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Influence of the interaction range on the thermostatistics of a classical many-body system

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HIGHLIGHTS

- Detailed molecular dynamics study for the HMF and the α-XY models is presented.
- Both short- and long-range regimes are analyzed and different behaviors are shown.
- For the short-range regime the results agree with standard statistical mechanics.
- In the long-range case the results points to nonextensive statistical mechanics.

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ABSTRACT

We numerically study a one-dimensional system of N classical localized planar rotators coupled through interactions which decay with distance as $1/r^{\alpha}$ ($\alpha \geq 0$). The approach is a first principle one (*i.e.*, based on Newton's law), and yields the probability distribution of momenta. For α large enough and $N \gg 1$ we observe, for longstanding states, the Maxwellian distribution, landmark of Boltzmann–Gibbs thermostatistics. But, for α small or comparable to unity, we observe instead robust fat-tailed distributions that are quite well fitted with q-Gaussians. These distributions extremize, under appropriate simple constraints, the nonadditive entropy S_q upon which nonextensive statistical mechanics is based. The whole scenario appears to be consistent with nonergodicity and with the thesis of the q-generalized Central Limit Theorem.

1. Introduction

More than one century ago, in his historical book *Elementary Principles in Statistical Mechanics* [1], J. W. Gibbs remarked that systems involving interactions such as Newtonian gravitation are intractable within the theory proposed by Boltzmann and himself, due to the divergence of the canonical partition function. This is of course the reason why no standard temperature-dependent thermostatistical quantities (*e.g.*, a specific heat at finite temperatures) can possibly be calculated for the free hydrogen atom, for example. Indeed, although the quantum approach of the hydrogen atom solves the divergence associated, for classical gravitation, with small distances, the divergence associated with large distances remains the same. More precisely, unless a box surrounds the atom, an infinite number of excited energy levels accumulate at the ionization value, which yields a divergent canonical partition function at any finite temperature. This and related questions are commented on in Ref. [2], for instance.

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Here we report a numerical study of the α-XY model [3], a many-body Hamiltonian system with two-body interactions whose range is controlled by a parameter of the model. More precisely, we assume a potential which decays with distance as $1/r^{\alpha}$ ($\alpha \geq 0$). This model recovers, when $\alpha = 0$, the Mean Field Hamiltonian (HMF), a fully coupled many-particle system [4], and recovers, in the $\alpha \to \infty$ limit, the first-neighbor XY ferromagnet, a model which is well defined within the traditional thermostatistical scenario of short-range interactions. Systems with long-range interactions have been attracting particular attention of the statistical-mechanical community in the last two decades. This renewed and increasing interest was launched by Antoni and Ruffo in 1995 [4] with their discussion of the HMF model, which in many aspects mimics traditional long-range systems while bypassing some of its difficulties.

The model focused on here was introduced some years later in Ref. [3]. It is a direct generalization of the HMF by including a power-law dependence on distance in order to control the range of the interactions.[1] We refer to short-range (long-range) interactions when the potential felt by one rotator of a d-dimensional system is integrable (nonintegrable), i.e., when $\alpha/d > 1$ ($0 \leq \alpha/d \leq 1$). A direct consequence of this fact is that the total energy is extensive when $\alpha/d > 1$, whereas it is superextensive if $0 \leq \alpha/d \leq 1$. As we shall numerically illustrate, for large values of α/d the system exhibits the standard behavior expected within Boltzmann–Gibbs (BG) statistical mechanics. However, we shall also exhibit that when long-range interactions become dominant, i.e., when $\alpha/d < 1$, the situation is much more complex. In 1988 a generalization of the BG statistical mechanics based on a different entropic functional [2,6,7] was proposed. Within this approach, the thermodynamical structure (free energy, temperature, etc.) can be extended [2,8–11]. Some of the numerical results presented in the next sections appear to be in close agreement with this theory.

2. The model

To transparently extract the deep consequences of Gibbs' remark, in the present paper we focus on the influence of the range of the interactions within an illustrative isolated classical system, namely the α-XY model [3]. This model consists of a d-dimensional hypercubic lattice of N interacting planar rotators, whose Hamiltonian is given by

$$\mathcal{H} = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} \frac{1-\cos(\theta_i-\theta_j)}{r_{ij}^{\alpha}} \quad (\alpha \geq 0), \tag{1}$$

with periodic boundary conditions. Each rotator is characterized by the angle $\theta_i \in [0, 2\pi)$ and its canonical conjugate momentum p_i. Without loss of generality we have considered unit moment of inertia, and unit first-neighbor coupling constant; r_{ij} measures the (dimensionless) distance between rotators i and j, defined as the minimal one given the periodic boundary conditions.

For $d = 1$, r_{ij} takes the values $1, 2, 3\ldots$; for $d = 2$, it takes the values $1, \sqrt{2}, 2, \ldots$; for $d = 3$, it takes the values $1, \sqrt{2}, \sqrt{3}, 2, \ldots$. Notice that, in contrast with Newtonian gravitation, the potential in Hamiltonian (1) does not diverge at short distances since the minimal distance, in any dimension, is always the unit. The kinetic term in (1), proportional to p_i^2, is the traditional one, but the interaction term is long-range for $\alpha \leq d$, which makes the internal energy per particle to diverge in the thermodynamic limit. Following [12], this property can be seen by realizing that the energy *per particle* of the interaction term varies with N like [13,14]:

$$\widetilde{N} \equiv \frac{1}{N}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} \frac{1}{r_{ij}^{\alpha}} = \sum_{j=2}^{N} \frac{1}{r_{1j}^{\alpha}}. \tag{2}$$

In the $\alpha \to \infty$ limit, $\widetilde{N} = 2d$. If $\alpha/d < \infty$, the discussion of the above sum can be conveniently replaced by the discussion of the following integral [3]:

$$d\int_{1}^{N^{1/d}} \mathrm{d}r\, \frac{r^{d-1}}{r^{-\alpha}} = \frac{N^{1-\alpha/d}-1}{1-\alpha/d}, \tag{3}$$

which behaves, when $N \to \infty$, like $N^{1-\alpha/d}/(1-\alpha/d)$ if $0 \leq \alpha/d < 1$, like $\ln N$ if $\alpha/d = 1$, and like $1/(\alpha/d-1)$ if $\alpha/d > 1$. In other words, the total internal energy is extensive (in the thermodynamical sense) for $\alpha/d > 1$, and nonextensive otherwise. In order to accommodate to a common practice, we can rewrite the Hamiltonian $\mathcal{H}$ as follows [3]:

$$\bar{\mathcal{H}} = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \frac{1}{2\widetilde{N}}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N} \frac{1-\cos(\theta_i-\theta_j)}{r_{ij}^{\alpha}} = K + V, \tag{4}$$

which can now be considered as "extensive" for all values of α/d, at the "price" that a microscopic two-body coupling constant becomes now, through $\widetilde{N}$, artificially dependent on N. However, as shown in Ref. [3], this corresponds in fact

[1] We refer the reader to the work by Chavanis and Campa [5], where a quite complete list of references about the evolution of this subject can be found.