Nonextensive scaling in a long-range Hamiltonian system

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The nonextensivity of a classical long-range Hamiltonian system is discussed. The system is the so-called $\alpha$-XY model, a lattice of inertial rotators with an adjustable parameter $\alpha$ controlling the range of the interactions. This model has been explored in detail over the last years. For sufficiently long-range interactions, namely $\alpha < d$, where $d$ is the lattice dimension, it was shown to be nonextensive and to exhibit a second order phase transition. However, conclusions in apparent contradiction with the previous findings have also been drawn. This picture reveals the fact that there are aspects of the model that remain poorly understood. Here we perform a thorough analysis, essaying an explanation for the origin of the apparent discrepancies.

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I. INTRODUCTION

Systems of many particles interacting via long-range forces, although ubiquitous, are not fully understood (see for instance [1]). Special interest in such systems has arisen recently in connection with the extension of standard statistical mechanics proposed by Tsallis [2]. As a prototype to study the dynamics and thermodynamics of long-range systems, both in equilibrium and non-equilibrium situations, a dynamical model with an adjustable interaction range has been introduced [3]. The model consists in $N$ interacting rotators moving on parallel planes and located on a periodical $d$-dimensional hypercubic lattice with unitary spacing. Each rotator is fully described by an angle $0 < \theta_i \leq 2\pi$ and its conjugate momentum $L_i$. The dynamics of the system is ruled by the Hamiltonian

\[ H = \frac{1}{2} \sum_{i=1}^{N} L_i^2 + \frac{J}{2} \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} \frac{1 - \cos(\theta_i - \theta_j)}{r_{ij}^{\alpha}} \equiv K + V, \]

where the coupling constant is $J \geq 0$ (we restrict our study to the ferromagnetic case where interactions are attractive) and, without loss of generality, moments of inertia equal to one are chosen for all the particles. Here $r_{ij}$ measures the minimal distance between rotators located at the lattice sites $i$ and $j$. One can associate to each rotator a “spin vector” $m_i = (\cos \theta_i, \sin \theta_i)$, which allows to define an order parameter $m = \frac{1}{N} \sum_{i=1}^{N} m_i$. The Hamiltonian (1), describing a classical inertial $XY$ ferromagnet, is usually referred to as $\alpha$-XY model. It includes as particular cases the first-neighbor ($\alpha \to \infty$) and the mean-field ($\alpha = 0$) models. Note that this is an inertial generalization of the well known $XY$ model of the statistical physics of magnetism: the time evolution is given by the natural dynamics governed by the Hamilton equations.

This prototype of complex long-range behavior has been thoroughly explored in the last few years (see for instance [3–5]). It has been shown that the model presents nonextensive behavior for $\alpha < d$ [3]. In that domain of $\alpha$ it displays a second order phase transition. This result has been exhibited first by means of numerical computations for the one-dimensional (1D) case [4] and later through analytical calculations for arbitrary $d$ using a scaled version of the Hamiltonian $H$ [5]. However, a recent work [6] draws conclusions that are in disagreement with the previous findings, claiming that the model is extensive for all $\alpha$ and that there is no phase transition. This apparent contradiction helps to put into evidence that there are aspects of the model that remain obscure. The lack of a comparative study as well as of a discussion on the origin of the discrepancies motivates the present work. It is the purpose of this paper to review and complement previous results to elucidate the question.

In order to do that, we use the following methodology. We start by solving the equations of motion associated to Hamiltonian $H$:

\[ \dot{\theta}_i = \frac{\partial H}{\partial L_i} = L_i, \]
\[ \dot{L}_i = -\frac{\partial H}{\partial \theta_i} = -J \sum_{j \neq i}^{N} \frac{\sin(\theta_i - \theta_j)}{r_{ij}^{\alpha}}, \quad i = 1, \ldots, N. \]

Numerical integration is performed by means of a symplectic fourth order algorithm [7] using a small time step to warrant energy conservation with a relative error smaller than $10^{-5}$. Equilibrium properties are analyzed by means of time averages (computed after a transient) that allow to mimic microcanonical averages. In Ref. [6], numerical results for the canonical ensemble were ob-
tained through standard Monte Carlo simulations. Due to ensemble equivalence [8], both methods are expected to yield the same macroscopic averages at thermal equilibrium. Simulations will be supplemented by analytical considerations.

II. EQUILIBRIUM THERMODYNAMICS OF THE $\alpha$-XY MODEL

Along this paper we will consider Hamiltonian (1) although many related works in the literature refer to a modified version of this Hamiltonian such that the interactions are scaled. Since there is a correspondence between both descriptions, we will discuss this point to take profit of all the pertinent results in the literature. To construct the scaled Hamiltonian, let us call it $\tilde{H}$, the coupling coefficient $J$ in $H$ is substituted by $J/N$, where $N$ is the upper bound of the potential energy per particle, that depends on $N$, $\alpha$, and $d$ according to $\tilde{N} = \frac{1}{N} \sum_1^N \sum_{j \neq i} \frac{1}{r_{ij}}$.

In the large $N$ limit one has [4,9]

$$\tilde{N}(N, \alpha/d) \sim \left\{ \begin{array}{ll}
N^{1-\alpha/d} & 0 \leq \alpha < d \\
\ln N & \alpha = d \\
\Theta(\alpha/d) & \alpha > d
\end{array} \right. \quad (3)$$

with $\Theta$ a function of the ratio $\alpha/d$ only, that goes to 2 as $\alpha/d$ goes to infinity. For $\alpha \leq d$, $\tilde{N}$ depends strongly on $N$. Then the representation given by $\tilde{H}$ may be considered artificial, since the microscopic coupling coefficient becomes $N$-dependent, that is, becomes fed with macroscopic information. Anyway, the thermodynamics and the underlying dynamics of $\tilde{H}$ can be trivially mapped onto those of $H$ by transforming energy-like quantities through $\tilde{E} \leftrightarrow E/N$ and characteristic times (as long as moments of inertia remain unitary) through $\tilde{\tau} \leftrightarrow \tau \tilde{N}^2$ [3]. The usual preference for the scaled form $\tilde{H}$ comes from the fact that the thermodynamic limit of $E/N$ is always finite and no further scalings of either thermodynamical or dynamical quantities are needed.

It has been analytically shown [5], through canonical calculations performed with Hamiltonian $\tilde{H}$, that the thermodynamics of systems with $\alpha < d$, at the final thermal equilibrium, is equivalent to that of its mean-field version (the so-called Hamiltonian Mean Field (HMF) [10]). Such systems display a second order phase transition, from a low-energy ferromagnetic state to a high-energy paramagnetic one, at a certain critical energy per particle $\tilde{\varepsilon}_c = \tilde{U}_c/N = 0.75J$. This important result for $\tilde{H}$ analytically confirms the previous findings [4] for the 1D case of the original Hamiltonian $H$, just by taking into account the simple mapping between $H$ and $\tilde{H}$. Since the equilibrium results of the HMF are universal for $\alpha < d$, we will summarize them. In terms of the magnetization, Hamiltonian $\tilde{H}$ leads to the following caloric curve

$$\tilde{U} = \frac{N}{2\tilde{\beta}} + \frac{JN}{2}[1 - m^2], \quad \text{with} \quad m = \frac{I_1(\tilde{\beta}Jm)}{I_0(\tilde{\beta}Jm)} \quad (4)$$

where $\tilde{\beta} \equiv 1/\tilde{T}$ (being $\tilde{T} = 2(\tilde{K})/N$ the temperature and having set the Boltzmann constant $k_B = 1$) and $I_n$ are the modified Bessel functions of order $n$. The consistency equation from which the magnetization is extracted can be found for instance through canonical calculations [10]. It has a stable solution $m = 0$ for $\tilde{\beta}J < 2$ while, for $\tilde{\beta}J > 2$, the zero magnetization solution becomes unstable and a non-vanishing $\tilde{\beta}$-dependent stable solution arises. From (4), it is clear that the critical value $\tilde{\beta}_cJ = 2$ corresponds to $\tilde{\varepsilon}_c = 0.75J$. Notice in Eq. (4) that, as $m^2 \leq 1$ and the inverse temperature $\tilde{\beta}$ does not depend on $N$, then the large $N$ limit of $E/N$ is always finite.

We will analyze the size dependence of thermal averages. We will focus on the range $0 \leq \alpha < 1$ of 1D lattices governed by Hamiltonian $H$. In Fig. 1(a), the average magnetization per particle $\langle m \rangle$ is represented as a function of the energy per particle $U/N$, for $\alpha = 0.5$ and different system sizes. Clearly, the energy per particle at which the system becomes disordered, i.e, at which the magnetization vanishes up to finite size corrections, grows with the system size. In Fig. 1(b), the same data are represented as a function of $U/N\tilde{N}$. Through this scaling, all data sets tend to the same curve in the thermodynamic limit, as it has already been shown previously [4]. In the inset of Fig. 1(b), a plot $\langle m \rangle$ vs. $N$, for $U/N\tilde{N} = 1.4$ and two values of $\alpha$, illustrate that the magnetization in the high energy regime decays with the system size as $1/\sqrt{N}$. Additionally, data sets for $N = 128$ and different values of $\alpha \in [0, 1]$ were included in Fig. 1(b) to show that the curve of magnetization vs. $U/N\tilde{N}$ is the same for any $\alpha$-XY system with $0 \leq \alpha < 1$, up to corrections of order $1/\sqrt{N}$. In particular, the universal curve coincides with the one for the HMF model ($\alpha = 0$), given by Eq. (4), once taken into account the mapping $\tilde{E} \leftrightarrow E/N$. Everything in agreement with the analytical results of Ref. [5]. However, concerning the phase transition, there is a risk to fall into an endless rhetorical discussion. Strictly speaking, there is no ferromagnetic transition, because the critical energy per particle $U_c/N = 0.75J\tilde{N}$ is divergent, as asserted in [6]. Nevertheless, the limit $N \to \infty$, despite being an idealized situation, must reflect the behavior of finite but large systems in order to be meaningful. Ultimately, we are interested in finite-size systems, as real systems are. For finite-size $\alpha$-XY systems, with $\alpha < 1$, as those that were simulated in this work, one can distinguish two regimes: One, at low energies, where the system is ordered with a magnetization significantly different from zero and independent from the system size, and another, a disordered one, with magnetization of order $1/\sqrt{N}$. A good, representative, thermodynamic limit, reflecting this situation,
can be defined by means of an appropriate scaling, the one allowing data collapse. In that case, it results a finite critical energy, \( U_c/N\bar{N} = 0.75J \), which plays the same role as the critical energy per particle in an extensive system.

If one extends the range of energies plotted (Fig. 1(e)), it becomes clear that data collapse does not hold any more through the \( N \)-scaling. Whereas, as before, it is the \( N\bar{N} \)-scaling the one which leads to data collapse in the full energy range (Fig. 1(f)). As an aside comment, note that, because the relation \( U \simeq 2(K) \) holds at low energies, data collapse would occur in that regime for any arbitrary scaling by \( \bar{N}^\gamma \), with \( \gamma \in \mathbb{R} \). In particular, this is true for \( \gamma = 1 \), as plotted in Fig. 1(d) (hence Fig. 1(e) at low energies) and for \( \gamma = 2 - \alpha \), as in Fig. 1(f) at low energies.

One can understand what is going on as follows. For very low energies, the dynamics is dominated by the quadratic terms of the potential. Thus, the system can be seen as a set of almost uncoupled harmonic oscillators (normal modes). One can also think of particles in a mean-field, a description that is exact in the infinite-range case. The particles effectively interact not through the full mean-field \( m \) but only through its fluctuations. If the mean-field were constant it would play the role of an external field and there would be no interactions. At low energies, where \( m \) is almost constant, the residual or effective interaction, that is the component coming from the fluctuations of \( m \), is small. This is consistent with the normal modes view, where interactions are very weak too. Therefore, in the limit of very low energies (as well as in the limit of very high energies) the system becomes non-interacting (hence, integrable). While at high energies, i.e., above the critical value, one has almost non-interacting rotators; at low energies, i.e., close to the ground state, one has almost non-interacting normal modes. Then, at low energies, from the virial theorem, the result \( \langle K \rangle \simeq \langle V \rangle \) arises trivially. The consequent relation \( U \simeq 2(K) = N/\beta \) indicates that the energy is extensive. A natural result since the interaction terms are not strong, contrarily to what was asserted in [6]. However, as the energy increases and anharmonicities grow, the correct scaling choice is no more that of an extensive system, as becomes evident in Fig. 1(e). Data collapse is actually obtained through the scaling by \( N\bar{N} \), as shown in Figs. 1(b) and 1(f). Moreover, this data collapse is expected to be universal for any \( \alpha \in [0, d) \) [5]. Hence, at criticality, we have the nonextensive behavior \( U_c \propto J N\bar{N} \) and also \( 1/\beta_c = T_c \propto J\bar{N} \).

Let us review the whole picture from the viewpoint of canonical ensemble calculations. We will consider the case \( \alpha = 0 \), but although tricky, a generalization to arbitrary \( \alpha \in [0, d) \) could be analytically performed [5]. The partition function of Hamiltonian (1) when \( \alpha = 0 \) is given by the following integral over phase space

\[
Z_K = \left( \frac{2\pi}{\beta} \right)^{N/2}
\]

and

\[
Z_V = e^{-\beta J N^2} \left( \frac{2\pi}{\beta} \right)^N \int_0^\infty dy e^{-N G(y)}.
\]

\[ (5) \]
where $Z_V$ has already been transformed by means of the Hubbard-Stratonovich trick and $G(y) = -\frac{1}{\beta} \ln y + \frac{y^2}{2\beta JN} - \ln I_0(y)$. The derivation is the same followed in [10] for the scaled Hamiltonian $\tilde{H}$, apart from an $N$-scaling that does not affect the procedure. The integration can be performed by means of the Gaussian approximation around the point $y_o$ verifying $G'(y_o) = 0$, that is, $y_o \simeq \beta J N^2 / I_0(y_o)$ and $G''(y_o) > 0$. In our case, the total energy results

$$U = -\frac{\partial \ln Z}{\partial \beta} = \frac{N}{2\beta} + \frac{JN^2}{2}(1 - m^2), \hspace{1cm} (6)$$

with

$$m = \frac{I_1(\beta J N m)}{I_0(\beta J N m)},$$

in correspondence with Eq. (4). For large $\beta J N$, from the consistency equation, one has $m^2 \simeq 1 - \frac{1}{\beta J N}$ for the stable solution, an approximation that is equivalent to considering $y_o \simeq \beta J N - 1/2$, as done in Ref. [6]. In fact, substitution of the above approximate expression for $m^2$ in (6), gives $U \simeq N/\beta$. Again one obtains that at low temperatures the energy is extensive. However, the approximation above is no longer valid as $\beta$ decreases. In this case, long-range couplings become effective and the nontrivial nonextensive behavior comes out. Then, the energy no longer scales with $N$ and one has to consider the more general Eq. (6). An analysis as that performed in Ref. [6], restricted to the very low temperature regime, misses most of the rich physics of the long-range interacting rotators. Of course, this discussion is meaningful as soon as $N$ is not excessively large. Recall that $1/\beta_c \sim JN$ for generic $\alpha$, hence $1/\beta_c \sim JN$ for $\alpha = 0$. Then $N$ has to be large enough so that the thermodynamic limit is a reasonable approximation but not so large as to drive the temperature scale out of a realistic range.

III. FINAL REMARKS

A double sum as in (1) indicates that, for interaction ranges $0 \leq \alpha/d < 1$, the total energy $U$ may grow as $N^\gamma$, with $\gamma > 1$, as occurs in the regimes of the $\alpha$–XY model where long-range couplings become relevant (see also [11]). Therefore, the large $N$ limit of $U/N$ is not well defined, in fact, the energy per particle diverges when $N \to \infty$. In that case, the energy is a nonextensive quantity [12]. Many systems in nature also display such kind of behavior, as illustrated by Thirring in the context of a discussion on the stability of matter [13]. In those cases, it is sometimes said that the thermodynamic limit does not exist. However, a proper thermodynamic limit can be effectively achieved by introducing a suitable $N$-dependent factor $N^* \sim N^{\gamma-1}$ such that the large $N$ limit of $U/N N^*$ results well defined [14]. Concerning criticality, for the $\alpha$–XY model, in the thermodynamic limit, there is no phase transition in the sense that a transition does never occur at a finite energy per particle. However for finite-size $\alpha$-XY systems, with $\alpha \in [0,d]$, one can distinguish two regimes: An ordered one at low energies and a disordered one above a “critical” energy that increases nonextensively with the system size (see Fig. 1(a)). Then, a different limit appears to be the relevant one. Indeed, application of an appropriate regularization procedure, namely, further scaling by $N^* = N$, allows to display a transition. By means of that scaling, a finite critical energy, $U_c/N N = 0.75J$, can be defined. In this way, a thermodynamic limit, representative of the behavior observed for large $N$ (although not exceedingly), which is not limited to the low energy clustered regime, is obtained.

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