Hamiltonian Dynamics Reveals the Existence of Quasistationary States for Long-Range Systems in Contact with a Reservoir

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We introduce a Hamiltonian dynamics for the description of long-range interacting systems in contact with a thermal bath (i.e., in the canonical ensemble). The dynamics confirms statistical mechanics equilibrium predictions for the Hamiltonian mean field model and the equilibrium ensemble equivalence. We find that long-lasting quasistationary states persist in the presence of the interaction with the environment. Our results indicate that quasistationary states are indeed reproducible in real physical experiments.

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The statistical mechanics of systems with long-range interactions is important for a variety of physical applications, including, e.g., gravitational systems, plasmas, and Bose-Einstein condensates [1]. In such systems, the interparticle interactions decay at large distances r as $1/r^\alpha$, with $\alpha \leq d$ (spatial dimension), and ordinary statistical mechanics assumptions are questioned by nontrivial effects, such as persistence of correlations and non-negligible interface energies. In particular, the Boltzmann transport equation picture for the approach to equilibrium is not valid [2], and long-range interacting systems may even display inequivalences among different equilibrium statistical ensembles [3,4]. Because of these subtleties, a privileged investigation tool is the microscopic Hamiltonian dynamical simulation. Hamiltonian dynamics at a fixed energy (microcanonical ensemble) for a paradigmatic long-range Hamiltonian (see below) directly connected with experiments [5] revealed the existence of long-lived quasistationary states (QSSs) that finally cross over to Boltzmann-Gibbs (BG) statistical equilibrium [6]. The question arises about the reproducibility of such QSSs in real physical experiments, where the environment introduces perturbations that cannot be taken into account in the microcanonical ensemble. If so, practical advantages could be obtained by knowing control mechanisms that improve or hinder this quasistationarity. The use of classical numerical prescriptions (such as the Nosé-Hoover or the Monte Carlo methods [7]) to perform such an investigation raises some subtle questions, since these methods implicitly assume the BG equilibrium. Here we propose a novel, physically transparent, microscopic Hamiltonian dynamics obtained by coupling the long-range system with a thermal bath (TB) which simulates the effect of the environment on the system itself. For sufficiently large time scales, such dynamics confirms the equilibrium canonical ensemble predictions. However, starting with out-of-equilibrium initial conditions, we discover that long-lived QSSs subsist in the presence of the TB, providing evidence in favor of the reproducibility of QSSs in real physical experiments. We also discuss the relaxation process following the QSS and the peculiar behavior of the Boltzmann's H function.

In a magnetic context, the Hamiltonian mean field (HMF) model [8] describes a set of M globally coupled XY spins with Hamiltonian

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

where $\theta_i \in [0, 2\pi)$ are the spin angles and $l_i \in \mathbb{R}$ their angular momenta (velocities). The presence of the kinetic term naturally endows the system of spins with an Hamiltonian dynamics. This Hamiltonian is considered "paradigmatic" for long-range interacting systems [9], since its equilibrium properties are analytically solvable both in the microcanonical and in the canonical ensemble [4,9] and it is representative of the class of Hamiltonians on a one-dimensional lattice in which the potential is proportional to $\sum_{i,j=1}^{M} [1 - \cos(\theta_i - \theta_j)]/r_{ij}^\alpha$, where r_{ij} is the lattice separation between spins and $\alpha < 1$ [10] [notice that the potential in Eq. (1) is recovered in the limit $\alpha \rightarrow 0$]. Also, direct connections with the problem of disk galaxies [9] and free electron laser experiments [5] have been established. Whereas it has been recently proven that (1) does not present microcanonical or canonical inequivalence at equilibrium [4], its unusual dynamical features received recently a lot of attention [6,9,11,12]. In fact, fixed-energy dynamical simulations starting with out-of-equilibrium initial conditions display the existence of long-standing (infinite-standing in the thermodynamic limit) QSSs appearing after a "violent relaxation" dynamics. During the QSS, phase functions such as the specific kinetic and potential energies fluctuate around stationary or quasistationary nonequilibrium average values. In this Letter, we introduce a microscopic setup where the HMF model is in contact with a short-range TB in such a way that the thermodynamic limit is achieved with a negligible interaction energy. Equilibrium dynamics confirms the equivalence between the microcanonical and the canonical ensembles for the HMF model. If the HMF-TB coupling is weak enough, the relaxation to equilibrium is still characterized by drastic slowing-down sequences (QSSs) where also the system energy fluctuates around quasistationary average values. We discuss in a separate paper [13] the details about the statistical mechanics of QSSs in the canonical ensemble, a question of considerable debate [6,9,11,12]. Here we report that in Gibbs's Γ space their statistical mechanics is obtained using the classical BG definition of the entropy.

The TB we consider is characterized by $N \gg M$ equivalent spins first neighbors coupled along a chain

$$H_{\rm TB} = \sum_{i=M+1}^{N} \frac{l_i^2}{2} + \sum_{i=M+1}^{N} [1 - \cos(\theta_{i+1} - \theta_i)], \quad (2)$$

with $\theta_{N+1} \equiv \theta_{M+1}$. The interaction between (1) and (2) is modulated by a coupling constant ϵ:

$$H_I = \epsilon \sum_{i=1}^{M} \sum_{s=1}^{S} [1 - \cos(\theta_i - \theta_{r_s(i)})], \quad (3)$$

where $r_s(i)$ are independent integer random numbers in the interval $[M+1, N]$. In this way, each HMF spin is in contact with a set of S different TB spins chosen randomly along the chain (see Fig. 1). This set is specified as the initial condition and remains fixed during the dynamics. The total Hamiltonian $H = H_{\rm HMF} + H_{\rm TB} + H_I$ defines then a microcanonical system (constant energy E), in which the energy of the HMF model can fluctuate. In our approach, the temperature is twice the specific kinetic energy, and we expect the TB to maintain a constant temperature about which the HMF model thermally equilibrates. By assuming a "surfacelike effect" $S \sim M^{\gamma-1}$ (with $0 < \gamma < 1$), we make sure that the interaction energy $E_I \sim M^{\gamma}$ satisfies $E_{\rm HMF} \sim M$ ($E_{\rm TB} \sim N \gg M$), thus ensuring a well defined thermodynamic limit. For the present results, we chose $N = M^2$ and $S = 10^5 M^{-1/2}$. To integrate the equation of motion, we use a velocity Verlet [7] algorithm with an integration step guaranteeing conservation of total energy within an uncertainty of $\Delta E/E \simeq 10^{-5}$.

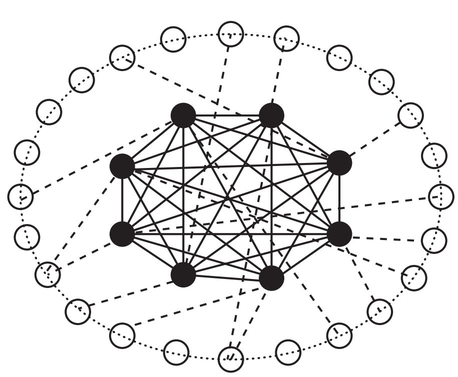

FIG. 1. Sketch of the interactions considered in our canonical setup. The dashed lines mimic the interactions between the HMF (solid circles) and the TB (empty circles) spins. The solid (dotted) lines represent the HMF (TB) couplings.

Let $e_{\rm HMF} \equiv E_{\rm HMF}/M = [k_{\rm HMF} + (1 - m_{\rm HMF}^2)/2]$, where $k_{\rm HMF} \equiv \sum_{i=1}^{M} l_i^2/2M$ and $m_{\rm HMF} \equiv |\sum_{i=1}^{M}(\cos\theta_i, \sin\theta_i)|/M$ are, respectively, the specific kinetic energy and the magnetization of the system. It is known that at $e_{\rm HMF} = 0.75$ and temperature $T_{\rm HMF} = 0.5$ (in natural dimensionless units) a continuous phase transition occurs, separating a disordered ($m_{\rm HMF} = 0$) phase from a ferromagnetic one [8,9]. Here we show that our Hamiltonian dynamics confirms such equilibrium predictions. The width T_0 of the Maxwellian probability density function (PDF) for the initial TB velocities $p_{\rm TB}(l, 0) = \exp(-l^2/2T_0)/\sqrt{2\pi T_0}$ is a control parameter through which we set the TB temperature. In fact, after a transient relaxation ($0 \le t < t^* \sim 100$), the TB reaches its own equilibrium at the target temperature T_0 [i.e., $2k_{\rm TB}(t) \simeq T_0\ \forall\ t > t^*$]. At $t = t^*$, we then switch on the HMF-TB coupling H_I by setting $\epsilon(t) = \epsilon^* \ge 0\ \forall\ t \ge t^*$. For $\epsilon^* = 0$, $H_I = 0$, and the scheme reproduces the microcanonical dynamics of the HMF. The setup was tested for many different initial conditions of the HMF model with $10^2 \le M \le 10^4$ and $0.005 \le \epsilon^* \le 0.1$. In all cases, for $t \gg t^*$, the system reaches the thermal equilibrium characterized by $2k_{\rm HMF}(t) \simeq T_0$ [Fig. 2(a)], a velocity PDF $p_{\rm HMF}(l, t) \simeq p_{\rm TB}(l, 0)$ [Fig. 2(b)], and an equilibrium magnetization. The relaxation to equilibrium could last very long and typically occurs through a number of drastic slowing-down sequences during which the average value

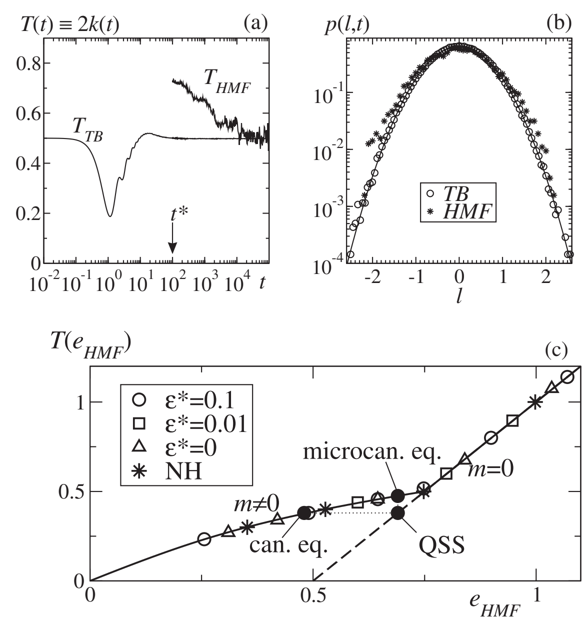

FIG. 2. (a) Time evolution of the $T_{\rm HMF}$ and $T_{\rm TB}$ temperatures for $M = 10^3$, $\epsilon = 0.01$, and $T_0 = 0.5$. Initially, $p_{\rm HMF}(l, 0) = \exp(-l^2/2T(t^*))/\sqrt{2\pi T(t^*)}$, with $T(t^*) = 0.7$. (b) Velocity PDF at $t \gg t^*$. The solid line is $p_{\rm TB}(l, 0)$. (c) Caloric curve. The solid line is the BG equilibrium, and the dashed line is the prolongation of the ordered phase to subcritical energies. The empty symbols are the average value of $e_{\rm HMF}(t)$ at equilibrium. The stars refer to Nosé-Hoover simulations. The solid circles correspond to the QSS studied in the Letter and to the microcanonical and canonical equilibrium obtained as $t \to \infty$.

of T_{HMF} is constant or almost constant [plateaux in Fig. 2(a)]. Similar effects were found in Ref. [14] using a stochastic dynamics (see also [9] for a stochastic canonical version of the HMF, named the Brownian mean field). By varying T_0, we obtain an estimate of the caloric curve in excellent agreement both with the BG equilibrium prediction and with the microcanonical simulation, even at the critical temperature and independently of ϵ^* [Fig. 2(c)]. These findings confirm the equilibrium ensemble equivalence [4] solely on the basis of Hamiltonian dynamics. For close to equilibrium initial conditions, the Nosé-Hoover dynamics [7] reproduces the caloric curve [Fig. 2(c)] as well.

We now turn to the nonequilibrium properties of the model by setting for the HMF system out-of-equilibrium initial conditions. In particular, at $t = t^*$, we consider a delta distribution for the angles [$p_{\mathrm{HMF}}(\theta, t^*) = \delta(0)$ so that $m^2_{\mathrm{HMF}}(t^*) = 1$] and a uniform distribution for the velocities $p_{\mathrm{HMF}}(l, t^*) = 1/2\bar{l}$, $l \in [-\bar{l}, \bar{l}]$, with $\bar{l} \simeq 2.03$ [$e_{\mathrm{HMF}}(t^*) \simeq 0.69$]. If $\epsilon^* = 0$, we verified the known result that for such initial conditions the system, after a fast process, is dynamically trapped into a QSS [6,9,11,12] [Fig. 3(a)]. The initial ($t \lesssim t^* + 1$) violent relaxation corresponds to a quick mixing of the spins in the single-particle μ space [9]. The QSS is then characterized by $m^2_{\mathrm{HMF}} \simeq 0$ ($T_{\mathrm{HMF}} = 0.38$) for $M \to \infty$ (zero force) and a lifetime t_x that increases as a power of M [6,12]. With respect to such QSSs,

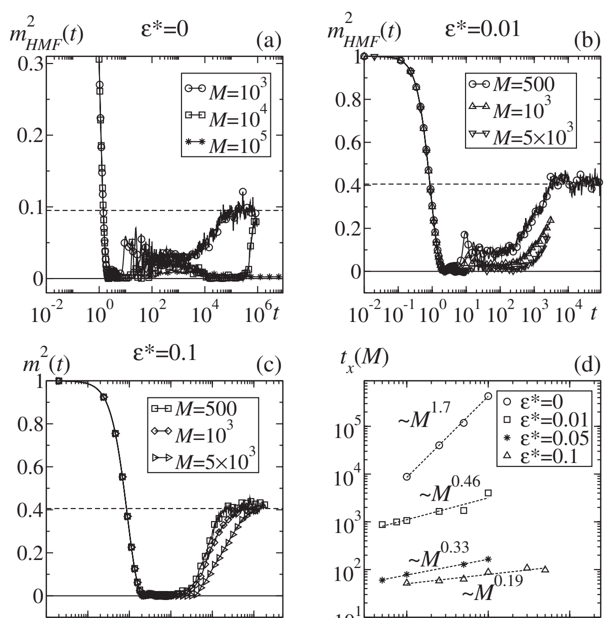

FIG. 3. (a) Microcanonical and (b),(c) canonical QSSs in terms of m^2_{HMF}. The curves have been obtained by averaging over a number I of initial conditions following the probability distributions described in the text. I varies from a maximum of 20 for small M down to 5 for big M. (d) Log-log plot of t_x as a function of the system size M. The QSS lifetime t_x has been defined as the time at which a phase function (T_{HMF} for $\epsilon^* = 0$ and e_{HMF} for $\epsilon^* \neq 0$) changes 10% of its stationary average value.

a crucial issue is to see whether they survive when the coupling between the HMF and the TB is switched on [11]. To address this point, we consider $\epsilon^* \neq 0$ but keep the nonequilibrium initial conditions described above. The TB temperature is first fixed at $T_0 = 0.38$. The time dependence of m^2_{HMF} [Figs. 3(b) and 3(c)] suggests that the QSSs indeed exist even in the canonical setup and independently of ϵ^* (if ϵ^* is small enough). Denoting by t_x the lifetime of the QSSs, we found that $t_x \sim M^\eta$, with η that tends to zero as ϵ^* increases and to the microcanonical estimate given in Ref. [12] as $\epsilon^* \to 0$ [Fig. 3(d)]. Preliminary evidences [15] suggest that t_x is also influenced by the "surface effect" parameter γ. We remark that during the QSS the long-range system does not thermalize with the TB. For example, a consistent change (10%) of T_0 does not alter T_{HMF} and even the subset of TB spins in direct contact with the HMF model remains at T_0 [13]. However, energy fluctuations are significantly larger than those due to the algorithm precision ($\Delta E_{\mathrm{HMF}}/E_{\mathrm{HMF}} \simeq 4 \times 10^{-2}$ for $M = 10^3$) [13]. This distinguishes the canonical QSSs from the microcanonical ones. During these QSSs, the HMF model is in a partial equilibrium state at a temperature (specific kinetic energy) which is not the one of the TB [13]. Perhaps this is one reason why a Nosé-Hoover dynamics with the same out-from-equilibrium initial conditions is not capable to reproduce the relaxation to equilibrium. In fact, we verified [15] that in such a case a Nosé-Hoover dynamics displays very strong fluctuations of the dynamical variables (e.g., E_{HMF}) that do not decay with time. Another important remark is that classical assumptions in mesoscopic stochastic equations seem to rule out the existence of such a canonical QSS. In fact, a stability analysis applied to a Fokker-Planck description of the HMF model in both ensembles (canonical and microcanonical) shows that anomalous velocity PDFs are (neutrally) stable only in the microcanonical ensemble [11].

The occurrence of canonical QSSs points towards an extension of the ensemble equivalence to some aspects of the nonequilibrium properties. We find, on the other hand, that there is a substantial microcanonical or canonical *inequivalence* in the relaxation to equilibrium process that follows the QSS. For example, the final equilibrium specific magnetization changes by a factor of 4 going from the microcanonical [Fig. 3(a)] to the canonical [Figs. 3(b) and 3(c)] simulations, independently of ϵ^*. A further indication of this inequivalence is given by the time evolution of the H function $H(t) \equiv -\int_{-\infty}^{+\infty} dl \int_0^{2\pi} d\theta\, p(l, \theta, t) \ln(p(l, \theta, t))$, in the two ensembles. Indeed, if during the microcanonical dynamics $H(t)$ on the average increases, reaching its maximum at equilibrium, in the $\epsilon \neq 0$ canonical ones it displays a maximum during the QSS and then *decreases* towards the $T_0 = 0.38$ equilibrium value (see Fig. 4). These unconventional behaviors with respect to the H theorem are consequences of the different relaxation dynamics in the two ensembles, i.e., fixed-energy and fixed-temperature [solid circles in Fig. 2(c)].

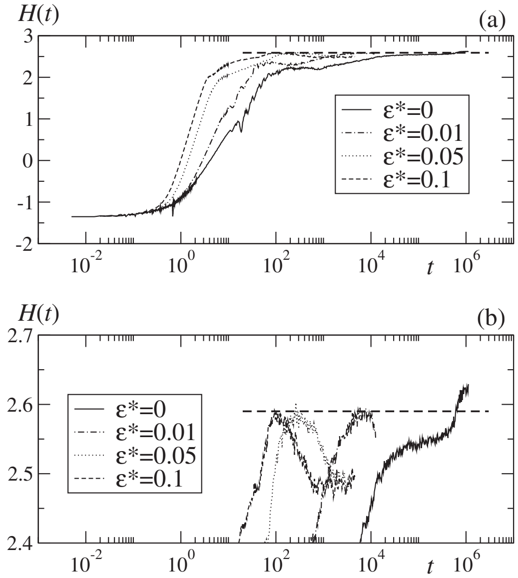

FIG. 4. Time dependence of the H function in the microcanonical ($\epsilon^* = 0$) and canonical ($\epsilon^* \neq 0$) ensembles for $M = 10^4$ and $T_0 = 0.38$. The dashed line indicates the common maximum of H for $\epsilon^* \neq 0$ reached during the QSS.

In summary, we introduced a Hamiltonian canonical setup for long-range interacting systems through a coupling with a short-range interacting TB. The coupling is described by a parameter that can be tuned continuously to provide a unified description of microcanonical and canonical ensembles. By applying our scheme to the HMF model, we verified its capability to reproduce the equilibrium BG statistics in both ensembles (ensemble equilibrium equivalence). The major feature of this setup is that it is based solely on microscopic Hamiltonian dynamics. This is a novelty with respect to previous approaches, which allows an unbiased dynamical description of the nonequilibrium properties of such system. As a result we found that, if the coupling with the TB is weak enough and we start from out-of-equilibrium initial conditions, the dynamics reveals the existence of quasistationary states in the canonical ensemble. These QSSs are reminiscent of the microcanonical ones [6,9,11,12] in the sense that, for example, their lifetime diverges with the system size M in a power law fashion. On the other hand, in the presence of the TB, the lifetime of the QSSs is influenced by the parameters controlling the interaction between a long-range system and a TB. This could be useful for an experimentalist who is willing to enhance or hinder the quasistationary behavior [5] and could also be of some importance in the understanding of the dynamical evolution of quasistationary structures, e.g., in galaxies [9] or in other long-range interacting systems. The presence of a canonical QSS extends the notion of ensemble equivalence from equilibrium to some nonequilibrium properties. A substantial microcanonical or canonical inequivalence is found in the relaxation to equilibrium process following the QSS, and it is clearly revealed by a dramatic change in the time dependence of the Boltzmann H function. Of course, a more detailed statistical description (and interpretation) of the canonical QSS is needed, and we are confident that our unbiased setup will be a useful tool for this achievement [13] not only with respect to the HMF model but also to other Hamiltonian long-range systems exhibiting either dynamical peculiar features [16] or equilibrium ensemble inequivalence [3].

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