Statistical Mechanics in the Extended Gaussian Ensemble

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The extended gaussian ensemble (EGE) is introduced as a generalization of the canonical ensemble. The new ensemble is a further extension of the Gaussian ensemble introduced by J. H. Hetherington [J. Low Temp. Phys. 66, 145 (1987)]. The statistical mechanical formalism is derived both from the analysis of the system attached to a finite reservoir and from the Maximum Statistical Entropy Principle. The probability of each microstate depends on two parameters $\beta$ and $\gamma$ which allow to fix, independently, the mean energy of the system and the energy fluctuations respectively. We establish the Legendre transform structure for the generalized thermodynamic potential and propose a stability criterion. We also compare the EGE probability distribution with the $q$-exponential distribution. As an example, an application to a system with few independent spins is presented.

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I. INTRODUCTION

The development of statistical mechanics based on ensemble theory is founded on the postulate of “equal a priori probabilities”, which is assumed to apply to all microstates consistent with the given macrostate of an isolated system [1]. The corresponding statistical ensemble is the so-called microcanonical ensemble. A representative system in this ensemble has all “mechanical” variables such as energy $E$, volume $V$, magnetization $M$ etc., fixed. For convenience in calculations, other ensembles are used which invariably suppose the existence of a subsidiary system or reservoir in contact with the actual system. For instance, in the canonical ensemble the walls of the system permit an exchange of energy with the reservoir while in the grand canonical ensemble, both energy and matter can be exchanged. In general, the different ensembles are constructed by allowing one or more mechanical variables to fluctuate. The exchange of each of these variables is controlled by a parameter which is a characteristic of the reservoir. For instance, in the case of the canonical ensemble, this parameter is precisely the temperature of the reservoir and determines the mean energy of the system. Actually, this is adequate when the reservoir is a very large system that can exchange arbitrary amounts of energy, without modification of its intensive properties. In practical situations, this is not always the case. However, very few studies have been devoted to analyse the consequences of possible deviations from these ideal reservoir properties.

In this paper, we develop the statistical mechanics of a system that can exchange energy with a finite reservoir characterized by two parameters: $\beta$ and $\gamma$. These parameters control independently the mean energy of the system and its energy fluctuations, respectively. The corresponding statistical ensemble represents a generalization of the canonical ensemble and will be called the extended gaussian ensemble (EGE). A similar ensemble was already developed, in a more restricted framework, by Hetherington [2]. The author considered that the sample system was in contact with a finite reservoir with size dependent properties. The so-called gaussian ensemble was introduced so that it is equivalent to the canonical ensemble in the limit of large systems, except in the energy range of a first-order transition. Interestingly, it enables a smooth interpolation between the microcanonical and the canonical ensembles. Taking into account these features, Challa and Hetherington [3] showed the interest of this ensemble for Monte Carlo simulation studies of phase transitions. They demonstrated a significant reduction in computer time (compared to standard simulations in the canonical ensemble) and, its adequacy for distinguishing second-order from first-order transitions. Compared to the EGE introduced in the present paper, the main difference arises from the fact that in the gaussian ensemble the sample and the reservoir are assumed to be statistically independent which implies the additivity of the corresponding entropies. This is not assumed in our formalism. The consequences are important and will be discussed in depth in this work.

The present formalism can be considered as an alternative to the statistical mechanics based on non-additive generalized entropies. Actually the study of such generalized entropies has generated a lot of interest in the past fifteen years. The motivation for the so called Tsallis statistical mechanics has been to extend the standard Boltzmann-Gibbs framework to include non-extensive systems [4]. Among different interpretations, it has been suggested that Tsallis formalism corresponds to an ensemble describing a system attached to a finite reservoir [5, 6]. Although a large number of papers have been published, the physical meaning of many related issues is
still open to discussion [8, 9]. The EGE formalism that we propose in this paper, provides a clear and consistent framework for the statistical mechanics with a finite reservoir.

The paper is organized as follows: in sections II and III the EGE is founded from the analysis of a contact with a finite reservoir and from the Maximum Statistical Entropy Principle respectively. In section IV the main thermodynamic relations are derived. In section V we highlight the non-additive nature of the thermodynamic formalism. In section VI a stability criterion is proposed. In section VII the equilibrium distributions of the EGE are compared with the $q$-exponential distributions. In section VIII we present an example of application to a system of independent spins. Finally, in section IX we summarize and conclude.

II. CONTACT WITH A FINITE RESERVOIR

Let us consider a system (that we will call the sample) in contact with a reservoir. Let us call the energy of the sample $E_1$ and the energy of the reservoir $E_2$. The sample and the reservoir together form an isolated system so that $E = E_1 + E_2$ is constant. Let us also define $\Omega_2(E_2)$ as the number of microstates of the reservoir. Following Callen [10], the probability that the system 1 is in a certain microstate with energy $E_1$ is given by

$$p_1(E_1) = \frac{\Omega_2(E - E_1)}{\Omega_{1+2}(E)},$$  \hspace{1cm} (1)

where $\Omega_{1+2}(E)$ is the total number of states available for the set $1 + 2$ (Note that we do not assume that $\Omega_{1+2}$ can be factorized as a product $\Omega_1 \Omega_2$ ). Let us define the entropy of the reservoir as:

$$S_2(E_2) = \ln \Omega_2(E_2),$$  \hspace{1cm} (2)

(all along the paper we choose the entropy units so that Boltzmann’s constant, $k_B = 1$.) Therefore:

$$p_1(E_1) = \frac{e^{S_2(E - E_1)}}{\Omega_{1+2}(E)}.$$  \hspace{1cm} (3)

The energy of the sample will, in general fluctuate. Let us call $U$ its mean (equilibrium) value. We can develop $S_2(E - E_1)$ around the equilibrium value $E - U$ as:

$$S_2(E - E_1) = S_2(E - U) + \left. \frac{dS_2}{dE_2} \right|_{E-U}(E_1 - E)$$

$$+ \frac{1}{2!} \left. \frac{d^2 S_2}{dE_2^2} \right|_{E-U}(E_1 - E)^2 + \mathcal{O}(E_1 - E)^3.$$  \hspace{1cm} (4)

The derivatives in the right hand side of this expression are quantities which depend only on the reservoir. We define

$$\left. \frac{dS_2}{dE_2} \right|_{E-U} = \beta,$$  \hspace{1cm} (5)

and

$$\left. \frac{d^2 S_2}{dE_2^2} \right|_{E-U} = -2\gamma.$$  \hspace{1cm} (6)

The standard canonical ensemble is characterized by a reservoir with constant $\beta$ (independent of $E_2$), which implies $\gamma = 0$ and there is no term beyond the first order term in the Eq. (6). However, in the present paper, we consider a more general reservoir for which $\gamma \neq 0$. Thus in this EGE, the reservoir is characterized by the pair of parameters $\beta$ and $\gamma$. The thermodynamic meaning of these parameters will be clarified in the following sections. To explicitly highlight the effects of this modification and also for the sake of simplicity, we assume that the cubic and higher order terms vanish. Then substituting (3) in (6) and denoting the energies of the microstates of the sample by $\epsilon_i (i = 1, ..., M)$, we obtain

$$p_i = \frac{1}{Z_G} \exp[-\beta(\epsilon_i - \gamma(\epsilon_i - U)^2)],$$  \hspace{1cm} (7)

where the normalization constant $Z_G$ is given by

$$Z_G = \sum_{i=1}^{M} \exp[-\beta\epsilon_i - \gamma(\epsilon_i - U)^2].$$  \hspace{1cm} (8)

The subscript $G$ only indicates the “gaussian” form of the probabilities. Note that $U$ is the mean energy and must be obtained self-consistently from the equation:

$$UZ_G = \sum_{i=1}^{M} \epsilon_i \exp[-\beta\epsilon_i - \gamma(\epsilon_i - U)^2].$$  \hspace{1cm} (9)

Eqs. (7), (8) and (9) reduce to the standard canonical ensemble definitions when $\gamma = 0$. Therefore, it is natural to relate the parameter $\gamma$ with the finite size of the reservoir.

III. MAXIMUM STATISTICAL ENTROPY PRINCIPLE

In this section, we derive the probability law of Eq. (7) from different arguments. This leads to a better understanding of the parameters $\beta$ and $\gamma$ as parameters characterizing the “equilibrium” distribution of the sample. To derive the probability distribution from the Maximum Statistical Entropy Principle, we maximize the standard Gibbs-Boltzmann-Shannon entropy given by

$$S_G = -\sum_{i=1}^{M} p_i \ln p_i,$$  \hspace{1cm} (10)

subject to the constraints of normalisation of the probability, the given mean value of the energy and the fixed
value of the fluctuations, respectively as
\[ \sum_{i=1}^{M} p_i = 1, \quad (11) \]
\[ \langle \epsilon_i \rangle \equiv \sum_{i=1}^{M} \epsilon_i p_i = U, \quad (12) \]
\[ \langle (\epsilon_i - U)^2 \rangle \equiv \sum_{i=1}^{M} (\epsilon_i - U)^2 p_i = W. \quad (13) \]
Then the maximization procedure is done by introducing the Lagrange multipliers $\lambda$, $\beta$, and $\gamma$, and maximizing the following functional $\mathcal{L}$:
\[ \mathcal{L} = -\sum_i p_i \ln p_i - \lambda \left( \sum_i p_i - 1 \right) - \beta \left( \sum_i \epsilon_i p_i - U \right) - \gamma \left( \sum_i (\epsilon_i - U)^2 p_i - W \right). \quad (14) \]
By requiring the condition:
\[ \frac{\partial \mathcal{L}}{\partial p_i} = 0, \quad (15) \]
it is easy to see that the optimum form of the probability distribution is given by the expression in Eq. (1). Therefore $\beta$ and $\gamma$, within this context, are simply Lagrange multipliers that allow to fix, self-consistently, a mean value of the energy $U = \langle \epsilon_i \rangle$ and a specific value of the variance $W = \langle (\epsilon_i - U)^2 \rangle$.

### IV. THERMODYNAMIC RELATIONS

We define a thermodynamic potential $\Phi(\beta, \gamma)$ as
\[ \Phi(\beta, \gamma) = \ln Z_G. \quad (16) \]
By differentiating Eq. (16), it can be straightforwardly obtained that:
\[ - \left( \frac{\partial \Phi}{\partial \beta} \right)_\gamma = U(\beta, \gamma), \quad (17) \]
\[ - \left( \frac{\partial \Phi}{\partial \gamma} \right)_\beta = W(\beta, \gamma). \quad (18) \]
The second derivative renders:
\[ - \left( \frac{\partial^2 \Phi}{\partial \beta^2} \right)_\gamma = - \left( \frac{\partial U}{\partial \beta} \right)_\gamma = \frac{1}{W^{-1}(\beta, \gamma) - 2\gamma}, \quad (19) \]
which represents a generalization of the standard formula for energy fluctuations in the canonical ensemble. It is natural to define the extended heat capacity as:
\[ C \equiv -\beta^2 \left( \frac{\partial U}{\partial \beta} \right)_\gamma = \frac{\beta^2 W}{1 - 2\gamma W}. \quad (20) \]
This equation is the same that was already derived in Ref. [1]. Note that, contrary to what happens in the standard canonical ensemble, the positivity of the fluctuations $W$ does not guarantee the positivity of $C$.

For $\gamma \to 0$, it is seen that the relations (17) and (18) go to the corresponding relations for the case of canonical ensemble. Also in this limit, from Eqs. (19) and (20) we get an interesting relation given by:
\[ \lim_{\gamma \to 0} \left( \frac{\partial \Phi}{\partial \gamma} \right)_\beta = \left( \frac{\partial^2 \Phi}{\partial \beta^2} \right)_\gamma, \quad (21) \]
which resembles in form with a diffusion equation.

The entropy $S_G$ as given by (10) is the inverse Legendre transform of $\Phi(\beta, \gamma)$, and can be expressed as:
\[ S_G(U, W) = \beta U + \gamma W + \Phi, \quad (22) \]
whereby $S_G$ is a function of the specified values of the constraints i.e. $U$ and $W$. Therefore we have the following thermodynamic relations
\[ \left( \frac{\partial S_G}{\partial U} \right)_W = \beta, \quad (23) \]
\[ \left( \frac{\partial S_G}{\partial W} \right)_U = \gamma. \quad (24) \]

### V. NON-ADDITIVITY

We remark that although the thermodynamics of a system in the EGE is well defined by the equations in the previous section, it is not straightforward to establish a mutual equilibrium condition for two different systems that would allow to establish a zeroth law (or, equivalently, an intensive temperature) [11]. This problem is due to the non additive character of the potential $\Phi(\beta, \gamma)$. Let us consider two systems 1 and 2 with hamiltonians $H_1$ and $H_2$. By applying the rules derived in the previous sections independently to the two systems, one can derive the thermodynamic potentials $\Phi_1(\beta, \gamma)$, $\Phi_2(\beta, \gamma)$ as well as the mean energies $U_1(\beta, \gamma)$ and $U_2(\beta, \gamma)$. One can then try to solve the composite system $1 + 2$ with hamiltonian $H_1 + H_2$. It is easy to verify that the new potential $\Phi_{1+2}(\beta, \gamma)$ satisfies:
\[ \Phi_{1+2}(\beta, \gamma) = \Phi_1(\beta, \gamma) + \Phi_2(\beta, \gamma) \]
\[ - \ln \left( e^{\gamma \left[ (H_1 + H_2 - U_{1+2})^2 - (H_1 - U_1)^2 - (H_2 - U_2)^2 \right]} \right), \quad (25) \]
where $U_{1+2}$ is the mean energy of the composite system. Note that $U_{1+2}$ as well as the average indicated by the angular brackets are computed with the probability distribution corresponding to the composite system $1 + 2$ which, in general, cannot be written as a product of probability distributions for systems 1 and 2.

The average values are, in general, non-additive ($U_{1+2} \neq U_1 + U_2$). But even if additivity of $U$ is imposed, the potential $\Phi$ remains non-additive. The correction term depends on the microscopic details of the two hamiltonians $H_1$ and $H_2$. 
This lack of additivity does not allow to define an equivalence relation of “mutual” equilibrium. Consider that two systems are known to be independently in equilibrium with a bath characterized by $\beta$ and $\gamma$. On putting the two systems in contact with bath simultaneously, their properties (probability distribution) will change. The parameters $\beta$ and $\gamma$ are, consequently, properties of the bath and cannot be considered as properties of the system, contrary to what occurs with the corresponding $\beta$ in the standard canonical ensemble.

VI. STABILITY CRITERION

In standard thermodynamics, the stability criterion $-\partial U / \partial \beta > 0$ is derived from the condition of maximum entropy. The derivation [10] considers a partition of an isolated system into any two subsystems. By allowing the two subsystems to alter their energies at fixed total energy, one can analyze the entropy change when the system is (virtually) displaced out of equilibrium. The condition of the maximum total entropy allows to deduce that the equilibrium state corresponds to a state with homogeneous $\beta$ (equilibrium condition) and with $-\partial U / \partial \beta > 0$ (stability condition). For the derivation, nevertheless, additivity of the entropy of the two subsystems must be used.

Within our new formalism, an additivity assumption cannot be used. Therefore it is not straightforward to establish a stability criterion. Although we cannot give a rigorous proof, in this section we provide some evidences that the same criterion ($-\partial U / \partial \beta > 0$) must hold.

First of all, it interesting to remark that the requirement of Eq. (28) would guarantee that this second derivative of $\Psi$ is negative and therefore the state of equilibrium corresponds to maxima of $\Psi(\beta, \gamma, U)$ with respect to $U$ displacements. Although, contrary to what happens in the standard canonical ensemble, the positivity of $W$ does not ensure the sign of $-\partial U / \partial \beta$ in general, at least we can derive that for small and positive values of $\gamma$:

$$0 < -\left(\frac{\partial U}{\partial \beta}\right)_\gamma = \left(\frac{\partial^2 \Psi}{\partial U^2}\right)_{\beta, \gamma} < 0. \quad (30)$$

Thus we suggest that this is the stability criterion to be used within the EGE, and we will use it in Section VIII for the analysis of some examples.

VII. COMPARISON WITH $q$-EXPONENTIAL DISTRIBUTIONS

$q$-exponential distributions are the central predictions of the generalized statistical mechanics proposed by Tsalilis [5]. These distributions have been considered as model distributions to describe various complex systems at their stationary states [12, 13, 14]. The general form of such distributions is given by $p(x) \sim e_q(x)$, where the $q$-exponential is defined as $e_q(x) = [1 + (1-q)x]^{1/(1-q)}$. This function goes to the usual $\exp(x)$ function for $q \rightarrow 1$. For definiteness, we restrict to the range $0 < q < 1$. In this section, we compare the $q$-exponential distributions with the equilibrium distributions of the EGE. But first, we show how to derive the $q$-exponential distributions by generalizing the canonical ensemble approach, along the lines of section VIII. We define a parameter which is in general, a function of the energy $E_2$ of the reservoir

$$\beta(E_2) = \frac{dS_2}{dE_2}. \quad (31)$$

At equilibrium, it attains the value given by Eq. (3). We impose that $\beta(E_2)$ satisfies:

$$\frac{d}{dE_2} \left(\frac{1}{\beta(E_2)}\right) = Q, \quad (32)$$

where $Q$ is a positive valued constant. From Eqs. (32) and (31), we obtain

$$\frac{d}{dE_2} \beta(E_2) = \frac{d^2 S_2}{dE_2^2} = -Q \beta^2(E_2). \quad (33)$$

In general, for all integer values of $n$

$$\frac{d^n S_2}{dE_2^n} = (n-1)! (-Q)^{n-1} \beta^n(E_2). \quad (34)$$
Now unlike in Eq. (1), if in the expansion of $S(E - E_1)$ around the equilibrium value $(E - U)$, we retain derivatives of $S_2$ up to all orders, then we have

$$S_2(E - E_1) = S_2(E - U) + \frac{1}{n!} \frac{d^n S_2}{dE_2^n} (U - E_1)^n.$$  \hspace{1cm} (35)

On applying Eq. (35) for the case of equilibrium, we can write

$$S_2(E - E_1) = S_2(E - U) + \frac{1}{n} (-Q)^n \beta^n (U - E_1)^n,$$  \hspace{1cm} (36)

where note that $\beta$ is given by its value at equilibrium. The equilibrium probability distribution is then given from (36) as

$$p(E_1) \sim \exp \left[ \sum_{n=1}^{\infty} \frac{1}{n} (-Q)^{n-1} \beta^n (U - E_1)^n \right].$$  \hspace{1cm} (37)

To compare Eq. (37) with the q-exponential distribution given by

$$p_q(E_1) \sim e_q[\beta(U - E_1)] = [1 + (1-q)\beta(U - E_1)]^{1/(1-q)},$$  \hspace{1cm} (38)

we rewrite the q-exponential as

$$e_q[\beta(U - E_1)] = \exp \left[ \frac{\ln[1 + (1-q)\beta(U - E_1)]}{(1-q)} \right],$$  \hspace{1cm} (39)

and expand the ln function using the series \(\ln[1 + x] = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + ...,\) provided that \(-1 < x \leq 1\). Thus we can write

$$e_q[\beta(U - E_1)] = \exp \left[ \sum_{n=1}^{\infty} \frac{1}{n} (-1-q)^{n-1} \beta^n (U - E_1)^n \right],$$  \hspace{1cm} (40)

for \(-1 < (1-q)\beta(U - E_1) \leq 1\). Thereby, on identifying $Q = (1-q)$ we may say that the general equilibrium distribution of Eq. (39) based on assumptions (31) and (32), is identical to a q-exponential distribution. Assuming that the relevant $q$ values are quite close to unity, we may keep terms only up to second order as done in Eq. (31). Then the equilibrium $q$-distribution for system 1 being in microstate $i$ of energy $\epsilon_i$ can be written as

$$p_q(\epsilon_i) = \frac{1}{Z_q} \exp \left[ -\beta \epsilon_i - \frac{1}{2} (1-q) \beta^2 (\epsilon_i - U)^2 \right],$$  \hspace{1cm} (41)

where $Z_q$ is the normalization constant.

On the other hand, for the case of EGE, instead of fixing the derivative of $\beta^{-1}$ (Eq. (32)), we fix the derivative of $\beta$ as follows:

$$\frac{d}{dE_2} \beta(E_2) = -2\gamma,$$  \hspace{1cm} (42)

where $\gamma$ is independent of $E_2$. This ensures that the higher order ($n > 2$) derivatives of $S_2$ vanish. On comparing (11) and (42), we note that $\beta^{-1}$ plays the role analogous to $\gamma$.

It may be remarked that if we identify parameter $\beta(E_2) = 1/(T(E_2))$ as the inverse temperature, then Eq. (42) implies that the heat capacity of the reservoir $C_q = dE_2/dT = Q^{-1}$. Recently, the $q$-exponential distributions have been discussed in the context of a reservoir with finite heat capacity $C_q$. On the other hand, following Gibbs’ approach to the canonical ensemble, but instead using the $q$-generalized Boltzmann entropy, $q$-exponential distributions were derived in Ref. [15].

VIII. APPLICATION TO A SYSTEM OF INDEPENDENT SPINS

A. Single Spin

As a first example of the EGE, we apply our formalism to the problem of a system with only two energy levels. Let us consider a single spin $s = \pm 1$ in the presence of a constant external magnetic field $B$. The Hamiltonian of the system reads:

$$H = -BS.$$  \hspace{1cm} (43)

The partition function is given by:

$$Z_G = e^{\beta B} e^{\gamma(-B-U)^2} + e^{-\beta B} e^{\gamma(B-U)^2},$$  \hspace{1cm} (44)

where the mean energy $U$ is the solution of the self-consistent equation:

$$U = -Be^\beta B e^{-\gamma(-B-U)^2} + Be^{-\beta B} e^{-\gamma(B-U)^2}.$$  \hspace{1cm} (45)

The dependence on $B$ can be easily overcome by defining the reduced units:

$$U^* = U/B, \quad \beta^* = \beta B, \quad \gamma^* = \gamma B^2.$$  \hspace{1cm} (46)

Thus, Eq. (45) becomes:

$$U^* = e^{-\beta^*} e^{-\gamma^*(1-U^*)^2} - e^{\beta^*} e^{-\gamma^*(1+U^*)^2}.\hspace{1cm} (47)$$

The numerical solution of this equation is plotted in Fig. 1. The behaviour of $U^*$ as a function of $1/\beta^*$ is shown for different values of $\gamma^*$. For $\gamma^* = 0$, one recovers the behaviour $U^* = \tanh(\beta^*)$ corresponding to the case of a system in contact with an infinite reservoir. For $\gamma^* \neq 0$, $U^*$ is smaller, indicating that it is more difficult to disorder the system by decreasing $\beta^*$. It is interesting to note that for $\gamma^* \approx 0.5$, there is a change in the behaviour at $\beta^* \to 0$. Above this value of $\gamma^*$, the system is not able to disorder completely anymore and always keeps a certain magnetization ($m = \langle s \rangle = -U^*$). This can be regarded as a “phase transition”, that occurs at $\beta^* = 0$. This change in the behaviour occurring at $\gamma^* \approx 0.5$ can also be seen by plotting the entropy $S$ as a function of $1/\beta^*$ for different values of $\gamma^*$. This is shown in Fig. 2. For $\gamma^* < 0.5$ the entropy tends to $\ln 2$ for $\beta^* \to \infty$, whereas it tends to a lower value for $\gamma^* > 0.5$. 


B. Two spins

As a second step, it is also very instructive to study a system of two independent spins. This will illustrate the non-extensive behaviour of the solution. In this case, the numerical solution of the self consistent equation (9) for the mean energy renders the behaviour shown in Fig. 3. For the values of $\beta^*$ and $\gamma^*$ for which more than one solutions are possible, we have used the stability criterion proposed in Section VI to decide which is the “equilibrium” solution. As can be seen, for $\gamma^* > 0.49$ a discontinuity occurs associated with a sudden loss of order in the system. Although the system is far from the thermodynamic limit, this change shares many similarities with a phase transition. Fig. 3 displays the behaviour of the corresponding energy fluctuations. It can be seen that $W^* = \langle (H^2) - U^2 \rangle / B^2$ exhibits a cusp at the transition for $\gamma^* \simeq 0.49$. For larger values of $\gamma^*$, the fluctuations exhibit a discontinuity. The discontinuities are associated with first-order phase transitions that display metastable behaviour. As an example, in Fig. 4 we show the detailed behaviour of $U^*$ as a function of $1/\beta^*$ for $\gamma^* = 0.6$. In the range $2.42 < 1/\beta^* < 2.86$, the numerical analysis of the self-consistent equation renders three solutions.

By analyzing the behaviour of the potential $\Psi(\beta^*, \gamma^*, U^*)$, shown in Fig. 6 it is easy to verify that two of such solutions are stable (correspond to local maxima of $\Psi$) whereas one is unstable (corresponds to a local minimum of $\Psi$ and is not plotted in Fig. 5).
C. Several spins

We have also performed a numerical study of systems with larger number of independent spins in the presence of an external field. An example is shown in Fig. 8, corresponding to a system with 4 spins (16 energy levels). A sequence of two consecutive phase transitions can be observed. As an interesting remark we want to note that in the case of \(N\) “non-interacting” spins \(s_k (k = 1, \ldots, N)\) in the presence of an external field, long-range forces will appear due to the finite size of the bath. This can be easily seen by writing the probabilities \(p_i\) for the microstates \((i = 1, \ldots, 2^N)\) of such a system:

\[
p_i = \exp \left[ \beta^* \sum_{k=1}^{N} s_k - \gamma^* \left( \sum_{k=1}^{N} s_k - U^* \right)^2 \right].
\]

(48)

Note that the development of the squared term in the exponent will lead to terms \(-\gamma^* s_k s_j\) which correspond to antiferromagnetic interactions among all spin pairs. A more detailed study of these examples is out of the scope of this paper.

IX. SUMMARY

We have presented the extended gaussian ensemble (EGE) as a generalization of the standard canonical ensemble. The ensemble statistics have been derived by two methods: first by considering a system in contact with a finite bath, secondly from the maximum statistical entropy principle by fixing the knowledge of both the mean energy and the energy fluctuations. The obtained probability law depends on two parameters \(\beta\) and \(\gamma\) which are properties of the bath. Thermodynamic re-
FIG. 8: Behaviour of the mean energy $U^*$ as a function of $1/\beta^*$ for several values of $\gamma^*$ in a system of 4 independent spins.

lations have been derived and a possible stability crite-

rion has been suggested. Nevertheless this point as well as the possibility for establishing a mutual equilibrium criterion will need further analysis in future works. We have also presented an application of the EGE formalism to the analysis of a system of one spin and two independent spins. Among other interesting results, the most remarkable one is the possibility for occurrence of a critical point or first-order phase transitions induced by the finite size of the reservoir. Further, comparisons of this new ensemble formalism with alternative extensions of statistical mechanics proposed for the study of nanosystems or for other non-extensive systems, are interesting problems for research.

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[1] R. K. Pathria, Statistical Mechanics (Butterworth Heinemann, Oxford, 1996), 2nd ed.
[2] J. H. Hetherington, J. Low Temp. Phys. 66, 145 (1987).
[3] M. S. S. Challa and J. H. Hetherington, Phys. Rev. Lett. 60, 77 (1988).
[4] M. S. S. Challa and J. H. Hetherington, Phys. Rev. A 38, 6324 (1988).
[5] C. Tsallis, J. Stat. Phys. 52, 479 (1988).
[6] M. P. Almeida, Physica A 300, 424 (2001).
[7] A. R. Plastino and A. Plastino, Phys. Lett. A 193, 140 (1994).
[8] M. Nauenberg, Phys. Rev. E 67, 036114 (2003).
[9] C. Tsallis, cond-mat/0304696 (2003).
[10] H. B. Callen, Thermodynamics and an Introduction to Thermostatistics (John Wiley & Sons, New York, 1985), 2nd ed.
[11] W. J. Hornix, in A Critical Review of Thermodynamics, edited by E. B. Stuart, B. Gal-Or, and A. J. Brainard (Mono Book Corp., Baltimore, 1970).
[12] S. Abe and Y. Okamoto, eds., Nonextensive Statistical Mechanics and Its Applications, Series Lecture Notes in Physics (Springer-Verlag, Heidelberg, 2001).
[13] G. Kaniadakis, M. Lissia, and A. Rapisarda, eds., Nonextensive Statistical Mechanics and Physical Applications, vol. 305, 1/2 of Physica A (2002).
[14] M. Gell-Mann and C. Tsallis, eds., Nonextensive Entropy - Interdisciplinary Applications (Oxford University Press, Oxford, 2003).
[15] S. Abe and A. K. Rajagopal, Europhys. Lett. 55, 6 (2001).
[16] T. L. Hill, Thermodynamics of Small Systems (Dover, New York, 1994).
[17] T.L.Hill, Nano Lett. 1, 111 (2001).
[18] T.L.Hill, Nano Lett. 1, 273 (2001).