Superdiffusion and Out-of-Equilibrium Chaotic Dynamics with Many Degrees of Freedoms

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We study the link between relaxation to the equilibrium and anomalous superdiffusive motion in a classical N-body Hamiltonian system with long-range interaction showing a second-order phase transition in the canonical ensemble. Anomalous diffusion is observed only in a transient out-of-equilibrium regime and for a small range of energy, below the critical one. Superdiffusion is due to Lévy walks of single particles and is checked independently through the second moment of the distribution, power spectra, trapping, and walking time probabilities. Diffusion becomes normal at equilibrium, after a relaxation time which diverges with N.

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Recently, there has been an increasing interest in physical phenomena which violate the central limit theorem such as anomalous diffusion and Lévy walks. These violations are not an exception in Nature and have been observed in many different fields and also in connection with deterministic chaos in low-dimensional systems [1–5]. The availability of more powerful computers has made it possible to study deterministic chaos and subdiffusive motion in systems with many degrees of freedom using nearest-neighbor coupled symplectic maps [6]. In a very recent paper, superdiffusive motion has been found in an N-body Hamiltonian system with long-range couplings [7]. The mechanism underlying this anomalous diffusion is similar to the one proposed by Geisel *et al.* [1] in "egg-crate" two-dimensional potentials.

In this Letter we present a novel study of superdiffusion and Lévy walks in a Hamiltonian system of N fully coupled rotors [called Hamiltonian mean field (HMF)] [8,9]. The new interesting result is that, in HMF, superdiffusion is connected to the presence of quasistationary nonequilibrium states, rather than to the mechanism proposed by Geisel *et al.* [1] and found also in [7]. Hamiltonian mean field has been used to investigate relaxation to thermodynamical equilibrium for systems with long-range interactions. It has been studied both at a macroscopic level, by means of the canonical formalism, and at a microscopic dynamical level. The canonical ensemble predicts a second-order phase transition from a clustered phase to a homogeneous one [8,9]. On the other hand, microcanonical simulations show strong chaotic behavior in the region below the critical energy; Lyapunov exponents and Kolmogorov-Sinai entropy reach a maximum at the critical point [9]. These results have been confirmed also for long but finite-range interactions [10]. Of particular importance for this Letter are the results obtained in Ref. [9] concerning the discrepancies between microcanonical results and canonical predictions. In fact, numerical simulations performed at constant energy reveal the existence of out-of-equilibrium quasistationary states (QSS) with an extremely slow relaxation to equilibrium. In Ref. [11] these QSS are shown to become stationary solutions in the continuum limit.

The main results of this letter are the following: (1) We find evidence of an anomalous superdiffusive behavior below the critical energy. Anomalous diffusion changes to a normal one after a crossover time τ_c, as also found by other authors [1,2,6,7,12,13]. Power spectra confirm the presence of the anomaly. (2) The superdiffusive behavior is connected to the presence of out-of-equilibrium QSS. We give substantial numerical evidence that the crossover time τ_c coincides with τ_r, the time needed for QSS to relax to canonical equilibrium. (3) We give an interpretation of our results in terms of Lévy walks, which are originated by chaotic transport of each rotor, which moves with an energy not constant in time and alternately sticks to the cluster, and has a quasiregular motion or undergoes free walks far from it with a constant velocity much greater than that of the cluster. Trapping time and walking time probability distributions show a power law behavior. The corresponding exponents can be related to the superdiffusion exponent using the model of Ref. [4] and are very similar to those found in the fluid flow experiment of Solomon *et al.* [2].

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In the following we recall the formalism and then we review the numerical results. The HMF describes a system of N classical particles (or rotors) characterized by the angles θ_i and the conjugate momenta p_i. Each rotor interacts with all of the others according to the following Hamiltonian:

$$H(\theta, p) = K + V, \tag{1}$$

where

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

are the kinetic and the potential energies. One can define a spin vector associated with each rotor $\mathbf{m}_i = [\cos(\theta_i), \sin(\theta_i)]$ and a total magnetization $\mathbf{M} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{m}_i$. The Hamiltonian then describes N classical spins similar to the XY model. This system has a ferromagnetic second-order phase transition from a clustered phase to a homogeneous one at a critical temperature $T_c = 0.5$ and a corresponding critical energy $U_c = E_c/N = 0.75$ (see Refs. [8,9]). The equations of motion for the N rotors are given by

$$\dot{r}_i = p_i, \qquad \dot{p}_i = -M \sin(\theta_i - \phi), \qquad i = 1, \dots, N, \tag{3}$$

where (M, ϕ) are, respectively, the modulus and the phase of the total magnetization vector $\mathbf{M}$. These equations are formally equivalent to those of a perturbed pendulum. To study relaxation to canonical equilibrium, we solve these equations on the computer using fourth-order symplectic algorithms (the details can be found in Ref. [9]). We start the system in a given initial distribution and we compute θ_i, p_i at each time step, and from them the total magnetization M and temperature T (through the relation $T = 2\langle K \rangle/N$). We consider systems with an increasing size N and different energies $U = E/N$.

Diffusion and transport of a particle in a medium or in a fluid flow are characterized by the average square displacement $\sigma^2(t)$ in the long-time limit. In general, one has

$$\sigma^2(t) \sim t^{\alpha} \tag{4}$$

with $\alpha = 1$ for normal diffusion. All processes with $\alpha \neq 1$ are termed anomalous diffusion, namely, subdiffusion for $0 < \alpha < 1$ and superdiffusion for $1 < \alpha < 2$.

In order to study anomalous diffusion in HMF we follow the dynamics of N rotors starting the system in a "water bag," i.e., a far-off-equilibrium initial condition obtained by putting all of the rotors at $\theta_i = 0$ and giving them a uniform distribution of momenta with a finite width centered around zero. We compute the variance of the one-particle angle θ according to the expression

$$\sigma_\theta^2(t) = \langle(\theta - \langle\theta\rangle)^2\rangle, \tag{5}$$

where $\langle\cdots\rangle$ indicate the average over the N particles, and we fit the value of the exponent α in Eq. (4). In Fig. 1 we plot on a log-log scale σ_θ^2 vs t for $N = 500$ at three different energies: $U = 0.2$, $U = 0.6$, and $U = 5$. The continuous lines are shifted fits and show a very clear power law over a few decades; the corresponding values for the slope α are indicated in the inset. The numerical results show clearly three different types of behavior: (1) No diffusion for very low energy, i.e., $U \leq 0.2$. In this case all of the particles belong to a single cluster and $\alpha = 0$. (2) A ballistic regime $\alpha = 2$ for U bigger than the critical energy ($U_c = 0.75$) (a short-time ballistic regime is obviously always present for all energies). (3) Superdiffusion with $\alpha = 1.38 \pm 0.05$ for $U = 0.6$, in the transient regime. After a crossover time $\tau_c \sim 7 \times 10^4$, a change to the slope $\alpha = 1$ (normal diffusion) is observed. The superdiffusive regime is present in the energy range $0.5 < U < 0.75$.

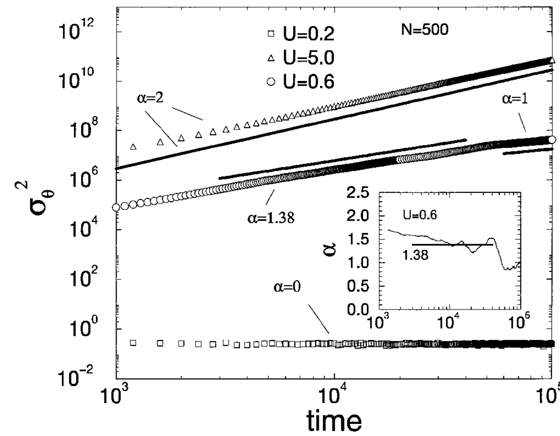

FIG. 1. For $N = 500$ we show three different behaviors: (1) no diffusion for $U = 0.2$; (2) ballistic diffusion for $U = 5$; and (3) superdiffusion for $U = 0.6$. In this last case we considered the average over 5 events. The straight full lines are shifted fits, and the relative slopes are also indicated. The relative errors obtained from the fits are $\sim 5\%$. We show in the inset the numerical evaluation of the slope α vs time for the case $U = 0.6$.

In Fig. 2 we study the dependence on N of the anomalous diffusion and the coincidence of crossover time τ_c with the relaxation time τ_r, i.e., the time the system needs to reach the canonical temperature [horizontal dotted line in panel (b)]. We report σ_θ^2 and temperature vs time for $N = 500$ and 2000 and $U = 0.69$. A slope $\alpha = 1.42 \pm 0.05$ is observed in a first time stage, in which the temperature is different from the canonical value. In fact, the temperature maintains for a very long period a constant value which corresponds to a QSS belonging to the continuation of the homogeneous phase at a subcritical energy (see, in particular, Fig. 1 of Ref. [9], and see also Ref. [11]). Indeed, the crossover time from anomalous to normal diffusion τ_c coincides with the relaxation time τ_r. This result has also been checked, changing the accuracy of the numerical simulation. The transient regime, in which QSS and anomalous diffusion are present, increases linearly with N [9]; consequently, for $N = 2000$,

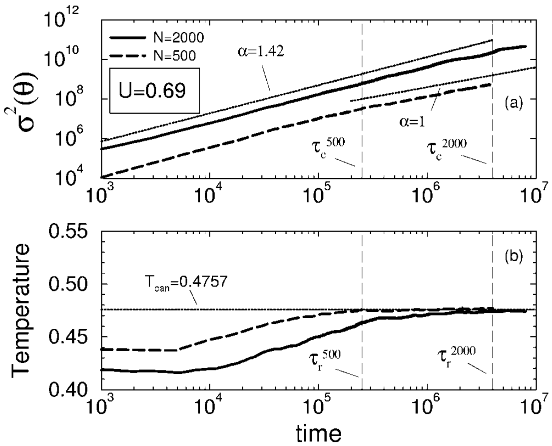

FIG. 2. Variance and temperature for two different sizes $N = 500$ (dashed lines) and 2000 (solid lines) at $U = 0.69$. Panel (a) shows that $\alpha \sim 1.4$ does not depend on N (within the accuracy of the calculations) and occurs only in a transient regime. Once the canonical temperature, shown in panel (b), is reached, diffusion becomes normal. The relaxation time τ_r is clearly larger for bigger N. The vertical dashed lines indicate $\tau_c \sim \tau_r$ for $N = 500$ and $N = 2000$.

one gets superdiffusion over almost three decades. On the other hand, the slope α does not seem to strongly depend on N, and, moreover, in the range $0.6 < U < 0.69$ it varies from 1.38 to 1.42. A similar scenario has been recently conjectured by Tsallis [14] for systems with long-term memory and slow relaxation to equilibrium, but to our knowledge this is the first time that it has been found in a numerical simulation.

The importance of noise and finite-size fluctuations in the crossover from anomalous to normal diffusion has been studied in detail in Refs. [12,13,7]. However, Kaneko and Konishi [6] claim that relaxation to normal diffusion is due to phase-space uniform sampling, which occurs asymptotically. Our results show that this relaxation occurs in coincidence with relaxation to the equilibrium of QSS, which is a quite close mechanism to the one proposed in Ref. [6]. However, at variance with these latter authors, our model displays superdiffusion, rather than subdiffusion, in the transient. Some important physical facts might be crucial in the observed differences. Superdiffusion occurs near a second-order phase transition in our case, while in the model of Ref. [6] no phase transition is present. The model of Ref. [7] has a first-order phase transition, and the particles performing correlated flights belong only to a distinct dynamical class or phase for $N \to \infty$. In our case this is not true: Close to the critical energy, fluctuations are maximal and do not disappear in the thermodynamical limit. Each particle regularly performs free walks and trapped oscillations until it forgets the initial condition and tends to a Brownian motion.

Evidence in favor of this mechanism is provided by the link of superdiffusion with Lévy walks. For low-dimensional chaotic Hamiltonian systems, superdiffusion has been interpreted as being due to the trapping of the particles by the cantori of the phase space; particles can eventually escape and walk freely before a new trapping occurs [5], and this mechanism prevents normal diffusion. An analogous situation occurs in the experiment of Solomon *et al.* for chaotic transport in a two-dimensional rotating flow [2]. In this case tracer particles are trapped and untrapped by a chain of six vortices. This last mechanism is very similar to ours. In Fig. 3 we report the time behavior of the angle θ and of the corresponding conjugate momentum p of a test particle in the transient anomalous diffusion regime [panels (a) and (b)] and in the equilibrium regime [panels (c) and (d)] for $U = 0.6$ and $N = 500$. Free walks and trapped motion are observed in the transient regime; the walks have an almost constant velocity corresponding to the separatrix between bounded and free motion ($\sim 2\sqrt{M}$) of the perturbed pendulum of Eqs. (3). In the equilibrium regime the test particle remains trapped in the cluster; it oscillates around its center and drifts together with it on a much longer time scale (for a study of cluster motion, see Ref. [8]). It is important to notice that the energy of the test particle is not conserved. The particle walks freely when it accidentally receives enough energy that allows it to escape from the mean field. In this sense the mechanism of anomalous diffusion in our case is similar to that of nonconservative systems. A quantitative difference between the two behaviors can be obtained by performing the power spectrum of the motion in Figs. 3(a) and 3(c). We get a power law with slope -2 for the equilibrium regime, as it should be for Brownian motion, and a slope smaller than -2 for the transient regime. To study the connection between Lévy walks and anomalous diffusion we evaluate trapping and walking time distributions.

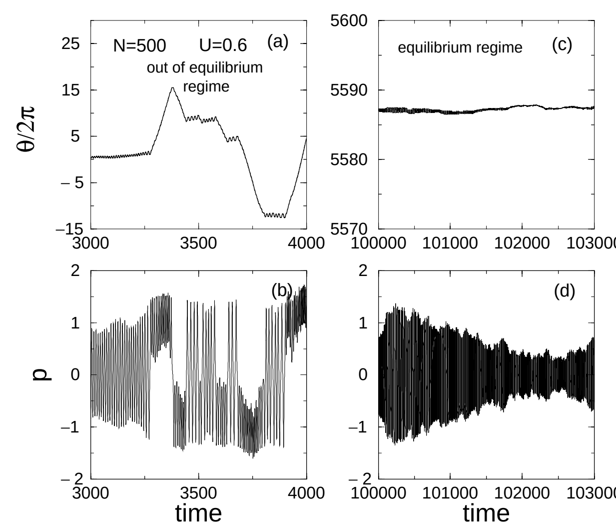

FIG. 3. Angle θ and momentum p of a typical particle for $U = 0.6$ and $N = 500$. Panels (a) and (b) refer to the transient regime, and (c) and (d) refer to the canonical equilibrium state. See text for more details.

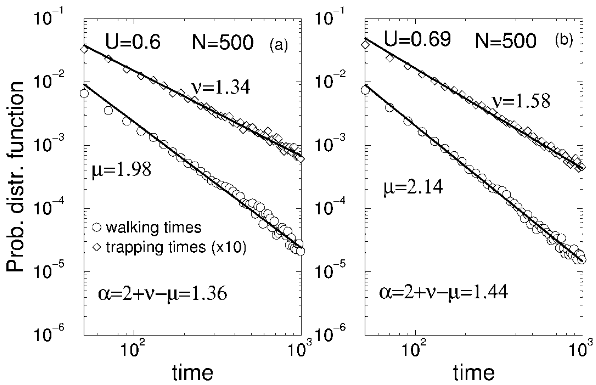

FIG. 4. For the cases $U = 0.6$ and $U = 0.69$, we show the probability distribution functions for trapping (open diamonds) and walking times (open circles) calculated in the transient regime ($2000 < t < 8000$). The corresponding fits and exponents are also indicated; see text for more details.

A free walk is identified by $\Delta\theta > 2\pi$. In Fig. 4 we consider, for $N = 500$ and two energies $U = 0.6$ and $U = 0.69$, the probability distribution of "walking times" and "trapping times." They show, as expected, a clear power law decay:

$$P_{\rm walk} \sim t^{-\mu}, \qquad P_{\rm trap} \sim t^{-\nu}. \tag{6}$$

The values of μ and ν obtained from the fitting are reported in the figure. Their value is crucial because the two exponents μ and ν can be related to the anomalous diffusion coefficient α. The following relationships, derived from Ref. [4], are the most appropriate for HMF:

$$\alpha = 2 + \nu - \mu, \qquad 2 < \mu < 3, \qquad \nu < 2, \tag{7}$$

$$\alpha = 4 - \mu, \qquad 2 < \mu < 3, \qquad \nu > 2. \tag{8}$$

These formulas are valid for a one-dimensional system under the assumption of walks with a constant velocity, separated by sticking events with no motion. In the case shown we get for $U = 0.69$ (0.6), $\mu = 2.14 \pm 0.1$ (1.98 ± 0.1), $\nu = 1.58 \pm 0.05$ (1.34 ± 0.05), and thus a value for $\alpha = 2 + \nu - \mu = 1.44 \pm 0.05$ (1.36 ± 0.05), which is consistent with the values obtained from the fits shown in Figs. 1 and 2, within our numerical accuracy (the relative error on the exponent α obtained by fitting the slope of the variance is $\sim$5%). As found in Ref. [2] we get for the trapping probabilities the exponent $\nu < 2$, which is not the usual case encountered in low-dimensional conservative maps. The reason for that is likely the nonconservation of energy for the test particle motion.

In conclusion, we have found superdiffusion and Lévy walks in a Hamiltonian system showing a second-order phase transition. This behavior occurs in a transient out-of-equilibrium regime in a range of energies slightly smaller than the critical energy where the system is strongly chaotic and QSS exist. We have also found that the equilibration time needed to reach the canonical temperature, which diverges with N, corresponds to the crossover to normal diffusion, confirming a recently proposed scenario [14]. This feature has been observed for the first time in a deterministic chaotic system with many degrees of freedom and could be relevant to understanding more realistic situations such as the anomalous diffusion observed in fluid flow experiments [2].

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