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

Vito Latora (a),(1)
Center for Theoretical Physics, Laboratory for Nuclear Sciences and Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
and
Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

Andrea Rapisarda (b),(2)
Dipartimento di Fisica, Università di Catania
and Istituto Nazionale di Fisica Nucleare, Sezione di Catania
Corso Italia 57, I-95129 Catania, Italy

Stefano Ruffo (c),(3)
Dipartimento di Energetica, Università di Firenze, INFN and INFN Via S. Marta 3, Firenze, Italy
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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.

In the recent years there has been an increasing interest for 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 [1–4]. The availability of more powerful computers has made possible to study deterministic chaos and subdiffusive motion in systems with many degrees of freedom using nearest-neighbour coupled symplectic maps [5]. In a very recent work superdiffusive motion has been found in a N-body Hamiltonian system with long-range couplings [6]. The mechanism underlying this anomalous diffusion is similar to the one proposed by Geisel [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) [7]. The new interesting result is that, in HMF superdiffusion is connected to the presence of quasi-stationary non-equilibrium states, rather than to the mechanism proposed by Geisel [1] and found also in [6]. HMF 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 a 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 Quasi-Stationary 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:

1) we find evidence of an anomalous superdiffusive behavior below the critical energy. Anomalous diffusion changes to normal one after a crossover time $\tau_c$, 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 $\tau_c$ coincides with $\tau_r$, the time needed for QSS to relax to canonical equi-
librium;
3) we give an interpretation of our results in terms of Lévy walks, that are originated by chaotic transport of each rotor, which moves with an energy not constant in time and alternately sticks to the cluster, which has a quasi-regular 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. [9] and are very similar to those found in the fluid flow experiment of Solomon et al. [2].

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

\[
H(\theta, p) = K + V,
\]

where

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

are the kinetic and potential energy. One can define a spin vector associated to 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 similarly 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 ref. [3]). The equations of motion for the \( N \) rotors are given by:

\[
\dot{\theta}_i = p_i, \quad \dot{p}_i = -M \sin(\theta_i - \phi), \quad i = 1, ..., N,
\]

where \( (M, \phi) \) are respectively modulus and 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. [3]). We start the system in a given initial distribution and we compute \( \theta_i, p_i \) at each time step, and from them the total magnetization \( \mathbf{M} \) and temperature \( T \) (through the relation \( T = 2 < K > /N \)). 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

\[
\sigma^2(t) \sim t^\alpha
\]

with \( \alpha = 1 \) for normal diffusion. All the 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 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 \( \theta \) according to the expression

\[
\sigma^2_\theta(t) = \langle (\theta - < \theta >)^2 \rangle,
\]

where \( < \cdot > \) indicate the average over the \( N \) particles, and we fit the value of the exponent \( \alpha \) in eq. (5). In fig.1 we plot on a log-log scale \( \sigma^2_\theta \) vs. \( t \) for \( N = 500 \) at three different energies: \( U=0.2, U=0.6, U=5 \). The continuous lines are shifted fits and show a very clear power law over a few decades; the corresponding values for the slope \( \alpha \) 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 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 transcient regime. After a crossover time \( \tau_c \sim 7 \cdot 10^4 \) a change to the slope \( \alpha = 1 \) (normal diffusion) is observed. The superdiffusive regime is present in the energy range \( 0.5 < U < 0.75 \).

In fig.2 we study the dependence on \( N \) of the anomalous diffusion and the coincidence of crossover time \( \tau_c \) with the relaxation time \( \tau_r \), i.e. the time the system needs to reach the canonical temperature (horizontal dotted line in panel b)). We report \( \sigma^2_\theta \) and temperature vs. time for \( N = 500, 2000 \) 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 Refs. [1] and Ref. [3]). Indeed, the crossover time from anomalous to normal diffusion \( \tau_c \) coincides with the relaxation time \( \tau_r \). 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 \( N \) [4], consequently for \( N=2000 \) one gets superdiffusion over almost 3 decades. On the other hand, the slope \( \alpha \) 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 [13] 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. [2,3,4]. On the contrary, Kaneko and Konishi [5] 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 equilibrium of QSS, which is a quite close mechanism to the one proposed in Ref. [7]. 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. [5] no phase transition is present. The model of Ref. [5] 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 favour of this mechanism is provided by the link of superdiffusion with Lévy walks. For low-dimensional chaotic Hamiltonian systems, superdiffusion has been interpreted as 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 [6], and this mechanism prevents from normal diffusion. An analogous situation occurs in the experiment of Solomon et al. for chaotic transport in a two-dimensional rotating flow [6]. 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 \( \theta \) 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 [6]). It is important to notice that the energy of the test particle is not conserved. The particle walks freely when accidentally it 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 non-conservative systems. A quantitative difference between the two behaviors can be obtained by performing the power spectrum of the motion in fig.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. To study the connection between Lévy walks and anomalous diffusion we evaluate trapping and walking time distributions. 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:

\[
P_{\text{walk}} \sim t^{-\mu}, \quad P_{\text{trap}} \sim t^{-\nu}.
\]

The values of \( \mu \) and \( \nu \) obtained from the fitting are reported in figure. Their value is crucial because, the two exponents \( \mu \) and \( \nu \) can be related to the anomalous diffusion coefficient \( \alpha \). The following relationships, derived in ref. [6], are the most appropriate for HMF:

\[
\alpha = 2 + \nu - \mu \quad 2 < \mu < 3, \quad \nu < 2
\]

and

\[
\alpha = 4 - \mu \quad 2 < \mu < 3, \quad \nu > 2.
\]

These formulae are valid for a one-dimensional system under the assumptions 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 \pm 0.1), \( \nu = 1.58 \pm 0.05 \) (1.34 \pm 0.05) and thus a value for \( \alpha = 2+\nu-\mu = 1.44\pm0.05 \) (1.36\pm0.05) 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 \( \alpha \) obtained by fitting the slope of the variance is \( \sim 5\% \)). As found in ref. [6] we get for the trapping probabilities the exponent \( \nu < 2 \), which is not the usual case encountered in low dimensional conservative maps. The reason of that is likely the non-conservation 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 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 of relevance to understand more realistic situations such as the anomalous diffusion observed in fluid flow experiments.

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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 $\alpha$ vs time for the case $U=0.6$.

FIG. 2. Variance and temperature for two different sizes N=500 (dashed lines),2000 (full 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 $\tau_r$ is clearly larger for bigger N. The vertical dashed lines indicate $\tau_c \sim \tau_r$ for N=500 and N=2000.
FIG. 3. Angle $\theta$ and momentum $p$ of a typical particle for $U = 0.6$ and $N = 500$. Panels (a) and (b) refer to the transient regime, (c) and (d) 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 correspondent fits and exponents are also indicated, see text for more details.