The role of energy in the dynamics of the HMF model

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Abstract. In this work we analyze the Hamiltonian Mean Field model, which consists of a set of $N$ interacting rotators that move around an unitary circle. This model presents a very complex dynamical behavior and, in particular, the canonical predictions do not necessarily coincide with the temporal averages obtained along numerical simulations. Recently, a topological explanation for the existence of these anomalies has been introduced. In this work we further analyze this hypothesis by considering the role of the energy of the system in the dynamics of the model.

The Hamiltonian Mean Field (HMF) model [1] can be considered a paradigmatic complex system. Despite its apparent extreme simplicity, its dynamical behavior has revealed a great amount of surprising outcomes, never expected before in a ferromagnetic infinite range model [2]. The system consists of $N$ rotators, each one moving on its own unitary circle. Mechanically, each rotator is completely described by the angle $\theta_i$ it forms with the $x$ axis and the corresponding generalized momentum $p_i$, and the system is ruled by the Hamiltonian

$$H = \frac{1}{2} \sum_{i=1}^{N} p_i^2 + \frac{1}{2N} \sum_{i,j=1}^{N} [1 - \cos (\theta_i - \theta_j)].$$

The first term represents the kinetic energy of the system and the second one the interacting potential energy. The second sum runs over all pairs of particles, indicating the infinite range character of these interactions. Note that, for fixed kinetic energy, this second term is minimized when all the particle rotate synchronously with the same angle.

This model is nothing but a kinetic version of the infinite range $XY$ ferromagnetic model. In that sense, one can associate to each rotator a planar local magnetization $\vec{m}_i = (\cos \theta_i, \sin \theta_i)$ and then define a global order parameter as, $\vec{M} = \frac{1}{N} \sum_{i=1}^{N} \vec{m}_i$. From a thermodynamical point of view, the free energy of the model can be very easily evaluated in the canonical ensemble [1] yielding a second order phase transition between a high temperature paramagnetic phase (characterized by $|\vec{M}| = 0$) and a low temperature ferromagnetic phase (whit $|\vec{M}| \neq 0$). The scenario is very different when considering its dynamical evolution. One can numerically integrate the Hamilton equations of motion, given by,

$$\dot{\theta}_i = \frac{\partial H}{\partial p_i} = p_i, \quad \dot{p}_i = -\frac{\partial H}{\partial \theta_i} = -\frac{1}{N} \sum_{j=1}^{N} \sin (\theta_i - \theta_j), \quad i = 1, \ldots, N.$$
and then compare the canonical predictions with temporal mean values of certain physical observables. Surprisingly, one finds that, depending on the initial preparation of the system, the expected equivalence fails to hold. This phenomenology has been observed for energies just below the critical transition, which occurs at $U_c/N = 3/4$ [1, 2]. Consider for instance the case of the temperature, which in true equilibrium must coincide with twice the kinetic energy per particle $T_k = 2k_BT/N$. Let us assume that the system is in thermal contact with a thermal bath at certain temperature $T$. The expected equivalence between the canonical results and those obtained through a microcanonical numerical integration is not always valid for the HMF model. When the simulations are performed with energies just below $U_c$ and start very far from equilibrium, the system can eventually get trapped into long standing out of equilibrium trajectories. A simple way of preparing the system far from equilibrium is by putting initially the system in a “water–bag” configuration, in which all the angles have the same value ($|\vec{M}| = 1$) while the momenta are chosen at random from an uniform distribution. Because $V/N = (1 - |\vec{M}|^2)/2$, the initial potential energy per particle is zero and the system has only kinetic energy $U = K$.

The time evolution of $T_k = 2 < K > /N$ shows an initial drastic cooling down, but instead of reaching the expected equilibrium value $T$, it attains a quasi-stationary value $T_{qs}(N) < T$ which depends on the system size $N$ in such a way that, if the system were infinitely large, it would get trapped into this quasi-stationary solutions forever [1, 2].

On the other hand, from a topological point of view, the potential energy per particle, $V/N$, foliates the configuration space of the system into the family $\{\Sigma_v\}_{\nu\in\mathbb{R}}$ of equipotential hypersurfaces, where $\Sigma_v = \{(\theta_1, \ldots, \theta_N) \in \mathbb{R}^N | V/N(\theta_1, \ldots, \theta_N) = v\}$ (with $0 \leq v \leq 1/2$). The configurational space is an $N$-dimensional torus parametrized by the $N$ angles. In the ordered phase the system is confined to move in half a torus, characterized by critical points that correspond to saddle nodes. At the critical value $v_c = 1/2$ a drastic topological change occurs and the systems can then visit the complete torus. This drastic change is precisely related to the second order phase transition the system suffers at $U_c/N = 3/4$. This approach, which has been vastly used in the context of critical phenomena to relate topological changes in configurational spaces with phase transitions in finite systems [3], is also connected to the anomalous dynamical behavior observed in the HMF model.

In [4, 5] it was showed that the complex nonequilibrium quasi-stationary regime observed just below the critical energy can also be understood in terms of the drastic topologic change observed at $v_c = 1/2$. In order to verify this hypothesis, the system was prepared in a water–bag initial configuration, with all the rotators aligned along the $x$ axis ($\theta_i = 0$ for all $i$), the momenta drawn from an uniform distribution (actually we used regularly spaced momenta) and energy per particle $U/N = 0.69$ (just below the transition point $U_c/N = 3/4$). Under these conditions, the system has initially zero potential energy and suddenly decreases its kinetic energy (temperature) as much as possible, settling at the flat top of its potential energy function ($v_c = 1/2$). Then, it starts to wander among different saddle nodes of the critical manifold $v_c = 1/2$, all of them characterized with only two negative directions and $N - 2$ marginal ones. To do this analysis, one has to evaluate at each time step of a numerical integration the modulus of the $N$ derivatives of $V/N$ and identify the maximum over $i = 1, \ldots, N$, through

$$\lambda = N \max_i \left| \frac{\partial(V/N)}{\partial \theta_i} \right|.$$  \hspace{1cm} (3)

Note that $\lambda = 0$ implies $\partial(V/N)/\partial \theta_i = 0$ for all the particles. In other words, each time $\lambda$ vanishes we can assert that the system passes over a critical point of $V/N$. These results confirmed that, in the quasi-stationary trajectories, the system is trapped in the critical submanifold $v_c = 1/2$. Moreover, the time $\Delta \tau$ elapsed between two successive critical points for fixed energy $U/N = 0.69$ has a power-law distribution, indicating a very complex pattern of wandering on the configurational space. A different scenario appears when the system is initially
prepared also in a water-bag configuration but with $U/N = 10.0$, in the disordered phase. Now one observes a periodic pattern of visits to the critical submanifold $v_c = 1/2$.

As mentioned above, in [4] only the cases $U/N = 0.69$ and $U/N = 10$ were considered. In this paper we extend the previous work [4] in order to analyze the role of the energy of the system. In particular, we consider here systems with different energies, ranging from $U/N = 0.60$ (in the ordered phase) to $U/N = 2.0$ (in the disordered phase) and follow the same protocol described in [4]. The initial momenta have been always chosen from an uniform random distribution and the angles were fixed along the $x$ axis. The numerical simulations were performed by using a fourth-order symplectic algorithm [6] in system of $N = 500$ rotators (we have verified that for larger sizes the behavior is the same). Along each simulation we evaluated $\lambda$ as a function of $t$ for a single sample.

In Fig. 1 we can clearly identify three different regimes. In the top plot we present the behavior of $\lambda(t)$ in the disordered phase, with energies per particle $U/N = 0.78, 1.0$ and $2.0$. We observe that the system periodically touches the critical submanifold $v_c = 1/2$ (each time $\lambda = 0$) and that the period $\Delta t$ decreases as $U/N$ increases. In the middle plot we describe the behavior observed just below the critical point. In the three cases analyzed, $U/N = 0.74, 0.71$ and $0.68$, the system wanders in the configurational space touching the critical submanifold. But, unlike the previous case, now the behavior of $\lambda$ has lost the periodicity. Instead we verify that the system has a complex pattern of wandering, as described in [4] for $U/N = 0.69$. In the bottom plot we present the behavior of $\lambda(t)$ also in the ordered phase but when the system is prepared with energies $U/N = 0.60, 0.63$ and $0.66$. Now, it is initially attracted to the critical submanifold $v_c = 1/2$ but after a few visits, it finally escapes. Once the system escapes, it will never again touch a critical point. At very low energies (which are not presented here) the system wanders always far away from the critical submanifold $v_c = 1/2$.

![Figure 1](image-url)

**Figure 1.** Time evolution of $\lambda$ for three different regimes and water–bag initial conditions: disordered phase (top), ordered phase with energies just below $U_c/N$ (middle) and ordered phase with intermediate energy values (bottom).

As described in the previous figure, in the high energy phase the system presents a regular pattern of wandering on the configurational space, touching the critical submanifold $v_c = 1/2$.
in a periodic manner. In Fig. 2 we present, in a log-log plot, a study on the dependency of the period $\Delta t$ on the energy of the system. We verify that, for large values of $U/N$, the period decays as a power law $\Delta t \propto t^{-\alpha}$, with $\alpha \approx 0.60$, indicating that the periodic behavior will always exist, independently of the energy of the system.

![Figure 2](image_url)

**Figure 2.** The period $\Delta t$ between two successive visits to the critical sub-manifold $v_c = 1/2$ as a function of $U/N$ in a log-log plot. The solid line corresponds to a power-law fitting of the last eight points.

Concluding, in this work we have extended the results presented in [4] by analyzing the role of the energy of the HMF in the behavior of $\lambda(t)$. Taking into account that each time the system touches the critical submanifold the parameter $\lambda$ equals zero (indicating that the system passes over a saddle node of the potential energy function per particle) we were able to identify four different regimes. First, in the high energy disordered phase, the system visits periodically the submanifold $v_c = 1/2$ and the period decreases as a power-law as $U/N$ increases. In the ordered phase we found three different behaviors. Just below the critical point $U_c/N$ the system visits the manifold $v_c = 1/2$ in a very irregular way. For intermediate values of $U/N$ the system is initially attracted by the critical sub-manifold but finally escapes. In the low energy regime the system wanders in the configurational space without visiting the critical submanifold.

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