Non-Gaussian equilibrium in a long-range Hamiltonian system

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We study the dynamics of a system of *N* classical spins with infinite-range interaction. We show that, if the thermodynamic limit is taken before the infinite-time limit, the system does not relax to the Boltzmann-Gibbs equilibrium, but exhibits different equilibrium properties, characterized by stable non-Gaussian velocity distributions, Lévy walks, and dynamical correlation in phase space.

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Though not always clearly stated, standard equilibrium thermodynamics [1–3] is valid only for sufficiently short-range interactions. This is not the case, for example, for gravitational or unscreened Coulombian fields, or for systems with long-range microscopic memory and fractal structures in phase space. The increasing experimental evidence of dynamics and thermodynamics anomalies in turbulent plasmas [4] and fluids [5–7], astrophysical systems [8–12], nuclei [13,14] and atomic clusters [15], granular media [16], glasses [17,18], and complex systems [19,20] found in the last years, provide further motivation for a generalization of thermodynamics.

In this paper, we consider a simple model of classical spins with infinite-range interactions [21–24], and we show that, if the thermodynamic limit is performed before the infinite time limit, the system does not relax to the Boltzmann-Gibbs (BG) equilibrium, but exhibits different equilibrium properties characterized by non-Gaussian velocity distributions, Lévy walks, dynamical correlation in phase space, and the validity of the zeroth principle of thermodynamics. Our results show some consistency with the predictions of a generalized nonextensive thermodynamics recently proposed [25,26]. The Hamiltonian mean-field (HMF) model describes a system of *N* planar classical spins interacting through an infinite-range potential [21]. The Hamiltonian may be written as

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

where θ_i is the ith angle and p_i the conjugate variable representing the angular momentum (or the rotational velocity since unit mass is assumed). The interaction is the same as in the ferromagnetic *X*-*Y* model [2], though the summation 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 ($V\sim N$ when $N\to\infty$) [25–28], since the energy remains nonadditive, i.e., the system cannot be trivially divided in two independent subsystems. The canonical analytical solution of the model predicts a second-order phase transition from a low-energy ferromagnetic phase with magnetization $M\sim 1$ (M is the modulus of $\mathbf{M}=(1/N)\Sigma_{i=1}^{N}\mathbf{m}_i$, where $\mathbf{m}_i=(\cos(\theta_i),\sin(\theta_i))$, to a high-energy one where the spins are homogeneously oriented on the unit circle and $M\sim 0$. The *caloric curve*, i.e., the dependence of the energy density $U=E/N$ on the temperature *T*, is given by $U=T/2+1/2(1-M^2)$ and shown in Fig. 1(a). The critical point is at energy density $U_c=0.75$ corresponding to a critical temperature $T_c=0.5$ [21]. The dynamical behavior of HMF may be investigated in the microcanonical ensemble by starting the system with the so-called water bag initial conditions (WBIC), i.e., $\theta_i=0$ for all $i(M=1)$ and velocities uniformly distributed, and integrating numerically the equations of motion [22]. As shown in Fig. 1(a), microcanonical simulations are in general in good agreement with the canonical ensemble, except for a region below U_c, where it has also been found a dynamics characterized by Lévy walks, anomalous diffusion [23], and a negative specific heat [24]. Ensemble inequivalence and negative specific heat have also been found in self-gravitating systems [8], nuclei, and atomic clusters [13–15], though in the present paper, such anomalies emerge as dynamical features [29,30]. In order to understand better this disagreement, we focus on a particular energy value, namely $U=0.69$, and we follow the time evolution of temperature, magnetization, and velocity distributions.

In Fig. 1(b), we report the time evolution of $2\langle K\rangle/N$, a quantity that, evaluated at equilibrium, is expected to coincide with the temperature ($\langle\cdot\rangle$ denotes time averages). The system is started with WBIC and rapidly reaches a metastable or quasistationary state (QSS) which does not coincide with the canonical prediction. In fact, after a short transient time, $2\langle K\rangle/N$ shows a plateau corresponding to a *N*-dependent temperature $T_{QSS}(N)$ (and $M_{QSS}\sim 0$) lower than the canonical temperature. This metastable state needs a long time to relax to the canonical equilibrium state with temperature $T_{can}=0.476$ and magnetization $M_{can}=0.307$.

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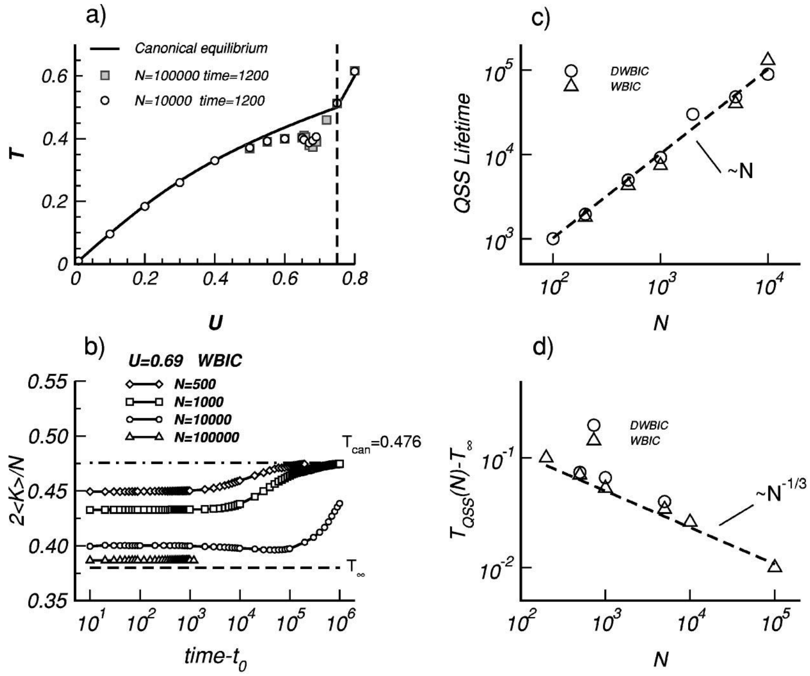

FIG. 1. (a) Caloric curve: microcanonical numerical results for $N=10\,000{,}100\,000$ are compared with equilibrium theory in the canonical ensemble. The dashed vertical line indicates the critical energy. Water bag initial conditions (WBIC) are used in the numerical simulations. Temperature is computed from $T=2\langle K\rangle/N$, where $\langle\cdot\rangle$ denotes time averages after a short transient time $t_0=10^2$ (not reported here). The time step used was 0.2 [22]. (b) Microcanonical time evolution of $2\langle K\rangle/N$, for the energy density $U=0.69$ and different sizes. Each curve is an average over typically $100-1000$ events. The dot-dashed line represents the canonical temperature $T_{can}=0.476$. The quantity $2\langle K\rangle/N$, which starts from an initial value 1.38 ($V=0$ and $K=UN$ in WBIC), does not relax immediately to the canonical temperature. The system lives in a quasistationary state (QSS) with a plateau *temperature* $T_{QSS}(N)$ smaller than the expected value 0.476. The lifetime of the QSS increases with N and the value of their temperature converges, as N increases, to the temperature $T_\infty=0.38$, reported as a dashed line. Log-log plot of the QSS lifetime (c) and $T_{QSS}(N)-T_\infty$ (d) are reported as a function of the size N. The lifetime diverges linearly with N, and $T_{QSS}(N)$ converges to $T_\infty=0.38$ as $N^{-1/3}$ (see fit shown as a dashed line). Note that from the caloric curve one gets $M^2=T+1-2U=T-0.38$. Therefore, from the behavior reported in panel (d), being $T_\infty=0.38$, one gets $M_{QSS}=N^{-1/6}$. Results are similar when we consider double water bag initial conditions (DWBIC), i.e., $\theta_i=0$ for all i and velocities uniformly distributed in $(-p_2,-p_1)$ and (p_1,p_2). In the figure, we report the case $p_1=0.8$, $p_2=1.51$.

The duration of the plateau increases with the size of the system: in particular, we have checked that the lifetime of QSS has a linear dependence on N, see Fig. 1(c). Therefore, the two limits $t\to\infty$ and $N\to\infty$ do not commute and if the thermodynamic limit is performed before the infinite time limit, the system does not relax to the BG equilibrium. This has been conjectured to be an ubiquitous feature in nonextensive systems [25], but it has also been found for spin glasses [17]. When N increases $T_{QSS}(N)$ tends to $T_\infty=0.380$, a value obtained analytically as the metastable prolongation (at energies below $U_c=0.75$) of the high-energy solution ($M=0$). We have also found that $[T_{QSS}(N)-T_\infty]\propto N^{-1/3}$ and $M_{QSS}\propto N^{-1/6}$, see Fig. 1(d). At the same time, we have checked that increasing the size, the largest Lyapunov exponent for the QSS tends to zero. In this sense, mixing is negligible and one expects anomalies in the relaxation process [31]. The fact that T_{QSS} converges to a nonzero value of temperature for $N\to\infty$ means that, when N is macroscopically large, systems may share the same temperature, though this equilibrium is not the familiar one. All this amounts to say that the zeroth principle of thermodynamics is stronger than what one might think through BG statistical mechanics, since it is true even when the system is not at the usual BG equilibrium. We have checked the robustness of the above results by changing the level of accuracy of the numerical integration and by adding small perturbations. We also verified that the QSS has a finite basin of attraction, by adopting different initial conditions, as for example, double water bag initial conditions (DWBIC). In Fig. 2, we focus on the velocity probability distribution functions (PDF's). The initial velocity PDF's (WBIC or DWBIC), reported in Fig. 2(a) , quickly acquire and maintain during the entire duration of the metastable state a *non-Gaussian shape*, see Figs. 2(b) and 2(c). 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 $p\sim1$ is consistent with the anomalous diffusion and the Lévy walks (with average velocity $p\sim1$) observed in the QSS regime [23]. The following rapid decrease for $p>1.2$ is due to conservation of total energy . The stability of the QSS velocity PDF may be explained by the fact that, for $N\to\infty$, $M_{QSS}\to0$ and thus the force on the spins tends to zero with N, being $F_i=-M_x\sin\theta_i+M_y\cos\theta_i$. Of course, for finite N, we have always a small random force, which makes the system

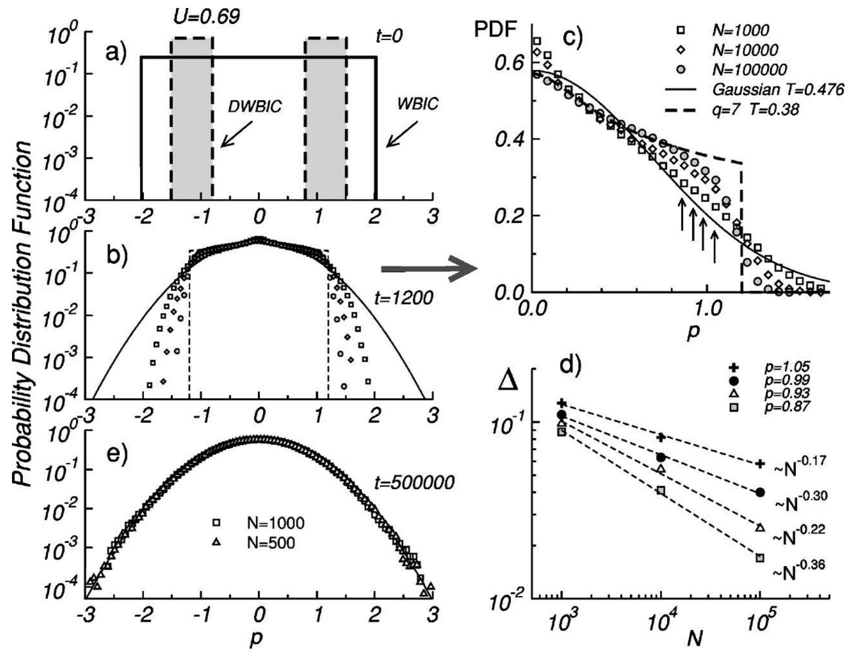

FIG. 2. Time evolution of the velocity probability distribution function (PDF) for $U=0.69$ and different sizes of the system. (a) At time $t=0$ we start with a single (WBIC) or a double (DWBIC) water bag velocity PDF. (b) In the transient regime where $2\langle K\rangle/N$ shows a plateau corresponding to $T_{QSS}(N)$ and the system lives in a quasistationary state (QSS), the velocity PDF's do not change in time and are very different from the Gaussian canonical equilibrium distribution (full curve). The PDF's at time $t=1200$ for $N=1000,10\,000,100\,000$ show a convergence towards a non-Gaussian distribution that can be fitted by means of a power-law analytical curve (dashed curve) consistent with the generalized nonextensive thermodynamics [25] proposed by Tsallis and characterized by $q=7$ and $T=0.38$, see text. The theoretical curve has been truncated with a sharp cutoff in order to have total probability equal to one, see text. (c) The same curves shown in (b) at $t=1200$ are reported in linear scale. (d) We show the difference, Δ, between the numerical results and the theoretical curve, as a function of N for the four values of p indicated by arrows in panel (c). (e) We show the numerical PDF's at $t=500\,000$ for $N=500$ and 1000. We get an excellent agreement with the Gaussian canonical equilibrium distribution at temperature $T=0.476$.

eventually evolve into the usual Maxwell-Boltzmann distribution after some time. We show this for small systems ($N=500,1000$) at time $t=500\,000$ in Fig. 2(e). When this happens, Lévy walks disappear and anomalous diffusion leaves place to Brownian diffusion [23]. A possible frame to reproduce the non-Gaussian PDF in Fig. 2(b) could be the nonextensive statistical mechanics recently proposed [25,26] with the entropic index $q\neq 1$. This formalism provides, for the canonical ensemble, a q-dependent power-law distribution in the variables p_i, θ_i. This distribution has to be integrated over all θ_i and all but one p_i in order to obtain the one-momentum PDF, $P_q(p)$, to be compared with the numerical one, $P_{num}(p)$, obtained by considering, within the present molecular dynamical frame, increasingly large N-sized subsystems of an increasingly large M system. Within the $M\gg N\gg 1$ numerical limit, we expect to go from the microcanonical ensemble to the canonical one (the cutoff is then expected to gradually disappear as indeed occurs in the usual short-range Hamiltonians), thus justifying the comparison between $P_q(p)$ and $P_{num}(p)$. The enormous complexity of this procedure made us turn instead to a naive, but tractable, comparison, namely that of our present numerical results with the following one-free-particle PDF [25] $P(p)=[1-(1/2T)(1-q)p^2]^{1/(1-q)}$, which recovers the Maxwell-Boltzmann distribution for $q=1$. This formula has been recently used to describe successfully turbulent Couette-Taylor flow [5] and non-Gaussian PDF's related to anomalous diffusion of *Hydra* cells in cellular aggregates [19]. In our case, the best fit is obtained by a curve with $q=7$, $T=0.38$ as shown in Figs. 2(b) and 2(c). 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 panel (d), where $\Delta=P_{th}-P_{num}$, the difference between the numerical results and the theoretical curve for $q=7$, 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 cutoff 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. Similar non-Gaussian PDF's have also been found in turbulence and granular matter experiments [5,16], though this is the first evidence in a Hamiltonian system. In Fig. 3, we verify, through the calculation of the fractal dimension D_2 [32], that a dynamical correlation emerges in the μ space before the final arrival to a quasiuniform distribution. During intermediate times some filamentary structures appear, a similar feature has recently been found also in self-gravitating systems [11], which might be closely related to the plateaus observed in Fig. 1(b). We learn from the curves in Fig. 3(c) that, since they do not

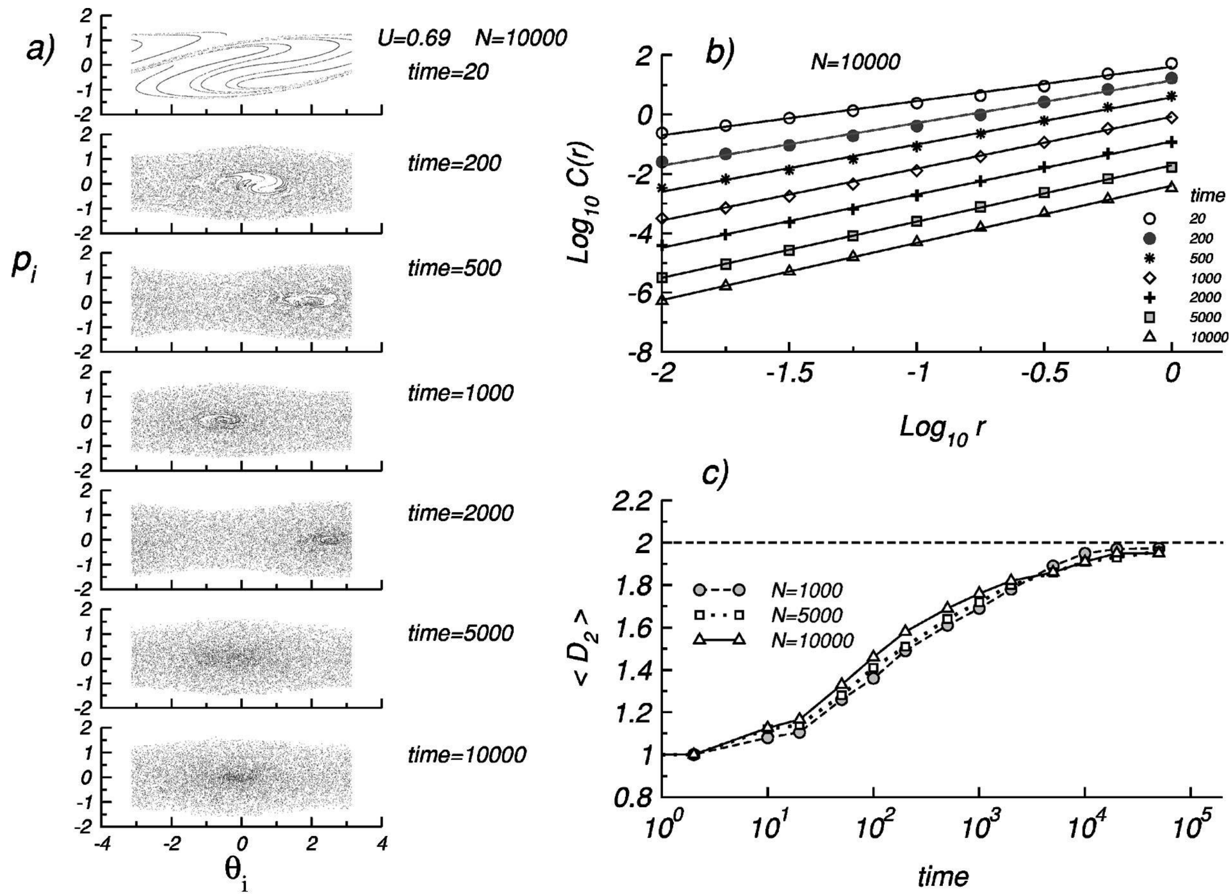

FIG. 3. Correlation in μ space. (a) We show the μ space, i.e., the angle and momenta of the N particles, for $U=0.69$ and $N=10\,000$ at different time scales, starting from WBIC. Although the initial configuration is uniform, structures emerge and persist for a very long time before dissolving again at equilibrium. A way to measure these correlations is by means of the correlation integral [32] $C(r) =(1/N^2)\Sigma_{i,j}^{N}\Theta(r-d_{i,j})$ where $d_{i,j}$ is the Euclidean distance between two points of the μ space. In general, $C(r)=r^{D_2}$, where D_2 is the correlation fractal dimension. (b) By reporting the logarithm of $C(r)$ vs the logarithm of r, a linear behavior over several decades is found. The fractal dimension thus extracted is reported in (c) vs time (an average over 50 events is considered). In the same time scale where we find the QSS, the correlation dimension is inbetween one and two. The particles are fully spread in the μ space only at equilibrium. As time increases, D_2 grows continuously from one to two.

sensibly depend on N, the possible connection does not concern the entire μ space, but perhaps only the small sticky regions between the ''chaotic sea'' and the quasiorbits [33].

Metastable states are ubiquitous in nature. Their full understanding is, however, far from trivial. They basically correspond to local, instead of global, minima of the relevant thermodynamic energy. The two types of minima are separated by activation barriers that at the thermodynamic limit, may be low, high, or infinite, all of them presumably occurring in nature. The last case yields of course to quite drastic consequences. Moreover, the local minimum may either make the system to live in a smooth part of the *a priori* accessible phase space, or it may force it to live in a geometrically more complex (e.g., multifractal) part of the phase space. The richness of such a situation is what makes the study of glasses, nuclei, atomic clusters, self-gravitating and other complex systems interesting. It is natural to expect for such systems that the infinite size and infinite time limits are not interchangeable. What has emerged quite clearly here is that thermodynamically large systems with long-range interactions belong to this very rich class. We have verified that the usual attributes of thermal equilibrium: *zeroth principle at finite temperatures, robustness associated with a finite basin of attraction in the space of the initial conditions, stable distribution of velocities*, are satisfied, but they *systematically differ from what* BG statistical mechanics have made familiar to us for the last 130 years. Our findings indicate some consistency with the predictions of nonextensive statistical mechanics [25], though a firm and unambiguous connection remains a challenge for future studies. In particular, we believe all these features not to be exclusive of the present HMF model. Similar scenarios are expected for systems with, for example, two-body interactions decaying like $r^{-\alpha}$ for $0\leqslant\alpha\leqslant\alpha_c$, where α_c is equal, for classical systems, to the space dimension [27,28].

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