Glassy phase in the Hamiltonian mean-field model

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We study the relaxation dynamics of a Hamiltonian system of N fully coupled XY spins. The thermodynamics of the system predicts a ferromagnetic and a paramagnetic phase. Starting from out-of-equilibrium initial conditions, the dynamics at constant energy drives the system into quasistationary states (QSSs) characterized by dynamical frustration. We introduce the spin polarization as an order parameter which allows us to interpret the dynamically generated QSS regime as a glassy phase of the model.

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The Hamiltonian mean-field (HMF) model, originally introduced in Ref. [1], has been intensively studied in the last years for its extreme richness and flexibility in exploring the connections between dynamics and thermodynamics in long-range many-body systems. In fact, on the one hand the model has an exact equilibrium solution; on the other hand, because of the presence of a kinetic energy term in the Hamiltonian, the dynamics can be studied by means of molecular dynamics simulations [1–4]. From these investigations, many interesting features have emerged which are common to other systems with long-range interactions [5–7]. One of the most intriguing characteristics of the dynamics is the existence of quasistationary states (QSS's)—i.e., dynamically created states—whose lifetime diverges with the system size N [8]. In such states anomalous diffusion [3], non-Gaussian velocity distributions [8], vanishing Lyapunov exponents [8], and ergodicity breaking and slow-decaying correlations [9,10] have been observed. These features have suggested a possible application of Tsallis generalized thermodynamics [8,11–14].

In this paper we show that the HMF model in the QSS regime behaves similarly to a glassy system. In fact, by means of an order parameter, it is possible to characterize the dynamically generated QSS's as a thermodynamics glassy phase of the model, despite the fact that neither disorder nor frustration are *a priori* present in the interaction. The main idea of the paper originated from the observation of slow relaxation and aging [9,10] in the QSS regime. Such a behavior is typical of frustrated systems, whose prototype are spin glasses [15]: in these systems, the impossibility to minimize simultaneously the interaction energies of all the couples of spins leads the system to a very complex energetic landscape. One might imagine it as consisting of large valleys separated by high activation energies. Each valley contains many local minima—i.e., metastable states—in which the system, after quenching in its low-temperature phase, can remain trapped for a very long time, showing those strong memory effects better known as aging behavior.

The HMF model describes a system of N fully coupled classical XY spins [1]:

$$\vec{s}_i = (\cos\ \theta_i, \sin\ \theta_i) \quad i = 1, \ldots, N. \tag{1}$$

The equations of motion derive from the Hamiltonian

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

where θ_i $(0 < \theta_i \leqslant 2\pi)$ is the angle and p_i the respective conjugate variable representing the rotational velocity (the mass is set equal to 1) of spin i. If we associate a particle, moving on the unit circle, to each spin, the model can be seen as a system of fully coupled *rotators*. Though the division of the potential by a factor N (the so-called Kac's prescription) makes the Hamiltonian formally extensive [4], the latter remains nonadditive due to the long-range nature of the interaction [12].

The equilibrium solution of the model in the canonical ensemble predicts a second-order phase transition from a high-temperature paramagnetic (PA) phase to a low-temperature ferromagnetic (FE) one [1]. The critical temperature is $T_c = 0.5$ and corresponds to a critical energy per particle $U_c = E_c/N = 0.75$. The order parameter of this phase transition is the modulus of the *average magnetization* per spin defined as $M = (1/N)|\Sigma_{i=1}^{N} \vec{s}_i|$. Above T_c, in the PA phase, the spins point in different directions and $M \sim 0$. Below T_c, in the FE phase, all the spins are aligned (the rotators are trapped in a single cluster) and $M \neq 0$.

The molecular dynamics simulations at constant energy (microcanonical ensemble) reveals interesting properties in the energy range $U = 0.5 - 0.75$. In fact, starting from out-of-equilibrium initial conditions [16], the system has an extremely slow relaxation to the equilibrium and shows the presence of metaequilibrium *quasistationary states* with the following properties.

(1) The temperature (calculated from the average kinetic energy) and the magnetization assume constant values for a time τ_{QSS}. Such values are different from the equilibrium ones and depend on the number of spins N.

(2) For large N, M vanishes (as $N^{-1/6}$) and T tends to an energy-dependent value so that the QSS's lie on the extension for $T < T_c$ of the high-temperature branch of the caloric curve.

(3) τ_{QSS} grows linearly with the system size N [2]. For this reason the QSS regime can be interpreted as the true equilibrium if the thermodynamic limit is taken before the infinite-time limit [8].

(4) The QSS's are characterized by non-Gaussian veloc-

ity distributions [8], Lévy walks, and anomalous diffusion [3].

(5) The largest Lyapunov exponent vanishes and the system resides in a restricted part of the *a priori* accessible phase space. Such a *weak-mixing* dynamics suggests a connection with the Tsallis generalized thermodynamics [8], but also the possibility of framing the QSS's within the so-called *weak-ergodicity-breaking* scenario [17], typical of glassy systems.

The last point has been recently corroborated by the discovery of aging in the QSS regime [9,10]. In the following we show how the analogy with glassy systems and the weak-ergodicity-breaking scenario can be made more stringent [18] by the introduction of an order parameter inspired by the microscopic dynamics of spin-glass models.

The materials that originally were called *spin glasses* are alloys formed by a noble metal support (gold, silver, copper) containing randomly distributed magnetic impurities (iron or manganese). Such a configuration determines a random distribution ("quenched disorder") of the interactions: according to the distance between each pair of spins, the interaction among them may be either ferromagnetic or antiferromagnetic, thus generating frustration. The first theoretical spin-glass model was the short-range *Edwards-Anderson* (EA) model [19]. However, the first solvable one was the *Sherrington-Kirkpatrick* (SK) model [20], where the spins are coupled by infinite-ranged interactions independently distributed according to a Gaussian. Depending on the temperature and the parameters of the Gaussian distribution, the SK model shows three different phases: namely, ferromagnetic, paramagnetic, and spin glass (SG). Since the magnetization M vanishes in the SG phase as well as in the PA one, an additional order parameter q_{EA}—called the *EA order parameter*—was proposed [19,20] in order to discriminate between spin-glass disorder and paramagnetism. The physical meaning of this order parameter is that of one quantifying the degree of freezing in the SG phase. In fact, the three phases are characterized by a different microscopic behavior. In order to get an intuitive picture of this behavior, let us imagine taking some snapshots of the spin configuration in each of the three phases [21]. If a snapshot is taken at one particular time, one easily would be able to recognize the FE phase, since all the spins are aligned and frozen in their equilibrium position. However, it would be impossible to distinguish between the PA and SG phases. In fact, in both of these phases the orientations of spins are random, due to the high thermal noise for the PA phase and to the quenched spatial disorder for the SG phase. Discrimination between these two phases is possible only if one takes a temporal sequence of snapshots. In fact, in the PA phase the orientation of each spin at successive instants of time would be random, so the sequence of snapshots shows every time a different spatial configuration. On the other hand, in the SG phase all the snapshots are identical, since each spin is frozen and retains the same orientation over very long periods of time.

As previously discussed, the HMF model at equilibrium has only two phases—PA and FE. The main goal of this paper is to show that the dynamically generated QSS's can be interpreted as a glassy phase of the model. For this reason, inspired by the arguments described above, we propose to introduce an order parameter, the *average polarization* p, in order to measure the extent of freezing of the system. The physical meaning of p is related to the elementary polarizations $\vec{p}_i$—i.e., the time averages of the successive positions of each elementary spin vector—defined as

$$\vec{p}_i = \langle \vec{s}_i(t) \rangle = \frac{1}{\tau} \int_0^\tau \vec{s}_i(t) dt, \quad i = 1, \ldots, N. \tag{3}$$

The average polarization is then obtained averaging the modulus of the elementary polarization over all the rotators:

$$p = \frac{1}{N} \sum_{i=1}^{N} |\vec{p}_i|. \tag{4}$$

Such an order parameter has to be compared to M, the modulus of the *average magnetization*, calculated as

$$M = \langle M(t) \rangle = \frac{1}{\tau} \int_0^\tau M(t) dt, \quad M(t) = \frac{1}{N} \left| \sum_{i=1}^{N} \vec{s}_i(t) \right|. \tag{5}$$

In the FE phase each elementary polarization vector coincides with the correspondent spin vector, both being frozen and parallel; then, the average polarization p keeps a nonzero value equal to M. In the PA phase the orientation of each spin vector at every time is completely random, so this continuous motion yields a zero value both for M and p. On the other hand, if the QSS's correspond to a glassylike phase of the model, we expect to find a zero value for M, as in the PA phase, and a nonzero value for p, as in the FE one. All these features are summarized in Table I.

TABLE I. Values of M and p in the three phases of the HMF model.

	M	p
Ferromagnetic phase FE	$\neq 0$	$\neq 0$
Paramagnetic phase PA	0	0
Glassy phase	0	$\neq 0$

In Fig. 1 we show the modulus of the elementary polarization for each spin i. We consider a system of $N=1000$ spins and different energy densities. The values of the average polarization p and the average magnetization M are also reported in the figure. In the simulation we have performed, the time averages of p and M are evaluated over an opportune time interval $\tau < \tau_{\mathrm{QSS}}$, in order to stay inside the temperature plateau for those energy values where the QSS regime appears ($U=0.5$ and $U=0.69$). In particular, we have used $\tau=2000$ and a transient of 1000 time units. The results do not depend significatively on τ. As usual in molecular dynamics simulations, in order to make our results independent of the specific dynamical realization, we have also taken averages over a set of different realizations (events) of the same out-of-equilibrium initial conditions. As expected, the two parameters p and M coincide and are close to 1 at low energy—e.g., $U=0.1$—while both of them tend to zero for U above the critical value $U_c=0.75$. The situation is different

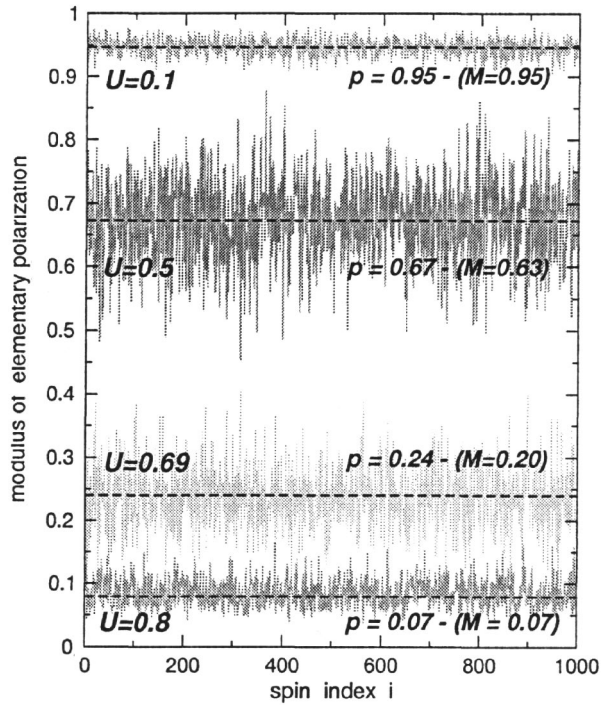

FIG. 1. The modulus of the elementary polarization $|\vec{p}_i| = |\langle \vec{s}_i(t) \rangle|$ for a system with $N=1000$ and different energies. The values of the average polarization p (dashed lines) and magnetization are also reported for comparison. Notes that only for $U=0.5$ and $U=0.69$ are we in the QSS regime. In the other cases, the system is at equilibrium.

for $U=0.5$ and for $U=0.69$, two energies at which the QSS's appear. In these cases the values of p and M are different: for $N=1000$, we have, respectively, $p=0.67$, $M=0.63$ and $p=0.24$, $M=0.20$. We have checked that the difference between p and M increases with the system size N. In particular, for large N, in the QSS regime, we expect a vanishing average magnetization M and an average polarization p different from zero.

In Fig. 2 we study the behavior of p and M with the size of the system. We report only the case $U=0.69$ where the anomalous effects of QSS's are more evident. As expected, while M vanishes as $N^{-1/6}$, p is independent of N (within the error) and equal to 0.24 ± 0.02.

Finally, in Fig. 3 we consider a system with $N=10\,000$ and we compare magnetization M and polarization p at equilibrium for different energies. In order to let the system reach equilibrium for the energy range $0.5 \leqslant U \leqslant U_c$ we ran the simulations for a time much larger than τ_{QSS}. In this way every trace of metastability, and consequently also of the glassy phase behavior, disappears. The numerical values of M and p reported in the figure coincide, in agreement with the previous statement about the equivalence between M and p in the pure FE and PA phases.

Our numerical results support the interpretation of the QSS regime as a dynamically created glassy phase of the HMF model. In the QSS regime the simulations show the formation of a dynamical clustering [10]. The rotators feel the attraction of the dynamically generated clusters in competition within each other. Each rotator remains trapped in a cluster for a while and then eventually succeeds in escaping from it [22]. This is also the cause of the anomalous diffusion and Lévy walks observed in Ref. [3]. Such a competition between the different clusters in the QSS regime therefore realizes a *dynamical frustration* that slows down the dynamics and prevents the system from exploring all potentially available phase space. Such a behavior is also related to the aging phenomenon observed in Refs. [9,10] and can be interpreted in the framework of the weak-ergodicity-breaking scenario [17]. When at the end of the QSS regime the system relaxes to the equilibrium of the pure FE phase, all the rotators concentrate in a single cluster which rotates with the same phase of the average magnetization vector—i.e., $\phi = \tan^{-1}(M_y/M_x)$ [23]—and all the anomalies disappear.

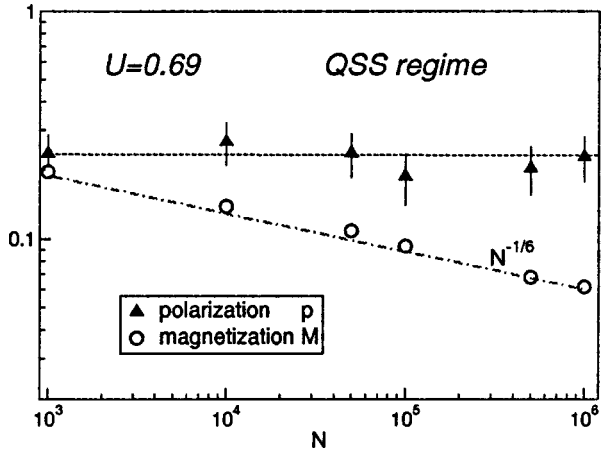

FIG. 2. We plot the values of the polarization p and the magnetization M calculated in the QSS regime for $U=0.69$ as a function of the size N of the system. While p assumes a constant value $\sim 0.24 \pm 0.02$, M decreases as $N^{-1/6}$.

In conclusion, the results of this paper show that the most remarkable features of the long-range HMF model—namely, the dynamically generated metastable states—can be interpreted as a thermodynamical glassy phase of the model. If

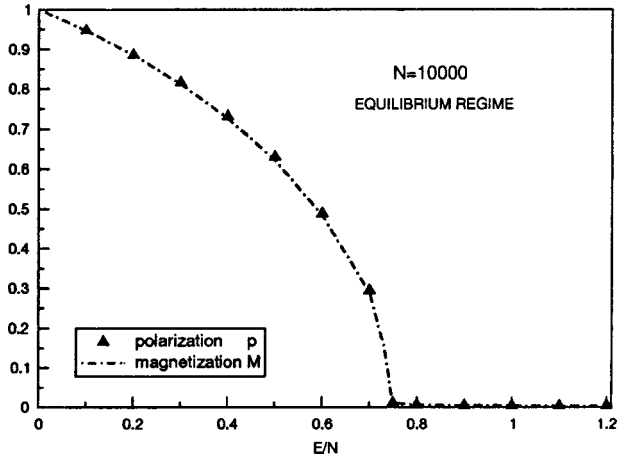

FIG. 3. For $N=10\,000$, we show the polarization p and magnetization M vs energy per particle U once the equilibrium regime has been reached.

the system is started sufficiently far from equilibrium, the long-range character of the interaction produces dynamically a very complex configurational landscape typical of glassy systems. We have introduced the polarization p as an order parameter to characterize the degree of freezing of the spins due to the presence of the dynamical competition among clusters in the metastable state. Considering that the HMF model is paradigmatic of a large class of long-range Hamiltonian systems, it seems very interesting to search for further connections with glassy dynamics, which likely could help understanding some of the open problems in this field.

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[22] Although the system has a long-range interaction, one can define clusters by considering rotators close in angle which move with almost the same velocity [3,10].
[23] In order to compute the elementary polarization of the spins, one should consider that also in the QSS regime the system is always moving with a global resulting motion that can be expressed by the phase of the average magnetization M. Then we have to subtract this phase from the spin angles. We implicitly assume this subtraction in all the simulations of the paper.