Microcanonical quasistationarity of long-range interacting systems in contact with a heat bath

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On the basis of analytical results and molecular dynamics simulations, we clarify the nonequilibrium dynamics of a long-range interacting system in contact with a heat bath. For small couplings with the bath, we show that the system can first be trapped in a Vlasov quasistationary state, then a microcanonical one follows, and finally canonical equilibrium is reached at the bath temperature. We demonstrate that, even out of equilibrium, Hamiltonian reservoirs microscopically coupled with the system and Langevin thermostats provide equivalent descriptions. Our identification of the key parameters determining the quasistationary lifetimes could be exploited to control experimental systems such as the free-electron laser, in the presence of external noise or inherent imperfections.

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In recent years, systems characterized by interactions that slowly decay at large distances have considerably attracted the attention of experimental and theoretical physicists. Plasmas, gravitational systems, two-dimensional vortices, and wave-matter interaction systems all fall in this category [1]. Of particular interest to what follows is the case of the free-electron laser (FEL), a source of coherent radiation which is expected to outperform traditional lasers thanks to the properties of a relativistic-electron lasing medium (see, e.g., [2] and references therein). For these systems, the prevalence of long-range interactions over mechanisms acting on short-range scales implies an inefficiency of fast collision processes. This is in contrast with the assumptions underlying Boltzmann's derivation of the transport equation and brings us to the fact that long-range interacting systems get easily stuck in (Vlasov) nonequilibrium quasistationary states (QSSs) [1,3–6]. For instance, the possible observation of QSSs in FEL experiments is predicted on the basis of molecular dynamics simulations of isolated (microcanonical) Hamiltonian systems capturing the essential features of the FEL dynamics [7]. From an experimental point of view, it is crucial to recognize if a stable nonequilibrium picture survives in the presence of an external environment (or inherent imperfections) acting on the system [8–10] and which are the parameters playing a key role in the determination of the QSS lifetimes. In addition, a basic theoretical issue is whether a stochastic dynamics simulating a thermal bath (TB)—e.g., of the Langevin type—reproduces the same nonequilibrium features of a Hamiltonian reservoir microscopically interacting with the long-range system.

While for short-range systems the equivalence between Hamiltonian and Langevin thermostats is well established, the connection between these two different descriptions for the nonequilibrium behavior of a long-range system is less clear, and recent simulations [11] recovered the same results for the two TBs only at equilibrium. Here we demonstrate that Hamiltonian and Langevin TBs provide in fact an equivalent description of the behavior of a paradigmatic long-range system also in nonequilibrium conditions. This is established, both analytically and numerically, analyzing the scaling properties of the QSS lifetimes. We recast the interaction between the system and a Hamiltonian TB in terms of an equivalent set of generalized Langevin equations. The damping coefficient γ determines the time scale t_{bath} for the relaxation to canonical equilibrium, achieved when the system and TB share the same temperature. However, even in the presence of a TB, correlations due to a slow collisional process determine another time scale t_{coll} (depending on system size N) which corresponds to a relaxation to a *microcanonical QSS*. Thus, for γ small enough and N not too large, our main result is the discovery of a rich picture for the transport to equilibrium: On a time scale $t_{dyn}\sim 1$ (in dimensionless units), a violent relaxation drives the system into a Vlasov QSS. Then, on a time scale $t_{coll}\sim N^{\delta}$ (with $\delta \geqslant 1$), the system reaches a microcanonical QSS. Finally, on a time scale $t_{bath}\sim 1/\gamma$, the system crosses over to canonical (thermal) equilibrium.

Thanks to its appealing (yet nontrivial) simplicity, a system which captured a paradigmatic interest among researchers is the Hamiltonian mean-field (HMF) model [1,4–6,8–10], which can be thought of as a set of N globally coupled XY spins with Hamiltonian

$$H_{HMF}=\sum_{i=1}^{N}\frac{l_i^2}{2}+\frac{1}{2N}\sum_{i,j=1}^{N}[1-\cos(\theta_i-\theta_j)], \qquad (1)$$

where $\theta_i\in[0,2\pi)$ are the spin angles and $l_i=\dot{\theta}_i\in\mathbb{R}$ their angular momenta (velocities). Defining the kinetic temperature $T\equiv\sum_{i=1}^{N}l_i^2/N$ as twice the specific kinetic energy and the specific magnetization as $m\equiv|\sum_{i=1}^{N}(\cos\theta_i,\sin\theta_i)|/N$, one obtains the exact relation $E/N=T/2+(1-m^2)/2$, where E is the total energy of the system. The free energy of the HMF model can be exactly mapped [7] onto that of the Colson-Bonifacio Hamiltonian model for the single-pass FEL [12]. In such a context, the variables l_i's are interpreted as the phase velocities relative to the center of mass of the N electrons and the θ_i's are the electron phases with respect to the copropagating wave [7]. Despite some dynamical and thermodynamic differences, analogies can also be found between the HMF model and the behavior of one-dimensional self-gravitating systems [13].

When the HMF model is isolated, in order to determine whether the system truly converges toward statistical equilibrium and the time scale of this relaxation, one must develop an appropriate kinetic theory. This is a classical problem addressed, e.g., in [14] and, more recently, in [9]. From the Liouville equation it is possible to derive the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy for the reduced joint probability density functions (PDFs) $p_j(\theta_1,\ldots,\theta_j,\dot{\theta}_1,\ldots,\dot{\theta}_j,t)$, with $j=1,2,\ldots,N$. In the thermodynamic limit $N\to\infty$, $E/N\sim 1$, and fixed volume $V=2\pi$, the hierarchy can be closed by considering a systematic expansion in powers of $1/N$ of the solutions of the equations [9]. At the order $1/N$, the distribution function $f=Np_1$ satisfies

$$\frac{\partial f}{\partial t}+\dot{\theta}\frac{\partial f}{\partial \theta}-\frac{\partial \phi}{\partial \theta}\frac{\partial f}{\partial \dot{\theta}}=\frac{1}{N}C_{coll}(f), \tag{2}$$

where $\phi(\theta,t)\equiv-\frac{1}{2\pi}\int_0^{2\pi}d\theta'\cos(\theta-\theta')\int_{-\infty}^{+\infty}d\dot{\theta}f(\theta',\dot{\theta},t)$. For $N\to+\infty$, the right-hand side (rhs) of Eq. (2) is negligible and we get the Vlasov equation [14]. For N finite, $C_{coll}(f)$ is a "collision" operator taking into account correlations between particles [9]. The scaling in Eq. (2) indicates that "collisions" (more properly correlations) operate on a very slow time scale, of the order Nt_{dyn} or even larger when $C_{coll}(f)=0$, as for a spatially homogeneous one-dimensional system [9]. It is precisely because of the development of correlations that the system reaches, on the "collisional" relaxation time t_{coll}, a microcanonical Boltzmann distribution. Since $t_{coll}(N)$ diverges for $N\to+\infty$ (different scalings $t_{coll}\sim Nt_{dyn}$, $N^{1.7}t_{dyn}$, and $e^N t_{dyn}$ have been reported depending on the initial conditions [15]), the domain of validity of the Vlasov equation is huge. Starting from an out-of-equilibrium initial condition, the Vlasov equation develops a complicated mixing process in the single-particle phase space, leading, in most cases, to a QSS [6,15]. This process is called violent relaxation since it takes place on a time scale $t_{dyn}\sim 1$. The QSS is a nonlinearly dynamically stable stationary solution of the Vlasov equation on a coarse-grained scale [9]. The Vlasov equation admits an infinite number of stationary solutions. The statistical theory of Lynden-Bell [16] predicts the "most probable" (most mixed) state [4,5]. However, in view of the possible occurrence of incomplete relaxations [4,9], there are cases in which the QSSs take forms different from those described by Lynden-Bell's theory.

The interaction of the system (1) with a reservoir has been studied in Refs. [8,9] introducing a Hamiltonian and a Langevin TB, respectively. In the latter case, the dynamics of the system is governed by a set of N coupled stochastic equations:

$$\ddot{\theta}_i=F_i-\gamma\dot{\theta}_i+\sqrt{2\gamma T_b}\xi_i(t), \tag{3}$$

where $F_i\equiv-\frac{1}{N}\sum_{j=1}^N\sin(\theta_i-\theta_j)$ is the long-range force experienced by the spin i, γ is a damping coefficient due to the interaction with the TB, T_b is the TB temperature, and ξ_i is a Gaussian white noise satisfying $\langle\xi_i(t)\rangle=0$ and $\langle\xi_i(t)\xi_j(t')\rangle=\delta_{ij}\delta(t-t')$. Equation (3) defines the so-called Brownian mean-field model (BMF) [9] (see also [10]). The evolution of the N-body PDF is governed in this case by the Fokker-Planck equation, from which a BBGKY-like hierarchy for

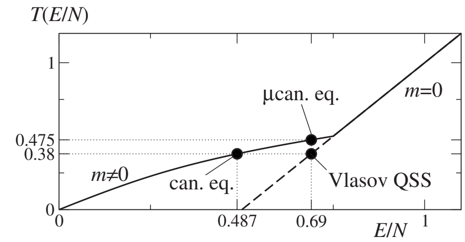

FIG. 1. Caloric curve of the HMF model (solid line). The dashed line is the prolongation of the ordered phase to subcritical energies. See text for details.

the p_j's can be derived. In the thermodynamic limit $N\to+\infty$, $T_b\sim 1$, $V=2\pi\sim 1$, the hierarchy can be closed by considering an expansion in powers of $1/N$. It is possible to see [9] that $p_2(\theta_1,\dot{\theta}_1,\theta_2,\dot{\theta}_2)=p_1(\theta_1,\dot{\theta}_1)p_1(\theta_2,\dot{\theta}_2)+O(1/N)$. Hence, for $N\to+\infty$, the equation for $f=Np_1$ becomes the mean-field Kramers equation

$$\frac{\partial f}{\partial t}+\dot{\theta}\frac{\partial f}{\partial \theta}-\frac{\partial \phi}{\partial \theta}\frac{\partial f}{\partial \dot{\theta}}=\gamma\frac{\partial}{\partial \dot{\theta}}\left(T_b\frac{\partial f}{\partial \dot{\theta}}+f\dot{\theta}\right)\equiv\gamma C_{bath}(f). \tag{4}$$

This equation relaxes to the canonical mean-field Maxwell-Boltzmann distribution $f(\theta,\dot{\theta})=\frac{1}{Z}e^{-(\dot{\theta}^2/2+\phi(\theta))/T_b}$ [with $\phi(\theta)=\lim_{t\to\infty}\phi(\theta,t)$] on a time scale $t_{bath}\sim 1/\gamma$, independent of N. For $\gamma=0$ one recovers the microcanonical situation in which the system is isolated. Correspondingly, the Fokker-Planck equation becomes the Liouville equation and the mean-field Kramers equation becomes the Vlasov equation.

The numerical integration of Eq. (3) exhibits a very rich transport-to-equilibrium picture [11]. In this paper, we show that the key point for understanding the nonequilibrium behavior of the system is the comparison between the time scales t_{dyn}, t_{coll}, and t_{bath}. We specifically analyze the time evolution of the magnetization of the system for simulations with random water bag initial conditions of the form $p_1(\theta,\dot{\theta},0)=\delta(\theta-0)[\vartheta(\dot{\theta}+\bar{l})+\vartheta(\dot{\theta}-\bar{l})]/2\bar{l}$ (ϑ being the Heaviside step function), where $\bar{l}\simeq 2.03$. We thus have $m(0)=1$, $E(0)/N\simeq 0.69$, and $T(0)=1.38$. These and similar nonequilibrium initial conditions have been largely studied in microcanonical simulations [5,6,15] and recently discussed in the presence of a TB [8,11]. The initial energy of the system is below the critical point $E_c/N=3/4$ (see Fig. 1). Microcanonical simulations ($\gamma=0$) display, in a time $t_{dyn}\sim 1$, a violent relaxation process in which the magnetization drops to $m\simeq 0+O(1/\sqrt{N})$ and the temperature to $T\simeq 0.38$. A QSS lasting a time of the order $t_{coll}\sim N^\delta$ follows the violent relaxation.[1] After the QSS, the isolated system warms up (at fixed energy) due to finite-size effects and finally reaches the microcanonical equilibrium state with $T\simeq 0.475$ and $m\simeq 0.31$. At variance, in a relaxation process at fixed temperature $T_b=0.38$ (canonical simulations with $\gamma\neq 0$), the system reaches a canonical equilibrium state with $T=T_b$, E/N

[1]For this $m(0)=1$ initial condition, the Vlasov QSS is not described by the Lynden-Bell theory because of incomplete relaxation (see [4,9]).

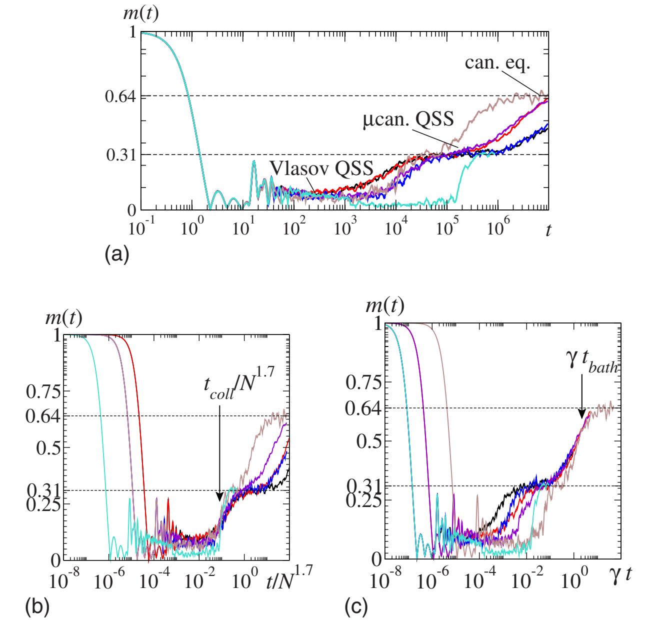

FIG. 2. (Color online) Time evolution of the magnetization with a Langevin TB. The control parameters $\gamma=10^{-7}$, 5×10^{-7}, 10^{-6} and $N=500, 1000, 5000$ satisfy $\gamma \ll 1/N^{1.7} \ll 1$. Plots are averages over at most ten runs. The system reaches a Vlasov QSS for $t \sim t_{dyn} \sim 1$, a microcanonical QSS for $t \sim t_{coll} \sim N^{1.7}$, and a canonical equilibrium for $t \sim t_{bath} \sim 1/\gamma$.

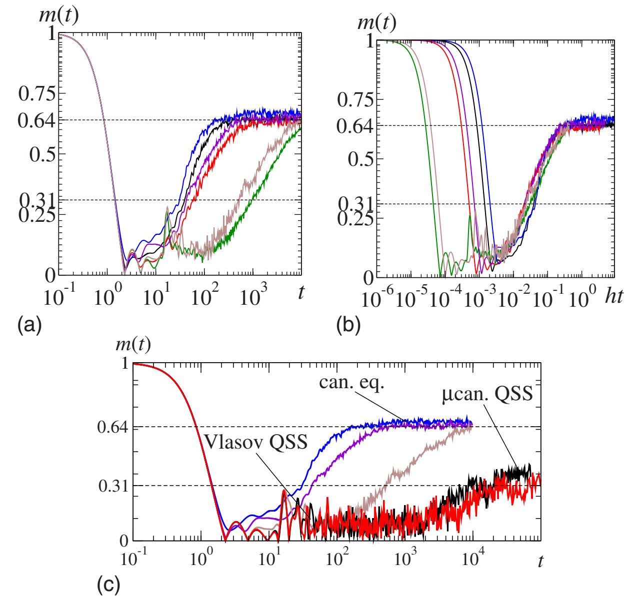

FIG. 3. (Color online) Time evolution of m with the Hamiltonian TB in Eqs. (5) and (6). In (a) and (b) the control parameters are $\epsilon=0.1, 0.05, 0, 01$, $N=500, 1000, 5000$, and $S=10^5 N^{-1/2}$. We found $h \equiv \epsilon^{3/2} S$. In (c) the longer simulations are with $\epsilon=10^{-3}$, 10^{-4} and $N=500$. Averages are over at most ten runs.

$\simeq 0.487$, and $m \simeq 0.64$ (see again Fig. 1). Hence, if we fix the TB temperature in Eq. (3) at $T_b=0.38$ and let $\gamma \to 0$, there is an apparent discontinuity in the final equilibrium value of the magnetization [11]. Actually, this paradox is solved by the presence of a second QSS which follows the Vlasov one. Indeed, for $t \ll t_{bath} \sim 1/\gamma$ the energy is relatively well conserved. Thus, if $t_{dyn} \ll t_{coll} \ll t_{bath}$ (i.e., $\gamma \ll 1/N^{\delta} \ll 1$), the magnetization of the system relaxes to the microcanonical value $m \simeq 0.31$ on the collisional time scale $t_{coll} \sim N^{\delta}$ (we find $\delta \simeq 1.7$, independently of γ). This is the reason why we call this second quasiequilibrium state the "microcanonical QSS." The equilibrium with the TB, and the consequent value $m \simeq 0.64$, is established only on the much larger time scale t_{bath}. On the contrary, for $t_{dyn} \ll t_{bath} \ll t_{coll}$ (i.e., $1/N^{\delta} \ll \gamma \ll 1$), the system first reaches a Vlasov QSS on a time scale t_{dyn}, then a canonical equilibrium state with temperature $T=T_b$ on a time scale t_{bath}, and does not form a microcanonical QSS. We note that in order to see the microcanonical QSS we need a very small noise level: $\gamma \ll 1/N^{\delta}$. There is a further interesting situation, obtained for $t_{bath} \ll t_{dyn}$ (i.e., $\gamma \gg 1$). In this latter case, the system reaches a canonical equilibrium state with temperature $T=T_b$, without forming any (Vlasov or microcanonical) QSS. This corresponds to the overdamped (Smoluchowski) regime studied in [9]. In conclusion, the limits $t \to \infty$, $N \to \infty$, and $\gamma \to 0$ do not commute. Depending on the order in which they are taken, the average value of the magnetization can be the Vlasov ($N \to \infty$ and $\gamma \to 0$ before $t \to \infty$), the microcanonical ($\gamma \to 0$ and $t \to \infty$ before $N \to \infty$), or the canonical ($N \to \infty$ and $t \to \infty$ before $\gamma \to 0$) one. The simulations reported in Fig. 2 demonstrate these features. In Fig. 2(a) curves with the same N almost coincide for $t < t_{coll}$. Those with the same γ collapse onto each other for $t > t_{coll}$. The presence of a microcanonical QSS following the Vlasov one is particularly evident in the rescaled plots of Figs. 2(b) and 2(c), which confirm the scaling properties of t_{coll} and t_{bath}.

The next step is to establish whether these microcanonical QSSs are an artifact of the mesoscopic stochastic dynamics (3) or if they are still present when we consider a Hamiltonian TB microscopically coupled with the long-range system. In Ref. [8] a first-neighbor coupled XY-spin TB has been introduced,

$$H_{TB} = \sum_{i=1}^{N_{TB}} \frac{l_i^{TB^2}}{2} + \sum_{i=1}^{N_{TB}} [1 - \cos(\theta_{i+1}^{TB} - \theta_i^{TB})], \qquad (5)$$

interacting with the HMF model through the potential

$$H_I = \epsilon \sum_{i=1}^{N} \sum_{s=1}^{S} [1 - \cos(\theta_i - \theta_{r_s(i)}^{TB})], \qquad (6)$$

where $r_s(i)$ are integer-independent random numbers in the interval $[1, N_{TB}]$. Each HMF spin is in contact with a set of S different TB spins chosen randomly along the chain, and the coupling constant $\epsilon \geq 0$ determines the interaction strength between the system and TB. The conditions [8] $N_{TB}=N^2$ and $S=10^5 N^{-1/2}$ assure that for large N the interaction, the system, and the TB energies are well separated. Molecular dynamics simulations of the Hamiltonian $H_{HMF}+H_{TB}+H_I$ were shown to agree with the Langevin ones at equilibrium [11], whereas the presence of QSSs with a lifetime depending on both ϵ and N (or, equivalently, S) has been detected [8,11].

In order to clarify this dependence we study a different Hamiltonian form for the TB and for its interaction with the system, which has the advantage of allowing an explicit analytical analysis. Following the approach outlined by Zwanzig [17] for short-range systems, our aim is to recast the Hamiltonian equations of motion in a form similar to Eq. (3). Hence, we replace Eqs. (5) and (6) with

$$H'_{TB} = \sum_{i=1}^{N_{TB}} \frac{l_i^{TB2}}{2}, \quad H'_I = \epsilon \sum_{i=1}^{N} \sum_{s=1}^{S} \left[\frac{\omega_{r_s(i)}}{4} (\theta_i - \theta_{r_s(i)}^{TB})^2 \right], \quad (7)$$

respectively, and consider the Hamiltonian $H_{HMF}+H'_{TB}+H'_I$. The TB in Eq. (7) describes a set of N_{TB} isochronous harmonic oscillators in their canonical coordinates, which interact with the system through a quadratic potential. This quadratic form can be thought of as a small-angle expansion of Eq. (6), and again each element of the HMF model interacts with S different TB oscillators. Using, for example, the Laplace transform and performing then an integration by parts, the Hamiltonian dynamics of the θ_i's becomes

$$\ddot{\theta}_i(t) = F_i - \int_0^t dt\, K(t-\tau)\dot{\theta}_i(\tau) + \xi'(t), \quad (8)$$

where $K(t) \equiv \epsilon \Sigma_{i=1}^{S} \omega_{r_s(i)}^2 \cos[\sqrt{\epsilon}\omega_{r_s(i)} t]$ and ξ' can be written explicitly in terms of the initial conditions.[2] Assuming a random distribution for the initial data, ξ' can be regarded as a stochastic term. On the other hand, K is a memory kernel which depends on ϵ, S, and the distribution of the frequencies $\omega_{r_s(i)}$. Specifically, when K reduces to a δ function, Eq. (8) recasts into Eq. (3) with $\gamma = h(\epsilon, S)$, and h a model-dependent function. The form of Eq. (8) suggests that the relaxation process in the presence of a general Hamiltonian TB should be analogous to that described by the stochastic Langevin equation (3), with the canonical equilibrium established on a time scale $t_{bath} = [h(\epsilon,S)]^{-1}$. In particular, by choosing sufficiently small ϵ's, the system should exhibit microcanonical QSSs also if coupled with a Hamiltonian TB. We verified these conclusions for the Hamiltonian TB in Eqs. (5) and (6). Figures 3(a) and 3(b) demonstrate that if we rescale the time by $h(\epsilon,S) = \epsilon^{3/2} S$, indeed the relaxation time to the thermal equilibrium obtained for different ϵ's and S's collapses onto the same value. Moreover, for $\epsilon \leq 10^{-3}$ microcanonical QSSs clearly appear [Fig. 3(c)].

In summary, we have shown that the nonequilibrium dynamics of a paradigmatic long-range system which can be mapped onto the one describing the single-pass FEL is characterized by the three time scales $t_{dyn} \sim 1$, $t_{coll} \sim N^{\delta}$, and $t_{bath} \sim 1/\gamma$. By acting on the initial conditions, on the system size N, or on the coupling with the heat bath γ, one can conceive experiments in which the system is either in equilibrium with the bath or in a quasiequilibrium state with a dynamical temperature which is different from the temperature of the thermal environment. This situation could inspire interesting applications and provides a control on the imperfections influencing a FEL and other long-range systems.

[2] $\xi'(t) \equiv \epsilon \Sigma_{i=1}^{S} \omega_{r_s(i)}^2 \{[\theta_{r_s(i)}^{TB}(0) - \theta_i(0)] f_1(t) + \dot{\theta}_{r_s(i)}^{TB}(0) f_2(t)\}$, where $f_1(t) \equiv \cos(\sqrt{\epsilon}\omega_{r_s(i)} t)$ and $f_2(t) \equiv \sin(\sqrt{\epsilon}\omega_{r_s(i)} t)/\sqrt{\epsilon}\omega_{r_s(i)}$.

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