Hamiltonian dynamics reveals the existence of quasi-stationary states for long-range systems in contact with a reservoir

Fulvio Baldovin and Enzo Orlandin

Dipartimento di Fisica and Sezione INFN, Università di Padova, Via Marzolo 8, I-35131 Padova, Italy

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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 quasi-stationary states persist in presence of the interaction with the environment. Our results indicate that quasi-stationary 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, Bose-Einstein condensates. In such systems, the inter-particle 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, like persistence of correlations and non-negligible interface energies. In particular, the Boltzmann transport equation picture for the approach to equilibrium is not valid and long-range interacting systems may even display inequivalences among different equilibrium statistical ensembles. Because of these subtleties a privileged investigation tool is the microscopic Hamiltonian dynamical simulation. Hamiltonian dynamics at fixed-energy (microcanonical ensemble) for a paradigmatic long-range Hamiltonian (see below) directly connected with experiments revealed the existence of long-lived quasi-stationary states (QSS) that finally cross over to Boltzmann-Gibbs (BG) equilibrium 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’ $H$-function.

In a magnetic context, the Hamiltonian Mean Field (HMF) model describes a set of $M$ globally coupled $XY$-spins with Hamiltonian

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

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 since its equilibrium properties are analytically solvable both in the microcanonical and in the canonical ensemble and it is representative of the class of Hamiltonians on a one-dimensional lattice in which the potential is proportional to $\sum_{i=1}^{M} \left[ 1 - \cos(\theta_i - \theta_j) \right] / r_{ij}^\alpha$, where $r_{ij}$ is the lattice separation between spins and $\alpha < 1$ (notice that the potential in Eq. (1) is recovered in the limit $\alpha \to 0$). Also, direct connections with the problem of disk galaxies and free electron lasers experiments have been established. Whereas it has been recently proven that $H$ does not present microcanonical/canonical inequivalence at equilibrium, its unusual dynamical features received recently a lot of attention. In fact, fixed-energy dynamical simulations starting with out-of-equilibrium initial conditions display the existence of longstanding (infinitesimal 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 quasi-stationary non-equilibrium average values. In this Letter we introduce a microscopic setup where the HMF model is in contact with a short-range thermal bath (TB) in such a way that the thermodynamic limit is achieved with a negligible interaction energy. Equilibrium dynamics confirms the microcanonical/canonical equivalence for the HMF.

*Electronic address: baldovin@pd.infn.it, orlandin@pd.infn.it
FIG. 1: Sketch of the interactions considered in our canonical setup. Dashed lines mimic the interactions between the HMF- (full circles) and the TB- (empty circles) spins. Full (dotted) lines represent the HMF (TB) couplings.

model. If the HMF-TB coupling is weak enough, the relaxation to equilibrium is still characterized by drastic slowing-downs (QSSs) where also the system energy fluctuate around quasi-stationary 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’ 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

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

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

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

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 initial condition and remains fixed during the dynamics. The total Hamiltonian \( H = H_{HMF} + H_{TB} + H_I \) defines then a microcanonical system (constant energy \( E \)), in which the energy of the HMF model can fluctuate. In our approach, the temperature is defined by (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 “surface-like effect” \( S \sim M^{\gamma-1} \) (with \( 0 < \gamma < 1 \)), we make sure that the interaction energy, \( E_I \sim M^\gamma \), satisfy \( E_{HMF} \sim M \) (\( E_{TB} \sim N \gg M \)), 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 \( \Delta E/E \approx 10^{-5} \).

Let \( e_{HMF} \equiv E_{HMF}/M = [k_{HMF} + (1 - m_{HMF}^2)]/2 \), where \( k_{HMF} \equiv \sum_{i=1}^{M} \varepsilon_i^2/2M \) and \( m_{HMF} \equiv \sum_{i=1}^{M} (\cos \theta_i, \sin \theta_i)/M \) are respectively the specific kinetic energy and the magnetization of the system. It is known that at \( e_{HMF} = 0.75 \) and temperature \( T_{HMF} = 0.5 \) (in natural dimensionless units) a continuous phase transition occurs separating a disordered (\( m_{HMF} = 0 \)) 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 PDF for the initial TB-velocities \( p_{TB}(l, 0) = \exp(-l^2/2T_0)/\sqrt{2\pi T_0} \) is a control parameter through which we set the TB temperature. In fact, after a transient relaxation \( (0 \leq t < t^* \sim 100) \) the TB reaches its own equilibrium at the target temperature \( T_0 \) (i.e. \( 2k_{TB}(t) \approx T_0 \forall t > t^* \)). At \( t = t^* \) we then switch on the HMF-TB coupling, \( H_I \), by setting \( \epsilon(t) = \epsilon^* \geq 0 \forall t \geq t^* \). 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 \( 10^2 \leq M \leq 10^4 \) and \( 0.005 \leq \epsilon^* \leq 0.1 \). In all cases, for \( t \gg t^* \), the system reaches the thermal equilibrium characterized by \( 2k_{HMF}(t) \approx T_0 \) (Fig. 2a) a velocity PDF \( p_{HMF}(l, t) \approx p_{TB}(l, 0) \) (Fig. 2b), and an equilibrium magnetization. The relaxation to equilibrium could last very long and typically occurs through a number of drastic slowing-downs during which the average value of \( T_{HMF} \) is constant or almost constant (plateaux in Fig. 2c).

FIG. 2: (a): Time evolution of the \( T_{HMF} \) and \( T_{TB} \) temperatures for \( M = 10^3, \epsilon = 0.01 \) and \( T_0 = 0.5 \). Initially, \( p_{HMF}(l, 0) = \exp((-l^2/2T_0))/\sqrt{2\pi T_0} \) with \( T(t^*) = 0.7 \). (b): Velocity PDF at \( t \gg t^* \). Solid line is \( p_{TB}(l, 0) \). (c): Caloric curve. Solid line is the BG equilibrium and dashed line is the prolongation of the ordered phase to subcritical energies. Empty symbols are the average value of \( e_{HMF}(t) \) at equilibrium. Stars refer to Nosé-Hoover simulations. Full circles correspond to the QSS studied in the paper and to the microcanonical and canonical equilibrium obtained as \( t \to \infty \).
Similar effects were found in [14] using a stochastic dynamics (see also [8] for a stochastic canonical version of the HMF, named 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 $\epsilon^*$ (if $\epsilon^*$ is small enough). Denoting by $t_x$ the life time of the QSSs we found that $t_x \sim M^\eta$, with $\eta$ that tends to zero as $\epsilon^*$ increases and to the microcanonical estimate given in [12] as $\epsilon^* \to 0$ (Fig. 3d). Preliminary evidences [13], suggest that $t_x$ is also influenced by the “surface effect” parameter $\gamma$. 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 ($\Delta E_{HMF}/E_{HMF} \approx 4 \times 10^{-2}$ for $M = 10^3$) [13]. This distinguishes the canonical QSSs from the microcanonical ones. During these QSSs, the HMF model are 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 [13] 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 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 (neutral) 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 non equilibrium properties. We find on the other hand that there is a substantial microcanonical/canonical inequivalence in the relaxation to equilibrium process that follows the QSS. For example, the final equilibrium specific magnetization changes by a factor 4 going from the microcanonical (Fig. 3c) to the canonical (Figs. 3a,b) simulations, independently of $\epsilon^*$. A further indication of this inequivalence is given by the time evolution of the H-function, $H(t) = -\int_\Omega p(l, \theta, t) \ln(p(l, \theta, t)) dl$, with $l \in [-L, L]$, $\eta = 2.03$ ($\epsilon_{HMF}(t^*) \approx 0.69$). 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, 8, 11, 12] (Fig. 3b). The initial $(t \lesssim t^* + 1)$ violent relaxation corresponds to a quick mixing of the spins in the single-particle $\mu$-space [6]. The QSS is then characterized by $m_{HMF}^2 \simeq 0$ ($T_{HMF} = 0.38$) for $M \to \infty$ (zero force) and a lifetime $t_x$ that increases as a power of $M$ [6, 11, 12]. With respect to such QSSs, 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 keeping the non-equilibrium initial conditions described above. The TB-temperature is first fixed at $T_0 = 0.38$. The time dependence of $m_{HMF}^2$ (Fig. 3c) suggests that the QSSs indeed exist even in the canonical setup and independently of $\epsilon^*$ (if $\epsilon^*$ is small enough).
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 quasi stationary states in the canonical ensemble. These QSSs are reminiscent of the microcanonical ones in the sense that, for example, their lifetime diverges with the system size $M$ in a power law fashion. On the other hand in presence of the TB, the life-time of the QSSs is influenced by the parameters controlling the interaction between long-range system and TB. This could be useful for an experimentalist who is willing to enhance or hinder the quasi-stationary behavior and could also be of some importance in the understanding of the dynamical evolution of quasi-stationary structures, e.g., in galaxies, or in other long-range interacting systems. The presence of canonical QSS extends the notion of ensemble equivalence from equilibrium to some non equilibrium properties. A substantial microcanonical/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 set up will be a useful tool for this achievement not only with respect to the HMF model, but also to other Hamiltonian long-range systems exhibiting either dynamical peculiar features or equilibrium ensemble inequivalence.

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