Metastable states in a class of long-range Hamiltonian systems

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Abstract

We numerically show that metastable states, similar to the Quasi Stationary States found in the so called Hamiltonian Mean Field Model, are also present in a generalized model in which $N$ classical spins (rotators) interact through ferromagnetic couplings decaying as $r^{-\alpha}$, where $r$ is their distance over a regular lattice. Scaling laws with $N$ are briefly discussed.

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1 Introduction

The study of the dynamical properties of systems with long-range interactions is important from a foundational point of view. It is well known that if the potential energy of a classical Hamiltonian system does not obey the so-called temperedness and stability conditions then the existence of a statistical mechanics is questionable [1]. If the potentials are well behaved it can be shown that the statistical thermodynamics of the system is extensive (i.e. the free energy density does not depend on the number of degrees of freedom) and additive (i.e. the free energy of the system as a whole can be expressed as the sum of the free energies of its component macroscopic parts) [2].

The good potentials are repulsive at short distances and decay sufficiently fast at large distances. Slowly decaying interactions may induce into the system spatial and temporal correlations leading to anomalous relaxations and to equilibrium distribution functions different from that of standard statistical mechanics. The nonextensive generalization of Boltzmann-Gibbs statistics, proposed by C. Tsallis [4, 5], is a powerful parametrization of the statistical mechanics of out-of-equilibrium states in open systems. The formulas in this approach are labelled by the so-called entropic index $q$, and in the limit $q = 1$ the Boltzmann-Gibbs expressions are recovered.

It has been also conjectured that this formalism could be applied to anomalous states of conservative Hamiltonian systems with long-range interactions [6]. The so-called quasi stationary states (QSS) of the Hamiltonian Mean Field model (HMF), originally introduced by Ruffo and Antoni [6], have been recently investigated and discussed in this perspective by Latora, Rapisarda and Tsallis [7, 8]. If particular initial conditions are chosen for the model, microcanonical simulations reveal anomalous properties [9]. For example anomalous diffusion is observed [10, 11, 12], single-particle velocity distribution functions are not gaussian [7, 8, 10, 13] and the temperature as a function of time is locked at a value which is dependent on $N$, and which is different from the canonical equilibrium.
one \[7, 8, 10, 12, 14\], established analytically \[14\]. After a characteristic lifetime, those non-usual properties relax toward the ones predicted by standard statistical mechanics. This relaxation has been appealing interpreted as the irreversible passage from a non equilibrium state, appropriately described by Tsallis’ statistics, toward the equilibrium Boltzmann-Gibbs state \[15\]. Since the lifetime of the QSS has been shown to diverge with \(N\), then in the thermodynamic limit the system is frozen forever in a state characterized by a \(q\) different from 1.

In this paper we give numerical evidence that the stationary states are also present in a system that generalizes the HMF model. In the system we consider classical spins interact with couplings that decay as \(r^{-\alpha}\), where \(r\) is the distance between two spins. If \(\alpha \geq d\), the euclidean dimension of the embedding space, then the interaction is short-ranged, if \(0 \leq \alpha < d\) it is long-ranged. The spins are fixed at the nodes of a \(d\)-dimensional lattice; this avoids the singularity of the potential terms at very short distances.

As we shall point out in sect. \[4\] the system can be made extensive through an appropriate rescaling function. Nevertheless, in the long-range case, additivity might not hold, and anomalous dynamical effects similar to those observed in the infinite range HMF model are expected.

The present study is the starting point of a project devoted to the investigation of the effects of the range of the interactions, as controlled by the exponent \(\alpha\), on the dynamical properties of a class of systems for which the HMF model is the infinite range limit.

## 2 The model

We consider the following classical hamiltonian

\[
H = \frac{1}{2} \sum_{i=1}^{N} L_i^2 + \frac{1}{2N} \sum_{i \neq j}^{N} \frac{1 - \cos(\theta_i - \theta_j)}{r_{ij}^\alpha}
\]

(1)

of planar rotators (XY spins) on a generic \(d\)-dimensional lattice. At each lattice site \(i\) conjugate canonical coordinates \((L_i, \theta_i)\) represent the angular momentum and the angular position of a rotator. Each of them has unit moment of inertia
and moves on a reference plane passing through its lattice site. Parameter $\alpha \geq 0$ tunes the interaction and periodic boundary conditions are enforced in the form of nearest image convention. For $\alpha = 0$ the hamiltonian of the HMF model is recovered. The rescaling parameter $\tilde{N}$ is a function of $\alpha, N, d$ and the lattice, and is defined as $\tilde{N} = \sum_{j \neq i} 1/r_{ij}^\alpha$. Because of periodicity the previous sum does not depend on the choice of the origin $i$. The presence of this rescaling is necessary to make the system extensive, i.e. to guarantee the existence of a bounded energy density in the thermodynamic limit [15].

The model, that we tend to call the $\alpha - XY$ model, has been introduced by Anteneodo and Tsallis [16]; its thermodynamics has been studied computationally for $d = 1$ [17] and its canonical partition function has been computed analytically [15, 18] in the case $\alpha < d$. These last studies have shown that, through a rescaling function $\tilde{N}$, the canonical statistical mechanics of the $\alpha - XY$ can be mapped on that of the HMF model. In particular, both models have a second-order phase transition between a supercritical disordered phase and a low energy ferromagnetic ordered phase, with the same critical energy $U_c = 3/4$.

The study of the chaotic properties of the supercritical $\alpha - XY$ model has remarkably shown a universal reduction of mixing in the thermodynamic limit, controlled by the parameter $\alpha/d$ [16, 18, 19]. These results have found a theoretical setting in a paper by Firpo and Ruffo [20].

### 3 Simulation details and results

We have decided to carry on the search for the existence of metastable states in the generalized model [11] along the same lines of the studies conducted on the HMF model. A previous brief inspection of the single-particle velocity distribution functions had revealed a non-Gaussian distribution, also for $\alpha \neq 0$ [18]. Here we focus on the behaviour of the instantaneous temperature $T(t)$ defined
as both a time and ensemble average:

$$T(t) = \langle \int_{t_0}^{t} dt' 2K(t')/N \rangle,$$

(2)

where $K$ is the total kinetic energy, $t_0$ is an equilibration time, and the external average $\langle \cdot \rangle$ is over different initial conditions, all of the "water-bag" form: $\theta_i = 0$ for all $i$ and $L_i$ uniformly distributed. We have simulated the system in dimension $d = 1$ for different $\alpha$ and $N$. The simulations are performed at fixed energy integrating the equations of motion through a $4^{th}$ order symplectic algorithm [21] with time-step $dt = 0.02$ which gives an energy conservation $\Delta E/E \sim 10^{-7}$. We chose $t_0 = 100$ and rescaled the velocities to fix the energy density value at $U = 0.69$. For short, we have followed the protocol that was successful in detecting metastable states in earlier works [7, 8, 9, 10, 11, 12, 13, 14, 22].

We have first run a few simulations for one fixed $\alpha = 0.4$, increasing $N$ up to $N = 2000$. The results are shown in Fig. 1. They indeed confirm the existence of a temperature plateau which, after a given time, relaxes towards the canonical temperature (known to be at $T = 0.476$). The length of the plateau increases for increasing $N$ and characterises therefore the lifetime $\tau$ of a true metastable (or "Quasi stationary" (QSS)) state. The height of plateau gives the "metaequilibrium" temperature $T_{QSS}$ and is found to decrease with increasing $N$ as in the HMF model [8]. However how these two quantities $\tau$ and $T_{QSS}$ scale with $N$ is not clear and still under investigation.

We have to remark that the computation of the quantity (2) is strongly affected by fluctuations. Both averages (time, ensemble) in formula (2) appear necessary to have a good statistics and thus a smooth curve. We have checked that averaging over a set of 100 initial conditions led to a definite smooth $T$ vs $t$ curves. Averaging over an increasing number of initial conditions has the effect of slightly shifting the curves, but $T_{QSS}$ and $\tau$ change within a few percent. For 100 averages the curve appears definite but only for averages over 1000 initial conditions the height of the plateau (but not the length) seems not to be
affected any more. We expect that at large $N$ one has to average over less initial conditions, but still the task is computationally expensive even if our integration of the forces is of order $N \ln N$, due to the use of Fast Fourier Transforms.

We decided then to fix the number of rotators at $N = 500$ and concentrate our computational resources to the study of the effects of changes in $\alpha$. We simulated ten values of $\alpha$ between 0 and 1 and averaged over 100 initial conditions. We report the resulting temperature curves in Fig. 2.

We observe slight discrepancies between our curve for $\alpha = 0$ and the one found in [7, 8] because the height of our plateau looks a bit higher. We think the difference is due to a poor average on initial conditions which as said before can affect this quantity.

From the curves in Fig. 2 we computed the lifetime $\tau$ of the metastable state for the various $\alpha$’s. We defined $\tau$ to be the point where a sharp increase in the curve is found. We point out that this definition is purely qualitative. Smoother data from a better (and harder) sampling should lead to a more precise definition and thus a better estimate of $\tau$. We report the results in Fig. 3. Note that $\tau$ at $\alpha = 0$ is around 1000, a value consistent with the HMF results (see fig. 1b of ref. (8) and fig. 2 of ref.(9)). As soon as $\alpha$ is increased, reducing the range of the interaction, an abrupt increase of $\tau$ is observed. From $\alpha = 0.1$ on $\tau$ decreases almost exponentially. It would be interesting to carefully investigate the effect of small $\alpha$s in a more extended study.

4 Discussion

In this paper we have shown that metastable states are also present in the $\alpha - XY$ model; this was quite expected. Qualitatively, the quasi stationary states behave similarly to those observed in the HMF model; in particular, from Fig. 1 we see that lifetimes tend to increase with $N$ and the plateau temperatures tend to decrease with $N$; we have checked with short runs up to $N = 100000$ and $\alpha = 0.9$ that the plateau tend to the same value of $T_\infty = 0.38$, that has been obtained extending the upper-critical universal caloric curve of the HMF.
model (corresponding to $\alpha = 0$) into the lower-critical region. From Fig. 3 we can say that the lifetime of the QSS tends to become very small as $\alpha$ tends to 1, and that confirms that the existence and stabilization of these states is due to the range of the interactions.

We have made efforts to rescale the data in Fig. 1 and Fig. 2 using the scaling factor $\tilde{N}$. Our aim was to show that the scaling laws observed in the HMF models are also valid in the $\alpha - XY$ model, but the simple ways we have attempted gave no result. In fact, the exponential fit in Fig. 3 shows that the lengths of the temperature plateau do not scale with $\tilde{N}$ (that is with $N^{1-\alpha}$). On the other hand we have to say that $\tilde{N}$ is a rescaling function that was successfully applied, as an "effective number of interacting degrees of freedom" to the computation of equilibrium canonical quantities. There is no reason that scaling by the same function should reveal some universality of the non-equilibrium dynamical features in this class of models. More work is needed to search for such a universal behaviour.

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Figure 1: $T$ vs $t$ for various $N$ and $\alpha = 0.4$. Lifetime of the metastable state increases with $N$ also for $\alpha \neq 0$. Plateau height also decreases in accordance with $\alpha = 0$ results. The $N = 200, 500, 1000, 2000$ curves are averaged respectively over 300, 100, 100, 50 initial conditions.
Figure 2: $T$ vs $t$ for various $\alpha$ and $N = 500$. Lifetimes of the metastable states and plateau height depend on $\alpha$, the latter also non-monotonically. All curves are averaged over 100 initial conditions.
Figure 3: QSS lifetime $\tau$ vs $\alpha$ as extracted from figure 2. The dashed line is an exponential fit.