Dynamics and thermodynamics of rotators interacting with both long and short range couplings

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Abstract

The effect of nearest-neighbor coupling on the thermodynamic and dynamical properties of the ferromagnetic Hamiltonian Mean Field model (HMF) is studied. For a range of antiferromagnetic nearest-neighbor coupling, a canonical first order transition is observed, and the canonical and microcanonical ensembles are non-equivalent. In studying the relaxation time of non-equilibrium states it is found that as in the HMF model, a class of non-magnetic states is quasi-stationary, with an algebraic divergence of their lifetime with the number of degrees of freedom $N$. The lifetime of metastable states is found to increase exponentially with $N$ as expected.

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1. INTRODUCTION

Hamiltonian systems with long-range interactions exhibit several peculiarities, both in their equilibrium properties and in the dynamical behavior. At equilibrium, it is often found that different statistical ensembles can be non-equivalent even in the thermodynamic limit. First discussed theoretically by Hertel and Thirring, this result has been confirmed in analytical and numerical studies (see, e.g., Refs. [3, 4, 5, 6, 7, 8, 9, 10, 11]), which pointed out that ensemble inequivalence is usually associated with the presence of a first order phase transition in the canonical ensemble.

Attention has also been focussed on the dynamics, in particular on the relaxation to equilibrium of a system initially prepared in a state which is far from equilibrium. Many studies have been devoted to the Hamiltonian Mean Field (HMF) model, a system of classical XY-rotators with infinite range ferromagnetic couplings. This model exhibits a second order transition to a magnetized state. It has been shown numerically in microcanonical simulations that for a large class of non-equilibrium initial conditions the model exhibits fast relaxation to another non-equilibrium state, in a fashion similar to the violent relaxation of astrophysical systems [13, 14]. After this transient the relaxation to Boltzmann-Gibbs equilibrium takes place in times that diverge with the number $N$ of rotators, according to a power law [12, 15, 16, 17]. The stability of these long-lived states, that have been called “quasi-stationary” states, has recently been analyzed in terms of Vlasov and Fokker-Planck equations [18, 19, 20, 21]. It should be emphasized that these quasi-stationary states are not metastable states in the thermodynamical sense, since they do not correspond to local maxima of the entropy (in the microcanonical ensemble) or local minima of the free energy (in the canonical ensemble). A similar effect has recently been observed in the Ising model with long and short range interactions, where the lifetime of the quasi-stationary states diverges logarithmically with $N$.

In this work we consider the robustness of the quasi-stationary states with respect to perturbations of the long-range Hamiltonian. This problem is of interest if one wants to ascertain the relevance of these states in realistic long-range systems, where a purely long-range Hamiltonian could be perturbed by external forces or by the presence of additional short-range terms in the potential energy. In particular, we generalize the HMF model to include nearest-neighbor interaction between the rotators, in addition to the long range...
interaction.

The paper is organized as follows: In Section 2 we introduce our model; in Section 3 we summarize the equilibrium properties of the model as obtained within the canonical and the microcanonical ensembles. In Sections 4 and 5 we report our numerical results on the relaxation time of quasi-stationary and metastable states, respectively. Concluding remarks are given in Section 6.

2. THE MODEL

We study a system of $N$ rotators characterized by phase variables $\theta_i$, whose Hamiltonian is given by:

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

The $N$ rotators are placed on a one-dimensional lattice with periodic boundary conditions ($\theta_{N+1} \equiv \theta_1$). The choice of a one-dimensional lattice is made for mathematical convenience, as it will be explained in the following Section. The parameter $K$ is the short-range (actually nearest-neighbor) coupling between rotators. For $K = 0$ this system reduces to the HMF model, that, for positive $J$, has a second order ferromagnetic transition at the critical temperature $T_c = 0.5J$, corresponding to the critical energy density $\epsilon_c = 0.75J$ [12]. Clearly in this case the topology of the lattice is irrelevant. The transition is characterized by the value of the order parameter given by the magnetization $m$:

$$m = \frac{1}{N} \sqrt{\left( \sum_{i=1}^{N} \cos \theta_i \right)^2 + \left( \sum_{i=1}^{N} \sin \theta_i \right)^2} = \sqrt{m_x^2 + m_y^2}. \quad (2)$$

In the $N \to \infty$ limit, $m$ is positive below the critical energy, approaching zero for $\epsilon \to \epsilon_c$; while $m$ is identically zero above $\epsilon_c$. It has been shown that for the HMF model microcanonical and canonical ensembles are equivalent [11]; this equivalence had been discussed before for a general class of magnetic systems with long range interactions [23]. Microcanonical simulations in which the system is initially prepared in an homogeneous state, i.e. with the angles $\theta_i$ uniformly distributed between 0 and $2\pi$ (and thus $m \approx 0$ at time $t = 0$) and the $p_i$’s uniformly distributed between $-p_0$ and $p_0$ (with $p_0$ determined by the energy) show the following: if the energy per particle is in a certain range below the critical energy, then the
system remains for a long time in this non-magnetic state, and it approaches the equilibrium magnetized state only after a time that diverges like $N^{1.7}$ \cite{18}. In the same subcritical energy range it is found that if the $\theta_i$’s are initially all equal, with the $p_i$’s uniformly distributed, there is a fast relaxation to a non-magnetic state, and again the equilibrium magnetized state is reached after a time diverging with $N$, although with a smaller power law \cite{17}.

In the following sections we study the equilibrium properties of system (1) for general values of $K$, and consider the dynamical properties at small values of $K$, when the system can be thought of as a perturbed HMF.

3. EQUILIBRIUM PROPERTIES

The canonical partition function and the microcanonical entropy of the model can be obtained by a straightforward generalization of the corresponding calculations of the HMF model \cite{11,12}. We will not report here the full details of these calculations, which we defer to a longer paper, but rather restrict ourselves to a brief sketch of the derivation. Without loss of generality we take $J = 1$ in (1).

We begin by considering the free energy per particle $f(\beta)$, obtained from the calculation of the canonical partition function. Applying the Hubbard-Stratonovich transformation, $f(\beta)$ can be written as

$$-\beta f(\beta) = \max_m \left[ -\frac{\beta(1 + m^2)}{2} + \ln \lambda(\beta m, \beta K) + \ln \frac{2\pi}{\beta} \right].$$

(3)

In this expression $\lambda(z, \alpha)$ is the largest eigenvalue of the transfer matrix given by the symmetric integral operator $\mathcal{T}$ defined as

$$(\mathcal{T} \psi)(\theta) = \int d\theta' \exp \left[ \frac{1}{2} z(\cos \theta + \cos \theta') + \alpha \cos(\theta - \theta') \right] \psi(\theta').$$

(4)

The energy density $\epsilon(\beta)$ is computed from (3) using standard expressions. The microcanonical entropy as a function of $\epsilon$ can be computed from the argument of maximization in (3) using the recipe introduced in Ref. \cite{7}, performing first a minimization over the inverse temperature $\beta$ before maximizing over the order parameter $m$

$$s(\epsilon) = \max_m \min_{\beta} \left[ \beta \epsilon + \ln \frac{2\pi}{\beta} - \frac{\beta(1 + m^2)}{2} + \ln \lambda(\beta m, \beta K) \right] \equiv \max_m s(\epsilon, m).$$

(5)

The value of $\beta$ corresponding to the solution of the optimization problem (5) gives the microcanonical temperature as a function of $\epsilon$. The phase-diagram in both the canonical
FIG. 1: The canonical and microcanonical \((K,T)\) phase diagram. In the canonical ensemble the transition is continuous (bold solid line) down to the tricritical point CTP where it becomes first order (dashed line). In the microcanonical ensemble the continuous transition coincides with the canonical one at large \(K\) (bold solid line). It persists at lower \(K\) (light solid line) down to the tricritical point MTP where it turns first order, with a branching of the transition line (dotted lines).

and the microcanical ensembles can be directly derived from the properties of free energy and entropy. For positive (i.e., ferromagnetic) nearest-neighbor couplings the system behaves in a way which is analogous to the HMF \((K=0)\) case: there is a second order ferromagnetic transition (at a \(K\) dependent critical temperature and energy), ensembles are equivalent and the temperature-energy relation (so-called caloric curve) is qualitatively similar to that of the HMF model. It is found that there exists a range of negative values of the short-range coupling \(K\) for which the system exhibits a first order phase transition in the canonical ensemble. This is a result of the competing effect of the mean-field potential and the antiferromagnetic short-range coupling. As expected, the canonical and the microcanonical ensembles are non-equivalent in this range of coupling. The \((K,T)\) phase diagram of the model is given in Fig. \(\text{II}\). For clarity the plot is restricted to the interesting negative \(K\) region. Starting from positive values and decreasing \(K\), the canonical critical line ends at the tricritical point (CTP) \(K = K_1 \approx -0.168, T = T_1 \approx 0.273\), where the canonical phase transition becomes first order. The dashed line in Fig. \(\text{II}\) shows the canonical transition temperature for \(K < K_1\). This line ends at \(K = -0.25, T = 0\). For smaller values of \(K\)
FIG. 2: Two examples of $s(\epsilon, m)$: (a) Local entropy minimum for a $m = 0$ quasi-stationary state; (b) Local entropy maximum for a metastable $m = 0$ state.

the system is disordered at any temperature and there is no transition. This can be easily understood by computing the energies of the staggered antiferromagnetic $m = 0$ state and that of the fully magnetized $m = 1$ state. For $K \leq -1/4$ the former is always favoured, even at zero temperature. In the microcanonical ensemble the critical line extends down to the microcanonical tricritical point (MTP) located at $K = K_2 \approx -0.182, T = T_2 \approx 0.234$, where the transition becomes first order. Below this point, a temperature jump between the two microcanonical temperatures given by the dotted lines appears. Again, for $K < -0.25$ there is no transition. The two ensembles are therefore non-equivalent for $-0.25 < K < K_1$.

4. QUASI-STATIONARY STATES

The equilibrium magnetization at a given energy $\epsilon$ is obtained by maximizing the entropy $s(\epsilon, m)$ with respect to $m$ (see Eq. (5)). Local maxima correspond to metastable states, that we consider in the next Section. For small $K$ values (both positive and negative) the entropy dependence on magnetization shows only a global maximum, at the equilibrium value of $m$. A typical entropy curve is given by the one shown in Fig. 2(a), which has $K = 0$ (HMF model); the entropy has a local minimum at $m = 0$. We are primarily interested in this case since we want to study the difference in the dynamical behavior induced by a perturbation of the HMF system, for which the long lifetime of quasi-stationary states, with $m$ close to 0, is strictly of dynamical origin \[18\]. We consider here only the case of initial homogeneous
non-magnetic states, with $\theta$ and $p$ both uniformly distributed.

We performed runs at different $K$ values. For each $K$ we have chosen a value of the energy density $\epsilon$ below the critical energy, $\epsilon = \epsilon_c(K) - \Delta\epsilon$, keeping $\Delta\epsilon = 0.06$ fixed. This distance is the same as for the simulations typically performed at $K = 0$ (HMF), where $\epsilon = 0.69$ is studied, with the critical energy density being at $0.75$ [18]. We have performed runs for a number of rotators $N$ ranging from 1024 to 32768.

It turns out that the escape from non-magnetic quasi-stationary states takes place after a time that fluctuates from run to run (corresponding to different realizations of the uniform initial distributions of $\theta$ and $p$), although these fluctuations are much smaller than those of the case of the thermodynamic metastable case discussed in the following Section. In Fig. 3 we plot the instantaneous magnetization as a function of time for the case $K = 0.05$ and $\epsilon = 0.7115$, and for the increasing $N$ values from left to right. These plots are obtained by averaging over several runs (the number of these runs for each $N$ value is reported in the caption). It is worth mentioning that for a given $N$ the lifetime of the quasi-stationary states is considerably shorter than that of the HMF model (see, e.g., Ref. [18]). To define this lifetime we have chosen the time at which, during the rise of the magnetization towards the equilibrium value, the magnetization has a value equal to the average between the plateau value in the quasi-stationary state and the equilibrium value. In order to smooth
FIG. 4: Growth of the lifetime of quasi-stationary states with $N$ for different values of $K$. From top to bottom the data refer to $K = 0$, $K = 0.0025$, $K = 0.05$, $K = 0.1$. Data for $K = 0$, with $\tau$ diverging as $N^{1.7}$, are taken from Ref. [18].

out fluctuations, we used a running average of the magnetization over a sliding time window of a conveniently chosen size. This definition of the lifetime is practically equivalent to that used in Ref. [18] through a more sophisticated fitting procedure. In Fig. 4 we plot the lifetime $\tau$ as a function of $N$, in a log-log plot for different $K$ values. It is evident that the lifetime $\tau$ increases with $N$, possibly diverging in the limit $N \to \infty$. This suggests that quasi-stationarity persists when short range interactions are added to the HMF model. A naive fit of the curves to the form $\tau \sim N^\gamma$ with $K$-dependent power-law exponents $\gamma(K)$ yields $\gamma(0.0025) \approx 0.65$, $\gamma(0.05) \approx 0.56$, $\gamma(0.1) \approx 0.45$. Thus the observed exponent $\gamma$ decreases with increasing $K$. For $K > 0.1$ we do not observe a plateau region in the magnetization at $m \approx 0$ and one cannot reasonably speak of quasi-stationarity. Clearly one cannot rule out the possibility that the seemingly $K$ dependence of $\gamma$ is just a finite size effect, which are evidently present in the up-bending of the smaller $K$ value curve in Fig. 4 and the down-bending of the other two. More extensive numerical simulations are necessary in order to assess the law of divergence with $N$. 

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5. METASTABLE STATES

In our system, thermodynamic metastable states are found for negative $K$ values, for which the microcanonical transition is first order. In Fig. 2(b) we show an example of an entropy function with a local maximum at $m = 0$, while the global maximum is at $m \neq 0$. The evolution of this $m = 0$ state was studied. In Fig. 5 we show a typical plot of the instantaneous magnetization $m$ as a function of time, for a system with $N = 150$ rotators. After a transient time spent in the metastable state, there is a sudden transition to the equilibrium magnetization. In Fig. 6 we plot the lifetime $\tau$ of the metastable state as a function of $N$. It should be pointed out that an average over many runs is necessary in order to obtain a sufficiently accurate determination of this value, since the differences from run to run are not small. We find that $\tau \sim e^{N\Delta s}$, where $\Delta s$ is the “entropy barrier”, i.e. the difference between the entropy at $m = 0$ and the one at the minimum (see Fig. 2(b)). Thus the transition is determined by the fluctuations at finite $N$, and the exponential divergence of the lifetime is governed by the entropy barrier. Analogous results have been found for other systems [24].
FIG. 6: Exponential growth of the lifetime of the metastable state of Fig. 3 with the number of rotators.

6. DISCUSSION

The model studied in this work offers another example of a long-range system with inequivalence of ensembles. When the long-range and the short-range interactions have a competing character (i.e., when $K$ is negative), we found that the microcanonical and the canonical ensembles yield different results, in a range of $K$ values.

The existence of quasi-stationary states seems to be a peculiar feature of long-range systems, and in this work our aim was to study their robustness with respect to perturbations of the long-range nature of the interaction. We found that if the perturbation is sufficiently small the divergence with $N$ of the lifetime of these states is preserved. This fact was not obvious a priori, since one could have argued that even small perturbations could have given rise to finite lifetimes also in the $N \to \infty$ limit. One could have hypothesized the finiteness of the lifetime on the basis of the fact that, when the rotators have also a short-range coupling, the $1/N$ expansion of the Vlasov equation, suitable for the HMF case [25], is no longer possible. It has to be inferred that, in spite of this fact, an approximate description of the system with a kinetic equation possessing out of equilibrium stable stationary states would still be possible. Its determination is one of the possible directions of development of this work. It is worth noting that in the case of the Ising model with both long and short range interactions, quasistationarity was found to exist, but with a universal logarithmic
divergence of the lifetime with $N^2$.

We have considered here only one class of initial conditions. As was found in the HMF model, other initial states may behave differently. It would be interesting to explore the dynamical behavior of other initial conditions. The model we have analyzed lives on a 1D lattice, but we believe that some basic dynamical features observed here should extend to higher dimensions.

It would of course be interesting to determine the range of validity, across different models, of the results presented in this paper; this could be relevant for the study of the dynamical properties, and in particular for the approach to equilibrium of open long-range systems, i.e., systems in interaction with external degrees of freedom. One could suppose that the open character of the system can be mimicked by a perturbation of the long-range Hamiltonian. Preliminary investigations of a simple magnetic system with these characteristics give results with features that are similar to those presented in this work.

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[1] Dynamics and Thermodynamics of Systems with Long-Range Interactions, edited by T. Dauxois, S. Ruffo, E. Arimondo, and M. Wilkens, Lecture Notes in Physics 602 (Springer-Verlag, New York, 2002).

[2] P. Hertel and W. Thirring, Ann. Phys. 63, 520 (1971).

[3] A. Torcini and M. Antoni, Phys. Rev E 59, 2746 (1999).

[4] I. Ispolatov and E. G. D. Cohen, Physica A 295, 475 (2000).

[5] R. S. Ellis, K. Haven, and B. Turkington, J. Stat. Phys. 101, 999 (2000).

[6] J. Barré, D. Mukamel, and S. Ruffo, Phys. Rev. Lett. 87, 030601 (2001).

[7] F. Leyvraz and S. Ruffo, J. Phys. A: Math. Gen. 35, 285 (2002).

[8] F. Gulminelli and Ph. Chomaz, Phys. Rev. E 66, 046108 (2002).
[9] R. S. Ellis, H. Touchette, and B. Turkington, Physica A 335, 518 (2004).
[10] M. Costeniuc, R. S. Ellis, and H. Touchette, J. Math. Phys. 46, 063301 (2005).
[11] J. Barré, F. Bouchet, T. Dauxois, and S. Ruffo, J. Stat. Phys. 119, 677 (2005).
[12] M. Antoni and S. Ruffo, Phys. Rev. E 52, 2361 (1995).
[13] D. Lynden-Bell, Mon. Not. Roy. Astron. Soc. 136, 101 (1967).
[14] T. Padmanabhan, Phys. Rep. 188, 285 (1990).
[15] V. Latora, A. Rapisarda, and S. Ruffo, Phys. Rev. Lett. 80, 692 (1998).
[16] V. Latora, A. Rapisarda, and S. Ruffo, Phys. Rev. Lett. 83, 2104 (1999).
[17] A. Pluchino, V. Latora, and A. Rapisarda, Physica A 340, 187 (2004).
[18] Y. Y. Yamaguchi, J Barré, F. Bouchet, T. Dauxois, and S. Ruffo, Physica A 337, 36 (2004).
[19] M. Y. Choi and J. Choi, Phys. Rev. Lett. 91, 124101 (2003); J. Choi and M. Y. Choi, J. Phys. A: Math. Gen. 38, 5659 (2005).
[20] C. Anteneodo and R. O. Vallejos, Physica A 344, 383 (2004).
[21] P. H. Chavanis and F. Bouchet, Astronomy and Astrophysics 430, 771 (2005); P. H. Chavanis and C. Sire, Physica A 356, 419 (2005); P. H. Chavanis, J. Vatteville, and F. Bouchet, European Physical Journal B 46, 61 (2005).
[22] D. Mukamel, S. Ruffo, and N. Schreiber, cond-mat/0508604.
[23] A. Campa, A. Giansanti, and D. Moroni, J. Phys. A: Math. Gen. 36, 6897 (2003).
[24] M. Antoni, S. Ruffo, and A. Torcini, Europhys. Lett. 66, 645 (2004); P. H. Chavanis, Astronomy and Astrophysics, 432 117 (2005).
[25] F. Bouchet and T. Dauxois, cond-mat/0407703.
[26] F. Baldovin and E. Orlandini, private communication.