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Fingerprints of nonextensive thermodynamics in a long-range Hamiltonian system

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Abstract

We study the dynamics of a Hamiltonian system of N classical spins with infinite-range interaction. We present numerical results which confirm the existence of metaequilibrium quasi stationary states (QSS), characterized by non-Gaussian velocity distributions, anomalous diffusion, Lévy walks and dynamical correlation in phase-space. We show that the thermodynamic limit (TL) and the infinite-time limit (ITL) do not commute. Moreover, if the TL is taken before the ITL the system does not relax to the Boltzmann–Gibbs equilibrium, but remains in this *new equilibrium state* where nonextensive thermodynamics seems to apply. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

Statistical thermodynamics is usually intended as the study of N -body systems at equilibrium. However only a few textbooks [1] state clearly that the validity of equilibrium ensembles as models of thermodynamics is not automatically granted, but depends crucially on the nature of the Hamiltonian of the N -body system. In particular the very same basic postulate of equilibrium statistical mechanics, the famous *Boltzmann principle* $S = k \log W$ of *microcanonical ensemble*, assumes that dynamics can be automatically (and kind of easily) taken into account. However this is not always

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justified [2,3].¹ On the other hand, the Boltzmann–Gibbs *canonical ensemble*, is valid only for sufficiently short-range interactions and does not necessarily apply for example to gravitational or unscreened Coulombian fields for which the usually assumed entropy additivity postulate is not valid [4,5]. In general, a series of thermodynamic anomalies [6–12], which seem to escape a common general framework of understanding, has been observed. A few years ago, a generalized thermodynamics formalism based on a nonextensive entropy formula was proposed [13]. The latter has been encountering a large number of successful applications in far-from-equilibrium situations, as for example, to cite only a few cases among the most recent ones, in plasma physics [14], heavy-ion collisions [15], turbulence [16], discrete maps [17] and even in interdisciplinary fields such as bio-physics [18] and linguistics [19]. Such a formalism is the best candidate to be the general framework for a thermodynamics when long-range correlations or fractal structures in phase space are important and time evolution is not trivial, in other words when *the dynamics plays a nontrivial role* [2,3]. In this paper we study the dynamics of relaxation to equilibrium in a Hamiltonian system of classical spins with infinite-range interactions [20–23]. We show that, for some values of the initial energy and a class of off-equilibrium initial conditions, the system does not relax to the Boltzmann–Gibbs equilibrium, but exhibits different equilibrium properties characterized by non-Gaussian velocity distributions which can be fitted by the probability distribution functions (pdfs) of nonextensive thermodynamics [13]. The present study, together with the results presented in [24], provide the first indication that the generalized nonextensive thermodynamics can be a good candidate to explain some of the anomalies found in Hamiltonian systems with long-range interactions.

2. Dynamics and thermodynamics of the HMF model

The model, usually called Hamiltonian mean field (HMF), consists of N planar classical spins interacting through an infinite-range potential [20]. The Hamiltonian is

$$H = K + V = \sum_{i=1}^N \frac{p_i^2}{2} + \frac{1}{2N} \sum_{i,j=1}^N [1 - \cos(\theta_i - \theta_j)], \quad (1)$$

where θ_i is the i th angle and p_i the conjugate variable representing the rotational velocity. Note that the summation in V is extended to all couples of spins and not restricted to first neighbors. Following tradition, the coupling constant in the potential is divided by N . This makes H only formally extensive, i.e., $V \propto N$ when $N \rightarrow \infty$ [13,25], since the energy remains nonadditive, that is *the system cannot be trivially divided into*

¹ Usually W is put equal to the number of complexions... In order to calculate W , one needs a *complete* (molecular-mechanical) theory of the system under consideration. Therefore it is dubious whether the Boltzmann principle has any meaning without a complete molecular-mechanical theory or some other theory which describes the elementary processes. $S = (R/N) \log W + \text{const.}$ seems without content, from a phenomenological point of view, without giving in addition such an *Elementartheorie* (translation: Abraham Pais, *Subtle is the Lord...*, 1982).

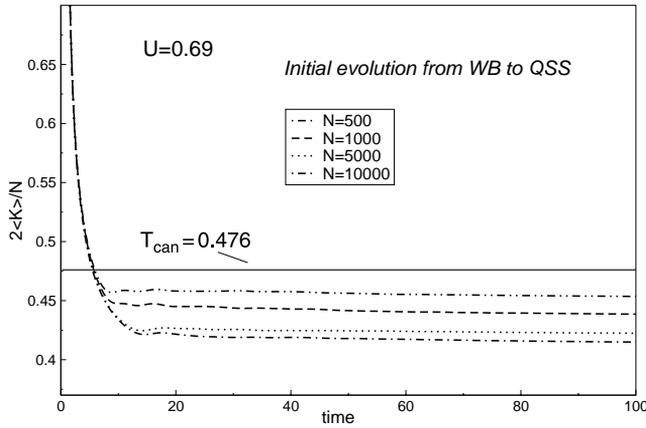


Fig. 1. The figure shows the initial time evolution from the water bag (WB) initial state to the QSS for different system sizes. The straight full line indicates the canonical equilibrium temperature.

two independent sub-systems. The model has an order parameter which is the magnetization M , i.e., the modulus of $\mathbf{M} = 1/N \sum_{i=1}^N \mathbf{m}_i$, where $\mathbf{m}_i = [\cos(\theta_i), \sin(\theta_i)]$. The canonical analytical solution of the model predicts a second-order phase transition from a low-energy ferromagnetic phase with magnetization $M \sim 1$, to a high-energy one, where the spins are homogeneously oriented on the unit circle and $M \sim 0$. The dependence of the energy density $U = E/N$ on the temperature T , usually called the caloric curve, is given by [20,21]

$$U = \frac{T}{2} + \frac{1}{2}(1 - M^2). \tag{2}$$

The critical point is at energy density $U_c = 0.75$ corresponding to a critical temperature $T_c = 0.5$ [20]. The dynamics of HMF can be investigated by starting the system with out-of-equilibrium initial conditions and integrating numerically the equations of motion [21]. In particular in Refs. [21,24] we have adopted water bag (WB) initial conditions, i.e., $\theta_i = 0$ for all i ($M = 1$), and velocities uniformly distributed. In a special region of energy values ($0.5 < U < U_c$) the results of the simulations show, for a transient regime which depends on the system size, a disagreement with the canonical ensemble. In this region the dynamics is characterized by Lévy walks and anomalous diffusion, while in correspondence the system shows a negative specific heat [23]. Ensemble inequivalence and negative specific heat have also been found in self-gravitating systems [6,7], nuclei and atomic clusters [9–11], though in the present model such anomalies emerge as dynamical features [26,27]. In this paper we focus on a particular energy value belonging to the anomalous region, namely $U = 0.69$, and we study the time evolution of temperature, magnetization, velocity distributions.

In Fig. 1 we report the time evolution of $2\langle K \rangle/N$, a quantity that coincides with the temperature ($\langle \cdot \rangle$ denotes time averages). The system, started with WB initial conditions, rapidly reaches a metastable quasi-stationary state (QSS) which does not coincide with the canonical prediction. In fact, after a short transient time, $2\langle K \rangle/N$ assumes a fixed

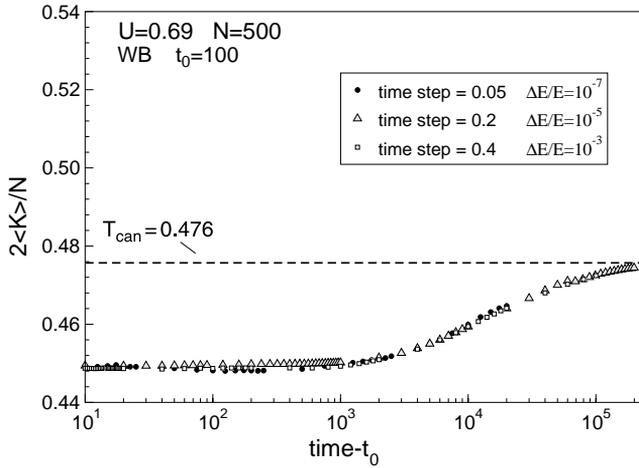


Fig. 2. For $N = 500$ we show the time evolution of the *temperature plateau* correspondent to the quasi stationary state (QSS) calculated with different accuracies, reported in the plot. The initial time interval $t_0 = 100$, shown in Fig. 1, has been subtracted for clearness.

value (the plateau in figure) corresponding to a N -dependent temperature $T_{QSS}(N)$ lower than the canonical prediction, also reported. In correspondence of this plateau one gets for the magnetization a value $M_{QSS} \sim 0$. If we want to observe relaxation to the canonical equilibrium state with temperature $T_{can} = 0.476$ and magnetization $M_{can} = 0.307$, we have to wait for a time longer than that shown in Fig. 1, as shown for example in Fig. 2 for the case $N = 500$. In Ref. [24] the following scaling relations have been found:

- (i) the duration of the plateau, the lifetime of the QSS τ , increases as $\tau \propto N$;
- (ii) $T_{QSS}(N) \rightarrow T_\infty = 0.380$, a value obtained analytically as the metastable prolongation, at energies below U_c , of the high-energy solution ($M = 0$) as $[T_{QSS}(N) - T_\infty] \propto N^{-1/3}$. This implies that $M_{QSS} \propto N^{-1/6}$ (see Fig. 1(c) of Ref. [24]).

These numerical results clearly indicate that

- the two limits, the infinite-time limit (ITL) $t \rightarrow \infty$ and the thermodynamic limit (TL) $N \rightarrow \infty$ do not commute;
- if the TL is performed before the ITL, the system does not relax to the BG equilibrium and lives forever in the QSS.

The robustness of the above results was checked in two different ways: (1) by adopting different initial conditions, as for example double water bag (DWB) initial conditions, and checking that we get the same QSS (see Ref. [24] for details); (2) by changing the level of accuracy of the numerical integration, as shown in Fig. 2. We expect these results to be ubiquitous in nonextensive systems as conjectured in Ref. [13].

In Fig. 3 we study the velocity pdfs. The initial velocity pdfs (WB or DWB initial conditions) quickly acquire and maintain during the entire duration of the metastable state a *non-Gaussian shape*. In Figs. 3(b) and (c) we see that the pdfs of the QSS do

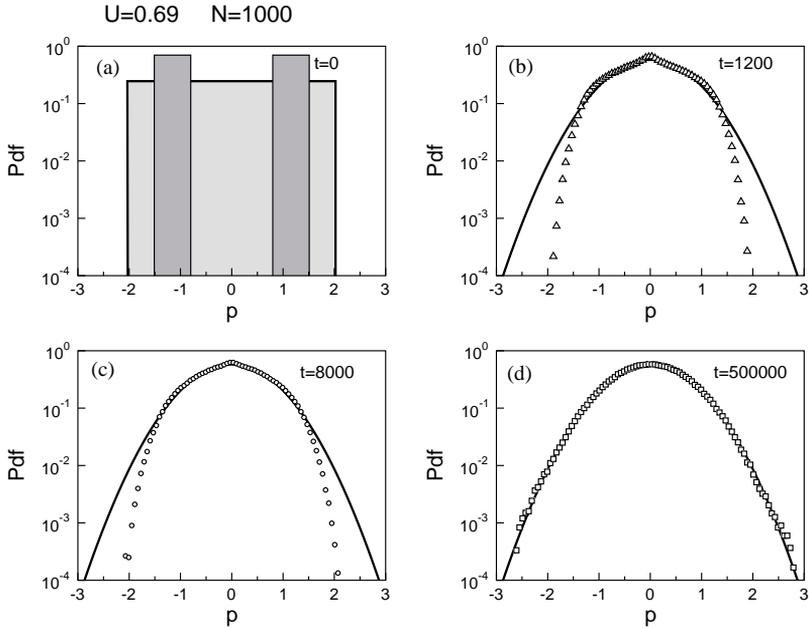


Fig. 3. Time evolution of numerical velocity pdfs for $N=1000$ starting from WB and DWB initial conditions, panel a). For comparison we show also the equilibrium Gaussian curve (full line) in the QSS regime, panel b–c) (time $t = 1200, 8000$), and in the equilibrium one, panel d) (time $t = 500000$).

not change up to a time $t = 8000$ for a system with $N = 1000$. The velocity pdf of the QSS is wider than a Gaussian for small velocities, but shows a faster decrease for $p > 1.2$. The enhancement for velocities around $p \sim 1$ is consistent with the anomalous diffusion and the Lévy walks observed in the QSS regime [22]. The following rapid decrease for $p > 1.2$ is due to conservation of total energy. From a dynamical point of view, the stability of the QSS velocity pdf can be explained by the fact that, for $N \rightarrow \infty$, $M_{QSS} \rightarrow 0$ and thus the force on the spins $F_i = (-M_x \sin \theta_i + M_y \cos \theta_i) \rightarrow 0$. On the other hand, when N is finite, we have always a small random force, whose strength depends on N , which makes the system eventually evolve into the usual Maxwell–Boltzmann distribution after some time. We show this for $N = 1000$ at time $t = 500000$ in Fig. 3(d). When this happens, Lévy walks disappear and anomalous diffusion leaves place to Brownian diffusion [22].

We fit the non-Gaussian pdf in Fig. 3(b) by using the one-particle prescription of the generalized thermodynamics (see Ref. [24] for more details):

$$P(p) = \left[1 - (1 - q) \frac{p^2}{2T} \right]^{1/(1-q)} . \tag{3}$$

This formula recovers the Maxwell–Boltzmann distribution for $q = 1$ and has been recently used to describe successfully turbulence [16] and non-Gaussian pdfs related to anomalous diffusion of *Hydra* cells in cellular aggregates [18].

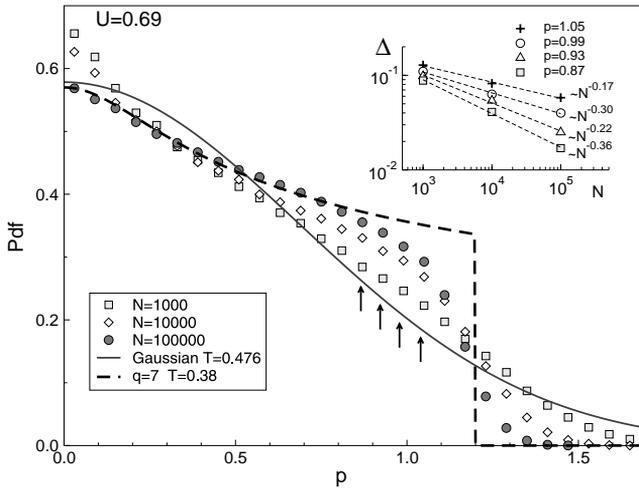


Fig. 4. Nonextensive theoretical pdf, with cut-off (dashed curve) in comparison with the numerical ones (points) and the gaussian equilibrium prediction (full curve). In the inset we report the scaling of $\Delta = P_{th} - P_{num}$ with N for those points indicated by the arrows.

In our case, the best fit is obtained by a curve with $q = 7$, $T = 0.38$ as shown in Fig. 4. The agreement between numerical results and theoretical curve improves with the size of the system. A finite-size scaling confirming the validity of the fit is reported in the inset, where $\Delta = P_{th} - P_{num}$, the difference between the theoretical points and the numerical ones, is shown to go to zero as a power of N (for four values of p). Since $q > 3$, the theoretical curve does not have a finite integral and therefore it needs to be truncated with a sharp cut-off (herein assumed to be discontinuous for simplicity) to make the total probability equal to one. It is however clear that, the fitting value $q = 7$ is only an effective nonextensive entropic index. Although similar non-Gaussian pdfs have been found previously, it was for dissipative systems [16], while this is the first evidence in a Hamiltonian system.

In order to investigate deeper the dynamics of the plateaux observed in Figs. 1 and 2, we have studied the Lyapunov exponent in the QSS regime. In Fig. 5 we show that, as expected, the largest Lyapunov exponent (LLE) tends to zero when N increases. The scaling behavior of the LLE can be understood following the same argument already applied in Ref. [21] in the overcritical region. It is known in fact that, when the Lyapunov can be estimated by the product of random matrices, the LLE scales with the power $\frac{2}{3}$ of the perturbation [28,21]. In our case the perturbation is given by the magnetization, for which we have the scaling law $M^2 \propto N^{-1/3}$ in the QSS regime [24], thus we get the scaling $LLE \propto M^{2/3} \propto (N^{-1/3})^{1/3} = N^{-1/9}$. The latter is in perfect agreement with the numerical results as shown in the figure. Since LLE tends to zero as the system is increasingly large, one can safely say that mixing is increasingly slower and the observed anomalies in the relaxation process are naturally expected in the sense predicted by Krilov [29]. We note finally that, emergence of

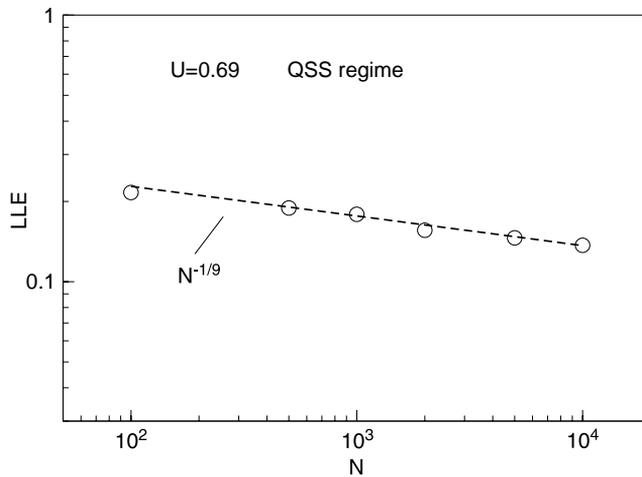


Fig. 5. Open points indicate the Largest Lyapunov Exponent (LLE) vs N for the QSS regime. An average over 10 runs is considered. Straight line indicates the theoretical prediction for LLE scaling, see text.

dynamical correlations and filamentary sticky structures in the μ -space have also been observed in the QSS regime [24].

3. Conclusions

In this paper we have studied a simple Hamiltonian system with long-range interaction. The dynamics of relaxation process is extremely rich and the system shows the existence of QSS different from the canonical equilibrium. These states satisfy the usual attributes of thermal equilibrium though they systematically differ from what BG statistical mechanics has made familiar to us. Our results provide a first verification of nonextensive statistical mechanics [13] in long-range Hamiltonian systems, and illustrate the correctness of the criticism that Einstein developed in his celebrated 1910 paper [2] about the possible nonuniversality of Boltzmann thermostatics, and the need of providing a mechanical basis to it (including naturally *time* in the discussion).

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