Anomalous diffusion and quasistationarity in the HMF model

Alessandro Pluchino and Andrea Rapisarda

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

Abstract. We explore the quasistationary regime of the Hamiltonian Mean Field Model (HMF) showing that at least three different classes of events exist, with a different diffusive behavior and with a relative frequency which depends on the size of the system. Along the same line of a recent work [1], these results indicate that one must be very careful in exchanging time averages with ensemble averages during the non-ergodic metastable regime and at the same time they emphasize the role of finite size effects in the evaluation of the diffusive properties of the system.

Keywords: Metastable phases, long-range interactions, complex systems
PACS: 64.60.My, 89.75.-k

INTRODUCTION

It is a common practice in statistical physics to exchange time averages with ensemble averages since it is usually assumed that the ergodic hypothesis is in general valid. Although the latter is very often verified, it is not always true, especially for complex systems. In a recent paper [1] we discussed one example where this happens in the context of the well known Hamiltonian mean field (HMF) model, a paradigmatic long-range system whose behavior has been very debated in the last decade [2, 3, 4, 5, 6]. Working in the same direction, in this paper we want to focus our attention on a controversial topic regarding the anomalous dynamics of the HMF model, i.e. its superdiffusive behavior observed in the metastable regime [5, 7, 8, 9, 10, 11, 12, 13, 14]. In particular, we present new numerical results which permit to clearly identify at least three classes of events in that regime, showing a different temperature evolution and a different diffusive behavior. The relative frequency of the three types of events strictly depends on the size of the system. These results indicate that one must be very careful in exchanging time averages with ensemble averages and at the same time they emphasize the role of finite size effects in the evaluation of the diffusive properties of the system.

MODEL AND ANOMALIES

The HMF model describes a system of $N$ fully-coupled classical inertial XY spins (rotators) $\hat{s}_i = (\cos \theta_i, \sin \theta_i)$, $i = 1, \ldots, N$, with unitary module and mass [15]. These spins can also be thought as particles rotating on the unit circle. The Hamiltonian can be
written as

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

where \( \theta_i \) is the angle and \( p_i \) the conjugate variable representing the rotational velocity of spin \( i \).

At equilibrium the model can be solved exactly and one has a second order phase transition from a high temperature paramagnetic phase to a low temperature ferromagnetic one \[15\]. The order parameter of this phase transition is the modulus of the average magnetization per spin defined as:

\[ M = \frac{1}{N} \left| \sum_{i=1}^{N} s_i \right| . \]

The transition occurs at a critical temperature \( T_c = 0.5 \), which corresponds to a critical energy per particle \( U_c = E_c/N = 0.75 \). Above \( T_c \), rotators point towards different directions and \( M \sim 0 \). Below \( T_c \), at variance, they are aligned and trapped into a single cluster, so that \( M \neq 0 \). The out-of-equilibrium dynamics of the model is also very interesting. In a range of energy densities between \( U \in [0.5, 0.75] \), special initial conditions called water-bag, with initial magnetization \( M_0 = 1 \) (i.e. with all the spins aligned and with all the available energy in the kinetic form), drive the system, after a violent relaxation, towards metastable Quasistationary States (QSS), where the system remains trapped for a while before slowly relaxing towards equilibrium. These QSS are characterized by a lifetime which diverges with the system size \( N \) \[3, 4, 5\] and by a temperature \( T_{QSS} \) which results to be lower than the canonical equilibrium one. In the thermodynamic limit, \( T_{QSS} \) tends to a limiting value \( T_{N \to \infty} \) which depends on the energy density.

Numerous dynamical anomalies characterize the QSS regime, e.g. vanishing Lyapunov exponents, non-Gaussian velocity distributions, slow decaying velocity correlations, fractal-like phase space structures, aging and anomalous diffusion \[3, 4, 5\]. Among them, the diffusive behavior of the rotators is one of the most debated. In order to study diffusion it is customary to consider the mean square displacement of phases \( \sigma^2(t) \) defined as

\[ \sigma^2(t) = \frac{1}{N} \sum_{j=1}^{N} (\theta_j(t) - \theta_j(0))^2 = \langle [\theta_j(t) - \theta_j(0)]^2 \rangle, \tag{2} \]

where the symbol \( \langle \ldots \rangle \) represents the average over all the \( N \) rotators. Following the one-dimensional generalized Einstein’s relation, the quantity \( \sigma^2(t) \), if it is finite, typically scales as \( \sigma^2(t) \sim t^\gamma \): the diffusion is normal when \( \gamma = 1 \) (corresponding to the well known law for Brownian motion) and ballistic for \( \gamma = 2 \) (corresponding to free motion). For different values of \( \gamma \) the diffusion is anomalous and in particular for \( \gamma > 1 \) one has superdiffusion.

Superdiffusion has been so far observed in the metastable regime of the HMF model for water-bag initial conditions with variable initial magnetization \( M_0 \). It has been found an exponent \( \gamma \) going progressively from \( 1.4 \sim 1.5 \) (for \( 0.4 < M_0 < 1 \)) to \( 1 \) for \( M_0 = 0 \) \[7, 8, 11\]. More recently, a general relationship between the slow decay of the velocity autocorrelation functions and the superdiffusive behavior, based on a theoretical result by Tsallis and Bukman \[16\], has been proposed \[7, 8\]. This formula has been the object of several controversies \[12, 13, 17\], also related to the possible application of the non-extensive statistical mechanics in this context. The main objection is that anomalous
diffusion in the QSS regime is likely only a finite size effect and therefore in an infinite system one should recover $\gamma \sim 1$. Furthermore, it has recently been claimed [17] that if in the QSS regime the velocity autocorrelation functions can be fitted by a $q$-exponential, then the diffusion should be normal, in apparent contradiction with the results of [5, 7, 8]. In the next section, supported by new numerical simulations, we shall discuss these points in detail.

**DISCUSSION OF NUMERICAL RESULTS**

In Fig. 1 we consider a system of $N = 15000$ rotators at the energy density $U = 0.69$. This energy density has been well studied in the past being the value at which the anomalies are most evident. We have adopted an initial magnetization $M_0 = 1$. In Fig. 1 (a) we plot the temporal evolution of temperature $T$ (calculated dynamically as $T(t) = \frac{1}{N} \sum p_i^2$) for three different realizations (events) of the initial conditions. The latter have been selected among many others as representative of three classes of events which are observed most frequently. Please see [4] for details about the HMF equations of motion and the integration algorithm adopted. In the figure, it is clearly visible that, after a short violent
relaxation stage, where the system suddenly relaxes from the initial high temperature state, in all the three cases the system enters into a longstanding metastable regime at a temperature $T_{QSS}$ lower than the canonical equilibrium one (for $U = 0.69$ one has the equilibrium temperature $T_{eq} \approx 0.476$) and only for $t > 10^5$ definitively relaxes towards equilibration. But the temperature plateaux appear very different in the three cases. In fact for the type 1 event, the temperature oscillates around $T \approx 0.41$ and starts to slowly relax towards equilibrium after $t \approx 10^5$; for the type 2 event, the temperature stays for a while around $T \approx 0.40$, then relaxes towards $T \approx 0.38$ (double plateau) and finally, after $t \approx 10^5$, slowly reaches the equilibrium value; for the type 3 event, the temperature stays around $T \approx 0.38$ (i.e. the limiting $T_{N \to \infty}$ for $U = 0.69$) up to $t \approx 10^6$ and then abruptly relaxes to equilibrium. The description of these three kinds of events refers to the case $N = 15000$ of Fig. 1, but we have found a similar behavior for a wide range of system sizes. So we can identify more generally three different classes of events

- **Type 1 event** - the system shows a single quasistationary plateau at temperature $T_{QSS}$ with $T_{N \to \infty} < T_{QSS} < T_{eq}$ where it remains for a long time before equilibration;
- **Type 2 event** - the system passes through two different quasistationary plateaux before equilibration: the first one is similar to that of type 1 event, while the second is at $T_{N \to \infty}$;
- **Type 3 event** - the system exhibits again a single plateau, but at temperature $T_{N \to \infty}$, where it stays for a longer time with respect to type 1 event and relaxes then abruptly to equilibrium.

Since in the literature the QSS temperature plateaux have been always calculated performing averages over many events, such a different behavior of single runs has been overlooked. Moreover, if one considers small system sizes, fluctuations can hide such a different behavior, which emerges very clearly only for large sizes $N \geq 10000$. The difference among these three main classes of events open new perspectives for the dynamical anomalies registered during the QSS regime, as we discuss immediately below.

In Fig. 1 (b), we plot the instantaneous diffusive exponent $\gamma(t)$ as a function of time, calculated for the same three events previously discussed by taking the logarithm of both sides of the Einstein’s generalized relation and differentiating with respect to $\ln t$:

$$\gamma(t) = \frac{d(\ln \sigma^2)}{d(\ln t)}. \quad (3)$$

Note that the time scales of the two panels of Fig. 1 are the same, so that it is possible to compare the transitions to the different regimes. It clearly appears that to the three types of events plotted in the top panel corresponds to a different diffusive behavior in the bottom one. After a common ballistic regime ($\gamma \sim 2$) between $t = 10^2 - 10^3$, in all the three cases $\gamma(t)$ starts to decrease; but only for the type 3 event it quite monotonically reaches the value $\gamma \sim 1$ indicating normal diffusion (and remains there apart a big peak due to the sudden temperature relaxation towards equilibrium). In fact, for the type 1 event $\gamma(t)$ stays around 1.5 (the same value found in [5, 7, 8]) up to $t \sim 10^6$, then - when the system equilibrates - definitely relaxes to $\gamma \sim 1$. Finally, the type 2 event shows a behavior oscillating between the previous two.
In Fig. 2 we repeat the same simulations of Fig. 1 but for a larger system of $N = 50000$ rotators, in order to reduce the fluctuations. The results seem to confirm, in an even more evident way, the previous picture: again we recover three types of events with a different diffusive behavior, and again only in the type 3 event, whose temperature directly stabilizes in the $T_{N \to \infty} \sim 0.38$ plateau, the system monotonically reaches the normal diffusion unitary value. On the contrary, in the type 1 event $\gamma(t)$ shows again a plateau around the value 1.5 for $t > 5 \cdot 10^4$, that persists also during the relaxation towards equilibrium. Finally, the intermediate type 2 event shows again a double QSS temperature plateau, much clearer than that shown in the $N = 15000$ case: this time $\gamma(t)$ firstly monotonically decays towards the value 1.65, where remains for $5 \cdot 10^4 < t < 1 \cdot 10^5$; then, when the temperature reaches the limiting value $T_{N \to \infty} \sim 0.38$, it slowly relaxes towards $\gamma \sim 1$. For this size of the system we do not plot the complete relaxations to equilibrium for the three events but they approximatively follow the behavior of Fig. 1, with $\gamma(t)$ that reaches in all the cases the value 1 when the temperature reaches its equilibrium value.

In order to clarify what is the relative weight of these different kinds of events when increasing the size of the system, we report in Fig. 3 the fraction of events of the three
FIGURE 3. Fraction of events of the three classes as a function of the size of the system \( N \), calculated over sets of 20 events for each size.

classes as a function of \( N \) (calculated over sets of 20 events for each size). As one could expect, the fraction of type 1 events (a), initially around 0.8, decreases with the size of the system and becomes null above \( N = 10^5 \) while, on the contrary, the fraction of type 3 events (c) increases with \( N \) and, above \( N = 10^5 \), starts to oscillate around 0.3. On the other hand, the fraction of type 2 events (b), those having the double QSS plateau, stays constant around 0.3 up to \( N \sim 10^4 \), then rapidly increases and stabilizes around 0.7 above \( N \sim 5 \cdot 10^5 \): this is quite surprising because, for great values of \( N \), we know that the ensemble averaged temperature should tend to the stable value \( T_{N \to \infty} \sim 0.38 \), thus one could expect that, increasing the size of the system, all the events should belong to the type 3 class.

The non vanishing fraction of type 2 events for any value of the studied \( N \) evidently indicates that the ensemble average of temperature, which yields single QSS plateaux at \( T_{N \to \infty} \sim 0.38 \) \([3, 4, 5]\), will not coincide with the time average over type 2 events, due to their double QSS plateau. Such a result is in perfect agreement with those of \([1]\), where it has been shown that, due to the non-ergodicity of the QSS regime, the inequivalence between ensemble averages and time averages holds for velocities Pdfs, and q-Gaussian attractors appear instead of the usual Gaussian ones predicted by the Central Limit Theorem when ergodicity applies. In this respect, the double plateau of the type 2 events seems to suggest the existence of two different attractors in the QSS regime, corresponding to the two different temperature values of the plateau.

At the same time, in order to answer to the criticism mentioned at the end of the previous section \([12, 13, 14, 17]\), the presented results also show that, even for \( N \to \infty \), anomalous diffusion persists at least in the first part (that one with the higher temperature) of the
QSS plateau in *type 2* events, thus it does not appear to simply be a finite size effect. The eventual convergence to normal diffusion is very slow and in most real physical cases, where both time and size are finite, it is not assured. On the other hand, the fact of having anomalous diffusion appears to contradict what found in Ref. [7, 8], according to Ref. [17]. However, in this latter paper, stationarity of the correlation function was assumed and this is in general not true, since ageing has been found in the QSS regime, see for examples Refs. [9, 10]. Finally, the different distributions plotted in Fig. 3 as a function of N indicate a sensible dependence on N and on the type of the event, a fact which was previously not clearly observed for small sizes. In this respect it is interesting to notice that the minimum sometimes observed in the last part of the QSS temperature plateau, when averaging over many events [18], could be now likely explained as the result of a mixture of events of the three types.

**CONCLUSIONS**

We have shown that three different classes of events exist in the metastable QSS regime of the HMF model, with a relative frequency which depends on the size of the system. Each class presents different details in the diffusive behavior and some anomalies, like superdiffusion and double QSS temperature plateau, persist also increasing the size of the system. These are only preliminary results: in a future study we will calculate more accurately the fraction of events of the three classes (using larger sets of events) and we will try also to estimate the crossover time between the two QSS plateaux in the *type 2* events as a function of the system size. However, we think that the present work contributes to clarify some controversial points about the anomalous behavior observed in the QSS regime of the HMF model.

**ACKNOWLEDGEMENTS**

We would like to thank Stefano Ruffo and Constantino Tsallis for interesting discussions. The numerical calculations here presented were done within the TRIGRID project. The authors acknowledge financial support from the PRIN05-MIUR project "Dynamics and Thermodynamics of Systems with Long-Range Interactions".

**REFERENCES**

1. A. Pluchino, A. Rapisarda and C. Tsallis, *Europhys. Lett.* **80**, 26002 (2007).
2. V. Latora, A. Rapisarda and S. Ruffo, *Phys. Rev. Lett.* **80**, 692–695 (1998).
3. V. Latora, A. Rapisarda and C. Tsallis, *Phys. Rev. E* **64**, 056134 (2001).
4. A. Pluchino, V. Latora and A. Rapisarda, *Physica D* **193**, 315–328 (2004).
5. A. Rapisarda and A. Pluchino, *Europhysics News* **36**, 202 (2005).
6. A. Antoniazzi, F. Califano, D. Fanelli and S. Ruffo, *Phys. Rev. Lett* **98**, 150202 (2007).
7. A. Pluchino and A. Rapisarda, *Progress in Theoretical Physics Supplement* **162**, 18 (2006).
8. A. Pluchino and A. Rapisarda, *Physica A* **338**, 60–67 (2004).
9. A. Pluchino, V. Latora, A. Rapisarda, *Physica D* **193**, 315–328 (2004).
10. A. Pluchino, V. Latora, A. Rapisarda, *Continuum Mech. Thermodyn.* **16**, 245–255 (2004).
11. V. Latora, A. Rapisarda and S. Ruffo, *Phys. Rev. Lett* **83**, 2104–2107 (1999).
12. Y.Y. Yamaguchi, *Phys. Rev. E* **68**, 066210 (2003).
13. F. Bouchet and T. Dauxois, *Phys. Rev. E* **72**, 045103(R) (2005).
14. L.G. Moyano and C. Anteneodo, *Phys. Rev. E* **74**, 021118 (2006).
15. M. Antoni and S. Ruffo, *Phys. Rev. E* **52**, 2361–2374 (1995).
16. C. Tsallis and D.J. Bukman, *Phys. Rev. E* **54**, R2197 (1996).
17. A. Antoniazzi, D. Fanelli and S. Ruffo, *this volume*.
18. D. Zanette and M.A. Montemurro *Phys. Rev. E* **67**, 031105 (2003).