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Metastability and weak mixing in classical long-range many-rotator systems

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We perform a molecular dynamical study of the isolated $d=1$ classical Hamiltonian $\mathcal{H}=\frac{1}{2}\sum_{i=1}^{N}L_i^2+\sum_{i\neq j}[1-\cos(\theta_i-\theta_j)]/r_{ij}^{\alpha}$; $(\alpha\geqslant 0)$, known to exhibit a second order phase transition, being disordered for $u\equiv U/N\tilde{N}\geqslant u_c(\alpha,d)$ and ordered otherwise $[U\equiv$ total energy and $\tilde{N}\equiv(N^{1-\alpha/d}-\alpha/d)/(1-\alpha/d)]$. We focus on the nonextensive case $\alpha/d\leqslant 1$ and observe that, for $u<u_c$, a basin of attraction exists for the initial conditions for which the system quickly relaxes onto a long standing metastable state (whose duration presumably diverges with N-like $\sqrt{\tilde{N}}$) which eventually crosses over to the microcanonical Boltzmann-Gibbs stable state. It is exhibited that the appropriately scaled maximal Lyapunov exponent $\lambda_{u<u_c}^{max}(\text{metastable})\propto N^{-\kappa_{metastable}}$;$(N\to\infty)$, where, for all values of α/d, $\kappa_{metastable}$ numerically coincides with *one third* of its value for $u>u_c$, hence decreases from 1/9 to zero when α/d increases from zero to unity, remaining zero thereafter. This simple *connection between anomalies above and below the critical point* reinforces the nonextensive universality scenario.

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The foundation of statistical mechanics, hence of thermodynamics, is a subtle and fascinating matter that has driven enriching controversies and clarifications since more than one century (see, for instance, Einstein's remark on the Boltzmann principle [1]). The field remains open to new aspects and proposals. One of these is nonextensive statistical mechanics, proposed in 1988 Ref. [2] (see [3] for reviews). This formalism is based on an entropic index q (which recovers usual statistical mechanics for $q=1$), and has been applied to a variety of systems, covering certain classes of both (meta)equilibrium and nonequilibrium phenomena, e.g., turbulence [4], hadronic jets produced by electron-positron annihilation [5], cosmic rays [6], motion of *Hydra viridissima* [7], and the edge of quantum chaos [8]. In addition to this, it has been advanced that it could be appropriate for handling some aspects of long-range interacting Hamiltonian systems. This possibility is gaining plausibility nowadays, as argued in Ref. [9] and elsewhere. Indeed, in molecular dynamical approaches of isolated systems, strongly non-Maxwellian velocity distributions have recently been observed that are consistent with such possibility [9]. A paradigmatic system in the realm of this discussion is the following classical Hamiltonian:

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

where (θ_i,L_i) is the angle and angular momentum conjugate pair. The inertial planar rotators (ferromagnetic XY-like model) are localized at the sites of a d-dimensional periodic lattice. As distance r_{ij} (measured in crystal units) for a given pair (i,j) we consider the shortest among all the possible ones (due to periodicity). For $d=1$ we have $r_{ij}=1,2,3,\ldots$; for $d=2$ we have $r_{ij}=1,\sqrt{2},2,\ldots$; for $d=3$ we have $r_{ij}=1,\sqrt{2},\sqrt{3},2,\ldots$, and so on. The so called Hamiltonian mean field system [10] is recovered for $\alpha/d=0$, and the first-neighbor model is recovered for $\alpha/d\to\infty$. Hamiltonian (1) is extensive if $\alpha/d>1$ and nonextensive if $0\leqslant\alpha/d\leqslant 1$. This can be seen as follows. If we define

$$\tilde{N}\equiv 1+d\int_1^{N^{1/d}}dr\,r^{d-1}r^{-\alpha}=\frac{N^{1-\alpha/d}-\alpha/d}{1-\alpha/d},\qquad(2)$$

it can be easily checked that the energy scales as $N\tilde{N}$, i.e., it is asymptotically proportional to N if $\alpha/d>1$, to $N\ln N$ if $\alpha/d=1$, and to $N^{2-\alpha/d}$ if $0\leqslant\alpha/d<1$. This Hamiltonian is sometimes presented in the literature in the following form:

$$\mathcal{H}'=\frac{1}{2}\sum_{i=1}^{N}L_i'^2+\frac{1}{\tilde{N}}\sum_{i\neq j}\frac{1-\cos(\theta_i-\theta_j)}{r_{ij}^{\alpha}}\quad(\alpha\geqslant 0),\qquad(3)$$

which artificially (see Ref. [11]) makes its energy to scale as N, $\forall(\alpha/d)$. The transformation from this form to the one presented in Eq. (1), adopted from now on in the present work, has been described in detail in Ref. [11]. This system has since long been shown [12] to obey Boltzmann-Gibbs (BG) statistical mechanics for $\alpha/d>1$. What happens for $0\leqslant\alpha/d\leqslant 1$ is a subtle question that is under intensive study nowadays [13–18]. In fact, several long-range-interacting systems are since long known [19–23] to present a variety of thermodynamical anomalies, such as negative specific heat and superdiffusion, among others. The molecular dynamics in the isolated Hamiltonian (1) with total energy U exhibits, for infinitely large time, the existence of a second order phase transition at $u\equiv U/N\tilde{N}=u_c(\alpha,d)$. For $u\geqslant u_c$ the sys-

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tem is disordered (paramagneticlike); otherwise, it is ordered (ferromagneticlike). It exhibits anomalies on both sides of the critical point.

For $u>u_c$ (i.e., in the disordered phase), after a quick transient, the one-particle distribution of velocities gradually becomes Maxwellian in the $N\to\infty$ limit, in accordance with what is expected within BG statistical mechanics. *However*, while N increases, the entire Lyapunov spectrum approaches zero, which is a quite anomalous behavior; indeed, no such weakening of chaos is expected or observed for $\alpha/d>1$. This weakening of the sensitivity can be characterized through the maximal Lyapunov exponent $\lambda^{max}_{u>u_c}$ (appropriately scaled as indicated in Ref. [11]) which, in the $N\to\infty$ limit, vanishes as $\lambda^{max}_{u>u_c}\propto N^{-\kappa_d}$ (d stands for disordered phase); κ_d decreases from 1/3 to zero while α/d increases from zero to unity (analytical approximations are available [16,17] for the $d=1$ case), and remains zero thereafter [15]. The fact that the sensitivity to the initial conditions becomes subexponential (possibly a power law) strongly reminds what has been observed [24–33] in a variety of low-dimensional maps, which are known to be adequately described within nonextensive statistical mechanical concepts.

For $u<u_c$, after a quick transient, the behavior depends on the initial conditions. Two wide basins of attraction exist in the space of the initial conditions. One of them (which includes Maxwellian velocity distribution and all angles equal) yields a standard BG microcanonical distribution that approaches the BG canonical one in the limit $N\to\infty$. The other one, which includes the uniform distribution of all velocities (that are possible at the chosen total energy) with all angles taken to be equal at $t=0$, yields a long standing metastable (quasistationary) state (whose associated magnetization is basically zero) and only at very large time joins the BG distribution (whose associated magnetization is nonzero). The duration of this metaequilibrium state diverges with N. It has been conjectured [34] that it does so as $\tau'\propto\tilde{N}$ if we use the Hamiltonian written as in Eq. (3), or equivalently (see Ref. [11]) as $\tau=\tau'/\sqrt{\tilde{N}}\propto\sqrt{\tilde{N}}$ if written as in Eq. (1). Recent results support this scaling; indeed, (i) for $\alpha=0$, this conjecture implies $\tau'\propto N$, which has been verified [9], (ii) for fixed N, it implies that τ' exponentially decays with α, which once again has been verified [18].

Our focus in this paper is on the metastable state of the $d=1$ model, which we study for typical values of (α,u,N). The time evolution of the model has been generated integrating the equations of motion through a fourth order symplectic algorithm [35] with a relative error in the total energy conservation less than 10^{-4}. We verify that the time evolution of the (scaled) average kinetic energy per particle (which plays the role of temperature) exhibits two plateaux, the first one being anomalous and the second one being of the BG class. This is illustrated in Fig. 1 for $\alpha=0.6$. In the same figure we show the time evolution of $\lambda^{max}_{u<u_c}$ (calculated with the method of Benettin *et al.* [36]). As in the $\alpha=0$ case, one expects also for $0<\alpha/d<1$ two plateaux in $\lambda^{max}_{u<u_c}(t)$. We can see, however, that for $\alpha=0.6$ the difference is almost unperceptively small; it might happen that this difference

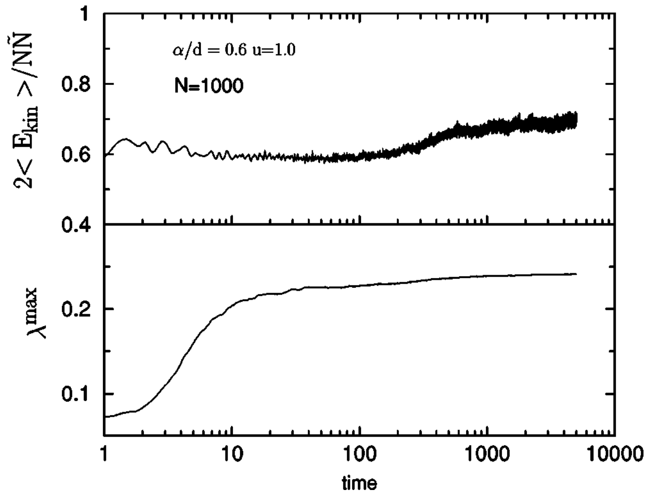

FIG. 1. Time evolution for twice the (scaled) average kinetic energy per particle $\langle E_{kin}\rangle/N\tilde{N}$ (which plays the role of temperature; upper curve) and the (scaled) largest Lyapunov exponent $\lambda^{max}_{u<u_c}$ (lower curve) for $\alpha=0.6$, $u=1$, and $N=1000$. We have averaged ten different initial conditions corresponding to a uniform velocity distribution for all the velocities compatible with the chosen total energy, all angles being initially set parallel to each other.

quickly decreases with an increase in α, as it is the case for τ, but such study is out of the scope of the present work. The systematic detection of both plateaux in the temperature enabled the calculation of the caloric curves, as illustrated in Fig. 2. We clearly see the existence of negative specific heat for the metastable state, just below u_c. Then, by focusing on small time (after the quick transient, nevertheless), it was possible to calculate the N dependence of $\lambda^{max}_{u<u_c}$(metastable) for typical values of α. The results are shown in Fig. 3. We verify that $\lambda^{max}_{u<u_c}(\text{metastable})\propto N^{-\kappa_{metastable}}$, where $\kappa_{metastable}$ decreases from 1/9 (thus confirming Ref. [37]) to zero, while α increases from zero to unity, and remains zero

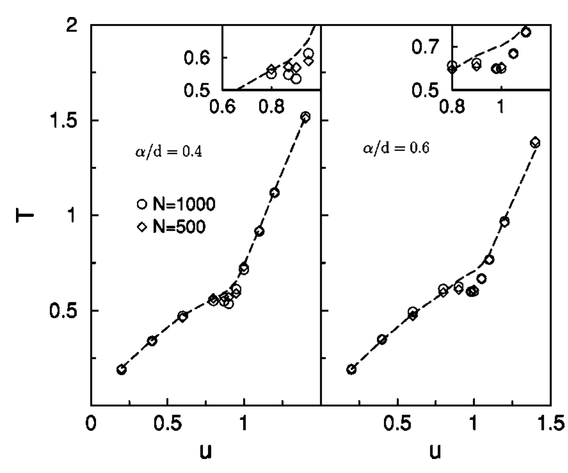

FIG. 2. Microcanonical caloric curves for typical values of α and N. The lower branch corresponds to the metastable state. The stable state is indicated by the dashed line. The size of the symbols in the insets characterizes the numerical errors at the chosen energies.

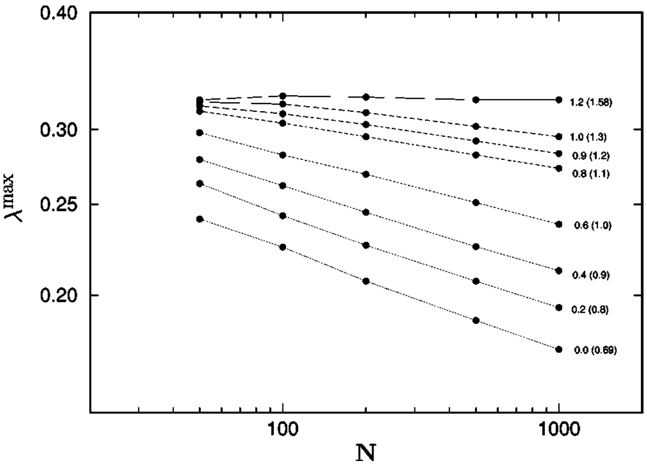

FIG. 3. N dependance of the rescaled largest Lyapunov exponent $\lambda^{max}_{u<u_c}$(metastable) [corresponding in fact to Hamiltonian (3), as shown in Ref. [11]] for α ranging from 0 to 1.2 (the values in parentheses are those for u, so chosen in order to be in all cases slightly below the critical point u_c, whose exact value can be obtained from Ref. [13] through a simple transformation). The average in the interval $10<t<3000$ has been considered as the metastable state value (the very slight increase of the Lyapunov exponent occasionally observed up to $t=3000$ is numerically without consequences).

thereafter. Furthermore, we numerically verify a remarkable property, namely (see Fig. 4)

$$\kappa_{metastable}=\frac{\kappa_d}{3}(\forall\alpha). \tag{4}$$

Summarizing, for $\alpha/d<1$, we observe the following scenario as times evolves. If $u>u_c(\alpha,d)$, for basically all initial conditions, after a transient, both the temperature (proportional to the average kinetic energy) and the maximal Lyapunov exponent attain their N-dependent equilibrium values. When N diverges, the temperature remains finite, whereas the Lyapunov exponent approaches zero. If $u<u_c(\alpha,d)$, two big basins of attraction exist for the initial conditions. One of them (which includes Maxwellian distribution of velocities) corresponds to the terminal BG equilibrium, for which both the temperature and the maximal Lyapunov remain finite while N diverges. The other one, which includes uniform distribution of velocities and all angles equal at $t=0$, corresponds to a metaequilibrium state, which eventually crosses over to the BG equilibrium. As N diverges, the duration of this (presumably nonergodic) metaequilibrium state diverges, its temperature remains finite and the maximal Lyapunov exponent vanishes.

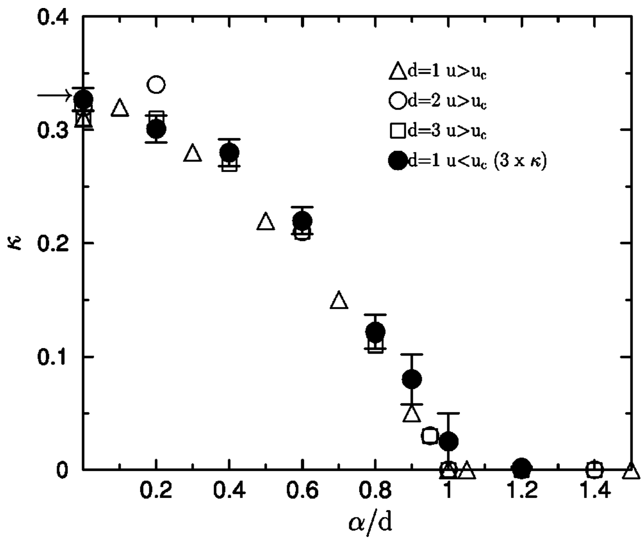

FIG. 4. α/d dependance of $3\times\kappa_{metastable}$ (full circles). Open triangles, circles, and squares, respectively, correspond to κ_d of the $d=1,2,3$ models [11,15]. The arrow points to 1/3, value analytically expected [16,17] to be exact for $\alpha=0$ and $u>u_c$.

Equation (4) constitutes the first connection found for this type of long-range-interaction models between the anomalies *below* and *above* the critical point. This is a conceptually important point, in spite of the unfortunate fact that we do not have general analytical arguments to prove it (see Ref. [37] for an argument for the $\alpha=0$ case). Indeed, if nonextensive statistical mechanics is relevant for such long-range interacting systems as the velocity distributions presented in Ref. [9] seem to suggest, one would expect the model to be somehow associated with a *single* value of the entropic index q for all energies, both below and above possible critical points. Equation (4) makes this possibility plausible. Before ending let us emphasize that no anomalies were detected or expected for $\lambda^{max}_{u<u_c}$(stable) (i.e., in the BG regime emerging at large time), which should gradually (as N increases) attain positive, N-independent values for all values of α. This is of course consistent with the picture (see more details in Ref. [3]) that $\lim_{t\to\infty}\lim_{N\to\infty}$ (anomalous thermodynamical metaequilibrium) and $\lim_{N\to\infty}\lim_{t\to\infty}$ (BG thermodynamical equilibrium) are *not* interchangeable if $0\leqslant\alpha/d\leqslant1$, whereas they are if $\alpha/d>1$.

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