Metastability and anomalous behavior in the HMF Model: connections to nonextensive thermodynamics and glassy dynamics

Alessandro Pluchino, Andrea Rapisarda, Vito Latora

Dipartimento di Fisica e Astronomia, Università di Catania, and INFN sezione di Catania, Via S. Sofia 64, I-95123 Catania, Italy

Abstract

We review some of the most recent results on the dynamics of the Hamiltonian Mean Field (HMF) model, a systems of N planar spins with ferromagnetic infinite-range interactions. We show, in particular, how some of the dynamical anomalies of the model can be interpreted and characterized in terms of the weak-ergodicity breaking proposed in frameworks of glassy systems. We also discuss the connections with the nonextensive thermodynamics proposed by Tsallis.

Key words: Hamiltonian dynamics; Long-range interactions; power-law correlations; anomalous diffusion.

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1 Introduction

Metastability, nonextensivity and glassy dynamics are features so ubiquitous in complex systems that are often used to characterize them or, more in general, to define complexity [1]. In this work we will discuss such features in the context of the so called Hamiltonian Mean Field (HMF) model, a system of inertial spins with long-range interaction. The model, originally introduced by Antoni and Ruffo [2], has been thoroughly investigated and generalized in the last years for its anomalous dynamical behavior [3,4,5,6,7,8,9,10,11,12,13]. With respect to systems with short-range interactions, the dynamics and the thermodynamics of many-body systems of particles interacting with long-range forces, as the HMF, are particularly rich and interesting. In fact, more and more frequently nowadays, the out-of-equilibrium dynamics of systems with long-range interactions or long-term correlations has shown physical situations which can be badly described within the ergodic assumption that is
at the basis of the Boltzmann-Gibbs thermostatistics. In all such cases it happens, for instance, that a system of particles kept at constant total energy $E$, does not not visit all the a-priori available phase space (the surface of constant energy $E$), but it seems to remain trapped in a restricted portion of that space, giving rise to anomalous distributions that differs from those expected. A few years ago, Tsallis has introduced a generalized thermodynamics formalism based on a nonextensive definition of entropy [14]. This nonextensive thermodynamics is very useful in describing all those situations characterized by long-range correlations or fractal structures in phase space [6,15,16]. On the other hand, the latter feature is also connected with the so called ”weak ergodicity breaking” scenario, which is at the basis of the long-term relaxation and aging observed in glassy systems. Such systems show competing interactions (frustration) and are characterized by a complex landscape and a hierarchical topology in some high dimensional configuration space [17], which, in turn, generates a strong increase of relaxation times together with metastable states and weak chaos.

The Hamiltonian Mean Field model, considered in this paper, is exactly solvable at equilibrium and exhibits a series of anomalies in the dynamics, as the presence of quasistationary states (QSS) characterized by: anomalous diffusion, vanishing Lyapunov exponents, non-gaussian velocity distributions, aging and fractal-like phase space structure. Furthermore, the model is easily accessible by means of both molecular dynamics and Monte Carlo simulations. Thus, it represents a very useful “laboratory” for exploring metastability and glassy dynamics in systems with long-range interactions. The model can be considered as a minimal and pedagogical model for a large class of complex systems, among which one can surely include self-gravitating systems [13] and glassy systems [10], but also systems apparently belonging to different fields as biology or sociology. In fact, we recently found similar features also in the context of the Kuramoto Model [19], one of the simplest models for synchronization in biological systems [20]. Moreover, the proliferation of metastable states in the vicinity of a critical point in the phase diagram seems to be responsible for the onset of complexity and diverging time calculation in many different kind of algorithms [18].

In this paper we focus on two different aspects of the HMF model: its glassy-dynamics and the possible connections with the generalized thermodynamics. The paper is divided into two parts. In Section 2.1 we investigate the model following the analogy with glassy systems and the ‘weak ergodicity breaking’ scenario. In previous works we have shown that the “thermal explosion”, characteristic of initial conditions with finite magnetization, drives the system into a metastable glassy-like regime which exhibits ‘dynamical frustration’. With the aim to characterize in a quantitative way this behavior, we have explicitly suggested to introduce a new order parameter, the ‘polarization’, able to measure the degree of freezing of the rotators (or particles). Here we present new numerical results reinforcing the glassy nature of the QSS’s metastability and the hierarchical organization of phase space. In Section 2.2 we investigate
the links with nonextensive thermostatistics. In ref. [11] we have found that, for a particular class of initial conditions with constant velocity distribution and finite magnetization, the velocity correlations obtained by integrating the equations of motion of the HMF model are well reproduced by q-exponential curves. Here, we show numerical evidences that the superdiffusion observed in the anomalous QSS regime (ref. [5]) can be linked with the q-exponential long-term decay of the velocity correlations, as analytically suggested by a formula obtained by Tsallis and Bukman [21] for a nonlinear Fokker-Planck (FP) equation, using an ansatz based on the generalized entropy.

2 Anomalous dynamics in the HMF model

The HMF model has been introduced originally in ref. [2] with the aim of studying clustering phenomena in N-body systems in one dimension. The Hamiltonian of the ferromagnetic HMF model is:

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

where the potential energy is rescaled by 1/N in order to get a finite specific energy in the thermodynamic limit \( N \to \infty \). This model can be seen as classical XY-spins (inertial rotators) with unitary masses and infinite range coupling, but it also represents particles moving on the unit circle. In the latter interpretation the coordinate \( \theta_i \) of particle \( i \) is its position on the circle and \( p_i \) its conjugate momentum (or velocity). Associating to each particle the spin vector

\[ \vec{s}_i = (\cos \theta_i, \sin \theta_i) , \]

it is possible to introduce the following mean-field order parameter:

\[ M = \frac{1}{N} |\sum_{i=1}^{N} \vec{s}_i| , \]

representing the modulus of the total magnetization.

The equilibrium thermodynamical solution in the canonical ensemble predicts a second-order phase transition from a low-energy condensed (ferromagnetic) phase with magnetization \( M \neq 0 \), to a high-energy one (paramagnetic), where the spins are homogeneously oriented on the unit circle and \( M = 0 \). The caloric curve, i.e. the dependence of the energy density \( U = H/N \) on the temperature \( T \), is given by \( U = \frac{T}{2} + \frac{1}{2} (1 - M^2) \) [2,5]. The critical point is at energy density
\( U_c = \frac{3}{4} \), corresponding to a critical temperature \( T_c = \frac{1}{2} \).

At variance with the equilibrium scenario, the out-of-equilibrium dynamics shows, just below the phase transition, several anomalies before complete equilibration. More precisely, if we adopt the so-called \( M1 \) initial conditions (i.c.), i.e. \( \theta_i = 0 \) for all \( i \) \( (M(0) = 1) \) and velocities uniformly distributed (water bag), the results of the simulations, in a special region of energy values (in particular for \( 0.68 < U < U_c \)) show a disagreement with the canonical prediction for a transient regime whose length depends on the system size \( N \). In such a regime, the system remains trapped in metastable states (QSS) with vanishing magnetization at a temperature lower then the canonical equilibrium one, until it slowly relaxes towards Boltzmann-Gibbs (BG) equilibrium, showing strong memory effects, correlations and aging. This transient QSS regime becomes stable if one takes the infinite size limit before the infinite time limit.

### 2.1 Dynamical frustration and hierarchical structure

As required by the discovery of correlations and aging, which in turn imply complex trajectories of the system in phase space, it is interesting to explore directly the microscopic evolution of the QSS. This can be easily done plotting the time evolution of the Boltzmann \( \mu \)-space, where each particle of the system is represented by a point in a plane characterized by the conjugate variables \( \theta_i \) and \( p_i \), respectively the angular position and the velocity of the \( i \)th particle.

It has been shown\[8\] that, during the QSS regime, correlations, structures and clusters formation in the \( \mu \)-space appear for the \( M1 \) i.c., but not for initial conditions with zero magnetization, the so called \( M0 \) i.c.: in the latter case both the angles and velocities distributions remain homogeneous from the beginning and a very slow mixing of the rotators has been observed. For the \( M1 \) case, the dynamics in \( \mu \)-space can be clarified through the concept of ”dynamical frustration”: the clusters appearing and disappearing on the unit circle compete one with each other in trapping more and more particles, thus generating a dynamically frustrated situation that put the system in a glassy-like regime.

In Fig.2.1 we show a molecular dynamics simulation where the complete distribution function \( f(\theta, p, t) \) is considered for different values of time. In fact, we plot - for \( M1 \) i.c., \( N=10000 \) and \( U=0.69 \) - a sequence of snapshots of \( f(\theta, p, t) \) for six different times: at the beginning of the simulation \( (t=0) \), in the QSS regime \( (t=50-500) \) and towards canonical equilibrium \( (t=10000) \). In the QSS region one clearly observes the presence of competing clusters, each cluster being composed by particles with both angles and velocity included in the same \( \mu \)-space cell (notice that, in our simulations, we considered a total of 100x100 cells for the \( \mu \)-space lattice). For \( t=10000 \), instead, any trace of macroscopic glassy behavior has disappeared.

In Fig.2 we show the power law behavior of the cluster size cumulative dis-
Fig. 1. Snapshots of $f(\theta, p, t)$ for $t=0$ (upper left), 50 (upper right), 100 (center left), 200 (center right), 500 (lower left) and 1000000 (lower right). In this case we considered $N=10000$ at $U=0.69$ and M1 i.c.. See text.

distributions calculated in the case $U = 0.69$ for several snapshots in the QSS regime at time $t=200, 350$ and 500. For each one of the 100x100 cells a sum over 20 different realizations (events) has been performed. Then, for each cluster size (greater than 5 particles) the sum of all the clusters with that size has been calculated and plotted. As one can see from 2, the distribution does not change significantly in the plateaux region as expected. We report also a power law fit (drawn as a straight dashed line above the data points) which indicates that the cluster distribution has an approximately exponent decay $-1.6$. The cluster size distribution reminds closely that of percolation at the
critical point, where a length scale, or time scale, diverges leaving the system in a self-similar state [22]. More in general, it has been also suggested [23] that, optimizing Tsallis’ entropy with natural constraints in a regime of long-range correlations, it is possible to derive a power-law hierarchical cluster size distribution which can be considered as paradigmatic of physical systems where multiscale interactions and geometric (fractal) properties play a key role in the relaxation behavior of the system. Therefore, we can say that the power-law scaling resulting in the distributions of Fig. 2 strongly suggests a non-ergodic topology of a region of phase space in which the system remains trapped during the QSS regime (for the M1 i.c.), thus supporting the weak-ergodicity breaking scenario. A weak breakdown of ergodicity, as originally proposed by Bouchaud for glassy systems [24], occurs when the phase-space is a-priori not broken into mutually inaccessible regions in which local equilibrium may be achieved, as in the true ergodicity-breaking case, but nevertheless the system can remain trapped for very long times in some regions of the complex energy landscape. In fact it is widely accepted that the energy landscape of a finite disordered (or frustrated) system is extremely rough, with many local minima corresponding to metastable configurations. Since the energy landscape is rough, these local minima are surrounded by rather high energy barriers and we thus expect that these states would act as "traps" which get hold of the system during a certain time $\tau$.

In ref. [24] such a mechanism has been proposed in order to explain the aging phenomenon, i.e. the dependence of the relaxation time on the history of the system, i.e. on its age $t_w$. Actually, it results that $\tau_{\text{max}} \approx t_w$, being $\tau_{\text{max}}$ the longest trapping time actually encountered during a waiting time $t_w$. In other
words, the deepest state encountered traps the system during a time which is comparable to the overall waiting time, a result that - in turn - allows to quantitatively describe the relaxation laws observed in glassy systems [17]. Aging phenomenon has been found also in the HMF model for $M1$ i.c., more precisely in the autocorrelation functions decay for both the angles and velocities [9] and for velocities only [8], thus reinforcing the hypothesis that a weak ergodicity-breaking could really occur in the metastable QSS regime and could be related to the complex dynamics generated by the vanishing of the largest Lyapunov exponent and by the dynamical frustration due to the many different small clusters observed in this regime. Such a scenario is in agreement also with the results about anomalous diffusion shown in ref.[4], where the probability distribution of the trapping times, calculated for a test particle in the transient QSS regime for $M1$ i.c., shows a clear power law decay

$$P_{\text{trap}} \sim t^{-\nu} ,$$

characterized by an exponent $\nu$ related to the anomalous diffusion coefficient. In the next section we will show that the anomalous diffusion coefficient can in turn be connected with the velocity correlations decay by means of the nonextensive formalism, thus suggesting a deeper link between the latter and the weak ergodicity breaking.

2.2 Nonextensive thermodynamics and HMF model

In previous works it was shown that the majority of the dynamical anomalies of the QSS regime, among which $\mu$-space correlations, clusters and dynamical frustration, are present not only for $M1$ initial conditions, but also when the initial magnetization $M(t = 0)$ is in the range $(0, 1)$ [11]. In order to prepare the initial magnetization in the range $0 < M \leq 1$, we distribute uniformly the particles into a variable portion of the unitary circle. In this way we fix the initial potential energy $V(\theta)$ and, in turn, the magnetization. Finally, we assign the remaining part of the total energy as kinetic energy by using a water bag uniform distribution for the velocities. The velocity correlations can be calculated by using the following autocorrelation function[11]

$$C(t) = \frac{1}{N} \sum_{j=1}^{N} p_j(t)p_j(0) ,$$

where $p_j(t)$ is the velocity of the $j$-th particle at the time $t$. In Fig.2.2-left, we plot the velocity autocorrelation function (4) for $N = 1000$ and $M(0) = 1, 0.8, 0.6, 0.4, 0.2, 0$. An ensemble average over 500 different realizations was
performed. For $M(0) \geq 0.4$ the correlation functions are very similar, while 
the decay is faster for $M(0) = 0.2$ and even more for $M(0) = 0$. If we fit these 
relaxation functions by means of the Tsallis’ $q$-exponential function

$$e_q(z) = [1 + (1 - q)z]^\frac{1}{1-q},$$  \hspace{1cm} (5)$$

with $z = -p_\tau$, and where $\tau$ is a characteristic time, we can quantitatively 
discriminate between the different initial conditions. In fact we get a $q$-exponential 
with $q = 1.5$ for $M(0) \geq 0.4$, while we get $q = 1.2$ and $q = 1.1$ for $M(0) = 0.2$ 
and for $M(0) = 0$ respectively. Notice that for $q = 1$ one recovers the usual ex-
ponential decay [15,5,6,8]. Thus for $M(0) > 0$ correlations exhibit a long-range 
nature and a slow power-law decay. This decay is very similar for $M(0) \geq 0.4$, 
but diminishes progressively below $M(0) = 0.4$ to become almost exponential 
for $M(0) = 0$.

In order to study diffusion, one can consider the mean square displacement of 
phases $\sigma^2(t)$ defined as

$$\sigma^2(t) = \frac{1}{N} \sum_{j=1}^{N} [\theta_j(t) - \theta_j(0)]^2 = \langle [\theta_j(t) - \theta_j(0)]^2 \rangle.$$ \hspace{1cm} (6)$$

where the symbol $\langle ... \rangle$ represents the average over all the $N$ rotators. 
The quantity $\sigma^2(t)$ typically scales as $\sigma^2(t) \sim t^\gamma$. The diffusion is normal 
when $\gamma = 1$ (corresponding to the Einstein’s law for Brownian motion) and 
ballistic for $\gamma = 2$ (corresponding to free particles). For different values of $\gamma$ the 
diffusion is anomalous, in particular for $1 < \gamma < 2$ one has superdiffusion. We
Fig. 4. In this figure we check the correctness of the $\gamma - q$ conjecture (see text) for the HMF model by plotting $\gamma$ as a function of the ratio $2/(3-q)$ for different initial conditions with variable magnetization. See text.

notice that the quantity $\sigma^2(t)$ can be rewritten by using the velocity correlation function $C(t)$ as

$$\sigma^2(t) = \int_0^t dt_1 \int_0^t dt_2 < p_j(t_2) p_j(t_1) > = 2 \int_0^t dt_1 \int_0^{t_1} dt_2 C(t_2),$$

(7)

where $C(t)$ is defined as in Eq.4.

Superdiffusion has been already observed in the HMF model for M1 initial conditions[4]. Recently we have also checked that, even decreasing the initial magnetization, the system continues to show superdiffusion [11]. We illustrate this behavior in Fig.2.2-right, where one sees that, after an initial ballistic regime ($\gamma = 2$) proper of the initial fast relaxation, the system shows superdiffusion in correspondence of the QSS plateau region and afterwards. The exponent goes progressively from $\gamma = 1.4 - 1.5$ for $0.4 < M(0) < 1$ to $\gamma = 1.2$ for M0. In the latter case, we have checked that, by increasing the size of the system, diffusion tends to be normal ($\gamma \sim 1$ for $N=10000$). The slow decay and the superdiffusive behavior illustrated in Fig.2.2 can be connected by means of a conjecture based on a theoretical result found in ref.[21] by Tsallis and Bukman. In fact in that paper the authors show, on general grounds, that non-extensive thermostatistics constitutes a theoretical framework within which the unification of normal and correlated (driven) anomalous diffusions can be achieved. They obtain, for a generic linear force $F(x)$, the physically relevant exact (space, time)-dependent solutions of a generalized Fokker-Planck (FP)
equation
\[ \frac{\partial}{\partial t} [p(x,t)]^\mu = -\frac{\partial}{\partial x} \{ F(x)[p(x,t)]^\mu \} + D \frac{\partial^2}{\partial x^2} [p(x,t)]^\nu \] (8)
by means of an ansatz based on the Tsallis entropy.
For our purpose, we remind here that such a FP equation, in the nonlinear "norm conservation" case ($\nu \neq 1$ and $\mu = 1$), generates Tsallis space-time distributions with the entropic index $q$ being related to the parameter $\nu$ by $q = 2 - \nu$. By means of the latter, and following again ref.[21], it is possible to recover the following relation between the exponent $\gamma$ of anomalous diffusion (being $\sigma^2 \propto t^\gamma$) and the entropic index $q$
\[ \gamma = \frac{2}{1 + \nu} = \frac{2}{3 - q} \] (9)
Hence, being in diffusive processes the space-time distributions linked to the respective velocity correlations by the relation (7), one could think to investigate if the relation (9) would be satisfied choosing the entropic index $q$, characterizing the correlation decay, and the corresponding anomalous diffusion exponent. This is done in Fig.4 where in order to check the latter hypothesis, that we call the $\gamma - q$ conjecture, we report the ratio $\frac{\gamma}{3 - q}$ vs the exponent $\gamma$ for various initial conditions ranging from $M(0)=1$ to $M(0)=0$ and different sizes at $U = 0.69$. Both $q$ and $\gamma$ have been taken from the results shown in Fig.2.2. Within an uncertainty of $\pm 0.1$, the data show that this ratio is always one, thus providing a strong indication in favor of this conjecture, which is satisfied for the HMF model.
Summarizing, we have shown numerical simulations which connect the superdiffusion observed in the anomalous QSS regime of the HMF model to the $q$-exponential long-term decay of the velocity correlations in the same regime. This new result is very interesting because opens a way to set a rigorous analytical link between the entropic index $q$ and the dynamical properties of nonextensive Hamiltonian many-body systems.

Conclusions

We have briefly reviewed some of the anomalous features observed in the dynamics of the HMF model, a kind of minimal model for the study of complex behavior in systems with long-range interactions. We have also discussed how the anomalous behavior can be interpreted within the nonextensive thermostatistics introduced by Tsallis, and in the framework of the theory glassy systems. The two pictures are not in contradiction and probably have more
strict links than previously thought, which deserve to be further explored in the future.

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