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Physica A 342 (2004) 112 – 118

PHYSICA A

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Nonextensive scaling in a long-range Hamiltonian system

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Received 31 October 2003; received in revised form 19 January 2004

Available online 12 May 2004

Abstract

The nonextensivity of a classical long-range Hamiltonian system is discussed. The system is the so-called α-*XY* model, a lattice of inertial rotators with an adjustable parameter α 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 findings above 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 to understand the origin of the apparent discrepancies.

PACS: 05.20.−y; 05.70.−a

Keywords: Nonextensivity; Phase transitions; Long-range interactions

1. Introduction

Systems of many particles interacting via long-range forces, although ubiquitous, are not fully understood (see for instance Ref. [1]). In recent years, special interest in such systems has arisen in connection with the extension of standard statistical mechanics proposed by Tsallis [2]. Then, as a prototype to study the dynamics and thermodynamics of long-range systems, both in equilibrium and nonequilibrium situations, a dynamical model with an adjustable interaction range, usually referred to as α-*XY*

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0378-4371/$ - see front matter
doi:10.1016/j.physa.2004.04.066

model, has been introduced [3]. It consists in N interacting XY rotators localized on a periodic d-dimensional regular lattice with unitary spacing. The model Hamiltonian is

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

where the angle θ_i and its conjugate momentum L_i are the coordinates of each rotator with unitary moment of inertia, the coupling constant is $J \geqslant 0$ (we restrict our study to the ferromagnetic case), r_{ij} measures the minimal distance between rotators located at the lattice sites i and j, and α controls the range of the interactions. This classical inertial XY ferromagnet 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 α 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 via analytical calculations for arbitrary d using a scaled version of 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 α 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 in an attempt 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:

$$\dot{\theta}_i = \frac{\partial H}{\partial L_i} = L_i, \quad \dot{L}_i = -\frac{\partial H}{\partial \theta_i} = -J\sum_{j\neq i}\frac{\sin(\theta_i-\theta_j)}{r_{ij}^{\alpha}}, \quad i = 1,\ldots,N \ . \tag{2}$$

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 mirocanonical averages. In Ref. [6], numerical results for the canonical ensemble were obtained 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.

2. Equilibrium thermodynamics of the α-XY model

Along this paper we will consider Hamiltonian (1) although many related works in the literature refer to a version where 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 $J/\tilde{N}$, where $\tilde{N}$ is the upper bound of the potential energy per particle, namely, $\tilde{N} = \frac{1}{N}\sum_i \sum_{j\neq i} \frac{1}{r_{ij}^{\alpha}}$. In the large N limit one has [4,9]

$$\tilde{N}(N,\alpha/d) \sim \begin{cases} N^{1-\alpha/d}, & 0 \leqslant \alpha < d\ , \\ \ln N, & \alpha = d\ , \\ \Theta(\alpha/d), & \alpha > d\ , \end{cases} \tag{3}$$

with Θ a function of the ratio α/d only. For $\alpha \leqslant d$, $\tilde{N}$ depends strongly on N. Then $\tilde{H}$ may be considered artificial, since the microscopic coupling coefficients are N-dependent, that is, are fed with macroscopic information. Anyway, the thermodynamics and the underlying dynamics of $\tilde{H}$ can be trivially mapped onto those of H by transforming energies via $\tilde{E} \leftrightarrow E/\tilde{N}$ and characteristic times (as long as moments of inertia remain of $\mathcal{O}(1)$) via $\tilde{\tau} \leftrightarrow \tau\tilde{N}^{\frac{1}{2}}$ [3]. The usual preference for the scaled form $\tilde{H}$ comes from the fact that the thermodynamic limit (TL) of the total energy per particle $\tilde{U}/N$ is finite and no further scalings of either thermodynamical or dynamical quantities are needed.

Canonical calculations for $\tilde{H}$ [5] show 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 critical specific energy $\tilde{U}_c/N = 0.75J$. This result analytically confirms the previous findings [4] for the 1D case of the original Hamiltonian H, just by taking into account the simple mapping between $\tilde{H}$ and H. Since the equilibrium results of the HMF are universal for $\alpha < d$, we will summarize them. One can associate to each particle a "spin vector" $\mathbf{m}_i = (\cos\theta_i, \sin\theta_i)$, which allows to define an order parameter $\mathbf{m} = \frac{1}{N}\sum_{i=1}^{N}\mathbf{m}_i$. In terms of the magnetization m, $\tilde{H}$ leads to

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

where $\tilde{\beta} \equiv 1/\tilde{T}$ (being $\tilde{T} \equiv 2\langle\tilde{K}\rangle/N$ 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 m is extracted can be found for instance by means of canonical calculations [10]. It has a stable solution $m = 0$ for $\tilde{\beta}J < 2$ (hence $\tilde{U}/N > 0.75J$) while, for $\tilde{\beta}J > 2$, the zero magnetization solution becomes unstable and a nonvanishing $\tilde{\beta}$-dependent stable solution arises. Note in Eq. (4) that, as $\tilde{\beta}$ does not depend on N and $m^2 \leqslant 1$, then the large N limit of $\tilde{U}/N$ is always finite for the scaled Hamiltonian $\tilde{H}$.

Here we will analyze the size dependence of thermal averages, focusing on the range $0 \leqslant \alpha < 1$ of 1D lattices governed by H. In Fig. 1(a), the average magnetization per particle $\langle m\rangle$ is represented vs. U/N, for $\alpha = 0.5$ and various system sizes. Clearly, the energy per particle at which the system becomes disordered, i.e., at which the magnetization vanishes within finite size deviations, grows with the system size. In Fig. 1(b), the same data are represented vs. $U/(N\tilde{N})$. Through this scaling, all data

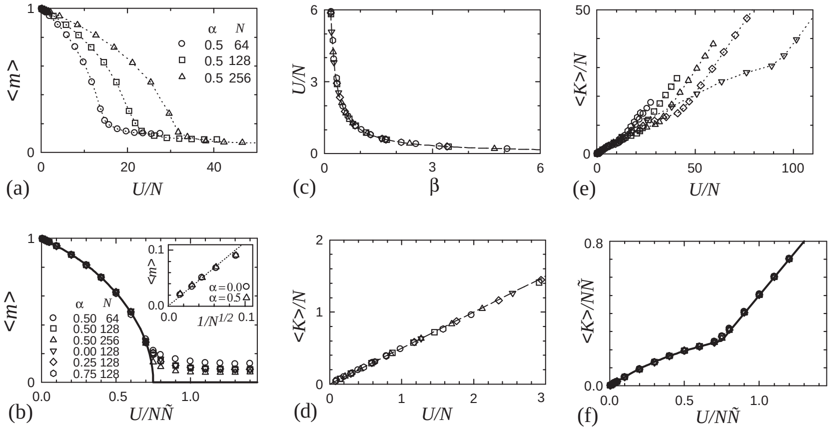

Fig. 1. (a) and (b) Average magnetization $\langle m \rangle$ vs. total energy U for different sets of parameters (α, N). The inset in (b) presents the magnetization vs. $1/\sqrt{N}$ for $U/(N\tilde{N}) = 1.4$. (c)–(f) Caloric curves. Recall that $1/\beta \equiv 2\langle K \rangle/N$ in all cases full lines correspond to the analytical result given by Eq. (4) and, dotted lines are guides to the eyes. Dashed lines correspond to $U/N = 1/\beta$ in (c) and to a straight line of slope $\frac{1}{2}$ in (d). Symbols (defined as in (b)) correspond to averages over 10 samples, computed over a time interval of order 10^3, after a transient ($t \approx 10^3$) has elapsed for "water-bag" [10] initial conditions. We have set $J = 1$. The lattice dimension is $d = 1$.

sets tend to the same curve in the TL, as previously shown in Ref. [4]. In the inset of Fig. 1(b), a plot $\langle m \rangle$ vs. N, for $U/(N\tilde{N}) = 1.4$, illustrates that $\langle m \rangle$ decays with the system size as $N^{-\frac{1}{2}}$, in the high energy regime. Additionally, data sets for different (α, N) were included in Fig. 1(b) to show that the curve of magnetization vs. $U/(N\tilde{N})$ is the same for any α-XY system with $0 \leqslant \alpha < 1$, within $\mathcal{O}(N^{-\frac{1}{2}})$ deviations. 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 $\tilde{E} \leftrightarrow E/\tilde{N}$. 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 Ref. [6]. Nevertheless, the limit $N \to \infty$, despite being an idealized situation, must reflect the behavior of sufficiently large but finite systems in order to be meaningful. Ultimately, we are interested in finite-size systems, as real systems are. For finite α-XY systems, with $\alpha < 1$, we have seen that there are 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 $\mathcal{O}(N^{-\frac{1}{2}})$ magnetization fluctuations. A good, representative TL, reflecting this picture, can be defined if one uses a suitable scaling, the one allowing data collapse. Then, it results a finite critical energy $U_c/(N\tilde{N}) = 0.75J$, analogous to the critical energy per particle in an extensive system.

Now let us focus on the relation between mean kinetic and total energies for various sets (α, N). In Fig. 1(c) we represent U/N vs. β, where $1/\beta \equiv T \equiv 2\langle K \rangle/N$. Perfect data collapse occurs, in agreement with [6], as can also be observed in the alternative representation exhibited in Fig. 1(d). However, these plots are restricted to *very low energies*. 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 $N\tilde{N}$-scaling the one which leads to data collapse in the *full energy range* (Fig. 1(f)). As an aside comment, because the relation $U \simeq 2\langle K\rangle$ holds at low energies, data collapse can be obtained in that regime for any arbitrary scaling by N^{γ}, with $\gamma \in \Re$. 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 $\mathbf{m}$ but only via its fluctuations. If the mean-field were constant it would play the role of an external field where particles do not interact among them. At low energies, where $\mathbf{m}$ is almost constant [11], the residual or effective interaction, that is the component coming from the fluctuations of $\mathbf{m}$, 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 noninteracting (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 $U \simeq 2\langle K\rangle = N/\beta$ indicates that the energy is extensive. A natural result since the interaction terms are not strong, contrarily to what was asserted in Ref. [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 by way of the $N\tilde{N}$-scaling, as shown in Figs. 1(b) and (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 $U_c \propto JN\tilde{N}$ and also $1/\beta_c = T_c \propto J\tilde{N}$.

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 $Z = \int \prod_{j=1}^{N} \mathrm{d}I_j\, \mathrm{d}\theta_j \exp \times (-\beta H) = Z_K Z_V$, which factorizes into the kinetic and potential contributions

$$Z_K = \left(\frac{2\pi}{\beta}\right)^{N/2} \quad \text{and} \quad Z_V = \mathrm{e}^{-\beta J N^2/2}\, \frac{(2\pi)^N}{\beta J} \int_0^{\infty} \mathrm{d}y\, y\, \mathrm{e}^{NG(y)}\,, \tag{5}$$

where Z_V has already been transformed by means of the Hubbard–Stratonovich trick and $G(y) = \ln I_0(y) - \frac{y^2}{2\beta JN}$. The integration can be performed by means of the Gaussian approximation around the point y_o that maximizes $G(y)$. The total energy results

$$U = -\frac{\partial \ln Z}{\partial \beta} = \frac{N}{2\beta} + \frac{JN^2}{2}(1 - m^2) \quad \text{with} \quad m = \frac{I_1(\beta JNm)}{I_0(\beta JNm)} \tag{6}$$

in correspondence with Eq. (4). For large βJN, from the consistency equation, one has $m^2 \simeq 1 - 1/(\beta JN)$, equivalent to considering $y_o \simeq \beta JN - \frac{1}{2}$, 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 ceases to be valid as β 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 $1/\beta_c \sim J\tilde{N}$ for generic α. Then N has to be large enough so that the TL is a reasonable approximation but not so large as to drive the temperature scale out of a realistic range.

3. Final remarks

A double sum as in Eq. (1) indicates that, for interaction ranges $0 \leqslant \alpha/d < 1$, the total energy U may grow faster than N, as occurs in the regimes of the α-XY model where long-range couplings become relevant (see also Ref. [12]). In such cases, the large N limit of U/N is not well defined, in fact, the energy per particle diverges when $N \to \infty$. Then the energy is a *nonextensive* quantity [13]. Many systems in nature also display such kind of behavior [14]. In those cases, it is sometimes said that the TL does not exist. However, a proper TL can be effectively achieved by introducing a suitable N-dependent factor N^* such that the large N limit of $U/(NN^*)$ does result *well defined* [15]. Concerning criticality, for the α-XY model, at the TL, there is no phase transition in the sense that a transition does never occur at a finite energy per particle. However for finite α-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 $N^* = \tilde{N}$, allows to display a transition. By means of that scaling, a finite critical energy, $U_c/(N\tilde{N}) = 0.75J$, can be defined. In this way, a TL representative of the behavior observed for large N (although not exceedingly), which is not limited to the low-energy clustered regime, is obtained.

Acknowledgements

I acknowledge S. Ruffo, F.A. Tamarit, C. Tsallis and R.O. Vallejos for enlightening discussions and Brazilian agency FAPERJ for financial support.

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