\beta'_z(t) \frac{\hat{p}_{z_n}^2}{2m} - \lambda_z \hat{z}_n^2 + \frac{\nu_z(t)}{2} \left(\hat{p}_{z_n}\hat{z}_n \mp \hat{z}_n \hat{p}_{z_n}\right) \cdot \\ & \exp \sum_n -\beta'_\perp(t) \frac{\vec{\hat{p}}_{\perp_n}^2}{2m} - \lambda_\perp \vec{\hat{r}}_{\perp_n}^2 + \frac{\nu_\perp(t)}{2} \left(\vec{\hat{p}}_{\perp_n} \cdot \vec{\hat{r}}_{\perp_n} + \vec{\hat{r}}_{\perp_n} \cdot \vec{\hat{p}}_{\perp_n}\right), \end{aligned} \tag{55}$$

where we have introduced the momentum $(\vec{\hat{p}}_{\perp_n})$ and coordinate $(\vec{\hat{r}}_{\perp_n})$ perpendicular to the deformation axis z. The distribution at a time t (55) is then function of the spatial deformation parameters $\lambda_z = \lambda_0 + 2\lambda_2$ and $\lambda_\perp = \lambda_0 - \lambda_2$. We can see that the kinetic energy is not determined by a unique temperature but by two different Lagrange parameters

$$\beta'_z(t) = \beta + 2(\lambda_0 (t-t_0)^2 + 2\lambda_2 (t-t_2)^2)/m \tag{56}$$

$$\beta'_\perp(t) = \beta + 2(\lambda_0 (t-t_0)^2 - \lambda_2 (t-t_2)^2)/m \tag{57}$$

Finally the deformed expansion parameters read

$$\nu_z(t) = 2(\lambda_0 (t-t_0) + 2\lambda_2 (t-t_2))/m \tag{58}$$

$$\nu_\perp(t) = 2(\lambda_0 (t-t_0) - \lambda_2 (t-t_2))/m. \tag{59}$$

The minimum biased density matrix (55) can also be written as a generalized equilibrium in the local rest frame

$$\hat{D}_{\beta,\lambda_0,\lambda_2}(t) = \frac{1}{Z_{\beta,\lambda_0,\lambda_2}} \exp \sum_n -\beta'_z(t) \frac{(\hat{p}_{z_n} - m h_z(t)\hat{z}_n)^2}{2m} - \lambda'_z \hat{z}_n^2 \tag{60}$$

$$\exp \sum_n -\beta'_\perp(t) \frac{\left(\vec{\hat{p}}_{\perp_n} - m h_\perp(t) \vec{\hat{r}}_{\perp_n}\right)^2}{2m} - \lambda'_\perp \vec{\hat{r}}_{\perp_n}^2 \tag{61}$$

where the Hubblian flow factors read

$$h_z = \frac{\nu_z(t)}{\beta'_z(t)}; \quad h_\perp = \frac{\nu_\perp(t)}{\beta'_\perp(t)}, \tag{62}$$

while the confining Lagrange multipliers are transformed into

$$\lambda'_z(t) = \lambda_z - \frac{m}{2}\frac{\nu_z^2(t)}{\beta'_z(t)}; \quad \lambda'_\perp(t) = \lambda_\perp - \frac{m}{2}\frac{\nu_\perp^2(t)}{\beta'_\perp(t)}. \tag{63}$$

Computing the exact time evolution of the density matrix (60), and using again the fact that for all k, representing both the particle and the axis labels, $\hat{p}_k^2$, $\hat{r}_k^2$ and $(\hat{p}_k\hat{r}_k + \hat{r}_k\hat{p}_k)$ form a closed Lie algebra, it is easy to demonstrate that the density matrix (60) is, at every time t, the exact solution of the dynamical evolution. For example, an ideal gas initially trapped in a quadrupoly deformed harmonic oscillator potential up to the time $t_0 = t_2$, and then freely expanding in the vacuum up to the time t exactly follows (60). The time t_2 start to play a role if the trapping potentials in different directions are not switched-off at the same time. For such a case the density (60) remains the exact solution.

It is interesting to note that the λ's are inversely proportional to the size of the system in coordinate space, and so are the produced flows. Thus the deformation in p space is larger in the narrower direction in the coordinate space.

Taking advantage of the commutator algebra of various functionals of the operators $\vec{\hat{p}}$ and $\vec{\hat{r}}$ this discussion can be generalized to more complex multipolar deformations and flows (see appendix A).

D. Role of an external potential

In many physical situations the Hamiltonian of the system does not reduce to a simple ideal gas, but also may contain explicitly a potential term $\hat{U} = \sum_n U\left(\vec{\hat{r}}_n\right)$, either coming from the interaction with some external field, or from a

self interaction treated at the mean-field level. In such a case the Hamiltonian becomes $\hat{H} = \sum_n \vec{\hat{p}}_n^2/2m + U\left(\vec{\hat{r}}_n\right)$. Considering the additional constraint $\vec{\hat{R}}^2$ it is easy to show that $\hat{B}_R^{(1)} = -\sum_n \frac{1}{m}\left(\vec{\hat{p}}_n \cdot \vec{\hat{r}}_n + \vec{\hat{r}}_n \cdot \vec{\hat{p}}_n\right)$ remains unchanged since $\left\{U\left(\vec{\hat{r}}_n\right), \vec{\hat{r}}_n^2\right\} = 0$. The difference starts at the second order, since in addition to the term $\sum_n 2\vec{\hat{p}}_n^2/m^2$, $\hat{B}_R^{(2)}$ contains

$$\{\hat{U}, \hat{B}_R^{(1)}\} = -\sum_n \frac{2\vec{\hat{r}}_n \cdot \vec{\nabla} U\left(\vec{\hat{r}}_n\right)}{m}.$$

For short time evolutions (up to the second order in $\delta t = t - t_0$) the minimum biased density matrix corresponds to a self similar flow in a modified potential

$$\hat{D}_{\beta,\lambda_0}(t) = \frac{1}{Z_{\beta,\lambda_0}} \exp \sum_n -\beta'(t) \left(\frac{\left(\vec{\hat{p}}_n - m h_0(t) \vec{\hat{r}}_n\right)^2}{2m} + \hat{U}' \right)$$

where the time dependent temperature β' and the Hubblian factor h_0 are given by eqs.(48),(51), and the effective potential $\hat{U}'$ is given by

$$\hat{U}' = \frac{\beta}{\beta'(t)}\hat{U} + \sum_n \frac{\lambda_0}{\beta'(t)}\vec{\hat{r}}_n^2 - \frac{\lambda_0 \delta t^2}{m\beta'(t)} \left(\frac{2\lambda_0 \vec{\hat{r}}_n^2}{\beta'(t)} + \vec{\hat{r}}_n \cdot \vec{\nabla} U\left(\vec{\hat{r}}_n\right) \right) \tag{64}$$

In the special case of an harmonic potential $U\left(\vec{\hat{r}}\right) = k\vec{\hat{r}}^2/2$ the solution can be exactly worked out at any arbitrary time. Indeed in this case the $\hat{B^{(p)}}$ operators read for $p \geq 1$

$$\begin{aligned} \hat{B}^{(2p)} &= \sum_n (-1)^p (2\omega)^{2p} \left(\frac{\vec{\hat{r}}_n^2}{2} - \frac{\vec{\hat{p}}_n^2}{2mk} \right) \\ \hat{B}^{(2p+1)} &= -\sum_n (-1)^p (2\omega)^{2p} \frac{\vec{\hat{p}}_n \cdot \vec{\hat{r}}_n + \vec{\hat{r}}_n \cdot \vec{\hat{p}}_n}{m} \end{aligned}$$

where $\omega^2 = k/m$. The distribution at time t reads

$$\hat{D}_{\beta',\lambda_0',\nu}(t) = \frac{1}{Z_{\beta',\lambda_0',\nu}} \exp \sum_n -\beta'(t) \frac{\vec{\hat{p}}_n^2}{2m} - \lambda_0'(t) \vec{\hat{r}}_n^2 + \frac{\nu(t)}{2m}\left(\vec{\hat{p}}_n \cdot \vec{\hat{r}}_n + \vec{\hat{r}}_n \cdot \vec{\hat{p}}_n\right),$$

where the temperature is oscillating in time

$$\beta'(t) = \beta - \frac{\lambda_0}{m} \frac{(\cos 2\omega(t - t_0) - 1)}{\omega^2}$$

as well as the effective constraining field

$$\lambda_0'(t) = \beta \frac{m\omega^2}{2} + \lambda_0 \left(1 + \frac{1}{2}(\cos 2\omega(t - t_0) - 1)\right)$$

and the collective radial velocity

$$\nu(t) = \lambda_0 \frac{\sin 2\omega(t - t_0)}{m\omega}.$$

Similar to the case of an ideal gas section IV B, this density matrix can be interpreted as a Gibbs equilibrium in the rest frame of a breathing system

$$\hat{D}_{\beta',\lambda'}(t) = \frac{1}{Z_{\beta',\lambda'}} \exp \sum_n -\beta'(t) \frac{\left(\vec{\hat{p}}_n - m h'(t) \vec{\hat{r}}_n\right)^2}{2m} - \lambda'(t) \vec{\hat{r}}_n^2 \tag{65}$$

where the Hubblian factor reads

$$h'(t) = \frac{\lambda_0}{\beta'(t)} \frac{\sin 2\omega (t - t_0)}{m\omega} \tag{66}$$

and the effective pressure is given by

$$\lambda'(t) = \lambda_0'(t) - \frac{\lambda_0^2}{2\beta'(t)} \frac{(\sin 2\omega (t - t_0))^2}{m\omega^2} \tag{67}$$

Due to the confining harmonic potential the distribution is periodic in time. The collective flow is oscillating but it is interesting to note that the velocity is at all times proportional to the radius. The expansion deviates from self similarity only in presence of an anharmonic potential or of finite range two body interactions, as it is shown in appendix B.

V. CONCLUSION

In this paper we have introduced an extension of Gibbs ensembles to account for time dependent constraints, in classical as well as in quantum mechanics. The formalism is developed for generic equations of motion and is illustrated on both Hamiltonian and dissipative time evolutions of the density matrix. We show that the time dependence imposes the introduction of new constraining observables. In the case of an Hamiltonian dynamics theses new relevant informations are the multiple commutators of the initial observable with $\hat{H}$. This leads to time odd constraints which can be interpreted as collective flows.

This formalism gives a statistical description of a system characterized by some relevant observables defined at a time at which the entropy has not reached its saturating value yet, as it may be the case in intermediate energy heavy ion reactions[26]. Another physical application concerns systems for which the relevant observables pertain to different times, as in high energy nuclear collisions where the kinetic energy seems to be still dissipated when the chemistry of the system is fixed[9] (i.e. systems presenting different freeze-out times for different observables).

An important result is that any statistical description of an unbound finite system must necessarily contain a local collective velocity term. Indeed the knowledge of the average spatial extension of the system at a given time, naturally produces a flow constraint at any successive times. This describes the dynamical expansion of the system. This is important for the transient unconfined systems formed in collisional processes which freely expand in vacuum. It may also describe out of equilibrium systems bound in a self consistent mean field or confined in traps. Conversely a collective flow measurement at a given time can be translated into an information on the system extension at a former time.

In the general case the time dependence of the density matrix can be accounted by introducing an infinite set of time even as well as time odd constraints and the relevant information (i.e. the number of independent relevant observables or state variables) rapidly increases with time. In some cases however the state variables form a closed Lie algebra, and the knowledge of a finite number of observables at a given time allows to predict the total density matrix at any successive time. This is notably the case of a system of particles interacting through polynomial one-body or two-body potentials. The simplest case is a system of particles or clusters thermalized in an harmonic oscillator which is suddenly taken off, and freely evolving in the vacuum afterwards. In this case the system experiences a self similar expansion at any successive time, and the exact time dependent density matrix is given by an isobar canonical Gibbs equilibrium in the local rest frame. This schematic example may have some relevance in the study of low energy nuclear collisions, where the so called freeze out hypothesis[23] describes the strongly interacting diluted nuclear system as an ideal gas of clusters[27]. The presented formalism provide a systematique treatment of the confinement and of the successive flow.

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VI. APPENDIX A: HIGHER MULTIPOLES DEFORMATIONS

The reasoning of section IV C can be extended to higher multipoles of rank k, typically considering the operators $\hat{B}_i^{(0)} = \sum_n \hat{r}_{i,n}^k$, where $\hat{r}_{i,n}$ is the ith component of the coordinate of the particle n. Then to have a complete

information on the system at any time we have to introduce k additional observables $\hat{B}_i^{(l)}, l = 1, \ldots, k$ given by

$$\hat{B}_i^{(l)} = \frac{(-1)^l}{(2m)^l} \frac{k!}{(k-l)!} \sum_n \sum_{s=0}^{l} \frac{l!}{s!(l-s)!} p_{i,n}^s r_{i,n}^{k-l} p_{i,n}^{l-s}$$

This produces non Hubblian flows and non Maxwellian local momentum distributions. For example a $\hat{B}^{(0)} = \sum_n \hat{x}_n^4$ tensorial deformation, which is part of an hexadecapole constraint, introduces the time dependent constraints $\hat{B}_x^{(1)} = -2\sum_n(\hat{p}_{x_n}\hat{x}_n^3 + \hat{x}_n^3\hat{p}_{x_n})/m$, $\hat{B}_x^{(2)} = 3\sum_n(\hat{p}_{x_n}^2\hat{x}_n^2 + 2\hat{p}_{x_n}\hat{x}_n^2\hat{p}_{x_n} + \hat{x}_n^2\hat{p}_{x_n}^2)/m^2$, $\hat{B}_x^{(3)} = -3\sum_n(\hat{p}_{x_n}^3\hat{x}_n + 3\hat{p}_{x_n}^2\hat{x}_n\hat{p}_{x_n} + 3\hat{p}_{x_n}\hat{x}_n\hat{p}_{x_n}^2 + \hat{x}_n\hat{p}_{x_n}^3)/m^3$, $\hat{B}_x^{(4)} = 24\sum_n p_n^4/m^4$. The first term can be interpreted as a cubic flow meaning that the expansion is non self-similar. The second term can be seen as a local reorganization of the temperature while the last one is an explicit deviation from the Gaussian distribution of velocities i.e. from a Maxwell distribution as expected from the Boltzmann factor of an ideal gas. The generalization to several dimensions, i.e. to constraints of the type $\hat{B}^{(0)} = \sum_n \hat{x}_n^{k_x}\hat{y}_n^{k_y}\hat{z}_n^{k_z}$ is tedious but straightforward. The $\hat{B}^{(l)}$ are linear combinations of products of $\hat{p}_x^i$, $\hat{p}_y^j$ and $\hat{p}_z^k$ with $\hat{x}^{i'}$, $\hat{y}^{j'}$ and $\hat{z}^{k'}$, with $i, j, k = 0, \ldots, l$ and $k_x = i' + i$, $k_j = j' + j$ and $k_z = k' + k$.

It is interesting to notice that considering a generic constraint $\hat{B}^{(0)} = \sum_n f(\vec{\hat{r}}_n)$, the first correction in time is $\hat{B}^{(1)} = -\frac{1}{2m}\sum_n \vec{\hat{p}}_n \cdot \vec{\nabla} f(\vec{\hat{r}}_n) + \vec{\nabla} f(\vec{\hat{r}}_n) \cdot \vec{\hat{p}}_n$ so that for short time fluctuations $(t - t_0) = \delta t$ the statistical ensemble reads (at the first order in δt)

$$\hat{D}_{\beta,\lambda}(t) = \frac{1}{Z_{\beta,\lambda}} \exp \sum_n -\beta \left(\frac{\left(\vec{\hat{p}}_n - \vec{A}\left(\vec{\hat{r}}_n\right)\right)^2}{2m} + U\left(\vec{\hat{r}}_n\right) \right)$$

with

$$\begin{aligned} \vec{A}\left(\vec{\hat{r}}_n\right) &= \delta t \vec{\nabla} U(\vec{\hat{x}}_n) \\ U\left(\vec{\hat{r}}_n\right) &= \frac{\lambda}{\beta} f(\vec{\hat{x}}_n) \end{aligned}$$

which is akin to an equilibrium of particles in the external scalar and vector field $\hat{U}$ and $\vec{\hat{A}}$.

VII. APPENDIX B: REAL GAS

Let us now study the case of a real gas with $\hat{H} = \hat{K} + \hat{V}$ with $\hat{V} = \sum_{nn'} V(\hat{r}_{nn'})$ a two body interaction depending only upon the relative distance $\hat{r}_{nn'} = \left|\vec{\hat{r}}_n - \vec{\hat{r}}_{n'}\right|$. Let us investigate the minimum biased distribution including a compactness observable $\vec{\hat{R}}^2$ known at a time t_R. V depending only upon $\hat{r}$, $\hat{B}_R^{(1)}$ remains unchanged: $\hat{B}_R^{(1)} = \{\hat{K}, \vec{\hat{R}}^2\} = -\frac{1}{m}\sum_n \vec{\hat{p}}_n \cdot \vec{\hat{r}}_n + \vec{\hat{r}}_n \cdot \vec{\hat{p}}_n$ while $\hat{B}_R^{(2)}$ contains an additional term

$$\{\hat{U}, \hat{B}_R^{(1)}\} = -\sum_{nn'} \frac{2\vec{\hat{r}}_n \cdot \vec{\nabla} V(\hat{r}_{nn'})}{m} = -\sum_{nn'} \frac{1}{m} \hat{r}_{nn'} \vec{\partial}_r V(\hat{r}_{nn'})$$

and thus reads

$$\hat{B}_R^{(2)} = \sum_n 2\vec{\hat{p}}_n^2/m^2 - \sum_{nn'} \frac{1}{m} \hat{r}_{nn'} \vec{\partial}_r V(\hat{r}_{nn'})$$

In case of an harmonic interaction the $\hat{B}_R^{(p)}$ operators only contain quadratic terms $\sum_n \vec{\hat{p}}_n^2$, $\sum_{nn'} \hat{r}_{nn'}^2$ and $\sum_{nn'} \vec{\hat{r}}_{nn'} \cdot \vec{\hat{p}}_{nn'}$, with $\vec{\hat{p}}_{nn'} = \vec{\hat{p}}_n - \vec{\hat{p}}_{n'}$. In this case the time evolution can be taken into account by a suitable time dependent reorganization of the temperature and the introduction of a time odd constraint, the radial flow. However, for any other interaction $\hat{B}_R^{(2)}$ modifies not only the temperature but also the two-body interaction. If we define $V'(\hat{r}) = V(\hat{r}) + \hat{r}\vec{\partial}_r V(\hat{r})/4$ and we work out the third order term:

$$\begin{aligned} \hat{B}_R^{(3)} &= \frac{2}{m^2} \sum_{nn'} \left\{ V(\hat{r}_{nn'}), \vec{\hat{p}}_n^2 \right\} - \frac{1}{2m^2} \sum_{nn'} \left\{ \vec{\hat{p}}_n^2, \hat{r}_{nn'} \vec{\partial}_r V(\hat{r}_{nn'}) \right\} \\ &= \frac{1}{m^2} \sum_{nn'} \vec{\hat{p}}_{nn'} \cdot \vec{\hat{r}}_{nn'} \frac{\vec{\partial}_r V'(\hat{r}_{nn'})}{\hat{r}_{nn'}} + \frac{\vec{\partial}_r V'(\hat{r}_{nn'})}{\hat{r}_{nn'}} \vec{\hat{r}}_{nn'} \cdot \vec{\hat{p}}_{nn'} \end{aligned}$$

we can see that the time dependence of the process induces an effective momentum dependent two-body interaction. An interesting phenomenon occurs at the level of the next order. Indeed while the kinetic energy term in the Hamiltonian leads to a first term in $\hat{B}_R^{(4)} = \{\hat{H}, \hat{B}_R^{(3)}\}$

$$\{\hat{K}, \hat{B}_R^{(3)}\} = \frac{1}{2m^3} \sum_{nn'} \left\{ \vec{\hat{p}}_n^2, \vec{\hat{p}}_n \cdot \vec{\hat{r}}_{nn'} \frac{\vec{\partial}_r V'(\hat{r}_{nn'})}{\hat{r}_{nn'}} + \frac{\vec{\partial}_r V'(\hat{r}_{nn'})}{\hat{r}_{nn'}} \vec{\hat{r}}_{nn'} \cdot \vec{\hat{p}}_n \right\}$$

which is again a akin to a two body interaction, the interaction part produces a three-body term

$$\begin{aligned}
\{\hat{V}, \hat{B}_R^{(3)}\} &= \frac{1}{m^2} \sum_{nn'n"} \left\{ V(\hat{r}_{nn"}), \vec{\hat{p}}_n \cdot \vec{\hat{r}}_{nn'} \frac{\vec{\partial}_r V'(\hat{r}_{nn'})}{\hat{r}_{nn'}} + \frac{\vec{\partial}_r V'(\hat{r}_{nn'})}{\hat{r}_{nn'}} \vec{\hat{r}}_{nn'} \cdot \vec{\hat{p}}_n \right\} \\
&= \frac{2}{m^2} \sum_{nn'n"} \vec{\partial}_r V(\hat{r}_{nn"}) \vec{\partial}_r V'(\hat{r}_{nn'}) \\
&= \frac{1}{m^2} \sum_{nn'n"} \vec{\partial}_r V(\hat{r}_{nn"}) \left(\frac{5}{4} \vec{\partial}_r V(\hat{r}_{nn'}) + \frac{\hat{r}_{nn'}}{4} \vec{\partial}_r^2 V(\hat{r}_{nn'}) \right)
\end{aligned}$$

VIII. APPENDIX C: DETAILS ABOUT THE RPA

In eq.(30) we have expressed the RPA matrix as $\mathcal{H} = \mathcal{W} - \mathcal{N}\mathcal{V}$ where the self consistent mean field is defined as $\mathcal{W} \parallel \cdot \gg = \parallel [W, \cdot] \gg$, the residual interaction $\mathcal{V} \parallel \cdot \gg = \parallel \frac{\partial W}{\partial \rho^T} \cdot \gg$ and the density operator $\mathcal{N} \parallel \cdot \gg = \parallel [\rho, \cdot] \gg$.

To show the hermiticity of these operators one should go back to the definition $\ll A \parallel \mathcal{B}^+ \parallel C \gg = (\ll C \parallel \mathcal{B} \parallel A \gg)^*$. In the case of $\mathcal{W}$ and $\mathcal{N}$, using $(TrC^+ [B, A])^* = TrA [B, C]$ valid when B is hermitian $B^+ = B$, we get $\ll A \parallel \mathcal{B}^+ \parallel C \gg = \ll A \parallel \mathcal{B} \parallel C \gg$. Concerning the residual interaction, using the hermiticity of $\hat{W}$ and its definition we can easily get an explicitly hermitian form $\mathcal{V}_{[1,2]} = \partial^2 E / \partial \hat{\rho}^*_{[1]} \partial \hat{\rho}^T_{[2]}$.

Then we have expressed the generalized constraints of the time dependent RPA problem in the small amplitude limit as

$$\hat{A}_\ell = a_{\upsilon_\ell} \hat{C}_{\upsilon_\ell} + a^*_{\upsilon_\ell} \hat{C}^+_{\upsilon_\ell} \tag{68}$$

$$\hat{B}_\ell = i\omega_{\nu_\ell} a_{\upsilon_\ell} \hat{C}_{\upsilon_\ell} - i\omega_{\nu_\ell} a^*_{\upsilon_\ell} \hat{C}^+_{\upsilon_\ell} \tag{69}$$

and we have interpreted $\hat{A}_\ell$ as a collective coordinate associated with the creation of a collective mode through the $\hat{C}^+_{\upsilon_\ell}$ operator, and $\hat{B}_\ell$ as the associated momentum.

Let us justify this interpretation.

If ω_ν is an eigenvalue of the RPA matrix correponding to the eigenstate $\delta\hat{\rho}_\nu$, it is easy to show that $\delta\hat{\rho}^+_\nu$ is solution of $\omega^*_\nu \parallel \delta\rho^+_\nu \gg = -\mathcal{H} \parallel \delta\rho^+_\nu \gg$ so that $\parallel \delta\rho^+_\nu \gg$ is also an eigenstate of the RPA matrix associated to $-\omega^*_\nu$. Thus RPA solutions can be grouped by pairs.

Then, because of the commutator structure of the dynamical equation, the RPA equation do not propagates the diagonal terms $\delta\hat{\rho}_{II}$, so we can focus on the off diagonal terms . Thus we can introduce a collective operator Q such that $\parallel \delta\rho \gg = \parallel [\rho, Q] \gg = \mathcal{N} \parallel Q \gg$. In fact the density variation $\delta\rho$ can be interpreted as produced by a unitary transformation generated by the operators Q and Q^+: $\hat{\rho} \to e^{-i\lambda(\hat{Q}+\hat{Q}^+)} \hat{\rho} e^{i\lambda(\hat{Q}+\hat{Q}^+)} = \hat{\rho} + i\lambda([\rho, Q] + [\rho, Q^+])$. Thus the relation holds $\omega_\nu \parallel Q_\nu \gg = \mathcal{N}^{-1}\mathcal{H}\mathcal{N} \parallel Q_\nu \gg$.

If $[W, \rho] = 0$, then $\mathcal{N}^{-1}\mathcal{H}\mathcal{N} = \mathcal{W} - \mathcal{V}\mathcal{N} = \mathcal{H}^+$ meaning that $\parallel Q_\nu \gg$ is an eigen vector of $\mathcal{H}^+$ associated with the eigenvalue ω_ν.This means that, when $[W, \rho] = 0$, ω^*_ν is also an eigenvalue of the RPA matrix and, since the RPA eigenvalues appears by pairs $-\omega_\nu$ is also a solution. Requiring the equality of these to solutions with the pair ω_ν and -ω^*_ν shows that ω_ν is real or purely imaginary and is associated with a second solution $-\omega_\nu$.

If we now introduce the dual basis $\ll C_\upsilon \parallel$ such that $\ll C_{\upsilon'} \parallel \delta\rho_\nu \gg = \delta_{\nu'\nu}$ and the associated closure relation $\sum_\nu \parallel \delta\rho_\nu \gg \ll C_\upsilon \parallel = 1$, the relation $\ll C_\upsilon \parallel \mathcal{H} = \omega_\nu \ll C_\upsilon \parallel$ is easily demonstrated. Then $\omega^*_\nu \parallel C_\nu \gg = \mathcal{H}^+ \parallel C_\nu \gg$ also holds showing that, when $[W, \rho] = 0$, $\hat{C}_\nu = \hat{Q}_\upsilon$ if ω_ν is real.

This shows that the dual of the eigenvector $\parallel \delta\rho_\nu \gg$ is the operator responsible of the excitation of the collective mode ω_ν as indicated in equation (69) with $a_{\upsilon_\ell} = \ll A_\ell \parallel \delta\hat{\rho}_\nu \gg$.

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[28] For infinite systems the discussion is now focused mainly on the issue of non-extensivity, linked to the introduction of entropies different from the Shannon one[2], and to the study of systems with long range interactions[3].

[29] When the system is finite the latter case deserves even more discussion since the factorization of the thermodynamics of the bath is not guaranteed out of the thermodynamic limit.

[30] For an isolated system described by an hamiltonian H, the ergodic picture defines a unique microcanonical equilibrium characterized by all the conserved quantities, the energy and other observable related to the symetries of H [8]. For a system in contact with a reservoir, we may get the different statistical ensembles depending on the conserved quantities characterizing the coupling with the bath.

[31] It should be noticed that in the Liouville space the measure is simply a projection $< \hat{A} >= \ll A \parallel \rho \gg$.

[32] Recall that if the unperturbed solution corresponds to a minimum in the energy surface and not to a maximum or to a saddle point, then the RPA eigenmodes are real[21].

[33] Writing eq.(40) we have implicitly assumed that the confining potential is known with an infinite accuracy. For realistic physical applications, the external potential should also be treated using information theory[15], and the statistical density matrix should be averaged over the distribution of k which minimizes the information (see appendix B).

[34] Depending upon the actual system studied, more observables describing its size or shape might be needed. Then, all those observables should be introduced as constraints in the minimization of the information in order to obtain an adequate statistical description.

[35] The ensemble of events dynamically prepared may be characterized by an information about size and shape more complex than the simple mean square root radius. In this case other constraints can be introduced such as $\hat{R}^4$ if the radii fluctuations are not maximal (i.e. are not maximizing the entropy, meaning that fluctuations are containing non-trivial information) or $\hat{Q}_2 = 2\hat{Z}^2 - \left(\hat{X}^2 + \hat{Y}^2\right)$ if the system is not spherical in average but has a finite quadrupole deformation.