Ensemble equivalence for non-extensive thermostatistics

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Abstract

We compute the internal energy of different Ising type models, both long–range and short–range, under Tsallis statistics using the microcanonical and the canonical ensembles and we discuss under which conditions both ensembles give equivalent results.

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1 Introduction

In this paper we study different Ising type systems in the microcanonical and the canonical ensembles under the generalized statistics introduced by Tsallis [1]. This is based upon the following alternative expression for the entropy:

$$S_q = \frac{1 - \sum_i p_i^q}{q-1}, \tag{1}$$

depending on a parameter q. A probability p_i is assigned to each of the $i = 1, \ldots, W$ microscopic configurations. The set of probabilities $\{p_i\}$ must be obtained maximizing S_q under the appropriate constraints. The physical observables associated to a microscopic dynamical function $\mathcal{O}$ are computed as statistical averages $\langle \mathcal{O} \rangle$ obtained using the rule[2]: $\langle \mathcal{O} \rangle = \sum_i O_i P_i$ with $P_i = p_i^q / \sum_j p_j^q$ and O_i is the value of $\mathcal{O}$ at the configuration i whose probability is p_i. Different statistical ensembles give rise to different probabilities p_i and we address in this paper the question of equivalence between the microcanonical (fixed energy) and the canonical (fixed average energy) ensembles. To be more specific we consider Ising type systems with Hamiltonian:

$$\mathcal{H} = \sum_{(n,m)} \frac{1 - s_n s_m}{r_{nm}^{\alpha}}. \tag{2}$$

Where $s_n = \pm 1$, and the indexes $n, m = 1, \ldots, N = L^d$ run over the distinct pairs of sites of a regular d-dimensional lattice of lattice spacing equal to 1 and with periodic boundary conditions; r_{nm} is the distance between the spins n and m, and the parameter α sets the interaction range. The energy of configuration i is ε_i (notice that the ground state has zero energy). The usual short range Ising model is recovered in the limit $\alpha \to \infty$ where $1/r_{nm}^{\alpha} \to 0$ unless n and m are nearest neighbors with $r_{nm} = 1$. For $\alpha \leq d$ the average energy per particle diverges in the thermodynamic limit and the system is said to be non–extensive. More precisely, a convenient scale for the average energy per spin in a finite system of size N is given by [3]: $E/N \sim \tilde{N} = \frac{N^{1-\alpha/d} - \alpha/d}{1-\alpha/d}$. We see that for $\alpha > d$ the average energy per spin scales as a constant in the limit of large N, whereas for $\alpha \leq d$, it grows with the system size, a non–extensive behavior. Throughout this paper we will be considering the following cases:

(a) $\alpha = \infty$, $d = 1$, the short range one dimensional Ising model.
(b) $\alpha = \infty$, $d = 2$, the short range two dimensional Ising model.
(c) $\alpha = 0.8$, $d = 1$, a non extensive, long range, one dimensional Ising model.
(d) $\alpha = 0$, the non extensive infinite range Ising model, whose properties are basically independent of the spatial dimension d.

For each of these cases we will compute the internal energy $E(T, N)$ (the average value of the Hamiltonian $\langle \mathcal{H} \rangle$) as a function of the temperature T and the number of particles N, in the microcanonical and the canonical ensembles. We will compare the results obtained in both ensembles using the standard definition of temperature as well as a recent proposal for a *physical* temperature [4].

2 The microcanonical ensemble

The microcanonical ensemble is defined by fixing the energy E and setting $p_i = 0$ to those configurations whose energy is not equal to E. The maximization problem for the original entropic form S_q given by Eq.(1) with the constraint of given energy E, and the normalization condition $\sum_i p_i = 1$, has the solution of equiprobability:

$$p_i = \begin{cases} \Omega(E, N)^{-1}, & \varepsilon_i = E, \\ 0, & \text{otherwise.} \end{cases} \tag{3}$$

$\Omega(E, N)$ is the number of configurations with energy E for a system with N particles. Using this solution, the entropy as a function of the energy is given by$S_q(E, N) = (\Omega(E, N)^{1-q} - 1)/(1 - q)$. Finally, the temperature is defined by the thermodynamic relation $\frac{1}{T} = \frac{\partial S_q}{\partial E} = \Omega(E, N)^{-q} \frac{\partial \Omega(E,N)}{\partial E}$. This relation allows us to plot the energy as a function of the temperature, $E(T, N)$.

We see that an essential ingredient in the microcanonical ensemble is $\Omega(E,N)$, the number of configurations having energy E for a system with N particles. The exact form of this function depends on the interaction range parameter α and on the spatial dimension d, although the total number of configurations is $\sum_E \Omega(E,N) = 2^N$ independent of α and d. We now specify this function in each of the four cases of interest:

(a) $\alpha = \infty$, $d = 1$. The possible energy levels are $E_k = 4k$, $k = 0,\dots,N/2$ (assuming that N is an even number) and their degeneracy is easily computed as: $\Omega(E_k,N) = 2\binom{N}{2k}$.

(b) $\alpha = \infty$, $d = 2$. The possible energy values are $E_k = 4k$, $k = 0,\dots,N$. No closed exact expression is known for the function $\Omega(E,N)$. However, the exact solution for the partition function of the $L \times M$ Ising model [5], has allowed Beale [6] to write a Mathematica program that can actually compute $\Omega(E,N)$ for moderate values of N. Using this program we have generated the exact values of $\Omega(E,N)$ for $N = 32^2$ or smaller.

(c) $\alpha = 0.8$, $d = 1$. This is the more complicated case, because no analytical expression or exact numerical values is available. For small values of N, up to $N = 34$ we have made a complete enumeration of the $W = 2^N$ configurations and their energies ε_i. For larger sizes, up to $N = 3000$, the values of $\Omega(E,N)$ have been obtained by using a numerical sampling method known as Histogram by Overlapping Windows (HOW)[7]. Details of the implementation of the method for this particular problem can be found in [8].

(d) $\alpha = 0$. This case is equivalent to consider the Bragg–Williams approximation to the solution of the Ising model [9]. The energy levels are $E_k = 2k(N-k)$, $k = 0,\dots,N/2$ (assuming again that N is an even number) and the number of states is: $\Omega(E_k,N) = 2\binom{N}{k}$ for $k = 0,1,\dots,N/2-1$ and $\Omega(E_k,N) = \binom{N}{N/2}$ for $k = N/2$.

3 The canonical ensemble

In the canonical ensemble we fix a value for the average energy $E = \langle \mathcal{H} \rangle$. Maximization of the entropy, Eq.(1), under this constraint and the normalization condition $\sum_i p_i = 1$, leads to the following solution for the probabilities P_i [2]:

$$P_i = \begin{cases} \dfrac{[1-(1-q)\varepsilon_i/T']^{\frac{q}{1-q}}}{\sum_j [1-(1-q)\varepsilon_j/T']^{\frac{q}{1-q}}}, & 1-(1-q)\varepsilon_i/T' > 0, \\ 0, & \text{otherwise.} \end{cases} \tag{4}$$

Where we have defined

$$T' = (1-q)\sum_j \varepsilon_j P_j + T(\sum_j P_j^{1/q})^{-q} \tag{5}$$

and T is the (inverse of the) Lagrange multiplier used to enforce the condition of fixed average energy in the maximization procedure. Finally, it is possible to show the validity of the the Legendre structure of the resulting thermodynamics formalism by proving the relation [10,2]: $1/T = \partial S_q / \partial E$.

Although Eqs.(4,5) form a closed set, it is very difficult to use them in that form because the number of terms in the sums is the number of microscopic configurations, or 2^N, an extremely large number. It is possible to simplify the calculations by rewriting those equations in terms of the number of states $\Omega(E, N)$. More precisely, one can replace the sum over microscopic configurations (with 2^N terms) by sum over energy levels (with an number of terms proportional to $N\tilde{N}$), $\sum_j \longrightarrow \sum_k \Omega(E_k, N)$. Using the function $\Omega(E, N)$ it is then possible to compute numerically the different sums and hence to compute the internal energy (and other quantities of interest) within the canonical ensemble formalism[8].

4 Results

In Fig.1 we plot the internal energy versus the temperature, in the microcanonical and the canonical ensembles obtained using the appropriate number of states $\Omega(E, N)$ for each case (a-d). It is shown that, within the accuracy displayed in that figure and in all cases, the microcanonical and canonical results agree for $q \leq 1$ but disagree for $q > 1$.

Recently [4] it has been suggested that an appropriate definition for a physical temperature is

$$T_{phys} = \left(1 + \frac{1-q}{k} S_q\right) \left(\frac{\partial S_q}{\partial U_q}\right)^{-1}. \tag{6}$$

In Fig. 2 we plot the internal energy as a function of this physical temperature in the four cases of interest (a-d). We can see from this figure that the results of the microcanonical ensemble collapse in a single curve for all values of q, i.e. the dependence on q disappears when using the physical temperature in the microcanonical ensemble. This collapse is in agreement with a recent theoretical analysis of the definition of physical temperature[11]. The results of the canonical ensemble show some zig-zags which should be repaired by using a Maxwell–type construction (although we have not been able to find an unambiguous way of performing such a construction). Those zig-zags have their origin in the necessary transformation to go from the parameter T' to the temperature T as given by Eq. (5), and a plot of T versus T' already shows that behavior. The mathematical origin of the zig-zags lies in the condition $1 - (1-q)\epsilon_i/T' > 0$ of Eq. 4: when we sweep along the values of T', the number of different energy levels with a non–zero probability increases in a discrete way, thus producing steps or zig-zags. The number of these steps is

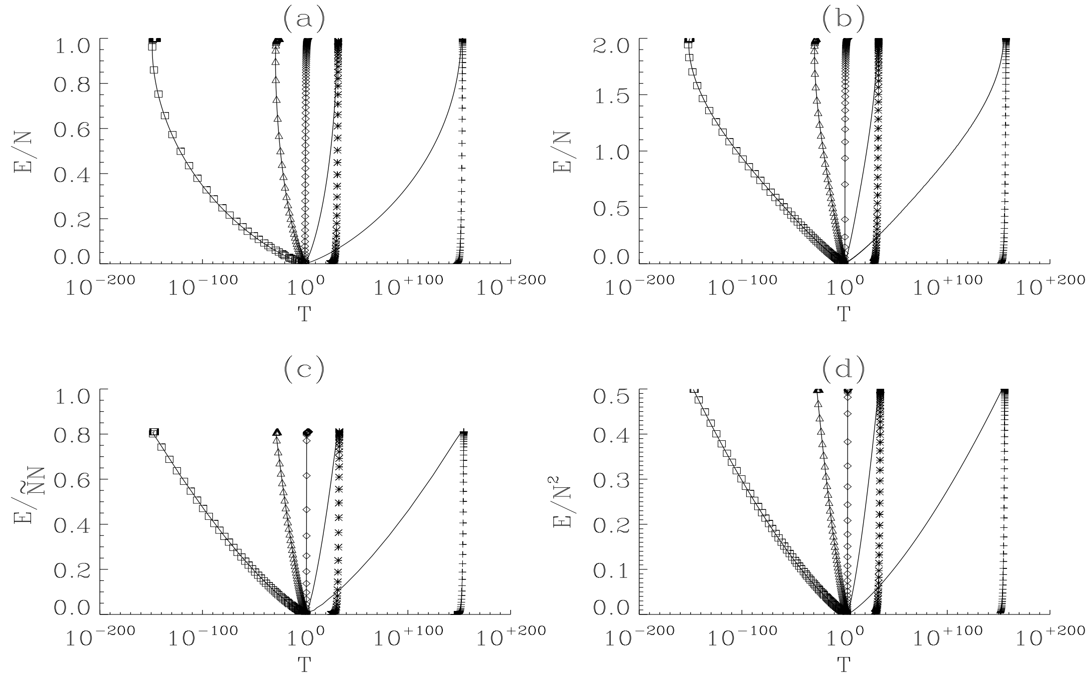

Fig. 1. Internal energy E as a function of the temperature T for the Ising model defined by (2) in the cases (a) $\alpha = \infty$, $d = 1$, (b) $\alpha = \infty$, $d = 2$, (c) $\alpha = 0.8$, $d = 1$, (d) $\alpha = 0$. The number of spins is $N = 1000$. Solid lines are the results obtained in the microcanonical ensemble, while symbols correspond to the canonical ensemble. From left to right curves, the values of q are $q = 0.5, 0.9, 1, 1.1, 1.5$.

proportional to $N\tilde{N}$, and in the thermodynamic limit we will get an almost continuous set of energy levels. These zig-zags are more pronounced the larger the interaction range. Except for this zig-zag behavior, we see again that the microcanonical and the canonical ensemble results agree for $q \leq 1$ and disagree for $q > 1$. The same conclusions are reached when studying the system magnetization instead of the internal energy. A more detailed study, beyond the scope of this paper, should consider also other properties such the heat capacity or the magnetic susceptibility.

Notice that the ultimate reason for not having equivalence between the two ensembles for $q > 1$, is that fluctuations of the energy in the canonical ensemble can not be neglected. We have checked that this is indeed the case by computing the energy fluctuations $\sigma(\mathcal{H}) = \sqrt{\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2}$ as a function of the system size. We have checked that the fluctuations, when normalized by the scale of energy, $N\tilde{N}$, do not decay to zero for increasing N in the range of temperatures for which the microcanonical and canonical ensemble do not agree. For $q \leq 1$ fluctuations do decay to zero with the system size in all the temperature range.

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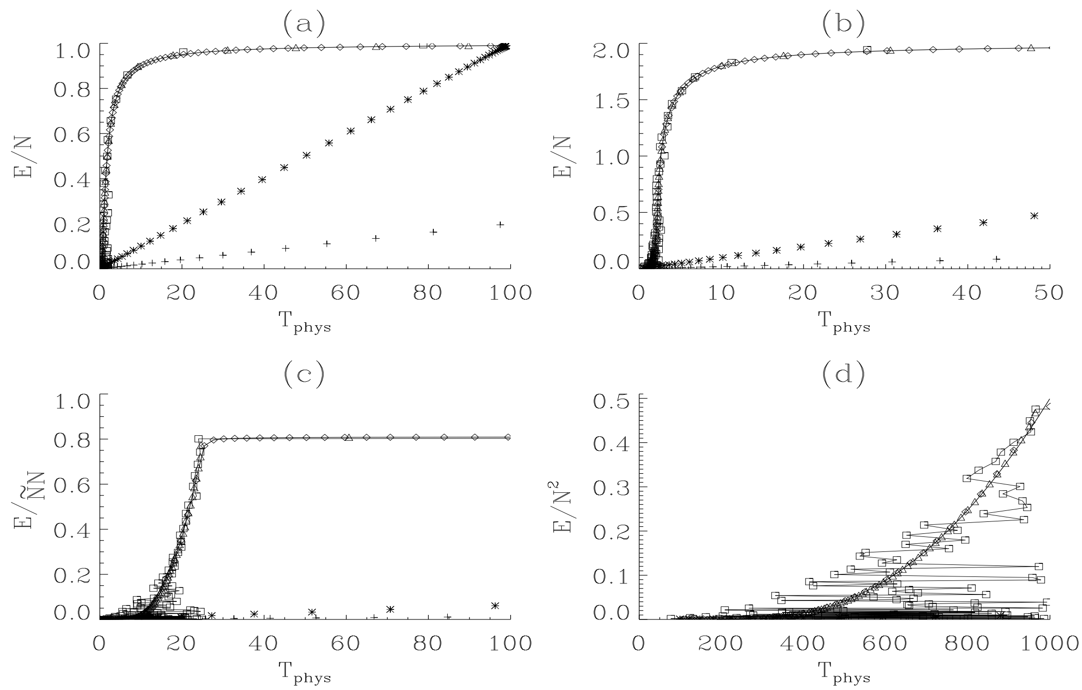

Fig. 2. Internal energy E as a function of the physical temperature T_{phys}. Same cases and symbol meanings as in Fig.1.

References

[1] C. Tsallis, *J. of Stat. Phys* **52**, 479 (1988). An updated bibliography on Tsallis statistics is available at http://tsallis.cat.cbpf.br/biblio.htm

[2] C. Tsallis, R.S Mendes, and A.R. Plastino, *Physica A* **261**, 534 (1998).

[3] P. Jund, S.G. Kim, and C. Tsallis, *Phys. Rev. B* **52**, 50 (1995).

[4] S. Abe, S. Martínez, F. Pennini, A. Plastino, *Phys. Lett.* A **281**, 126 (2001).

[5] B. Kaufman, *Phys. Rev.* **76**, 1232 (1949).

[6] P.D. Beale, *Phys. Rev. Lett.* **76**, 78 (1996).

[7] G. Bhanot, R. Salvador, S. Black, P. Carter, and R. Toral, *Phys. Rev. Lett.* **59**, 803 (1987) and references therein.

[8] R. Salazar and R. Toral, *Physica A* **290**, 159 (2001).

[9] See, for instance, P.M. Chaikin and T.C Lubensky, *Principles of Condensed Matter Physics*, Cambridge U. Press (1995).

[10] A. Plastino and A.R. Plastino, *Phys. Lett. A* **226**, 257 (1997).

[11] R. Toral, preprint cond-mat/0106060.