On the dynamical anomalies in the Hamiltonian Mean Field model

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We study the \( N \)-dependence of the thermodynamical variables and the dynamical behavior of the well-known Hamiltonian Mean Field model. Microcanonical analysis revealed a thermodynamic limit which defers from the \textit{a priori} traditional assumption of the \( N \)-dependence of the coupling constant \( g \) as \( \sim 1/N \) to tend \( N \to \infty \) keeping constant \( E/N^3 \) and \( g/N \), prescription which guarantees the extensivity of the Boltzmann entropy. The analysis of dynamics leads to approximate the time evolution of the magnetization density \( \mathbf{m} \) by means of a Langevin equation with multiplicative noise. This equation leads to a Fokker-Planck’s equation which is \( N \)-independent when the time variable is scaled by the \( N \)-dependent time constant \( \tau_{\text{mac}} = \sqrt{TN}/g \), which represents the characteristic time scale for the dynamical evolution of the macroscopic observables derived from the magnetization density. This results explains the origin of the slow relaxation regimen observed in microcanonical numerical computations of dynamics of this model system. Connection with the system self-similarity is suggested.

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I. INTRODUCTION

The present effort is devoted to study the \( N \)-dependence in the thermodynamical variables and dynamical behavior of the well-known Hamiltonian mean field model. This model describes a system of \( N \) planar classical spins interacting through an infinite-range potential.

\[
H_N (\theta, L; I, g) = K_N (L; I) + V_N (\theta; g)
\]

\[
= \sum_{i=1}^{N} \frac{1}{2} I_i^2 + \frac{1}{2} g \sum_{i,j=1}^{N} [1 - \cos (\theta_i - \theta_j)],
\]

(1)

where \( \theta \) is the \( i \)-th angle and \( L_i \) the conjugate variable representing the angular momentum, \( I \) is the moment of inertia of the rotator and \( g \) the coupling constant. This is an inertial version of the ferromagnetic X-Y model, which interaction is not restricted to first neighbors but is extended to all couples of spins.

Traditionally the coupling constant \( g \) is suppose to be \( N \)-dependent:

\[
g = \frac{\gamma}{N},
\]

(2)

assumption which makes \( H \) formally extensive (\( V \propto N \) when \( N \to \infty \)), since the energy remains non-additive and the system can not be trivially divided in independent subsystems. A fundamental observable of this model system is the magnetization density \( \mathbf{m} \), which is given by:

\[
\mathbf{m} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{m}_i,
\]

(3)

where \( \mathbf{m}_k = [\cos \theta_k, \sin \theta_k] \) is the intrinsic magnetization of the \( k \)-th particle.

The canonical analysis of the model predicts a second-order phase transition from a low-energy ferromagnetic phase with magnetization \( m \approx 1 \) to a high-energy paramagnetic phase with \( m \approx 0 \). The dependence of the energy density \( U = E/N \) on the temperature \( T \), the caloric curve, is given by:

\[
U = \frac{T}{2} + \frac{1}{2} [1 - m^2(T)]
\]

(4)

(\( U \) and \( T \) in units of \( \gamma \)) and this is shown at the Fig.1. The critical point is at the energy \( U_c = 0.75 \) corresponds to the critical temperature of \( T_c = 0.5 \).

The dynamical behavior of the HMF has been extensively investigated. Microcanonical simulations of dynamics are in general in good agreement with the canonical solution, except for a region below \( U_c \), where some anomalous phenomena have been observe, such as ensemble inequivalence and the slow relaxation regimen towards the Boltzmann-Gibbs’ equilibrium.

This ensemble inequivalence, characterized by the existence of a negative specific heat, appears as a dynamical feature. The origin of this anomaly is explained by the
existence of certain quasi-stationary state which is not the canonical one and depends on the initial conditions in the microcanonical numerical computation of the dynamics. In this case, the system needs a long time to relax to the canonical equilibrium state because of the duration of this metastable state has a linear dependence with $N$. This fact has been interpreted by Tsallis as the non-commutativity of the thermodynamic limit ($N \to \infty$) with the infinite time limit ($t \to \infty$): when the first is performed before the second, the system will not relax to the Boltzmann-Gibbs’ equilibrium.

Recent studies have shown that the slow-relaxation regime at long times is clearly revealed by numerical realizations of the model, but no traces of quasistationarity are found during the earlier stages of the evolution. This fact suggested the nonergodic properties of this system in the short-time range, which could make the standard statistical description unsuitable.

However, it there could be a mistake in the understanding of the macroscopic description of this model. There are many studies in long-range Hamiltonian system where the validity of the thermodynamical description in the thermodynamic limit is intimately related to the scaling with $N$ of the thermodynamic variables and potentials. The problems with the nonextensive nature of those systems are avoided using the Kac prescription in which the coupling constants are scaled by some power of $N$ in order to deal with an extensive total energy $E$. It is well-known that this kind of assumption affected the time scale of the system evolution, so that, its application should be taken with care.

II. MICROcanonical ANALYSIS

M. Antoni, H. Hinrichsen and S. Ruffo carried out the microcanonical analysis of the HMF in the ref.2. However, in their work they considered the equivalence of the microcanonical with the canonical ensemble in the thermodynamic limit, which depends on the validity of the canonical solution. In this section we will perform this analysis working directly on the microcanonical ensemble.

The microcanonical states density $\Omega$ is calculated as follows:

$$\Omega (E, N; I, g) = \frac{1}{N!} \int \frac{d^N \theta d^N L}{(2\pi \hbar)^N} \delta [E - H_N (\theta, L, I, g)] .$$

The integration by $d^N L$ yields:

$$\Omega (E, N; I, g) = \frac{1}{N!} \left( \frac{2\pi I}{\hbar^2} \right)^N \frac{1}{N!} \int \frac{d^N \theta}{(2\pi \hbar)^N} \left[ E - V_N (\theta; g) \right]^{N-1} .$$

The microcanonical accessible volume $W$ is expressed as $W = \Omega g/2^1$. We are interested in describing the large $N$ limit, where $W$ is given by:

$$W \simeq \left( \frac{2\pi I g}{N \hbar^2} \right)^N \int d^2 m \left[ m^2 + 2U - 1 \right]^{N-1} f (m; N) ,$$

where it was introduced the dimensionless parameter $U$:

$$E = g N^2 U,$$

and the function $f (m; N)$:

$$f (m; N) = \int \frac{d^N \theta}{(2\pi)^N} \delta \left[ m - \frac{1}{N} \sum_{k=1}^N m_k \right] .$$

We estimate the function $f (m; N)$ for large $N$ by using the steepest decent method. Expressing the delta function by mean of the Fourier’s integral representation, the Eq (9) is rewritten as follows:

$$f (m; N) \simeq N^2 \int \frac{d^2 k}{(2\pi)^2} \exp \left[ i Nk \cdot m \right] \left[ J_0 \left( -i \sqrt{N^2} k \right) \right] .$$

where $k = k + ix$, $x \in \mathbb{R}^2$, and $J_0 (z)$ is the modified Bessel function of zero order. It is easy to obtain the main contribution of the integral when $N \to \infty$ maximizing the integral function via the parameter $x$. That is:

$$f (m; N) \simeq N^2 \exp \left\{ -N \left[ x m - \ln J_0 (x) \right] \right\} .$$

where $x = |x|$ is related with $m = |m|$ by:

$$m = m (x) = \frac{I_1 (x)}{I_0 (x)} .$$

It is necessary to say that the validity of the steepest decent procedure is ensured by the positivity of the argument of the logarithmic term in the Eq.10.

1 For continuous variables, $W$ is only well-defined after a coarse grained partition of phase space, which is the reason why it is considered an small energy constant $\delta \varepsilon$ in order to make $W$ dimensionless. However, during the thermodynamic limit $N \to \infty$, the selection of $\delta \varepsilon$ does not matter if it is small.
The main contribution to the entropy per particle \( s(U, N; I, g) = \ln W/N \) for \( N \) large can be obtained by using again the steepest decent method as follows:

\[
s_o(U, N; I, g) = \frac{1}{2} \ln \left( \frac{2\pi Ig}{N^2} \right) + \max_x \left\{ \frac{1}{2} \ln \left[ m^2(x) + \kappa \right] - x m(x) + \ln I_0(x) \right\},
\]

where \( \kappa = 2U - 1 \). The maximization yields:

\[
\frac{m(x)}{x} - m^2(x) - \kappa \frac{x}{m^2(x) + \kappa} \frac{d}{dx} m(x) = 0,
\]

which represents the energy dependence of magnetization density for the bulk matter:

\[
U = \frac{1}{2} m(x) \bigg/ \frac{x}{x + \frac{1}{2} \left[ 1 - m^2(x) \right]} \bigg\} \text{ with } x \in [0, \infty), \quad \text{and } m = 0 \text{ if } U \geq U_c = 0.75.
\]

The caloric curve (14) is obtained from the canonical parameter \( \beta \):

\[
\beta = \frac{1}{T} = \frac{\partial s_0(U, N; I, g)}{\partial U} = \begin{cases} x/m(x) & \text{with } 0 \leq U < 0.75, \\ 1/(2U - 1) & \text{if } U \geq 0.75. \end{cases}
\]

This is the same result found by M. Antoni, H. Hinrichsen and S. Ruffo in the ref. [9]. Therefore, the subsequent analysis will be equivalent to their work. The microcanonical analysis confirms the existence of a second-order phase transition at the critical energy \( U_c = 0.75 \) with a critical temperature of \( T_c = 0.5 \).

It is interesting to note that although the main term of the entropy per particle is \( N \)-independent, there is an additional contribution which is \( N \)-dependent and makes the Boltzmann entropy nonextensive for an arbitrary \( N \)-dependence of the coupling constant \( g \). Although the selection of the \( N \)-behavior of the coupling constant does not change the thermodynamical picture in the microcanonical ensemble, it affects the extensive or nonextensive character of the energy in the thermodynamic limit, as well as the temporal scale in the dynamical behavior of this model system (see in the next section).

In order to deal with an extensive Boltzmann entropy is necessary to assume the following thermodynamic limit for the Hamiltonian mean field model:

\[
N \to \infty, \text{ keeping constant } \frac{E}{N^3} \text{ and } \frac{g}{N}.
\]

This assumption defers from the one used by other investigators, where the \( N \)-dependence of the coupling constant chosen in order to deal with an extensive energy.

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**FIG. 1: Microcanonical description of the HMF model in thermodynamic limit.** Here it is clearly shown a second-order phase transition at \( U_c = 0.75 \), where \( T_c = 0.5 \) and \( m = 0 \).

### III. THE ORIGIN OF THE SLOW RELAXATION REGIMEN

According to the Hamiltonian of the model, its motion equations are given by:

\[
\dot{\theta}_k = \frac{1}{L_k} k, \\
\dot{L}_k = g N (m_g \cos \theta_k - m_x \sin \theta_k),
\]

where \( k = 1, 2, \ldots N \) and it was used the expression given in Eq. (3). It is convenient to introduce the following characteristic units for time and momentum:

\[
\tau_0 = \sqrt{\frac{1}{gN}} \quad \text{and} \quad L_0 = \sqrt{1gN}.
\]

Note that, according to the thermodynamic limit (16), the characteristic time \( \tau_0 \) decreases with the \( N \) increasing as \( \tau_0 \propto 1/N \), while the characteristic momentum \( L_0 \) increases as \( L_0 \propto N \). However, when it is assumed the \( N \)-dependence (2) for the coupling constant, the characteristic time \( \tau_0 \) is \( N \)-independent. The time scale of \( \tau_0 \) gives the characteristic time scale for the evolution of each rotator, so that, this time units is relevant to microscopic level. In the numerical computation of the dynamics this characteristic time scale should be taken into account in order to ensure a great accuracy of the energy conservation.

Using the above characteristic units, as well as introducing the tridimensional vectors \( \mathbf{m}_k = (\cos \theta_k, \sin \theta_k, 0) \) and \( \mathbf{o}_k = (0, 0, L_k) \), the motion equations (14) are rephrased as follows:

\[
\dot{\mathbf{m}}_k = \mathbf{o}_k \times \mathbf{m}_k, \quad \dot{L}_k = \mathbf{m}_k \times L_k.
\]
The magnetization density obeys the following dynamical equation:

$$\dot{m} = Y = \Omega \times m + \Lambda m,$$

(20)

where $Y$ is the velocity of change of the magnetization density, $\Omega$, the angular velocity which characterizes the dynamical behavior of the $m$ orientation, while $\Lambda$ characterizes the behavior of its modulus. These quantities are given by:

$$Y = \frac{1}{N} \sum_{k=1}^{N} o_k \times m_k,$$

(21)

$$\Omega = \frac{1}{Nm} \sum_{k=1}^{N} (m_k \cdot m) o_k, \Lambda = \frac{1}{Nm} \sum_{k=1}^{N} o_k \times m_k \cdot m.$$ (22)

Since $o_k \times m_k$’s do not have a definite sign, the magnetization velocity of change $Y$ is a fast fluctuating quantity with a vanishing short time average (a time average along temporal interval comparable with the characteristic time of rotators evolution $\tau_0$) and standard deviation $\sigma_Y \sim 1/\sqrt{N}$. This fact provokes that the short time average of the magnetization $m$ varies slowly in comparison with the characteristic time scale of rotators evolution. Thus, there is two time scales in the dynamical evolution of the system: the microscopic time scale, $\tau_{mic} = \tau_0$, which is given by the characteristic time of the rotators evolution, and the macroscopic time scale, $\tau_{mac}$, which is given by the characteristic time of the short time average of magnetization density evolution, being this last considerably greater than the first time scale, $\tau_{mac} \gg \tau_{mic}$.

We are interested in studying the dynamical evolution of the macroscopic observables for temporal scale comparable with $\tau_{mac}$. Since $\tau_{mac} \gg \tau_{mic}$, at first approximation the dynamical evolution of $m$ could be modeled by a Langevin equation with multiplicative noise [10, 11]:

$$\dot{m} = Y = \sigma_1 (m; U) \xi_1 (t) e_1 + \sigma_2 (m; U) \xi_2 (t) e_2.$$ (23)

whose parameters $\sigma_1 (m; U)$ and $\sigma_2 (m; U)$ could be estimated by using a microcanonical average with fixed magnetization density. This last estimation is a reasonable approximation since the magnetization density only exhibits very small fluctuations around its short time average for $N$ large along time intervals comparable with $\tau_{mic}$. Here, $e_1$ and $e_2$ are unitary vectors in the parallel and perpendicular directions of $m$ respectively, being $e_3 = e_1 \times e_2 \equiv (0, 0, 1)$, the unitary vector along the third axis. $\xi_1 (t)$ and $\xi_2 (t)$ are Gaussian processes:

$$\langle \xi_i (t) \xi_j (t') \rangle = \tau_i \delta_{ij} \delta (t - t')$$ (24)

being $\tau_i$ the correlation times. The presence of $\delta_{ij}$ is due to the vanishing of the microcanonical average of $\langle Y_i Y_j \rangle = \langle e_i \cdot Y e_j \cdot Y \rangle$, with fixed magnetization density, which is easily proved by mean of a procedure anologue to the one used in the previous section for the determination of Boltzmann entropy. As already mentioned, the standard deviations of the components of the vector $Y$ depend on $N$ as $\sigma_j (m; U) \sim 1/\sqrt{N}$.

It is not difficult to understand that the correlation times $\tau_i$ are comparable with the microscopic time scale $\tau_{mic}$: the correlation times possess the same temporal scale of the characteristic time where the differentiable character of $Y$ is perceived, which is precisely characteristic time scale of rotators evolution.

According to the general theory, to this equation is associated the Fokker-Planck equation of the form:

$$\frac{\partial}{\partial t} F = \partial_{m_o} \left\{ \frac{1}{2} \tau_j \sigma_j \partial_{m_o} \left[ \sigma_j \partial_{m_o} F \right] \right\},$$ (25)

which describes the dynamics of the magnetization density distribution function $F = F (m, t; U)$. In this expression, the $\sigma_j$’s represent the components of $e_j$. Taking into account the $N$-dependence of $\sigma_j$, the right hand of the equation [20] decreases as $1/N$ during the $N$ increasing. Scaling the time scale as $t \rightarrow t = N t'$, the Fokker-Planck equation becomes $N$-independent. This means that the characteristic time scale for the dynamical evolution of $F (m, t; U)$, as well as all those macroscopic observables derived from $m$, have a linear dependence on $N$ during the increasing of system size (in $\tau_0$ units).

This is precisely the result which was observed in the numerical computation of the dynamics, where the relaxation time for the dynamical temperature $T_D (t) = 2K (t)/gN^2 = 2U - 1 + m^2 (t)$ grows proportional to $N$ with the $N$ increasing. As already mentioned, the time scale of such dynamical behaviors is precisely the macroscopic time scale $\tau_{mac}$:

$$\tau_{mac} \sim \tau_0 N = \sqrt{\frac{4N}{g}}.$$ (26)

Thus, when the thermodynamil limit [10] is taken into account, the relaxation time is finite when $N$ is tended to infinity. Therefore, no anomalous dynamical behavior will be observed: the thermodynamic limit ($N \rightarrow \infty$) necessary for the ensemble equivalence between the microcanonical ensemble with the canonical one, will commute with the infinite time limit ($t \rightarrow \infty$) necessary for the equilibration of the temporal average of the physical observables. Thus, the slow relaxation regimen observed in the microcanonical numerical computation of dynamics appears as consequence of the consideration of the $N$-dependence of the coupling constant [24]. The above analysis shows that the $N$-dependence of the coupling constant which ensures the extensivity of the Boltzmann entropy is more appropriate than the one which guarantees the extensivity of the energy. The first allows us to carry out a well-defined macroscopic description for the
Hamiltonian mean field model, instead, the second leads to the existence of dynamical anomalies.

IV. CONCLUDING REMARKS

As already showed, the microcanonical analysis revealed a thermodynamic limit \([16]\) which defers from the traditional assumption of the \(N\)-dependence of the coupling constant \([2]\). This thermodynamic limit is intimately related with the existence of the following self-similarity scaling behavior of the thermodynamical variables of the Hamiltonian mean field model:

\[
\begin{align*}
N \to N (\alpha) &= \alpha N, \\
E \to E (\alpha) &= \alpha^3 E, \\
g \to g (\alpha) &= \alpha g, \\
I \to I (\alpha) &= I,
\end{align*}
\]

\Rightarrow W (\alpha) = \mathcal{F} [W (1), \alpha] \quad (27)

where the functional \(\mathcal{F} [W, \alpha]\) defines an exponential self-similarity scaling laws for the microcanonical volume \(W\):

\[
\mathcal{F} [W, \alpha] = \exp [\alpha \ln W], \quad (28)
\]

being

\[
W (\alpha) = W [E (\alpha), N (\alpha); g (\alpha), I (\alpha)], \quad (29)
\]

where \(\mathcal{F} [W, \alpha]\) satisfies the self-similarity condition:

\[
\mathcal{F} [\mathcal{F} [W, \alpha_1], \alpha_2] = \mathcal{F} [W, \alpha_1 \alpha_2]. \quad (30)
\]

The reader may understand that this self-similarity scaling behavior is a generalization of the extensive properties exhibited by the traditional systems. As already discussed in our previous works, this self-similarity properties could be crucial in order to develop a well-defined thermodynamical description for a Hamiltonian nonextensive system \([12, 13, 14]\). We showed in the ref. \([14]\] how self-similarity can be used in order to analyze the necessary conditions for the validity of Tsallis’ Nonextensive Statistics \([13]\). The results obtained in the present paper seem to be consistent with this idea too.

In future works we hope to obtain an analytical expression for the parameters appearing in the Fokker-Planck equation \((25)\) in order to carry out a comparative study of this equation with the numerical computation of dynamics, since in this work we only concentrate on the analysis of their \(N\)-dependence.

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MICROCANONICAL DESCRIPTION

- **Caloric curve**
- **Magnetization curve**