Remarks about the thermostatistical description of the HMF model
Part I: Equilibrium Thermodynamics

L. Velazquez$^1$ and F. Guzman$^2$

$^1$Departamento de Física, Universidad de Pinar del Río, Martí 270, Esq. 27 de Noviembre, Pinar del Río, Cuba.
$^2$Departamento de Física Nuclear, Instituto Superior de Ciencias y Tecnología Nucleares, Carlos III y Luaces, Plaza, La Habana, Cuba.

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Abstract

In this series of papers we shall carry out a reconsideration of the thermodynamical behavior of the called HMF model, a paradigmatic ferromagnetic toy model exhibiting many features of the real long-range interacting systems. This first work is devoted to perform the microcanonical description of this model system: the calculation of microcanonical entropy and some fundamental thermodynamic observables, the distribution and correlation functions, as well as the analysis of the thermodynamical stability and the relevant thermodynamic limit.

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I. INTRODUCTION

The present effort deals with the macroscopic description of a toy model with a great conceptual significance: the called Hamiltonian Mean Field (HMF) model [1,2,3]. Despite the HMF model is enough amenable for allowing an accurate numerical and analytical characterization, it exhibits many features observed in more realistic long-range interacting systems such as: violent relaxation, persistence of metastable states, slow collisional relaxation, phase transition, anomalous diffusion, etc [4,5,6,7,8,9,10,11,12,13,14,15,16]. This reason explains why the present system is considered as a paradigmatic toy model in the understanding of the dynamical behavior of the HMF model with the aim to obtain a better understanding of its remarkable dynamical behavior. As expected, we begin to address the equilibrium thermodynamical properties of this model system by using the microcanonical description. As elsewhere discussed, the microcanonical ensemble is just a dynamical ensemble associated to the ergodic character of the many-body nonlinear Hamiltonian dynamics. Thus, the use of this statistical ensemble allows to keep a close relationship with the dynamical behavior of the HMF model studied by means of numerical microcanonical simulations. Besides the entropy and some relevant thermodynamical parameters, the magnetic susceptibility, the particles distribution and the two-body correlation function will be also obtained. Two novel aspects accounted for at the end of the present discussion are the analysis of thermodynamical stability and the relevance of the thermodynamic limit.

II. EQUILIBRIUM THERMODYNAMICS

The thermodynamical description of the HMF model by using the mean field approximation was considered in refs. [13,16]. We shall perform in this section the microcanonical description directly working on the $N$-body phase space. As usual, the microcanonical expectation value of any microscopic observable $A(X)$ is obtained from the expression:

$$A_m = \frac{1}{\Omega} \sum_p \delta (E - H_N) \langle A(X) \rangle,$$

where $\Omega$ is microcanonical states density, $\Omega = \sum_p \delta (E - H_N)$, while $\sum_p \delta (E - H_N)$ represents the $N$-body phase space integration:

$$\sum_p \delta (E - H_N) = \int dx_1 \ldots dx_N \prod_{i=1}^{N} \delta (E - H(x_i))$$
where the factorial term considers the particles identity.

The integration by $dW$ yields:

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

The accessible volume $W$ tends to infinity as follows:

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

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

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

The integration by $d^N L$ yields:

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

The main contribution of the integral when $N$ tends to infinity is obtained by using the steepest descend method:

$$f (m; N) \simeq \exp \left\{ -N \left[ x m - \ln I_0 (x) \right] - \frac{1}{2} \ln \left[ \left(\frac{2\pi}{N}\right)^2 \kappa_1 (x) \kappa_2 (x) \right] \right\},$$

where the functions $\kappa_1 (x)$ and $\kappa_2 (x)$ are given by:

$$\kappa_1 (x) = \frac{2m (x)}{x} + \frac{d}{dx} (x m (x) > 0, \ k_2 = \frac{m (x)}{x} > 0.$$

The main contribution to the entropy per particle $s (u, N; I, g) = \ln W/N$ when $N$ tends to infinity can be obtained by using again the steepest descend method as follows:

$$s (u, N; I, g) = s_0 + \max_x \left\{ \frac{1}{2} \ln \left[ m^2 (x) + \kappa \right] - x m (x) + \ln I_0 (x) \right\} + O \left( \frac{1}{N} \right).$$

The validity of the above approximation is ensured by the positivity of the argument of the logarithmic term in Eq. (12). The derivation of this expression appears in the appendix A. Notice that the integration function of Eq. (10) only depends on the modulus of $\mathbf{m}$, and therefore, the microcanonical expectation value of $\mathbf{m}$ identically vanishes as a consequence of the nonexistence of a preferential direction of this vector. Nevertheless, the expectation value of $\mathbf{m}$ can differ from zero as a consequence of the occurrence of a spontaneous symmetry breaking (see in the next subsection).

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The caloric curve is obtained from the canonical parameter $\eta = gN \beta = \partial s (u, N; I, g) / \partial u$:
FIG. 1: Microcanonical description of the HMF model in the thermodynamic limit: the caloric \( T(u) \) (solid line) and magnetization \( m(u) \) (dash line) curves clearly reveal the existence of a second-order phase transition at \( u_c = 0.75 \) with \( T_c = 0.5 \). The divergence of the correlation function \( g(u) \) (dash-dot line) manifests the existence of a long-range order at the critical point \( u_c \).

Thus, the heat capacity \( C(u) = (dT/du)^{-1} \) undergoes a discontinuity at \( u_c \):

\[
C(u_c^+) - C(u_c^-) = 2, \quad (23)
\]

being \( C(u) = 1/2 \) when \( u > u_c \).

The results obtained so far are in a total agreement with the one derived from the mean field approximation carried out in ref. [13]. As already evidenced, the thermodynamical features of the HMF model does not essentially differ from the ones exhibited by other ferromagnetic systems in the mean field approximation [17]. Therefore, the solution above provided should lost its validity in the neighborhood of the critical point \( u_c \) [13, 18, 19]. In order to show this fact, let us consider the second derivative of the maximization problem [15] which allows to check the stability of the stationary solution [17]:

\[
h(x; u) = \left( m'(x) - \frac{\kappa}{m^2(x) + \kappa^2} \right) m'(x). \quad (24)
\]

We have used the recurrence relations [10] and [11] in order to express the first derivative of the magnetization as \( m'(x) = 1 - m(x)/x - m^2(x) \). The stationary condition [16] allows to substitute the relation \( \kappa = \kappa(x) \equiv m(x)/x - m^2(x) \) into [24]. Thus, the second derivative [24] is negative everywhere with the exception of the stationary solution \( x = 0 \) corresponding to the paramagnetic phase:

\[
h(x = 0; u) \approx -\frac{u - u_c}{2u - 1}, \quad (25)
\]

which turns unstable when \( u < u_c \). The function \( h(x; u) \) is related to the average square dispersion of the magnetization throughout the expression:

\[
\langle \delta m^2 \rangle \simeq \langle m'(x) \delta x \rangle^2 \simeq -\frac{(m'(x))^2}{Nh(x; u)}, \quad (26)
\]

which diverges at the critical point of the second-order phase transition \( u_c \), yielding:

\[
\langle \delta m^2 \rangle = \frac{1}{4N} \frac{2u - 1}{u - u_c}, \quad (27)
\]

when \( u > u_c \). Since the average magnetization square dispersion is directly related to the correlation functions \( g_{ij} = \langle m_i \cdot m_j \rangle - \langle m_i \rangle \cdot \langle m_j \rangle \) via the formula:

\[
N \langle \delta m^2 \rangle \equiv \frac{1}{N} \sum_{ij} g_{ij} = g(u), \quad (28)
\]

the divergence of \( \langle \delta m^2 \rangle \) implies the existence of a long-range order at \( u_c \) [20] (see also in FIG. 1). It is well-known that the existence of such a phenomenon significantly modifies the behavior of the thermodynamical quantities close to the critical point \( u_c \).
B. Magnetic susceptibility

The Hamiltonian of the HMF model is invariant under the translation operation $\theta_k \rightarrow \theta_k + \psi$, which is equivalent to the $U(1)$ rotational symmetry acting on the rotator directions, whose existence implies the vanishing of the expectation value of the magnetization $m$. The $U(1)$ symmetry is broken by modifying the Hamiltonian with the incidence of an external magnetic field $H$ as follows:

$$H_N \rightarrow H_N^* = H_N - gN \sum_k H \cdot m_k. \quad (29)$$

The vector $H$ introduces now a preferential direction for the average magnetization, which leads to a modification of Eq.(1) as follows:

$$W \propto \int d^2m \, f \left( m; N \right) \left( m^2 + \kappa + 2H \cdot m \right)^{\frac{3}{2} N - 1}, \quad (30)$$

as well as the following dependences of the caloric and magnetization curves:

$$\varepsilon \left( x; H \right) = \frac{m \left( x \right) + H}{2x} + \frac{1}{2} \left[ 1 - m^2 \left( x \right) \right] - hm \left( x \right), \quad (31)$$

$$\eta = \frac{1}{T} = \frac{x}{m \left( x \right) + H}, \quad m \left( x \right) = \frac{I_1 \left( x \right)}{I_0 \left( x \right)}, \quad (32)$$

where $-H \leq \varepsilon \leq +\infty$, $0 \leq T \leq +\infty$, $0 \leq m \leq 1$ when $x$ goes from the infinity to zero, being $H = |H|$. Notice that we have distinguished between the dimensionless total energy $\varepsilon = u - Hm$ associated to the modified Hamiltonian and the dimensionless internal energy $u$ of the Hamiltonian. These curves are represented in FIG.2 by considering different values of the external field $H$. Thus, the system exhibits a nonvanishing magnetization $m$ for every finite energy $u$, as well as there is now a smooth dependence between $T$ and $\varepsilon$.

The caloric and magnetization curves are obtained from (31) and (32) when $H \rightarrow 0$. The expectation value of the magnetization drops to zero with the vanishing of $H$ when $u > u_c$, and therefore, the system recovers the original $U(1)$ symmetry. However, a nonzero magnetization along the direction of the external field survives when the vanishing of $H$ is carried out by keeping fixed its orientation. It means that the initial symmetry $U(1)$ is spontaneously broken when $u < u_c$.

Let us now obtain the magnetization dependence for low values of $H$ when $\varepsilon > u_c$. Since $m \left( x \right)$ and $x$ simultaneously vanish when $H \rightarrow 0$, we are able to use the power expansion in order to obtain the power expansion of the $H$ in terms of $x$ starting from Eq.(31):

$$H = 2x \left( \varepsilon - u_c \right) + x^3 \left( 2\varepsilon - \frac{19}{16} \right) + O \left( x^4 \right), \quad (33)$$

whose inversion leads to the expression:

$$x = \frac{1}{2} \frac{1}{\varepsilon - u_c} H - \frac{1}{4} \frac{32\varepsilon - 19}{\left( \varepsilon - u_c \right)^2} H^2 + O \left( H^3 \right). \quad (34)$$

We finally obtain the $m$ versus $H$ dependence by substituting this latter expansion into Eq.(19), yielding:

$$m \left( \varepsilon; H \right) = \frac{1}{4 \left( \varepsilon - u_c \right)} H - \frac{36\varepsilon - 22}{4 \left( \varepsilon - u_c \right)^2} H^2 + O \left( H^3 \right). \quad (35)$$

Thus, the microcanonical susceptibility $\chi^{(m)}_H$ when $u > u_c$ is given by:

$$\chi^{(m)}_H = \left( \frac{\partial m}{\partial H} \right) = \frac{1}{4 \left( \varepsilon - u_c \right)} - \frac{3}{4 \left( \varepsilon - u_c \right)^2} H^2 + O \left( H^3 \right), \quad (36)$$

which diverges at the critical energy $u_c$.

The dependence of the magnetization $m$ on the external field $H$ when $\varepsilon < u_c$ can be represented as $m = m \left( x_H \right)$, where $x_H = x \left( \varepsilon; H \right)$ is the solution of the problem:

$$\varepsilon \left[ x_H; H \right] = \varepsilon < u_c, \quad (37)$$

being $x \left( H, \varepsilon \right)$ the function defined by Eq.(31). The solution for small values of $H$ can be obtained by using the power expansions:

$$x_H = x + c_1 \left( x \right) H + c_2 \left( x \right) H^2 + \ldots, \quad (38)$$

$$m_H = m \left( x_H \right) = m \left( x \right) + \chi_1 \left( x \right) H + \chi_2 \left( x \right) H^2 + \ldots. \quad (39)$$
being $\varepsilon(x,0) = \varepsilon$ and $\chi_1(x) = m'(x)c_1(x)$, $\chi_2(x) = \frac{m''(x)}{4}c_1(x)^2 + m'(x)c_2(x)$, and so on. The substitution of Eqs. (38) and (39) into (37) yields the following results for the function $\chi_1$:

$$\chi_1(x) = \frac{m'(x)(m(x) - \frac{1}{x})}{(-m(x)m'(x) - \frac{m(x)}{2x} + \frac{1}{2}m'(x))}, \quad (40)$$

and $\chi_2 = p_1(x)/p_2(x)$, being:

$$p_1(x) = \chi_1(x) + \frac{1}{2}\chi_2'(x) - \frac{2}{x^3}(\frac{\chi_1(x)}{m'(x)})^2 + \frac{1}{2}\frac{\chi_1(x)}{x^2m'(x)}(\chi_1(x) + 1), \quad (41)$$

$$p_2(x) = -m(x) + \frac{1}{2x} - \frac{1}{2x^2}m'(x). \quad (42)$$

The function $\chi_1(x)$ represents the zero-order approximation of the power expansion for the microcanonical susceptibility $\chi_H^{(m)}(x,H)$ in terms of the magnetic field $H$. It is possible to show that $\chi_H^{(m)} \simeq \chi_1$ also diverges at $u_c$ as follows:

$$\chi_H^{(m)} \simeq \frac{1}{8}(u_c - \varepsilon), \quad (43)$$

when $\varepsilon < u_c$.

The above estimations of the microcanonical susceptibility $\chi_H^{(m)}$ are only applicable when $|\chi_1H| << 1$. In general, the magnetic susceptibility can be obtained from the formula:

$$\chi_H^{(m)} = m'(x)\left(\frac{\partial x}{\partial H}\right)_x. \quad (44)$$

which yields:

$$\chi_H^{(m)} = m'(x)'\left(m - \frac{1}{2x}\right)\left(\frac{m' + H}{2x} - \frac{m + H}{2} + \frac{m'}{x}\right)^{-1}. \quad (45)$$

The microcanonical susceptibility $\chi_H^{(m)}$ was also represented in FIG. 2 for different values of the external field $H$. Notice that $\chi_H$ remains almost constant at negative value $\chi_H^{(m)} \simeq -0.46$ when $\varepsilon < u_1 = 0.5$. The susceptibility begins to grow beyond the point $u_1$ and vanishes at $u_2 \approx 0.61$ independently of the value of the external field $H$. The behavior provoked by the presence of the factor $m(x) - 0.5/x$. The system exhibits a large susceptibility under the influence of a very small external magnetic field in the energetic range $(u_2, u_c)$, which is related to the existence of the second-order phase transition at $u_c$.

It worth to remark that the microcanonical susceptibility $\chi_H^{(m)}$ also admits negative values when $\varepsilon < u_2$. According to the well-known theorem derived from the canonical description:

$$\chi_H^{(c)} = \frac{\partial \langle M \rangle}{\partial H} = \beta G_c, \quad (46)$$

being $G_c = \langle \Delta M^2 \rangle$, the average square dispersion of the magnetization within this ensemble, the magnetic susceptibility should be nonnegative. Actually, the microcanonical susceptibility $\chi_H^{(m)}$ obtained in this subsection provides a measure of the magnetic sensibility of the system at constant energy instead of at constant temperature. It can be shown that the microcanonical counterpart of the identity (46) in the thermodynamic limit [21] is given by:

$$\chi_H^{(m)} = \frac{\partial \langle M \rangle}{\partial H} = \beta G_m + \langle M \rangle \frac{\partial \langle M \rangle}{\partial E}, \quad (47)$$

which clarifies that the negative values of $\chi_H^{(m)}$ come from the term $M\partial M/\partial E$ since usually $\partial M/\partial E < 0$ in the ferromagnetic phase.

C. Distribution functions

Let us now obtain the microcanonical n-body distribution functions of this model: $F_m^{(n)}[y] = F_m^{(n)}(y_1, \ldots, y_n)$:

$$F_m^{(n)}[y] = \frac{1}{\Omega}Sp[\delta(y_1 - x_1) \ldots \delta(y_n - x_n) \delta(E - H_N)], \quad (48)$$

where $x_k = (\theta_k, L_k)$. We shall assume that in the ferromagnetic phase there is a nonvanishing magnetization $\mathbf{m} = (m, 0)$, which could be obtained by considering the Hamiltonian (29) with $H = (H, 0)$ and sending $H$ to zero.

The state density $\Omega$ can be rephrased in a functional form $\mathcal{F}$ as follows:

$$\Omega \propto \mathcal{F}[\psi, N] = \int d^2\mathbf{m} f(\mathbf{m}, N)[\psi^2]^{N-1}, \quad (49)$$

where $\psi = \psi(\mathbf{m}; N) = 2u - 1 + \mathbf{m}^2$ (see in Eq. (6)). It is easy to see that the n-body distribution functions can be also rephrased by using this same functional form as follows:

$$F_m^{(n)} \propto \frac{\mathcal{F}[\psi + \delta\psi_n; N - n]}{\mathcal{F}[\psi, N]}, \quad (50)$$

where $\delta\psi_n$ is given by:

$$\delta\psi_n = -\frac{2}{N} \left(\sum_{k=1}^n \tilde{e}_k\right) + \frac{1}{N^2} \left(\sum_{k=1}^n \delta\mathbf{m}_k\right)^2, \quad (51)$$
being \( \mathbf{m}_k = \mathbf{m} (\theta_k) = (\cos \theta_k, \sin \theta_k) \) the magnetization vector, \( \delta \mathbf{m}_k = \mathbf{m}_k - \mathbf{m} \), the corresponding dispersion, and \( \delta \varepsilon_k - \mathbf{m} \cdot \mathbf{m}_k \equiv \varepsilon_k \) the energy of the \( k \)-th rotator. We also consider for convenience the dimensionless momentum \( p_k = L_k / L_0 \) by introducing the characteristic unit \( L_0 = \sqrt{\eta N} \).

The expression (50) suggests to perform a perturbative expansion in power series of \( 1 / N \) of the functional \( \ln \mathcal{F} (\psi + \delta \psi; N - n) \) by taking into account the Gaussian localization of these integrals when \( N \) tends to infinity. We obtain after some algebra the following result:

\[
F_n^{(m)} [y] \propto \int d^2 \mathbf{m} f (\mathbf{m}, N - n) \psi^{(N-n)-1} F^{(n)} [y; \mathbf{m}],
\]

where \( F^{(n)} [y; \mathbf{m}] \):

\[
\simeq \exp \left\{ -n \sum_{k=1}^{n} \varepsilon_k \right\} \left\{ 1 + \frac{1}{N} \left[ \frac{1}{2} \eta \left( \sum_{k=1}^{n} \delta \mathbf{m}_k \right)^2 + \right. \right.
\]

\[
\left. \left. - \eta^2 \left( \sum_{k=1}^{n} \varepsilon_k \right)^2 + (n + 2) \eta \sum_{k=1}^{n} \varepsilon_k \right\} + \mathcal{O} \left( \frac{1}{N} \right), \tag{53}
\]

being \( \eta = \psi^{-1} \), the dimensionless inverse temperature.

The progressive calculation demands a refinement of the steepest descend method in order to account for the \( 1 / N \)-contribution obtained beyond of the Gaussian estimation (see in appendix A 2).

The zero-order approximation of the one-body distribution function is given by:

\[
f_m (\theta, p; u) = C \exp (-\eta \varepsilon), \tag{54}
\]

where \( \varepsilon = \varepsilon (\theta, p) = \frac{1}{2} p^2 - \mathbf{m} \cdot \mathbf{m} (\theta) \), the normalization constant is given by:

\[
C^{-1} = \sqrt{\frac{2\pi \eta}{2\pi I_0 (\eta \varepsilon)}}, \tag{55}
\]

and the magnetization vector \( \mathbf{m} \) satisfied the self-consistent relation:

\[
\mathbf{m} = \int d\theta dp \mathbf{m} (\theta) f_m (\theta, p; u). \tag{56}
\]

Fig. 3 shows the angular distribution function \( \rho (\theta; u) \) for different energies:

\[
\rho (\theta; u) = \int dp f_m (\theta, p; u) = \frac{\exp (x \cos \theta)}{2\pi I_0 (x) \cdot \text{exp} (x \cos \theta)}, \tag{57}
\]

where the relation \( x \equiv \eta \varepsilon \) was taken into account. Notice that the ferromagnetic states with \( u > u_c \) are characterized by the existence of a clustered distribution of the angular variables \( \theta_k \) around the direction of the magnetization vector \( \mathbf{m} \), while a uniform distribution is observed in the paramagnetic phase with \( u > u_c \). This is the reason why the ferromagnetic states are referred as a clustered phase, while the paramagnetic ones are referred as a homogeneous phase.

The terms of the two-body correlation function \( g_m^{(2)} (x_1, x_2) = F_m^{(2)} (x_1, x_2) - F_m^{(1)} (x_1) F_m^{(2)} (x_2) \) surviving the first-order approximation are given by:

\[
g_m^{(2)} (x_1, x_2) \simeq \frac{1}{N} f_1 f_2 \left[ \Phi_{12} + \eta^2 g (u) \Theta_{12} \right] + \mathcal{O} \left( \frac{1}{N} \right); \tag{58}
\]

where \( f_i = f_m (\theta_i, p_i; u) \) is the zero-order approximation of the one-body distribution function (54), \( g (u) = N \left( \Delta \mathbf{m}^2 \right) \), the correlation function derived from the average magnetization dispersion \( \left( \Delta \mathbf{m}^2 \right) \) showed in Fig. 3 and \( \Phi_{12} \) and \( \Theta_{12} \), two new form factors given by:

\[
\Phi_{12} = \eta \delta \mathbf{m}_1 \cdot \delta \mathbf{m}_2 - 2\eta^2 \delta \varepsilon_1 \delta \varepsilon_2, \tag{59}
\]

\[
\Theta_{12} = (2\eta \delta \varepsilon_1 + \delta \mathbf{m}_1) \cdot (2\eta \delta \varepsilon_2 + \delta \mathbf{m}_2). \tag{60}
\]

The quantities \( \delta \varepsilon_i = \varepsilon_i - \langle \varepsilon \rangle \) and \( \delta \mathbf{m}_i = \mathbf{m}_i - \mathbf{m} \) represent the energy and magnetization deviations respectively. The presence of the function \( g (u) \) in Eq. (58) leads to the divergence of the two-body correlation function at the critical point \( u_c \). The spacial two-body correlation function in the homogeneous phase is given by \( g (\theta_1, \theta_2) = (2\pi)^{-2} c_2 (\theta_1, \theta_2; u) \), where the function:

\[
c (\theta_1, \theta_2) = \left( 1 + \frac{1}{4} \frac{1}{u - u_c} \right) \frac{1}{2u - 1} \cos (\theta_1 - \theta_2), \tag{61}
\]
diverges at the critical point of terms in the inverse temperature \( \eta \) as follows \( \simeq 4 (\eta_c - \eta)^{-1} \cos (\theta_1 - \theta_2) \). This
asymptotic behavior is consistent with the one estimated in the refs. [13, 18, 19], but (61) is now the exact microcanonical result within the first-order approximation.

The inexistence of three-body terms in Eq. (53) straightforwardly leads to the vanishing of the three-body correlation function \( g_m^{(3)} (x_1, x_2, x_3) \):

\[
g_m^{(3)} (x_1, x_2, x_3) = F_m^{(3)} (x_1, x_2, x_3) - g_m^{(2)} (x_1, x_2) F_m^{(1)} (x_3) - g_m^{(2)} (x_2, x_3) F_m^{(1)} (x_1) - g_m^{(2)} (x_3, x_1) F_m^{(1)} (x_2),
\]

in the first-order approximation, and hence, the three-body correlations are just \( O (1/N) \) size effects. Such a microcanonical result will be taken into consideration during the derivation of suitable dynamical equations for the distribution and correlation functions based on the well-known BBGKY hierarchy.

### III. THERMODYNAMIC STABILITY

Thermodynamic stability concerns the question about when a given admissible macrostate characterized by a certain energy and magnetization is stable or unstable under thermal fluctuations associated to the thermodynamic equilibrium where the temperature and the magnetic field act as constant control parameters. Such a question is also intimately related to the nature of the correspondence between the control parameters \((\eta, H)\) and the controlled system observables \((u, m)\) (internal energy \(u\) and the projection of the magnetization \(m\) along the magnetic field), that is, the existence or inexistence of the ensemble equivalence.

The analysis starts from the consideration of the partition function \( Z = \int dX_N \exp \left[ -\beta H_N^* \right] \) and the introduction of the Planck thermodynamical potential per particle \( p (\eta, H) = -\ln Z (\eta, H) / N \), which can be rephrased as follows:

\[
\exp \left[ -Np (\eta, H) \right] \propto \int d\mu_d \exp \left[ -Np (\eta, H, u, m) \right],
\]

where \( p (\eta, H, u, m) = \eta u + \lambda m - s (u, m) \) with \( \lambda = -\beta H \) and the detailed entropy \( s (u, m) \) given in a parametric form by:

\[
s (u, m) = s_0 + \frac{1}{2} \ln \left( \kappa + m^2 (x) \right) - m (x) + \ln J_0 (x)
\]

within the approximation provided by the steepest descend method. The exponential function of the integral (63) exhibits sharp peaks around its maxima when \( N \) is large enough, a behavior that allows to rephrase the integral (63) within the Gaussian approximation as follows:

\[
\sim \sum_k \exp \left[ -Np_k \right] \int \exp \left[ \frac{1}{2} NB (u, m; u_k, m_k) \right] d\mu_d,
\]

where \( p_k = p (\eta, H; u_k, m_k) \) and the bilinear form \( B (u, m; u_k, m_k) = H_{uu} \Delta u_k^2 + (H_{um} + H_{mm}) \Delta u_k \Delta m_k + H_{mm} \Delta m_k^2 \) with \( \Delta u_k = u - u_k \) and \( \Delta m_k = m - m_k \) obtained from the entropy \( H_{ij} \):

\[
H_{ij} = \begin{pmatrix} H_{uu} & H_{um} \\ H_{um} & H_{mm} \end{pmatrix} = \begin{pmatrix} \partial^2 s/\partial u^2 & \partial^2 s/\partial u \partial m \\ \partial^2 s/\partial u \partial m & \partial^2 s/\partial m^2 \end{pmatrix},
\]

evaluated at the \( k \)-th stable stationary point:

\[
\beta = \frac{\partial s (u_k, m_k)}{\partial u}, \quad \lambda = \frac{\partial s (u_k, m_k)}{\partial m},
\]

which satisfies the negative definition of the Hessian matrix (60). From the thermodynamical point of view, such maxima represent the coexisting macrostates or phases appearing for given values of \( \beta \) and \( H \). Obviously, there is ensemble inequivalence when there exist only one maximum representing a unique stable phase with given values of \((u, m)\). The greatest peak during the phase coexistence corresponds to the stable phase, while the other represent metastable states. The greatest peak corresponding to the stable phase provides the main contribution of the integral (63) allowing to estimate the Planck thermodynamic potential per particle as follows:

\[
p (\eta, H) = \inf \left\{ \eta u + \lambda m - s (u, m) \right\}.
\]

This is just the Legendre transformation which constitutes a fundamental stone of the thermodynamic formalism [20]. All those admissible macrostates of the system satisfying the stationary condition (67) but do not obey the negative definition of the entropy Hessian matrix (60) are precisely the unstable macrostates.

Performing the calculations, the canonical parameters:

\[
\beta = \frac{\partial s}{\partial u} = \frac{1}{\kappa + m^2 (x)}, \quad \lambda = \frac{\partial s}{\partial m} = \frac{m}{\kappa + m^2 (x)} - x,
\]

allow to express the magnetic field \( H \) and the temperature \( T = \beta^{-1} \) in terms of the macroscopic observables \( \kappa \) and \( m, m^2 \leq 1 \). The regions of stability in the plane \((\kappa, m)\) are determined from the entropy Hessian:

\[
H_{ij} = \beta^2 \begin{pmatrix} 2 & -2m \\ -2m & \kappa - m^2 - a (\kappa + m^2)^2 \end{pmatrix},
\]

being \( a^{-1} = m^2 (x) \equiv 1 - m (x) / x - m^2 (x) \). The determinant \( D = \det H_{ij} = -2 (\kappa + m^2)^3 \left[ 1 - a (\kappa + m^2) \right] \) vanishes at the boundary of the unstable region, a curve which is parametrically represented as:

\[
[k (x), m (x)] = \left[ 1 - \frac{m (x)}{x} - 2 m^2 (x), m (x) \right].
\]
the critical point $C$ observed in several systems [22] in terms of the thermodynamic potentials like the microcanonical entropy per particle $s(\varepsilon, H)$ or the Helmholtz Free energy per particle $f(\beta, H) = \inf_{\varepsilon} \{ \varepsilon - T s(\varepsilon, H) \}$ or $\inf_{u,m} \{ u - H m - T s(u, m) \}$ at the critical point $C$ can be related to the bifurcation of the magnetization curve shown in FIG.4 or caloric curve show in FIG.5 for $H = 0$. The system is unable to follow the "trajectory" $BCA$ with $m = 0$ since the branch $CA$ is located inside the region of ensemble inequivalence where there exist anomalous macrostates with $\chi_H^{(c)} < 0$. The large thermodynamic fluctuations existing there provoke a sudden change of the original tendency $BCA$ following in this way anyone of the stable symmetric branches $CP$ or $CQ$ with a nonvanishing magnetization $m \neq 0$, and consequently, the occurrence of a spontaneous symmetry breaking [20].

IV. SOME FINAL REMARKS

As already illustrated, the thermodynamic properties of the HMF model do not essentially differ from the other ferromagnetic models with short-range interactions. We have previously shown that the relevant microcanonical thermodynamic variable is $u = E/gN$, and the characteristic energy is $E_0 = gN^2$. The thermodynamic limit is carried out when $N$ is sent to the infinity by keeping fixed the dimensionless energy $u$. This is the same thermodynamic limit introduced in ref. [13] in order to perform the mean field description of this model. However, our analysis reveals that the entropy per particles is ill-defined in the thermodynamic limit: while the term of $s(u, N; I, g)$ containing the relevant thermodynamical variable $u$ is $N$-independent, the $N$-dependent additive constant $s_0 = \frac{1}{2} \ln (2\pi e^2 I g / N)$ diverges when $N \to \infty$. The lost of analyticity in the thermodynamic limit of the well-known thermodynamical identity $\chi_H^{(c)} = \beta \langle \delta M^2 \rangle$, but which is microcanonically admissible. Actually, it possesses the same anomalous character of the macrostates with a negative heat capacity $C = dE/dT < 0$ observed in several systems [22] in terms of the thermodynamical identity $C = \beta^2 \langle \delta E^2 \rangle$. The unstable region (dark zones in the plane ($\kappa, m$) shown in FIG.4) is characterized by the presence of negative values of the magnetic susceptibility at constant temperature $\chi_H^{(c)} = \langle \partial M / \partial H \rangle_T$, a behavior canonically anomalous for this kind of model system in terms of the critical point of the continuous phase transition $C$: $(\kappa_c, 0)$ with $\kappa_c = 2u_c - 1 = 0.5$ is just a bifurcation point of the magnetization curves located at the endpoint of the metastable region which touches also the stable and the unstable regions, and therefore, it is a point of marginal stability.

These results are summarized in FIG.4 and FIG.5: The curve $PAQ$ is the boundary of the physically admissible macrostates. The thick solid lines represent the magnetization curves at $H = 0$. The stable branch $PCQ$ constitutes the boundary between the stable and metastable regions. The critical point of the continuous phase transitions $C$: $(\kappa_c, 0)$ with $\kappa_c = 2u_c - 1 = 0.5$ is just a bifurcation point of the magnetization curves located at the endpoint of the metastable region which touches also the stable and the unstable regions, and therefore, it is a point of marginal stability.

The unstable region (dark zones in the plane ($\kappa, m$)) shown in FIG.4 is characterized by the presence of negative values of the magnetic susceptibility at constant temperature $\chi_H^{(c)} = \langle \partial M / \partial H \rangle_T$, a behavior canonically anomalous for this kind of model system in terms of the well-known thermodynamical identity $\chi_H^{(c)} = \beta \langle \delta M^2 \rangle$, but which is microcanonically admissible. Actually, it possesses the same anomalous character of the macrostates with a negative heat capacity $C = dE/dT < 0$ observed in several systems [22] in terms of the thermodynamical identity $C = \beta^2 \langle \delta E^2 \rangle$. The lost of analyticity in the thermodynamic limit of the thermodynamic potentials like the microcanonical entropy per particle $s(\varepsilon, H) = \sup_m \{ s[u = \varepsilon + H m, m] \}$ or the Helmholtz Free energy per particle $f(\beta, H) = \inf_{\varepsilon} \{ \varepsilon - T s(\varepsilon, H) \}$ or $\inf_{u,m} \{ u - H m - T s(u, m) \}$ at the critical point $C$ can be related to the bifurcation of the magnetization curve shown in FIG.4 or caloric curve show in FIG.5 for $H = 0$. The system is unable to follow the "trajectory" $BCA$ with $m = 0$ since the branch $CA$ is located inside the region of ensemble inequivalence where there exist anomalous macrostates with $\chi_H^{(c)} < 0$. The large thermodynamic fluctuations existing there provoke a sudden change of the original tendency $BCA$ following in this way anyone of the stable symmetric branches $CP$ or $CQ$ with a nonvanishing magnetization $m \neq 0$, and consequently, the occurrence of a spontaneous symmetry breaking [20].
The imposition of the thermodynamic limit affects the system dynamical behavior during the characteristic temporal scales. Therefore, any scaling acting on the dynamical evolution of a given system, and to the statistical independence or separability of a large system in independent subsystems appearing as a consequence of the existence of short-range forces. Obviously, such a microscopic picture is outside the context within intrinsic nonextensive nature.

The HMF model could be considered as a limit case with \( \alpha \to 0 \) of a parametric family of ferromagnetic models on a square lattice [25] whose potential energy is given by:

\[
V_{\alpha} = \frac{1}{2} g \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{1}{r_{ij}^{\alpha}} [1 - \cos (\theta_i - \theta_j)],
\]

where \( r_{ij} \) is the lattice distance between the \( i \)-th and \( j \)-th rotator. The integral estimation of potential energy per particle in the paramagnetic phase (where the averages open brackets \( \langle \cos (\theta_i - \theta_j) \rangle \) close brackets \( = 0 \) by using a lattice with spacing \( a \) and linear dimension \( R \propto \sqrt{N} \):

\[
v_{\alpha} = V_{\alpha}/N \sim a^{-2} \int_{0}^{R} \frac{2\pi r dr}{r^{\alpha}} = 2\pi \left( (\alpha - 2)^{-1} (a^{2-\alpha} - R^{2-\alpha}) \right) \frac{\alpha \neq 2}{\ln (R/a)} \alpha = 2
\]

allows to understand that such as models are extensive in the thermodynamic limit when \( \alpha > 2 \) and nonextensive elsewhere. As a consequence of the existence of long-range correlations, the nonextensive system cannot be trivially divided in independent subsystems, and therefore, there is no physical reason to justify the imposition of the extensive character of the total energy in this case.

The using a suitable scaling dependence for the coupling constants in order to regularize the thermodynamic parameters and potentials of a given system in the thermodynamic limit might be applicable in some way that also ensures a well-defined dynamical behavior characterized by the commutativity of the limits \( \lim_{N \to \infty} \) and \( \lim_{T \to \infty} \). Generally speaking, all that it is necessary to demand is the non divergence of the relaxation timescale \( \tau_{eq} \) when \( N \to \infty \). With some recent exceptions [11, 12], most of numerical studies of the microscopic dynamics of the HMF model revealed a characteristic relaxation timescale for the HMF model given by \( \tau_{eq} = \tau_{mic} N \), being \( \tau_{mic} = \sqrt{TN/g} \) the characteristic microscopic time of the rotators evolution [3, 5, 7, 8, 10]. It is easy to realize that the imposition of the scaling \( g/N = \gamma = const \) ensures both the well-defined behavior of the additive constant of the entropy per particle \( s_0 = \frac{1}{2} \ln (2\pi e^2 \gamma g/N) \) and the relaxation timescale \( \tau_{eq} = \sqrt{TN/g} \) when \( N \to \infty \). This ansatz leads to a power-law growing of the characteristic energy \( E_0 \propto N^3 \), which does not involves in principle any physical inconsistency since the HMF model is nonextensive. We shall return to this discussion in the forthcoming papers.

APPENDIX A: DEMONSTRATIONS

1. Derivation of Eq.(12)

We perform the power expansion up to the second order approximation of \( k \) for the complex number \( z \):

\[
z = -i \sqrt{\textbf{K}^2} = x + i n \cdot \textbf{k} = \frac{1}{2x} k^2 - \frac{1}{2x} (n \cdot k)^2 + O \left( |k|^2 \right),
\]

being \( x = |x| \) and \( n = x/|x| \). Let us now carry out the power expansion for the function \( I_0 (x + \Delta z) \) in terms of the variable \( \Delta z \) up to the second order approximation, being \( \Delta z = z - x \):

\[
\ln I_0 (x + \Delta z) = + m (x) \Delta z + \frac{1}{2} \frac{dm (x)}{dx} (\Delta z)^2 + O \left( (\Delta z)^2 \right),
\]

\[
(m (x))_{|x|} = \frac{1}{2 \pi} \frac{d}{dx} \left[ \int_{0}^{2\pi} e^{-|x| \cos \theta} d\theta \right] = \frac{x}{|x|^2} \frac{d}{dx} \left( 1 - \frac{1}{2} \text{Re} \left( \frac{1}{i \text{Im} (x)} \right) \right)
\]

\[
(m (x))_{|x|} = \frac{1}{2 \pi} \frac{d}{dx} \left[ \frac{1 - e^{-2|x|}}{|x|^2} \right] = \frac{1}{2 \pi} \frac{d}{dx} \left( \frac{1}{|x|^2} \right) = 0
\]

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(m (x))_{|x|} = \frac{1}{2 \pi} \frac{d}{dx} \left( \frac{1}{|x|^2} \right) = 0
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\]
where \( m(x) = I_1(x) / I_0(x) \). Thus, the exponential function:

\[
\exp [N \mathbf{k} \cdot \mathbf{m} + \ln I_0(z)],
\]

can be rewritten by dismissing the terms \( O(|k|^2) \) as follows:

\[
\simeq \exp (-N [xm - \ln I_0(x)]) \times \exp \left\{ -\frac{N}{2} \left[ \kappa_1(x) k_1^2 - \kappa_2(x) k_2^2 \right] \right\},
\]

where \( x \parallel \mathbf{m} \) and \( m = |\mathbf{m}|; k_1^2 = (\mathbf{n} \cdot \mathbf{k})^2 \) and \( k_2^2 = k^2 - (\mathbf{n} \cdot \mathbf{k})^2 \); while \( \kappa_1(x) = 2m(x)/x + dm(x)/dx \) and \( \kappa_2(x) = m(x)/x \). Since \( m(x) \) is an odd monotonic increasing function, with \( m(x) \geq 0 \) when \( x \geq 0 \), the functions \( \kappa_1(x) \) and \( \kappa_2(x) \) are always nonnegative. The integration of the expression \( \text{[A4]} \) leads to the result shown in Eq. \( \text{[A2]} \).

2. Refinement of the steepest descend method

The calculation of the first-order approximation of the correlation functions involves a little refinement of the steepest descend method. The aim is the determination of the \( 1/N \)-contributions of the average of a physical quantity \( A(x) \) as follows:

\[
\langle A \rangle \Omega = \int A(x) \exp [Ns(x;a)] d^nx,
\]

where the partition function \( \Omega \) is given by:

\[
\Omega = \int \exp [Ns(x;a)] d^nx.
\]

Firstly, we perform the power expansion of the function \( s(x) \) around its maximum point \( x_0 \) as follows:

\[
s(x) \simeq s(x_0) + c_2 \cdot (\Delta x)^2 + R(\Delta x; x_0),
\]

where the higher-order contributions \( R(\Delta x; x_0) \) are denoted by:

\[
R(\Delta x; x_0) = \sum_{m=3}^{\infty} c_m \cdot (\Delta x)^m.
\]

Hereafter, we shall consider the following convention in order to simplify the notation during the calculation. For example, the term \( c_m \cdot (\Delta x)^m \) represents the tensorial product:

\[
c_m \cdot (\Delta x)^m = \frac{1}{m!} \sum_{\{i\}} \frac{\partial^m s(x_0)}{\partial x^{i_1} \partial x^{i_2} \ldots \partial x^{i_m}} \Delta x^{i_1} \Delta x^{i_2} \ldots \Delta x^{i_m}.
\]

Eq. \( \text{[A7]} \) allows to express the exponential function as follows:

\[
\exp [Ns(x)] = \exp [Ns(x_0)] \exp \left[ -\frac{1}{2} \omega \cdot (\Delta x)^2 \right] F(\Delta x; x_0),
\]

where \( \omega = -2Nc_2 \) and the function \( F(\Delta x; x_0) = \exp [NR(\Delta x; x_0)] \) is given by:

\[
F(\Delta x; x_0) = \sum_{k=0}^{\infty} \frac{1}{k!} N^k R^k(\Delta x; x_0).
\]

This latter result can be conveniently rewritten as a power series expansion:

\[
F(\Delta x; x_0) = \sum_{m=0}^{\infty} \kappa_m \cdot (\Delta x)^m,
\]

where

\[
\kappa_m = \sum_{\{j\}} \delta \left( m - \sum_{k=3}^{\infty} k j_k \right) \prod_{k=3}^{\infty} \frac{N\kappa c_k^k}{j_k!}.
\]

being \( \delta(n) \) an integer function defined by:

\[
\delta(n) = \begin{cases} 1 & n = 0 \\ 0 & n \neq 0 \end{cases}.
\]

It can be checked that the first 10 coefficients of the power expansion \( \text{[A12]} \) are given by:

\[
\kappa_0 \equiv 1, \quad \kappa_1 \equiv \kappa_2 = 0, \quad \kappa_3 \equiv Nc_4, \quad \kappa_4 \equiv Nc_5,
\]

\[
\kappa_5 \equiv Nc_5, \quad \kappa_6 \equiv Nc_6 + \frac{1}{2!} N^2 c_3^2, \quad \kappa_7 \equiv Nc_7 + N^2 c_3 c_4,
\]

\[
\kappa_8 \equiv Nc_8 + N^2 \left( c_3 c_5 + \frac{1}{2!} c_1^2 \right),
\]

\[
\kappa_9 \equiv Nc_9 + N^2 \left( c_3 c_6 + c_4 c_5 \right) + \frac{1}{3!} N^3 c_3^3,
\]

\[
\kappa_{10} \equiv Nc_{10} + N^2 \left( c_3 c_7 + c_4 c_6 + \frac{1}{2!} c_5 c_5 \right) + \frac{1}{2!} N^3 c_3^3 c_4.
\]

Taking into account that in the Gaussian integration:

\[
\langle (\Delta x)^n \rangle = N_0 \int d^nx \exp \left[ -\frac{1}{2} \omega \cdot (\Delta x)^2 \right] (\Delta x)^k,
\]

survive only the odd dispersions, denoting by \( g_{2k} = N^k \langle (\Delta x)^{2k} \rangle \), being \( N_0 = \sqrt{\det \left( \frac{1}{2\pi} \omega \right)} \) the normalization constant, the first-order approximation of the partition function \( \Omega \) is given by:

\[
\Omega = \Omega_0 \left\{ 1 + \frac{1}{N} \left( c_4 g_4 + \frac{1}{2} c_3^2 g_6 \right) \right\},
\]

where \( \Omega_0 = \exp [Ns(x_0)] / N_0 \) is the zero-order approximation of the partition function.
The calculation of the integral \( \langle A \rangle \) is carried out by performing the power expansion of the quantity \( A(x) \) around the maximum point \( x_0 \)

\[
A(x) = \sum_{m=0}^{\infty} A^{(m)} \cdot (\Delta x)^m,
\]

(A18)

being:

\[
A^{(m)} \cdot (\Delta x)^m = \frac{1}{m!} \sum_{\{i\}} \frac{\partial^m A(x_0)}{\partial x_{i_1} \partial x_{i_2} \ldots \partial x_{i_m}} \Delta x_{i_1} \Delta x_{i_2} \ldots \Delta x_{i_m},
\]

(A19)

which allows to rewrite:

\[
A(x) F(\Delta x; x_0) = \sum_n B_n (\Delta x)^n,
\]

(A20)

being:

\[
B_n = \sum_{m=1}^{n} A^{(m)} \kappa_{n-m}.
\]

(A21)

Thus, the first-order approximation of the integral \( \langle A \rangle \) is given by:

\[
\langle A \rangle \Omega = \Omega_0 \left\{ A^{(0)} + \frac{1}{N} \left( A^{(2)} g_2 + \right. \right. + \left. \left. \left( A^{(0)} c_4 + A^{(1)} c_3 \right) g_4 + \frac{1}{2} A^{(0)} c_3^2 \right) \right\},
\]

(A22)

which leads to the following result

\[
\langle A \rangle = A^{(0)} + \frac{1}{N} \left( A^{(2)} g_2 + A^{(1)} c_3 g_4 \right).
\]

(A23)

Restoring now the ordinary notation, we finally obtain:

\[
\langle A \rangle = A(x_0) + \frac{1}{2!} \sum_{i_1 i_2} \partial^2 A(x_0) \left( \Delta x_{i_1} \Delta x_{i_2} \right) + \cdot \cdot \cdot
\]

(A24)

where \( \langle \Delta x_{i_1} \Delta x_{i_2} \rangle \propto 1/N \) and \( \langle \Delta x_{i_1} \Delta x_{i_2} \Delta x_{i_3} \Delta x_{i_4} \rangle \propto 1/N^2 \).

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