Scaling functions for Tsallis non–extensive statistics.

R. Salazar and R. Toral

Instituto Mediterráneo de Estudios Avanzados (CSIC-UIB)[†] *and Departament de Física*
Universitat de les Illes Balears, E-07071 Palma de Mallorca, Spain

We study the one-dimensional Ising model with long-range interactions in the context of Tsallis non-extensive statistics by computing numerically the number of states with a given energy. We find that the internal energy, magnetization, entropy and free energy follow non-trivial scaling laws with the number of constituents N and temperature T. Each of the scaling functions for the internal energy, the magnetization and the free energy, adopts three different forms corresponding to $q > 1$, $q = 1$ and $q < 1$, being q the non-extensivity parameter of Tsallis statistics.

It is generally assumed that Thermodynamics and Statistical Mechanics necessarily imply that the entropy, the internal energy and other thermodynamic potentials are extensive quantities. For instance, the internal energy E as a function of temperature T and number of constituents N scales usually as:

$$E(N,T) = Ne(T). \tag{1}$$

Within the theoretical framework of Statistical Mechanics, this is indeed a widespread consequence when the intermolecular potentials are short-range. For the so called *normal* systems [1], the number of microscopic states with a given energy scales as $\Omega(E,N) = \exp(Ns(E/N))$, from where it follows the entropy behavior $S(E,N) = \ln\Omega = Ns(E/N)$ [2]. The thermodynamic relation $T^{-1} = \left(\frac{\partial S}{\partial E}\right)_N$ leads then to the scaling law (1) for the internal energy. However, it has been also realized that long-range potentials can lead to non-extensive behavior and, recently, there has been some interest in finding the correct scaling laws for the thermodynamic potentials for systems whose non-extensive behavior arises from a long-range interaction [3,4]. Let us be more specific and consider the ferromagnetic Ising model with long-range interactions:

$$\mathcal{H} = \sum_{i,j=1}^{N} \frac{1 - S_i S_j}{r_{i,j}^{\alpha}}, \qquad (S_i = \pm 1, \ \forall i), \tag{2}$$

where indexes i, j run over the N sites on a d-dimensional lattice and $r_{i,j}$ is the distance between sites i and j. It can be easily shown that the energy levels scale as

$$NN^* \equiv N \frac{N^{1-\alpha/d} - 1}{1 - \alpha/d}. \tag{3}$$

In the case of $\alpha > d$, N^* tends to a constant in the limit of large N and the energy recovers its usual extensive behavior, whereas in the case $\alpha \le d$ the behavior is non–extensive (for $\alpha = d$ the limit $N^* = \ln N$ is assumed). Therefore one expects the failure of the scaling law (1) for $\alpha \le d$. This is indeed the case as Cannas and Tamarit [4] have shown by performing Monte-Carlo simulations of the Hamiltonian (2) in a d=1 system. Their results show that the Boltzmann-Gibbs canonical ensemble statistics leads to the following scaling laws for the internal energy, spontaneous magnetization, entropy and free energy:

$$E(N,T) = NN^* e(T/N^*), \tag{4}$$
$$M(N,T) = Nm(T/N^*), \tag{5}$$
$$S(N,T) = Ns(T/N^*), \tag{6}$$
$$F(N,T) = NN^* f(T/N^*). \tag{7}$$

The argument justifying these scaling laws can be summarized as follows [3]: the internal energy and the entropy appear in the definition of the Helmholtz free energy as $F = E - TS$, therefore one expects that E and TS should have the same behavior for large N. Since E scales as NN^* and S scales as N one obtains that T must scale as N^* thus leading to the previous scaling ansatzs.

Although the above scaling laws have been verified in [4] by application of the Boltzmann-Gibbs statistics, it has been argued that the appropriate frame to describe systems with long–range interactions should be that of Tsallis non-extensive statistics, since non-extensivity properties appear in this formulation in a natural way [5]. Tsallis statistics depends on a parameter q in such a way that the limit $q = 1$ retrieves the results of Boltzmann–Gibbs statistics whereas for $q < 1$, the entropy is super-extensive and for $q > 1$ it is sub-extensive.

The aim of this paper is to derive and compute numerically the scaling laws for the entropy, internal energy, free energy and magnetization that follow form the application of Tsallis statistics to the long–range d=1 Ising model defined by (2) in the non-extensive regime $\alpha \le d$. Our main result is that we can write scaling laws (see Eqs.(15)–(18) below) that depend on appropriate scaling factors $A_q(N)$, $A_q^E(N)$, $A_q^S(N)$ and N^*. In the limit $q \to 1$ the scaling laws for Boltzmann–Gibbs statistics (4)-(7) are recovered. Furthermore, the scaling functions e_q, m_q and f_q depend on the parameter q in such a way that they collapse onto only three scaling functions for each magnitude: those of $q > 1$, $q = 1$ and $q < 1$.

Let us remind briefly which are the basic ingredients of Tsallis statistics. Each of the W system configurations ($W = 2^N$ for the Ising model used here) is assigned a probability p_i, which is obtained by finding the extrema of the generalized entropy

$$S_q \equiv \frac{1 - \sum_{i=1}^{W} p_i^q}{q-1}, \tag{8}$$

subject to appropriate constraints. Once the p_i's have been obtained, the quantities of interest are computed as generalized averages of microscopic functions O_i [6]:

$$\langle O \rangle_q \equiv \frac{\sum_{i=1}^{W} p_i^q O_i}{\sum_{i=1}^{W} p_i^q}. \tag{9}$$

In the canonical ensemble, the main constraint (besides the normalization condition $\sum_i p_i = 1$) is that the mean value of the energy is fixed to a given value E_q. This variational problem has the implicit solution for the configuration probabilities:

$$p_i = \frac{[1-(1-q)\beta' \epsilon_i]^{\frac{1}{1-q}}}{\sum_{j=1}^{W}[1-(1-q)\beta' \epsilon_j]^{\frac{1}{1-q}}}, \tag{10}$$

where ϵ_i is the energy of the i-th configuration. We have used the notation

$$\beta' = \frac{\beta}{(1-q)\beta \sum_{i=1}^{W} p_i^q \epsilon_i / \sum_{i=1}^{W} p_i^q + \sum_{j=1}^{W} p_j^q} \tag{11}$$

and the Lagrange multiplier $\beta \equiv 1/T$ (the equivalent of the inverse temperature for the Boltzmann-Gibbs canonical ensemble) has to be found by imposing that the mean value of the Hamiltonian is equal to the given value $E_q = \langle \mathcal{H} \rangle_q$. The usual procedure, however, is to give a value for $T = 1/\beta$ and to derive, using equations (10) and (11), the probabilities $p_i(\beta)$ as a function of the (inverse) temperature β and then compute the mean value $E_q(\beta) = \sum_{i=1}^{W} p_i(\beta)^q \epsilon_i / \sum_{i=1}^{W} p_i(\beta)^q$.

Now the main problem arises in Tsallis statistics that we do not have the solution for the probabilities $p_i(\beta)$ in a closed form, since the non–linear coupled equations (10)–(11) have no explicit solution. Of course, in the case of $q = 1$ we do know the solution (up to a normalization factor) which is nothing but the celebrated Boltzmann factor: $p_i(\beta) = \mathcal{Z}^{-1} \mathrm{e}^{-\beta\epsilon_i}$ where $\mathcal{Z}$ is the partition function. The explicit knowledge of the probabilities $p_i(\beta)$ in the case $q = 1$ allows the use of Monte–Carlo techniques for the numerical calculation of the averages (9). In its simplest version [7], the Metropolis algorithm proposes a new configuration j by randomly flipping one spin in configuration i. The new configuration j is accepted with a probability $\min(1, p_j/p_i) = \min(1, \mathrm{e}^{-\beta(\epsilon_j - \epsilon_i)})$. Notice that the partition function cancels out in the calculation of the acceptance probabilities. Unfortunately, since for $q \neq 1$ the probabilities p_i are not known as a function of β, there is no trivial generalization of the Monte–Carlo method to perform the averages in (9) at fixed temperature β. One can perform Monte-Carlo simulations at fixed β' [8], but then the physical temperature β is not known. Another interesting approach (close in spirit to our method here) is that of Lima et al. [9] who have used the broad histogram method [10] to study the 2-d short-range Ising model, focusing mainly on the possibility of the existence of a phase transition for $q \neq 1$.

We overcome these problems by using a method of histogram by overlapping windows initially devised to study short-range lattice models [11]. In this method, one computes numerically the number $\Omega(E, N; \delta E)$ [12] of microscopic states whose energy lies in the interval $(E, E + \delta E)$. The histogram by overlapping windows method performs a microcanonical simulation by fixing the energy in a window $(E, E + \Delta E)$ and computing the ratios $\Omega(E_1, N; \delta E)/\Omega(E_2, N; \delta E)$ for energies E_1, E_2 within this window. Once those ratios have been computed with a given accuracy, we perform another microcanonical simulation in a different window $(E', E' + \Delta E)$ which overlaps the previous energy window. The method proceeds until the windows have swept over all the possible energy values. The exact knowledge of the degeneracy for the ground state $\Omega(E_0, N) = 2$ allows the recursive calculation of the number of states $\Omega(E, N; \delta E)$ for all values of E. For the long-range Ising model, the size of the window ΔE has to been chosen carefully in order to avoid the lack of ergodicity. A full account of the method details will be given elsewhere [13]. Here we just report on the results we obtain for the aforementioned scaling laws.

Using this method we have computed the number of states $\Omega(E_k)$ for the d=1 Hamiltonian defined in (2) with α=0.8 and system sizes N = 34, 100, 200, 400, 1000. Once the number of states $\Omega(E_k)$ is known, one can use a recursive method [15] to solve Eqs.(10)-(11) in order to find the probabilities $p_i(\beta)$. Equivalently, one can compute the probabilities $p_i(\beta')$ as a function of the parameter β' using (10), where the sum over configurations is now replaced by a sum over all possible energy bins of size δE. The entropy, $S_q(\beta')$, the internal energy $E_q(\beta')$ and the magnetization $M_q(\beta')$ [14] are computed in the same way as a function of β' using relations (8) and (9). The physical temperature $T = 1/\beta$ can be obtained by inverting (11):

$$\beta = \beta' \frac{1-(q-1)S_q(\beta')}{1-(1-q)\beta' E_q(\beta')}, \tag{12}$$

thus allowing a parametric plot of the internal energy, entropy and magnetization as a function of the temperature T. We have also computed the free energy defined as $F_q = E_q - TS_q$. It is important to remark that, in the case of $q < 1$, and for large values of system size N the raw data show a loop with temperature. This is similar to what happens in the short-range Ising model and we have adopted the same criterion than in [15]: to use a Maxwell-type construction that replaces the loop of the curve by a straight line joining the two points with the same value of the free energy.

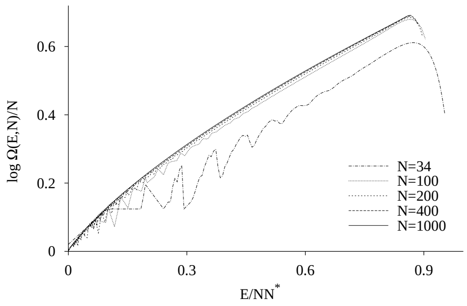

FIG. 1. Number of states $\Omega(E, N)$ plotted to check the scaling law (13). The results for $N = 34$ have been obtained by an exact enumeration of the $W = 2^{34}$ possible states, whereas the results for the other system sizes have been obtained by the histogram by overlapping windows method described in the text [16].

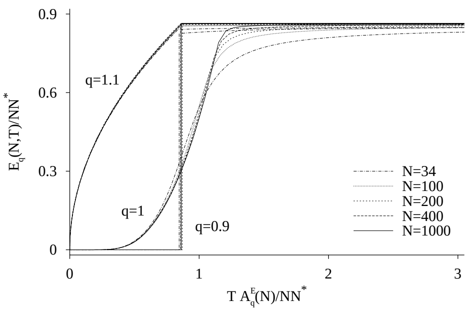

FIG. 2. Internal energy plotted to check the scaling relation (15) by using different values of q and system sizes N. The scaling factors used are those defined in (14) and (19).

In Fig.(1) we plot the computed values for the number of states $\Omega(E, N)$ as a function of the energy E for different systems sizes. In this figure, the data have been scaled to show that the number of states follows the scaling law that one would expect given that the total number of states scales as 2^N and the energy levels scale as NN^*, namely:

$$\Omega(E, N) = \exp(N\phi(E/NN^*)). \tag{13}$$

In order to generalize the scaling functions for the thermodynamic potentials in the case of Tsallis statistics, we notice that, in the case of equiprobability (corresponding to very high temperature) (8) implies that the entropy scales as $S_q(N) \sim A_q(N)$, where

$$A_q(N) = \frac{1 - 2^{N(1-q)}}{q - 1}. \tag{14}$$

Keeping in mind that the energy scales as NN^* and assuming that E_q and TS_q scale in the same way we derive that the temperature must scale as $NN^*/A_q(N)$ and hence we are led to the ansatz:

$$E_q(N, T) = NN^* e_q(TA_q^E(N)/NN^*), \tag{15}$$

$$M_q(N, T) = Nm_q(TA_q^E(N)/NN^*), \tag{16}$$

$$S_q(N, T) = A_q(N)s_q(TA_q^S(N)/NN^*), \tag{17}$$

$$F_q(N, T) = NN^* f_q(TA_q(N)/NN^*). \tag{18}$$

Here, in view of later results, we have introduced new scaling factors $A_q^E(N)$ and $A_q^S(N)$. The previous argument would imply simply $A_q^E(N) = A_q^S(N) = A_q(N)$. Notice that in the limit $q \to 1$ it is $A_1(N) \sim N$ and the scaling laws Eqs.(4)–(7) are recovered.

In figures (2) and (3) we scale the energy, magnetization and entropy data by using factors $A_q(N)$, $A_q^E(N)$, $A_q^S(N)$ and N^* as implied by Eqs.(15)-(18). In figure (2) we concentrate in the validity of scaling for different values of N, whereas in figure (3) we compare the scaling functions for different values of q using the scaling functions obtained for the largest value $N = 1000$. These figures give evidence that in the case $q \le 1$, scaling is well satisfied by using $A_q^E(N) = A_q^S(N) = A_q(N)$ as argued before. However, the data for $q > 1$ do not follow this scaling description. In order to obtain a good scaling for $q > 1$ one observes numerically that it is necessary to assume instead the limits $A_q^E(N) \sim 2^{N(1-q)}/(q-1)$ and $A_q^S(N) \sim 2^{N(q-1)}/(q-1)$. A unifying description that reproduces the required limits for all values of q is:

$$A_q^S(N) = \frac{2^{N|1-q|} - 1}{|\, 1 - q \,|}, \qquad A_q^E(N) = \frac{A_q(N)^2}{A_q^S(N)}. \tag{19}$$

and these expressions have been used to scale data as shown in the figures. We observe, see Fig.(2) for the internal energy, that the quality of the scaling is rather good and improves, as expected, with increasing system size. A very interesting feature is that, as shown in Fig.(3) the scaling functions group into three different forms corresponding to $q < 1$, $q = 1$ and $q > 1$. The only exception is that of the entropy for which the collapse for $q > 1$ is very poor. This is easily understood by noticing that the low temperature limit of the entropy for infinite system size is $S_q(T = 0) = (1 - 2^{1-q})/(q - 1)$ whereas the high temperature limit is $S_q(T \to \infty) = 1/(q - 1)$ and those two finite values can not be rescaled simultaneously. The scaling for the free energy follows directly from its definition $F_q = E_q - TS_q$. For $q \le 1$ it is $f_q(x) = e_q(x) - xs_q(x)$, whereas for $q > 1$ and in the limit of large N, the scaling function is given simply by $f_q(x) = e_q(0) - x s_q(\infty) = -x$.

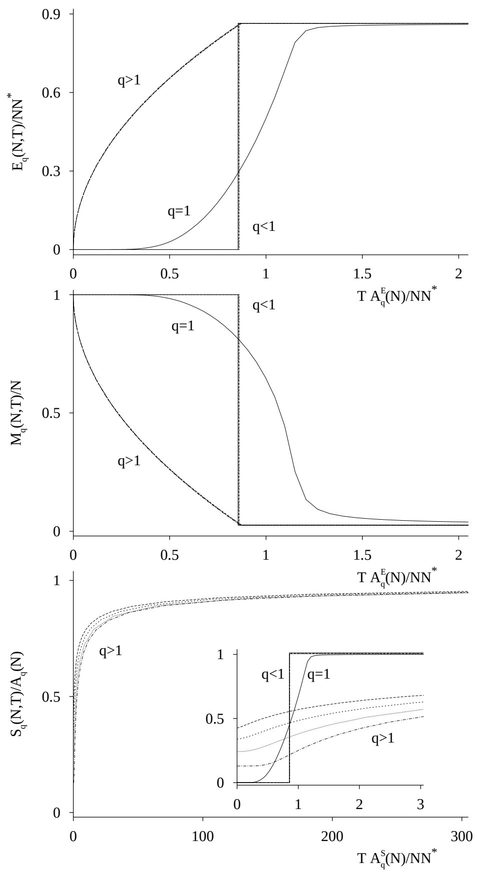

FIG. 3. Internal energy (top graph), magnetization (middle graph) and entropy (lower graph) plotted in order to check the proposed scaling behavior. We have used in all the curves the value $N = 1000$ and varied the parameter q. For clarity, in the entropy curve, the insert shows all the values of q, whereas the main plot takes only $q > 1$. The curves with $q > 1$ include $q = 1.2,\ 1.4,\ 1.6,\ 1.8$ and the curves with $q < 1$ include $q = 0.2,\ 0.4,\ 0.6,\ 0.8$, although the different curves are almost indistinguishable with the resolution of this figure.

In summary, the scaling laws given by Eqs.(15)-(18) work for all values of q when one uses the scaling factors given by Eqs.(14), and (19). Moreover, the scaling functions e_q, m_q and f_q adopt only three different forms for each magnitude: one valid for $q > 1$, one valid for $q = 1$ and another valid for $q < 1$.

Several final comments are in order. First, it is distressing the fact that the scaling forms for $q > 1$ do not follow the scaling ansatz that follows naively from the argument that T should scale as $E_q/S_q \sim NN^*/A_q(N)$. We have not been able to find a convincing argument that reproduces the scaling forms found in this paper for $q > 1$. It seems that the transformation $\beta' \to \beta$ given by Eq.(12) has two special points where the slope changes abruptly and which scale precisely as $NN^*/A_q^S(N)$ and $NN^*/A_q^E(N)$, although the exact implication for the scaling functions is not clear to us at this moment. Second, the fact that the scaling functions adopt very different forms (for $q < 1$, $q = 1$ and $q > 1$) might allow to conclude easily whether classical Boltzmann-Gibbs or Tsallis statistics should be used when analyzing experimental data. Finally, we would like to stress the power of the histogram by overlapping windows method to study numerically systems with long-range forces.

We thank A.R. Plastino for stimulating discussions. This work is supported by DGES (Spain) projects PB94-0167, PB97-0141-C02-01.

† `http://www.imedea.uib.es/PhysDept`

[1] See, for example, R.Kubo,*Statistical Mechanics*, North-Holland (1965)

[2] We use throughout the paper dimensionless units such that the Boltzmann constant is $k_B = 1$.

[3] C. Tsallis, Fractals **3**, 541 (1995).

[4] S.A. Cannas and F.A. Tamarit, Phys. Rev. **B54** R12661 (1996).

[5] C. Tsallis, J. Stat. Phys. **52**, 479 (1988). For a recent review, see C. Tsallis, Braz. J. Phys. **29**, 1 (1999).

[6] C. Tsallis, R.S Mendes, and A.R. Plastino, Physica **A261**, 534 (1998).

[7] M. Kalos and P. Whitlock, *Monte-Carlo Methods*, John Wiley and Sons (1986).

[8] I. Andricioaei and J.E. Straub, Phys. Rev. **E53**, R3055 (1996).

[9] A.R. Lima, J.S. Sá Martins, and T.J.P. Penna, Physica A **268**, 553 (1999).

[10] P.M.C. de Oliveira, T.J.P. Penna and H.J. Herrmann, Braz. J. Phys. **26**, 677 (1996); *ibid*, Eur. Phys. J. **B1**, 205 (1998).

[11] G. Bhanot, R. Salvador, S. Black, P. Carter, and R. Toral, Phys. Rev. Lett. **59** 803 (1987); G. Bhanot, S. Black, P. Carter, and R. Salvador, Phys. Lett. **B183**, 331 (1987); G. Bhanot, K. Bitar, S. Black, P. Carter, and R. Salvador, Phys. Lett. **B187**, 381 (1987); G. Bhanot, K. Bitar and R. Salvador, Phys. Lett. **B188**, 246 (1987).

[12] For clarity of notation, we write indistinctly $\Omega(E)$, $\Omega(E,N)$ or $\Omega(E,N;\delta E)$ to stress in each context the relevant variables upon which the number of states Ω depends.

[13] R. Salazar and R. Toral, to be published.

[14] We have used the usual definition $M = \mid N^{-1} \sum_{i=1}^{N} S_i \mid$.

[15] A.R. Lima and T.J.P. Penna. Phys. Lett. A **256**, 221 (1999).

[16] We have checked that for $N = 34$ the histogram by overlapping method reproduces accurately the exact results.