Generalized Gibbs canonical ensemble: 
A possible physical scenario

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Abstract

After reviewing some fundamental results derived from the introduction of the generalized Gibbs canonical ensemble, \( \omega(E) = \exp\left[-\frac{\eta \Theta(E)}{Z(\eta)}\right] \), such as the called thermodynamic uncertainty relation \( \langle \delta \beta \delta E \rangle = 1 + \left( \frac{\partial^2 S}{\partial E^2} \right) \langle \delta E^2 \rangle \), it is described a physical scenario where such a generalized ensemble naturally appears as a consequence of a modification of the energetic interchange mechanism between the interest system and its surrounding, which could be relevant within the framework of long-range interacting systems.

Key words: Classical ensemble theory, Geometry and Thermodynamics, Negative heat capacities, Fluctuation theory.

Introduction

Conventional Thermodynamics and the standard Statistical Mechanics are inadequate to deal with the called nonextensive systems. Loosely speaking, the non extensive systems are all those systems non necessarily composed by a huge number of constituents, that is, they could be small or mesoscopic, where the underlying interactions have a long-range comparable with or larger than the characteristic linear dimension of the system, leading in this way to the existence of long-range correlations which do not support the statistical independence or separability of the large short-range interacting (extensive) systems. The available and increasingly experimental evidences on anomalies presented in the dynamical and macroscopic behavior in plasma and turbulent fluids [1234], astrophysical systems [56789], nuclear and atomic clusters [101112], granular matter [13] glasses [1415] and complex systems [16] constitute a real motivation for the generalization of these fundamental physical theories.
The present paper addresses a simple generalization scheme of the Statistical Mechanics for the Hamiltonian systems which starts from the Boltzmann-Gibbs Statistics and the consideration of geometric features of the microcanonical ensemble. As already shown in previous papers [17,18,19,20,21,22], such ingredients allow us a simple generalization of the formalism of the conventional Thermodynamics which is able to overcome all those difficulties related to the ensemble inequivalence phenomenon or the presence of negative heat capacities. This results have found an immediately application in the enhancing of the available Monte Carlo methods based on the canonical ensemble in order to deal with the existence of the first-order phase transitions [23,24]. The main interest of this work is to describe a possible application scenario of this generalized framework in the context of the open Hamiltonian systems.

The paper is organized as follows. Firstly, I shall consider in the next section a brief review of the present generalization scheme and some of their fundamental results, such as the concept of reparametrization invariance, the generalized Gibbs canonical ensemble, the thermodynamic uncertainty relation and its application for the enhancing of the available Monte Carlo methods based on the standard Statistical Mechanics. A possible physical scenario for the nature appearance of the generalized Gibbs canonical ensemble is analyzed in the section 2. Finally, some conclusions are given in the section 3.

1 A review of fundamental concepts and results

Let us limited in the sake of simplicity to the special case of classical Hamiltonian systems whose thermodynamic description can be performed starting from microcanonical basis by considering only the total energy $E = H_N (X)$ (defined on every point $X$ of the N-body phase space $\Gamma$). Let $\Theta_N (X) = \Theta [H_N (X)]$ be a bijective and differentiable function of the Hamiltonian $H_N (X)$. It is said that the function $\Theta = \Theta (E)$ is just a reparametrization of the energy. It is easy to verify that the microcanonical distribution function $\hat{\omega}_M (X)$ is reparametrization invariant [17,18,19]:

$$\hat{\omega}_M (X) = \frac{1}{\Omega (E)} \delta [E - H_N (X)] \equiv \frac{1}{\Omega (\Theta)} \delta [\Theta - \Theta_N (X)] .$$

The demonstration of the above identity follows directly from the properties of the Dirac delta function:

$$\delta [\Theta - \Theta_N (X)] = \left( \frac{\partial \Theta (E)}{\partial E} \right)^{-1} \delta [E - H_N (X)] \Rightarrow \Omega (\Theta) = \left( \frac{\partial \Theta (E)}{\partial E} \right)^{-1} \Omega (E) ,$$
where $\Omega (\Theta) = Sp \left\{ \delta [\Theta - \Theta_N (X)] \right\}$ is the microcanonical partition function in the $\Theta$ energy reparametrization, and $Sp [A (X)] = \int A (X) dX$, the phase space integration.

A direct consequence of this symmetry is the reparametrization invariance of the whole Physics within the microcanonical description, i.e.: the microcanonical average $\langle A \rangle = Sp \left\{ \hat{\omega}_M (X) A (X) \right\}$ of any microscopic observable $A (X)$ is reparametrization invariant, $\langle A \rangle (E) \equiv \langle A \rangle (\Theta)$. The microcanonical partition function $\Omega$ allows us the introduction of an invariant measure:

$$d \mu = \Omega (E) dE = \Omega (\Theta) d\Theta,$$

which leads to an invariant definition of the microcanonical entropy $S = \log W_\alpha$, being $W_\alpha = \int_{C_\alpha} d\mu$ and $C_\alpha$ a subset belonging to a suitable coarsed grained partition $\mathcal{Z}$ of the phase space $\Gamma$, $\mathcal{Z} = \left\{ C_\alpha \subset \Gamma; \bigcup_\alpha C_\alpha = \Gamma \right\}$, i.e.:

$$C_\alpha \equiv \left\{ X \in \Gamma : E_\alpha - \frac{1}{2} \delta \varepsilon \leq H_N (X) < E_\alpha - \frac{1}{2} \delta \varepsilon \right\}.$$

The coarsed grained na-ture of the microcanonical entropy can be dismissed whenever the interest system is large enough ($\delta \varepsilon \ll E$), so that, such a thermodynamic potential could be considered as a continuous scalar function $S (E) = S (\Theta)$. The above reasonings allow us to claim that the microcanonical description can be performed by using any reparametrization of the total energy since this geometrical feature does not involve a modification of the underlying Physics within this ensemble.

The convex or concave character of any scalar function depends on the specific reparametrization use for describe it. A trivial example is the concave function $s (x) = \sqrt{x}$ with $x > 0$, which turns a convex function $s (y) = y^2$ under the reparametrization change $x = y^4$ with $y > 0$. This remarkable observation allows us to claim that the convex or concave character of the entropy is not a property microcanonical relevant since the concavity can be arbitrarily modified by the consideration of energy reparametrizations.

However, the convex character of the microcanonical entropy in terms of the total energy has taken always as an indicator of the ensemble inequivalence within the Gibbs canonical ensemble:

$$\hat{\omega}_C (X) = \frac{1}{Z (\beta)} \exp \left[-\beta H_N (X)\right],$$

which obviously does not obey the reparametrization invariance of the microcanonical ensemble [11]. The discrepancy between them is explained by the different underlying physical conditions: microcanonical description corresponds to an isolated system, while the canonical one corresponds to an open system.

Inspired on the reparametrization invariance of the microcanonical descrip-
tion, some consequences of assuming the energy reparametrizations within the framework of the Boltzmann-Gibbs statistics were analyzed in previous papers \[18,19,20,21\], as example, the following generalization of the Gibbs canonical ensemble:

\[
\hat{\omega}_{GC}(X) = \frac{1}{Z(\eta)} \exp[-\eta \Theta_N(X)].
\]

(5)

A simple but remarkable consequence of the reparametrization invariance of the microcanonical description is the reparametrization invariance of the formal structure of the thermodynamic formalism \[21\], which could be easily shown throughout the relation between the canonical partition function \(Z\) and the microcanonical partition function \(\Omega\):

\[
Z(\eta) = \int \exp[-\eta \Theta(E)] \Omega(E) dE \equiv \int \exp[-\eta \Theta] \Omega(\Theta) d\Theta,
\]

(6)

which leads when the interest system is large enough to the following Legendre transformation in terms of the energy reparametrization \(\Theta\):

\[
P(\eta) \simeq \inf_{\Theta} \{\eta \Theta - S(\Theta)\},
\]

(7)

being \(P(\eta) = -\log Z(\eta)\) the Planck thermodynamic potential associated to the generalized Gibbs canonical ensemble \(5\). This result shows that many results of the Gibbs canonical ensemble \[14\] can easily extended to the generalized ensemble with a simple change of reparametrization \((E, \beta) \rightarrow (\Theta, \eta)\). Particularly, the ensemble inequivalence is now associated to the existence of convex regions of the microcanonical entropy \(S\) in terms of the energy reparametrization \(\Theta, \partial^2 S(\Theta) / \partial \Theta^2 < 0\). Obviously, this result clearly shows us that those inaccessible regions within the canonical description \(4\) become accessible within the generalized canonical ensemble \(5\) by using a suitable energy reparametrization \(\Theta(E)\). An direct application of this idea is just the generalization of the Metropolis importance sample algorithm \[25\] in order to deal with the ensemble inequivalence (see below).

A preliminary vision about the underlying physical conditions leading to the generalized canonical ensemble \(5\) is found in terms of the Information Theory \[26\]. The generalized ensemble follows from the use of the well-known Shannon-Boltzmann-Gibbs extensive entropy:

\[
S_e[p] = -\sum_k p_k \log p_k,
\]

(8)

and the imposition of the constrain:

\[
\langle \Theta \rangle = \sum_k \Theta(E_k) p_k,
\]

(9)

a viewpoint recently developed by Toral in the ref.\[20\]. The analogy with the Gibbs canonical ensemble clearly suggest us that the generalized canonical
ensemble (5) can be associated to the influence of certain *external apparatus* performing a control process on the interest system by keeping fixed the average (9) instead of the usual energy average with $\Theta(E) = \bar{E}$. In this case, the external control apparatus is just a more sophisticated version of the Gibbs thermostat, where the parameter $\eta$ plays a role completely analogous to the inverse temperature $\beta$.

Despite of the mathematical analogies, the physical relevance of the energy reparametrization $\Theta(E)$ and the generalized canonical parameter $\eta$ of the external control apparatus in general is unclear. A suitable way to understand their meaning is unexpectedly obtained when the generalized ensemble (5) is used during the Metropolis simulation [25] of the interest system: the use of the generalized canonical weight $\exp[-\eta \Delta \Theta]$ instead of the usual $\exp[-\beta \Delta E]$, where $\Delta \Theta = \Theta(E + \Delta E) - \Theta(E)$. Since $\Delta E \ll E$ when the interest system is large enough, $\Delta \Theta \simeq \partial \Theta(E)/\partial E \Delta E$, so that, the acceptance probability of a Metropolis move can be given by $p(E|E + \Delta E) \simeq \min \{1, \exp[-\tilde{\beta} \Delta E]\}$, where:

$$\tilde{\beta} = \eta \frac{\partial \Theta(E)}{\partial E}, \quad (10)$$

This result clearly indicates that in terms of the energetic interchange with the interest system, the *external control apparatus* (or generalized thermostat with parameter $\eta$) is almost equivalent to a Gibbs thermostat with an effective fluctuating inverse temperature $\tilde{\beta}$. Obviously, such an external control apparatus possesses a more active role than the usual Gibbs thermostat. It can be shown that the usual equilibrium condition between the inverse temperature $\hat{\beta}$ of the thermostat and the corresponding inverse temperature $\beta$ of the interest system takes place only in average, $\langle \beta \rangle = \langle \beta \rangle$, being:

$$\hat{\beta} = \frac{\partial S(E)}{\partial E}, \quad (11)$$

the microcanonical inverse temperature of the interest system [22].

A very important result is obtained by analyzing the correlation function between the effective inverse temperature $\beta$ of the generalized thermostat and the total energy $E$ of the interest system. The dispersion $\delta \beta = \beta - \langle \beta \rangle$ can be estimated when the interest system is large enough by using the equation (10) as follows:

$$\delta \beta = \eta \frac{\partial^2 \Theta(\bar{E})}{\partial E^2} \delta E \Rightarrow \langle \delta \beta \delta E \rangle = \eta \frac{\partial^2 \Theta(\bar{E})}{\partial E^2} \langle \delta E^2 \rangle, \quad (12)$$

where $\bar{E} = \langle E \rangle$, and $\delta E = E - \langle E \rangle$ is the energy dispersion of the interest.
system, which is related with the dispersion \( \delta \Theta = \Theta - \langle \Theta \rangle \) as follows:

\[
\langle \delta \Theta^2 \rangle = \left( \frac{\partial \Theta}{\partial E} \right)^2 \langle \delta E^2 \rangle. \tag{13}
\]

The reparametrization invariance allows us to derive the parameter \( \eta \) and the dispersion \( \langle \delta \Theta^2 \rangle \) from the microcanonical entropy in the reparametrization \( \Theta \) as follows:

\[
\eta = \frac{\partial S}{\partial \Theta}, \quad \langle \delta \Theta^2 \rangle = -\left( \frac{\partial^2 S}{\partial \Theta^2} \right)^{-1}, \tag{14}
\]

where \( \bar{\Theta} = \langle \Theta \rangle = \Theta \left( \bar{E} \right) \), and therefore:

\[-\left( \frac{\partial \Theta}{\partial E} \right)^2 \frac{\partial^2 S}{\partial \Theta^2} \langle \delta E^2 \rangle = 1 \text{ and } \langle \delta \beta \delta E \rangle = \frac{\partial^2 \Theta}{\partial E^2} \frac{\partial S}{\partial \Theta} \langle \delta E^2 \rangle. \tag{15}\]

The using of the transformation rule of the entropy Hessian:

\[
\frac{\partial^2 S}{\partial E^2} = \left( \frac{\partial \Theta}{\partial E} \right)^2 \frac{\partial^2 S}{\partial \Theta^2} + \frac{\partial^2 \Theta}{\partial E^2} \frac{\partial S}{\partial \Theta}, \tag{16}\]

allows us to condense the results expressed in the equation (15) in a final remarkable form:

\[
\langle \delta \beta \delta E \rangle = 1 + \frac{\partial^2 S}{\partial E^2} \langle \delta E^2 \rangle. \tag{17}\]

The thermodynamic relation (17) constitutes by itself a fundamental result which generalizes the fluctuation theory of the standard Statistical Mechanics. Generally speaking, the Thermodynamics theory deals with equilibrium situations where the total energy \( E \) of the interest system (microcanonical description) or the inverse temperature \( \beta \) of the thermostat (canonical description) is fixed. However, the equation (17) clearly shows that the generalized canonical ensemble (5) is just a natural theoretical framework for consider physical situations where both \( \beta \) and \( E \) fluctuate around their equilibrium values.

Taking into account the microcanonical extension of the heat capacity \( C \):

\[
C = \frac{dE}{dT} = -\left( \frac{\partial S}{\partial E} \right)^2 \left( \frac{\partial^2 S}{\partial E^2} \right)^{-1}, \tag{18}\]

the reader can understand that the relation (17) constitutes a suitable generalization of the well-known relation \( C = \beta^2 \langle \delta E^2 \rangle \) of the conventional Thermodynamics, which allows us to consider all those microcanonical states with a negative heat capacity \( C < 0 \) associated to the convex character of the microcanonical entropy. Ordinarily, such anomalous macrostates are hidden by
the ensemble inequivalence, which takes place as a consequence of the *incompatibility* of the ordinary restriction $\delta \beta = 0$ within the convex regions of the microcanonical entropy, $\partial^2 S / \partial E^2 > 0$. The thermodynamic relation in these cases leads to the following inequality:

$$\langle \delta \beta \delta E \rangle > 1,$$

which allows us to claim two remarkable conclusions: (1) *The anomalous macrostates with a negative heat capacity can be only accessed by using a generalized thermostat with a fluctuating inverse temperature*; (2) *The total energy of the interest system $E$ and the inverse temperature of the thermostat $\tilde{\beta}$ behave as complementary thermodynamical quantities within the regions of ensemble inequivalence*: the energy fluctuations $\delta E$ can not be reduced there without an increasing the fluctuations of the inverse temperature $\delta \beta$ of the generalized thermostat, and vice versa. This is the reason why the result expressed in the equation (17) can be referred as *thermodynamic uncertainty relation* [21], since it imposes obviously certain restriction to the determination of the microcanonical caloric curve $\beta$ versus $E$.

The reader can appreciated that the thermodynamic uncertainty relation (17) does not make any reference to the energy reparametrizations $\Theta (E)$, that is, there is no reference to the underlying geometric formalism where this result was derived from. Such a remarkable feature suggests us the general applicability of the thermodynamic relation (17) to the thermodynamic equilibrium between the interest system under the influence of thermostat. This far-reaching conclusion has a paramount importance in the generalization of all the available Monte Carlo methods based on the canonical ensemble in order to overcome all the difficulties related to the presence of the first-order phase transitions [24]. Apparently, the using of a generalized thermostat with a fluctuating inverse temperature can be easily combined with any Monte Carlo algorithm based on the canonical ensemble in order to account for all those thermodynamic states with a negative heat capacity.

A numerical evidence suggesting the generality of this idea is shown in the FIG[1] It shows a comparative study among the caloric curve $\beta (\varepsilon) = \partial s (\varepsilon) / \partial \varepsilon$ and the curvature $\kappa (\varepsilon) = \partial^2 s (\varepsilon) / \partial \varepsilon^2$ curves associated to the $q = 10$ states Potts model [27]:

$$H_N = \sum_{(ij)} (1 - \delta_{\sigma_i, \sigma_j}),$$

on a square lattice $N = L \times L$ with periodic boundary conditions and only nearest neighbor interactions by using different Monte Carlo methods ($\varepsilon = E / N$ and $s = S / N$ are the energy and the entropy per particles respectively). While the Swendsen-Wang cluster algorithm [28] is unable to account for the anomalous regions with a negative heat capacity by using the ordinary Gibbs thermostat, the use of a generalized thermostat with a fluctuating inverse temperature overcomes this difficulty. The reader can appreciated the remarkable
Fig. 1. Caloric $\beta(\varepsilon)$ and curvature $\kappa(\varepsilon)$ curves obtained from the Metropolis algorithm and the Swendsen-Wang cluster algorithm using thermostats associated to the generalized canonical ensemble (GCE) as well as the canonical ensemble (CE) for the $q = 10$ states Potts model with $L = 25$.

agreement between the results obtained from the use of the Metropolis importance sample and Swendsen-Wang cluster algorithm.

The presence of such anomalous regions in the thermodynamical description of the short-range interacting systems is an indicator of the occurrence of first-order phase transitions or phase coexistence phenomenon [10]. This feature is clearly illustrated in the FIG.2a where the coexisting phase are revealed as the bimodal character of the energy distribution function associated to the canonical description in the neighborhood of the critical temperature. Horizontal lines represent here the constancy of the inverse temperature of the Gibbs thermostat, $\tilde{\beta} = \text{const}$. Only those interception points of such horizontal lines with the microcanonical caloric curve $\beta(\varepsilon)$ exhibiting a nonnegative heat capacity are accessible within the canonical description. The constancy of the inverse temperature is replaced in the generalized canonical ensemble by the constancy of the generalized canonical parameter $\eta$, which leads to a dependence of the effective inverse temperature $\tilde{\beta} = \eta \partial \Theta(E)/\partial E$ of the generalized thermostat on the instantaneous value of the total energy of the interest system $E$, which is represented in the FIG.2b. The reader can notice that such a behavior of the generalized thermostat ensures the interception of only one point of the microcanonical curve, which eliminates the multimodal character of the energy distribution functions within this ensemble. Besides, all those inaccessible macrostates for the canonical ensemble become accessible by using the present generalized description. This remarkable observation allows us to claim that the phase coexistence phenomenon appears as a consequence of an inefficient control of the external apparatus (thermostat) which is unable to
Fig. 2. Caloric curve and energy distributions functions of the $q = 10$ states Potts model: Panel a) Phase coexistence phenomenon and regions of ensemble inequivalence within the Gibbs canonical description; Panel b) None of these features appear within the Generalized canonical description. The first-order phase transitions are avoidable anomalies within a thermodynamical description involving energy reparametrizations!

Access to all those admissible microstates of the isolated system (microcanonical description). Thus, the first-order phase transitions becomes avoidable thermodynamical anomalies whenever the energy reparametrizations are involved in the thermodynamical description, a fact explaining the success of any Monte Carlo algorithms based on the generalized canonical ensemble.
2 A possible physical scenario

Generally speaking, the generalized canonical description of a given system is very easy to simulate by using Monte Carlo methods. However, such a description could be more difficult to implement experimentally since the usual physical conditions of the environment lead to the relevance of the Gibbs canonical ensemble \([4]\) in the framework of the short-range interacting systems.

The previous reasonings do not mean that we can not conceive the applicability of the generalized canonical ensemble \([5]\) in certain experimental setup whenever the external ”control apparatus” performs a more active role than the one exhibited by the Gibbs thermostat (while the thermodynamical state of the Gibbs thermostat is practically unperturbed by the influence of the interest system under control, the generalized thermostat changes its effective inverse temperature \(\tilde{\beta}\) with the fluctuations of the total energy \(E\) of the interest system). In principle, there is not \textit{a priori} objection to the designing of certain experimental arrangement for the implementation of the generalized canonical ensemble \([5]\).

The way in which the surrounding affect the interest system is crucial for the relevance of the canonical description \([4]\). The well-known Gibbs argument is based on the separability among the interacting subsystem, which is supported by the presence of short-range interactions. The energetic contributions associated to the interactions among the subsystems are considered here as boundary effects which could be neglected when these subsystems are large enough. Obviously, \textit{none of the above conditions can be applicable whenever long-range correlations are involved.}

While the observation of the equilibrium thermodynamical states with a negative heat capacity in the short-range interacting systems can be only performed by considering special experimental conditions simulating a thermostat with a fluctuating inverse temperature, there exist a natural physical scenario where such an anomaly becomes a very usual behavior: \textit{the astrophysical systems.} The existence of equilibrium thermodynamical states with a negative heat capacity is well-known in the astrophysical context since the famous Lyndel-Bell work \([29]\).

The usual way to access to such anomalous macrostates is by using the microcanonical description, since they are hidden behind of the ensemble inequivalence of the Gibbs canonical description. The microcanonical ensemble is the natural thermostatistitical description corresponding to the thermodynamic equilibrium of an isolated system. However, many astrophysical objects where negative heat capacities are observed do not correspond necessarily to isolated systems. Contrary, most of these objects can be considered as open
systems driven under the gravitational influence of other astrophysical objects which are able to interchange energy and particles with the first one, i.e.: the globular clusters under the influence of the nearby galaxy [30]. Contrary to the short-range interacting systems, the above observation clarifies us that the negative heat capacities are also relevant for an open astrophysical system under the influence of its surrounding. Therefore, the framework of the \textit{long-large interacting systems} could be a natural scenario for the relevance of the generalized Gibbs canonical ensemble (5).

Despite of the existence of long-range correlations, the generalized ensemble presupposes certain kind of \textit{separability} of the interest system from its surrounding. A natural separability appears when the whole degrees of freedom of the closed system (system + environment) are divided into internal and collective degrees of freedom. Let us denote the physical quantities of the interest system and the surrounding by the subindexes \( A \) and \( B \) respectively. The separability allows us to discompose the total energy contribution of the closed system \((AB)\) as follows:

\[
\hat{H}_{AB} \simeq \hat{H}_A [a_{AB}] + \hat{H}_B [a_{AB}] + \hat{V}_{AB}.
\]  

The terms \( \hat{H}_A [a_{AB}] \) and \( \hat{H}_B [a_{AB}] \) represent the energy contribution of the internal degrees of freedom of the interest system \( A \) and the environment \( B \) respectively, where the dependence \([a_{AB}]\) represents certain parametric influence of the collective degrees of freedom on the internal degrees of freedom.

Finally, the term \( \hat{V}_{AB} \) consider the pure energy contribution of the collective degrees of freedom. A simple consequence of the above assumptions is that the energy interchange between the interest system \( A \) and its surrounding \( B \) takes place by means of the influence of the collective degrees of freedom. While the internal degrees of freedom obey to a chaotic behavior, I shall assume that the collective degrees of freedom obey to a quasi-regular dynamics which depends on the energetic stage of the internal degrees of freedom.

According to the previous hypothesis, the number of microscopic configurations of the internal degrees of freedom can be estimated by:

\[
\Omega_A (E_A; a_{AB}) \Omega_B (E_B; a_{AB}) dE_A dE_B,
\]  

where \( E_A \) and \( \Omega_A (E_A; a_{AB}) \) represents the internal energy and the density of states of the interest system, as well as \( E_B \) and \( \Omega_B (E_B; a_{AB}) \), the respective quantities of the surrounding. The total energy of the closed system can be expressed as follows:

\[
E (E_A, E_B; a_{AB}) = E_A + E_B + \omega (a_{AB}; E_A, E_B),
\]  

where \( \omega (a_{AB}; E_A, E_B) \) represent the energy contribution of the collective degrees of freedom which drives the energy interchange between the interest
system and its surrounding. Notice that a dependence of this term on the energetic stage of the internal degrees of freedom, which appears as a consequence of the influence of the internal degrees of freedom on the quasi-regular dynamics of the collective degrees of freedom. Such a term is dismissed in the framework of the short-range interacting systems because the interactions between the interest system and the surrounding are just a boundary effect, which is not the case of the long-range interacting systems. Taken together all the above assumptions, the number of configurations $W$ of the close system is given by:

$$W (E; a_{AB}) = \int \delta \{ E - E (E_A, E_B; a_{AB}) \} \Omega_A (E_A; a_{AB}) \Omega_B (E_B; a_{AB}) dE_A dE_B, \quad (24)$$

The energy $E_B$ can be expressed in terms of the variables $E_A$, $E$ and the parameters $a_{AB}$ as follows:

$$E_B = E - E_A - \omega (a_{AB}; E_A, E_B) \equiv E - \Theta (E_A; E, a_{AB}), \quad (25)$$

where the function $\Theta (E_A; E, a_{AB})$ is just the solution of the problem:

$$\Theta = E_A + \omega (a_{AB}; E_A, E - \Theta). \quad (26)$$

The integration by $dE_B$ leads to the following expression:

$$W [E; a_{AB}] = \int \Omega_A (E_A; a_{AB}) \Omega_B [E - \Theta (E_A; E, a_{AB}); a_{AB}] \nu (E_A; E, a_{AB}) dE_A, \quad (27)$$

where:

$$\nu (E_A; E, a_{AB}) = 1 - \frac{\partial \Theta (E_A; E, a_{AB})}{\partial E}. \quad (28)$$

The approximations $\nu \approx 1$ and:

$$\frac{\Omega_B [E - \Theta (E_A; E, a_{AB}); a_{AB}]}{\Omega_B [E; a_{AB}]} \simeq \exp [ - \eta \Theta (E_A; E, a_{AB})], \quad (29)$$

are fully justified by considering the ordinary condition $\Theta (E_A; E, a_{AB}) \ll E$, where $\eta = \partial \log \Omega_B (E; a_{AB}) / \partial E$ is the microcanonical inverse temperature associated to the internal degrees of freedom of the surrounding. The normalization condition of the generalized canonical ensemble:

$$Z (\eta; a_{AB}) = \int \exp [ - \eta \Theta (E_A)] \Omega (E_A; a_{AB}) dE_A, \quad (30)$$

is obtained by introducing the reparametrization $\Theta (E_A) \equiv \Theta (E_A; E, a_{AB})$ and the partition function $Z (\eta; a_{AB}) = W (E; a_{AB}) / \Omega_B (E; a_{AB})$, which allows us to express the generalized canonical ensemble as follows:

$$\dot{\omega} (\eta, a_{AB}) = \frac{1}{Z (\eta; a_{AB})} \exp \left\{ - \eta \Theta \left( \hat{H}_A [a_{AB}] \right) \right\}. \quad (31)$$
The present derivation of the generalized canonical ensemble is based on a separation of internal and collective degrees of freedom of the closed system, a procedure that could be relevant within the astrophysical context. However, the reader can notice that all that is actually needed in order to support the natural appearance of the generalized ensemble is certain modification of the mechanism of energy interchange between the interest system ($A$) and its surrounding ($B$). Such a modification is provided in the present framework by the presence of the term $\omega(a_{AB}; E_A, E_B)$, which leads to an effective energy reparametrization $\Theta(E)$ whenever exists a nonlinear energetic dependence of this function.

The effective inverse temperature of the generalized thermostat associated to the generalized canonical ensemble:

$$\tilde{\beta} = \eta \frac{\partial \Theta (E_A)}{\partial E},$$

depends directly on the microcanonical inverse temperature associated to the internal degrees of freedom on the surrounding $\eta = \partial \log \Omega_B(E; a_{AB}) / \partial E$, but this quantity is affected by the incidence of the energetic interchange mechanism leading to the reparametrization of the internal energy $E_A$ of the interest system. This feature introduces the following modification of the equilibrium condition:

$$\langle \tilde{\beta} \rangle \equiv \left\langle \frac{\partial \Theta (E_A)}{\partial E} \right\rangle \frac{\partial \log \Omega_B(E; a_{AB})}{\partial E} = \frac{\partial \log \Omega_A(E_A; a_{AB})}{\partial E_A} \equiv \langle \hat{\beta} \rangle,$$

which drops to the usual one whenever the energy contribution $\omega(a_{AB}; E_A, E_B)$ can be neglected:

$$\omega(a_{AB}; E_A, E_B) / E_A \approx 0 \Rightarrow \partial \Theta (E_A) / \partial E \approx 1.$$

As already commented, this is the case of the extensive systems where the energy contribution characterizing the interaction between the interest system and its surrounding is just a boundary effect which becomes negligible in comparison to the internal energy of the interest system. The energy contribution $\omega(a_{AB}; E_A, E_B)$ could be comparable to the energy $E_A$ of the interest system in the case of long-range interacting systems, and therefore, the influence of the surrounding may become equivalent to a generalized thermostat with a fluctuating inverse temperature $\tilde{\beta}$.

3 Conclusions

The geometric framework derived from the reparametrization invariance of the microcanonical ensemble provides a suitable generalization of the stan-
dard Statistical Mechanics and Thermodynamics which is able to deal with
the phenomenon of ensemble inequivalence and the existence of equilibrium
thermodynamical states with a negative heat capacity [18,19,20,21,22]. Such
a development have found an immediately application to enhance the potential-
tialities of the available Monte Carlo methods based on the consideration of
the canonical ensemble [23,24].

While the usual physical conditions of the environment in the real life appli-
cations of the equilibrium Thermodynamics leads to the applicability of the
Gibbs canonical ensemble (or the Boltzmann-Gibbs distributions), the prac-
tical implementation of the generalized canonical ensemble [5] demands the
consideration of a special experimental setup. Nevertheless, a framework where
long-range interactions are involved becomes a possible physical scenario for
the natural appearance of the generalized canonical description. As already
suggested in this paper, the incidence of long-range correlations could pro-
voke a significant modification of the mechanism for the energetic interchange
between the interest system and its surrounding. Such a mechanism could be
relevant in the astrophysical context, where the existence of equilibrium states
with negative heat capacities is a very usual phenomenon, in spite of most of
astrophysical structures can be considered as open systems.

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\[ E > 1 \]

1.20
1.25
1.30
1.35
1.40
1.45
1.50
1.55
1.60

\[ \delta \beta = 0 \]

unstable

critical

coexisting phases

generalized canonical ensemble
(with \( \beta \) fixed)

generalized canonical ensemble
(with \( \eta \) fixed)

canonical ensemble
(with \( \beta \) fixed)
