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Numerical determination of the distribution of energies for the XY-model

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Abstract

We compute numerically the distribution of energies $\Omega(E, N)$ for the XY-model with short- and long-range interactions. We find that in both cases the distribution can be fitted to the functional form: $\Omega(E, N) \sim \exp(N\phi(E, N))$, with $\phi(E, N)$ an intensive function of the energy. © 2002 Elsevier Science B.V. All rights reserved.

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In 1988 Tsallis introduced a generalised q -entropy given by [1]

$$S_q = \frac{\sum_{i=1}^W p_i^q - 1}{1 - q}, \quad (1)$$

where p_i , ($i = 1, \dots, W$) is the probability of the microscopic configuration i , and the parameter q characterises the degree of non-extensivity of S_q .¹ Non-extensive systems with long-range interparticle interactions are good candidates to be studied under the generalised thermostatistics derived from this q -entropy [2]. One such system which has

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¹ A quantity is said to be non-extensive if its asymptotic dependence on the system's size N is non-linear. On the contrary, extensive quantities exhibit a linear dependence on N .

received special attention recently [3–6] is the XY model with long-range interparticle interactions. This model is described by the Hamiltonian

$$\mathcal{H} = \sum_{(i,j)}^N \frac{1 - \cos(\theta_i - \theta_j)}{r_{ij}^\alpha}, \quad (2)$$

where $\{\theta_i\}_{i=1,\dots,N}$ are angle-type variables, and the sum runs over all distinct pairs of sites on a d -dimensional regular lattice of lineal size $L = N^{1/d}$ with periodic boundary conditions. The distance between the sites i and j is r_{ij} , and the parameter α sets the interaction range. The short-range interaction XY model is recovered in the limit $\alpha = \infty$. To determine the range of parameters leading to non-extensive features, it is instructive to consider the scaling behaviour of the mean energy per particle [7],

$$\frac{E}{N} \sim \tilde{N} \equiv 1 + d \int_1^L dr r^{d-1} r^{-\alpha} = \frac{N^{1-\alpha/d} - \alpha/d}{1 - \alpha/d}. \quad (3)$$

Therefore, for $\alpha > d$ (including the limiting case $\alpha = \infty$) the energy scales as $E \sim N$ and the system behaves linearly, whereas in the non-extensive regime $\alpha < d$, the energy scales as $E \sim N^{2-\alpha/d}$. In the limiting case $\alpha = d$ the energy per site scales as the logarithm of the system size: $E \sim N \ln N$. The number of microscopic configurations with energy between E and $E + \delta E$ is equal to $\Omega(E, N) \delta E$, where $\Omega(E, N)$ is the density of states. Our aim here is to compute numerically $\Omega(E, N)$ in order to study its asymptotic dependence on N .

Recent numerical studies of a dynamical version of the long-range XY model (endowed with appropriate kinetic energy terms) have shown the existence of metastable states exhibiting a Tsallis' maximum entropy distribution of velocities [5,6]. The lifetime of these metastable states increases with the system size, thus suggesting that it diverges in the thermodynamic limit.

Here, we are going to consider an angle of this subject involving a recently conjectured relation [8] between (i) the range of applicability of Tsallis Statistics and (ii) the functional form of the density of states $\Omega(E, N)$. For most systems studied so far one has $\Omega(E, N) \sim \exp(N\phi(E, N))$, with $\phi(E, N)$ an intensive function, implying that the natural expression for an extensive entropy is the well known Boltzmann–Gibbs entropic form $S = \ln(\Omega(E, N))$. However, things might be different if, instead, the behaviour of $\Omega(E, N)$ were as $\Omega(E, N) \sim \varphi(E, N)N^\mu$ (again with $\varphi(E, N)$ an intensive function). In such a case it is conjectured that the relevant entropic form is the one determined by Eq. (1), $S_q = (\Omega(E, N)^{1-q} - 1)/(1 - q)$, with $\mu(1 - q) = 1$. Our intention is to present briefly some results about the form of $\Omega(E, N)$ for the XY model with long-range interactions. It is shown that an unrestricted counting of states leads to a functional form $\Omega(E, N) \sim \exp(N\phi(E))$. Therefore, if ergodicity is satisfied, the Boltzmann–Gibbs entropic form is the appropriate one. This suggests, in accord with the results reported in Refs. [5,6], that transient regimes (during which the system is not able to explore the whole range of energy values) may constitute an appropriate field of application of the non-extensive thermostatistics (see also Ref. [2]). The number of states $\Omega(E, N)$ has been numerically computed using the so-called histogram by overlapping windows (HOW) method [9–11]. Briefly, the HOW method works by confining the energy histogram generation to a suitably small

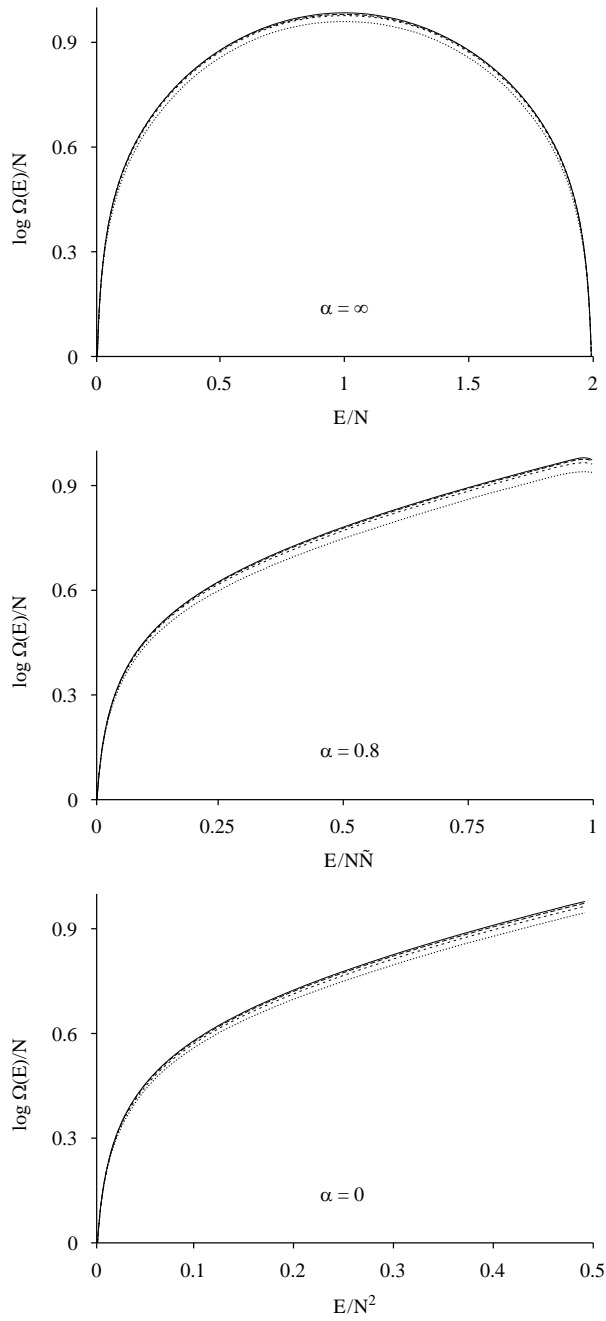


Fig. 1. Scaling relations of the number of states $\Omega(E, N)$ of the one-dimensional XY model, Eq. (2), for different values of the parameter α and $N = 50, 100, 200, 400$.

energy interval $[E_i, E_i + \Delta E]$, such that the values of the number of states for each energy in that interval are comparable. The process is repeated varying E_i until the full energy range is covered. We have also applied a method recently developed by Wang and Landau [12] which samples the function $\Omega(E, N)$ autoconsistently. Both methods give the same results within errors. We have obtained numerically $\Omega(E, N)$ for the one-dimensional XY model defined in Eq. (2), for different system sizes $N = 50, 100, 200, 400$. Our results are shown in Fig. 1 in three cases: (i) the extensive, short-range limit $\alpha = \infty$, (ii) the non-extensive case with $\alpha = 0.8$, and (iii) the non-extensive case with infinite range limit $\alpha = 0$. It is clear from Fig. 1 that in all the cases considered the generic behaviour is $\Omega(E, N) \sim \exp(N\phi(E, N))$ with an intensive function $\phi(E, N) = \phi(E/N\tilde{N})$ in which the energy appears rescaled according to Eq. (3). In each case of the Fig. 1 the energy axis cover the whole possible energy spectrum. We found that the last two cases of Fig. 1 have an abrupt ending around the maximum value of the system energy in a similar way to the α -Ising model [10,11].

We note that the scaling functions $\phi(x)$ appears to be independent of α in the range $0 \leq \alpha < d$. This equivalence for this range of values of α was also observed with other properties of the model in Refs. [3,4] where it was shown that a mean-field description holds in this case.

In conclusion and according to the above conjecture, we found for this model that the *equilibrium* properties of the system would be described by the standard canonical ensemble while the results of Refs. [5,6] apply to the metastable states developed during the transient dynamics. In this way, these two descriptions are completely compatible.

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References

- [1] C. Tsallis, J. Stat. Phys. 52 (1988) 479. (For an updated bibliography on Tsallis Statistics see <http://tsallis.cat.cbpf.br/biblio.htm>.)
- [2] S. Abe, Y. Okamoto (Eds.), Nonextensive Statistical Mechanics and Its Applications, Springer, Berlin, Heidelberg, 2001.
- [3] F. Tamarit, C. Anteneodo, Phys. Rev. Lett. 84 (2000) 208.
- [4] A. Campa, A. Giansanti, D. Moroni, Phys. Rev. E 62 (2000) 303.
- [5] V. Latora, A. Rapisarda, C. Tsallis, Phys. Rev. E 64 (2001) 056134.
- [6] V. Latora, A. Rapisarda, C. Tsallis, preprint cond-mat/0109056.
- [7] C. Tsallis, Fractals 3 (1995) 541.
- [8] C. Tsallis, Discussion at the NEXT 2001 conference in Cagliari, May 2001.
- [9] G. Bhanot, R. Salvador, S. Black, P. Carter, R. Toral, Phys. Rev. Lett. 59 (1987) 803.
- [10] R. Salazar, R. Toral, Physica A 290 (2001) 159.
- [11] R. Salazar, R. Toral, Phys. Rev. Lett. 83 (1999) 4233.
- [12] F. Wang, D.P. Landau, Phys. Rev. Lett. 86 (2001) 2050.