We study the Hamiltonian Mean Field (HMF) model, a system of \( N \) fully coupled particles, in the microcanonical ensemble. We use the previously obtained free energy in the canonical ensemble to derive entropy as a function of energy, using Legendre transform techniques. The temperature-energy relation is found to coincide with the one obtained in the canonical ensemble and includes a metastable branch which represents spatially homogeneous states below the critical energy. “Water bag” states, with removed tails momentum distribution, lying on this branch, are shown to relax to equilibrium on a time which diverges linearly with \( N \) in an energy region just below the phase transition.

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I. INTRODUCTION

In a pioneering work Fermi, Pasta and Ulam\(^*\) showed that in a Hamiltonian system with short-range interactions the relaxation time to thermodynamical equilibrium can be extremely long if the energy is small enough. This striking feature triggered an intense research activity and, nowadays, the relation between macroscopic thermodynamical properties and microscopic dynamics is actively investigated in a large variety of physical systems.\(^\dagger\) The common belief that microcanonical time averages coincide with equilibrium ensemble averages after a possibly quite long transient is confirmed by several numerical experiments (see Refs. \(^\ddagger\) for reviews). Therefore, although the rigorous proof of ergodicity is restricted to a few rather abstract dynamical systems (e.g. the Sinai billiard), it is nevertheless believed, and confirmed numerically,\(^*\ddagger\), that time averages of thermodynamic functions (temperature, internal energy, specific heat) converge to their equilibrium values, at least in the regime of strong chaos.

The case of long-range forces is quite less explored from this point of view. The study of relaxation to thermal equilibrium is here made more complex by the consequences of the inequivalence of statistical ensembles. Indeed, it is well known that the impossibility to isolate a small sub-system from a large thermal bath, due to the presence of long-range forces, prevents the derivation of canonical from microcanonical ensemble.

Exactly solvable toy models\(^\ddagger\) with weak long-range forces explicitly display ensemble inequivalence and the presence of negative specific heat in the microcanonical ensemble. Similar phenomena were also obtained for gravitational models\(^\dagger\). These toy models show a first order phase-transition in the canonical ensemble, which corresponds to the presence of a concave region of the entropy-energy curve in the microcanonical ensemble. This feature is present also in microcanonical molecular dynamics simulations of short-range models without hard-core,\(^\ddagger\) where one observes, in the phase-transition region, a high-density clustered phase coexisting with a low-density gaseous phase. More recently, microcanonical Monte-Carlo simulations have shown similar properties for the diluted three-state Potts model\(^\dagger\).

All the previous remarks concern equilibrium properties, but it is known that long-range interacting systems show also extremely slow relaxation to equilibrium. A remarkable example is the one-dimensional self-gravitating potential, where the study of long transients and quasi-equilibria has been undertaken by many groups.\(^\ddagger\) More recently, a scaling law for the relaxation to equilibrium has been proposed for gravitational systems based on diffusion in phase-space\(^\ddagger\).

The Hamiltonian Mean Field (HMF) model\(^\dagger\) has been introduced with the aim of studying clustering phenomena in \( N \)-body systems in one dimension. The original motivation was to consider a truncated Fourier series development of the one-dimensional gravitational and charged sheet models. Its canonical ensemble exact solution predicts a second-order phase transition from a clustered phase to a gaseous one. HMF is an infinite range interacting system and one would naturally expect unusual thermodynamical behaviour. However, microcanonical simulations of HMF show that “carefully” prepared initial states lead to a good agreement with canonical analytical results for the energy-temperature relation\(^\ddagger\). On the other hand, “water bag” initial states, \( ie. \) states with momentum distribution on a finite support, are metastable and show an extremely slow
relaxation to equilibrium near the critical energy [3].

In this paper, we derive analytically the entropy-energy relation of the HMF model in the microcanonical ensemble. We further study the properties of metastable states corresponding to the low energy extension of the high energy gaseous phase. The relaxation time of these states to canonical equilibrium is also investigated, showing that it increases linearly with the number of particles \( N \) near the critical energy.

II. THE MODEL

The Hamiltonian Mean Field model describes the dynamics of \( N \) classical and identical particles confined to move on the unit circle [2]. Its Hamiltonian writes

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

where \((\theta_i, p_i)\) are canonically conjugated coordinate and momentum variables with \( \theta_i \in [0, 2\pi] \). \( K \) is the kinetic energy and the potential energy \( V \) corresponds to the first harmonic of the one-dimensional self-gravitating potential \( V = \sum_{i < j} |\theta_i - \theta_j| \) (up to scaling constants). Total momentum \( \sum_i p_i \) is also conserved and always set to zero without loss of generality.

In the canonical ensemble, model (1) undergoes a second-order phase transition at the inverse temperature value \( \beta_c = T_c^{-1} = 2 \) [12], corresponding to a critical specific energy \( U_c = E_c/N = 3/4 \). The free energy

\[
F(\beta) = -\frac{1}{\beta} \lim_{N \to \infty} \left[ \frac{1}{N} \ln Z(\beta, N) \right], \tag{2}
\]

where

\[
Z(\beta, N) = \prod_i dp_i d\theta_i \exp(-\beta H), \tag{3}
\]

has been obtained using saddle-point techniques [12], giving

\[
-\beta F = \frac{1}{2} \ln \left[ \frac{2\pi}{\beta} \right] - \frac{\beta}{2} + \max_x \left[ X(x, \beta) \right], \tag{4}
\]

where

\[
X(x, \beta) = \ln(2\pi I_0(x)) - \frac{x^2}{2\beta}, \tag{5}
\]

\( I_0 \) being the zero order modified Bessel function. The maximization of \( X \) is performed by solving the consistency equation

\[
x = \frac{I_1(x)}{I_0(x)} \beta. \tag{6}
\]

whose unique solution at small \( \beta \) is \( x = 0 \), while at large \( \beta \), i.e. low temperature, a pair of symmetric non vanishing solutions is present. The bifurcation (of pitchfork type) occurs at \( \beta_c = 2 \) and at this temperature the value of the free energy \( F \) has a discontinuity in the second order derivative, which is the signature of a second-order phase transition. This is also confirmed by the calculation of the order parameter

\[
M = \frac{1}{N} \left( \sum_{i=1}^{N} \cos \theta_i \right) \left( \sum_{i=1}^{N} \sin \theta_i \right) = M \left( \cos \Phi, \sin \Phi \right), \tag{7}
\]

which vanishes continuously at \( \beta_c \), remaining zero in the whole high temperature phase. At low temperatures, \( M \) measures the degree of clustering of the particles.

The equations of motion derived from model (1), written in terms of \( M \), show that each particle has a pendulum like motion

\[
\ddot{\theta}_i = -M \sin(\theta_i - \Phi), \tag{8}
\]

which makes explicit the self-consistent nature of the dynamics, since each particle moves in the \( M \)-field, which is itself determined by the position \( \theta_i \) of all the particles. This has led [12] to the interpretation of the phase transition as a dynamical process of particle evaporation from the cluster. Moreover, this approach follows the idea that the study of self-consistent \( N \)-body dynamics is simplified by an “effective” reduction of the number of degrees of freedom [4].

III. ENTROPY - ENERGY RELATION.

The free energy \( F(\beta) \) in the canonical ensemble is readily computed once one knows the dependence of entropy \( S \) on specific energy \( U = E/N \) in the microcanonical ensemble. One begins from the relation

\[
Z(\beta, N) = \int_0^{\infty} \omega(E, N) e^{-\beta E} dE, \tag{9}
\]

where

\[
\omega(E, N) = \int \prod_i dp_i d\theta_i \delta(E - H) \tag{10}
\]

is the microcanonical phase-space density at energy \( E \). The lower limit of the integral in (9) is given by the energy of the ground state, which vanishes in our model (in this case all of the particles are at the same position with zero momentum). After rescaling by \( N \) and exponentiating \( \omega \) Eq. (3) becomes

\[
Z(\beta, N) = N \int dU \exp\left( N(-\beta U + \frac{1}{N} \ln(\omega(E, N))) \right). \tag{11}
\]
This integral is then solved by the saddle-point technique in the $N \to \infty$ limit, which implies taking the maximum of the argument of the exponential. Using the definition of entropy

$$S(U) = \lim_{N \to \infty} \left[ \frac{1}{N} \ln \omega(U N, N) \right]$$

(12)

and recalling the definition of free energy (3), one finally gets

$$- \beta F(\beta) = \max_U [ -\beta U + S(U) ] .$$

(13)

Entropy $S$ and free energy $F$ are thus related by a Legendre transform. Assuming now that $S$ is concave (i.e. downward bended), one can invert (13) and obtain

$$S(U) = \min_{\beta > 0} [ \beta (U - F(\beta)) ] .$$

(14)

This assumption is not innocent and the inversion (14) can be safely used only for second order phase transitions, as it is for our model. On the contrary, it is well known that for first-order phase transitions entropy has a concave region (3), which is responsible for the negative specific heat in the microcanonical ensemble. A generalization of model (6) to particle motion on the two-dimensional torus (15) does have a first-order phase transition, making the inversion impossible in this case.

The calculation of entropy in the microcanonical ensemble is then reduced to the min-max procedure

$$S(U) = \min_x \max_{\beta > 0} [ \beta U + \frac{1}{2} \ln \left( \frac{2 \pi}{\beta} - \frac{\beta}{2} + X(x, \beta) \right) ] ,$$

(15)

with $X$ given by (3). For $\beta > \beta_c = 2$ the max is at $x = 0$ and the min at $\beta = 1/(2U - 1)$, which gives the entropy function

$$S(U) = \frac{1}{2} \ln (2U - 1) + \text{const} .$$

(16)

This is plotted in fig. 1 with full line above $U = U_c = 3/4$ and with dashed line for $1/2 < U < U_c$ (below $U = 1/2$ the temperature $T = 1/\beta$ becomes negative and the solution meaningless). This solution corresponds to the high temperature Homogeneous Phase (HP) with $M = 0$ for $U > U_c$ and to the MetaStable (the meaning is clarified below) Homogeneous Phase $MS_{HP}$ below $U_c$. Both phases are present also in the canonical solution and while in this latter context the $MS_{HP}$ corresponds to a local, but not global, minimum of the free energy, in the microcanonical context the entropy of the $MS_{HP}$ is not maximal. Indeed, the solution which maximizes the entropy bifurcates continuously from this one at $U_c$.

Below this energy the equilibrium solution is related to the two symmetric solutions with $x \neq 0$ of the consistency equation (3). They give the new maximum value of $X$ in (3) and the numerical search of the minimum in $\beta$, which is unique, allows to compute the stable branch of $S(U)$ below $U_c$. The latter is plotted in fig. 1 with the continuous line and labelled $CP$, because it corresponds to the Clustered Phase, which is characterized by a non vanishing value of $M$. The temperature $T$ can also be derived from the standard relation $\delta S / \delta U = T^{-1}$ and is reported in fig. 1. The stable solution $S(U)$ (full line) is continuous with its derivative. The discontinuity is in the second derivative, which gives a jump in the specific heat $C_v = (\partial T / \partial U)^{-1}$.

To summarize, our results suggest that the microcanonical solution is fully consistent with the one in the canonical ensemble, and we can therefore conclude that the two ensembles lead to equivalent results for model (6).

IV. METASTABILITY

However, the dynamics reveals a quite peculiar behavior of the microcanonical metastable branch. We have performed numerical simulations in microcanonical fixed-energy conditions by integrating the equations of motion (5), starting from appropriately chosen initial states. We have used a fourth order symplectic algorithm (19) with a time step 0.1, allowing relative energy conservation as good as $10^{-5}$. We have checked the energy-temperature curve, defining temperature as twice the time average of the kinetic energy: $T = 2 < K >$. The equilibrium energy-temperature solution is reached from generic initial states over most part of the energy range. However, for $1/2 < U < U_c$ relaxation to equilibrium becomes very slow. We have started the runs in this range with the particles homogeneously distributed on the circle ($M = 0$) and with a “water bag” momentum distribution: the momenta are uniformly distributed in an interval around zero such that the variance of the distribution coincides initially with the temperature of the metastable branch $T = 2U - 1$.

The relaxation of the initial “water bag” to the equilibrium state proceeds through the slow development of Maxwellian tails in the velocity distribution. In the literature one can already find indications that the relaxation time to equilibrium grows linearly with $N$ (13) (the authors used as a criterion the convergence to the Boltzmann entropy of the Maxwellian). We have decided to consider directly the time evolution of the temperature of the $MS_{HP}$ states. The initial temperature lies below the equilibrium one (see dashed line in fig. 1) and relaxes to a fixed threshold temperature $\sigma T_{\text{eq}}$ after a time $t_{\text{relax}}$, where $\sigma < 1$ is the threshold amplitude and $T_{\text{eq}}$ is the microcanonical equilibrium temperature represented

\footnote{We thank an anonymous referee for this remark.}
by the full line in fig. 1. Considering different initial states, we have observed that the fluctuations of $t_{relax}$ are Poissonian and that a well defined average exists. This average relaxation time $t_{av,relax}$ is plotted in fig. 2 for $\sigma = 0.9$ as a function of $N$ for different values of $U$. For $U < 0.56$, $t_{av,relax}$ is almost independent of $N$ whereas for larger values of $U$, $t_{av,relax}$ increases approximately as $N$. Nothing substantially changes using different thresholds by changing the value of $\sigma$. We are therefore able to confirm, for a different observable and a better statistics (we have considered up to 3600 initial conditions for the points in fig. 2), the results of Ref. 13 on the linear divergence of the relaxation time with $N$, at least in a restricted energy interval just below $U_c$. The existence of such divergence implies that performing the $N \to \infty$ limit before the $t \to \infty$ limit, the system will stay indefinitely out of equilibrium and the momentum distribution will never develop Maxwellian tails. This has attracted the attention of Tsallis 17, who argues that his entropy definition should be appropriate to describe the thermodynamical properties of such metastable states in the thermodynamic limit (in particular it would possibly describe the power law tails of the momentum distribution). It should however be remarked that what we have tested here is not the divergence of the lifetime of such states, but that of the relaxation time. However, recent numerical simulations performed by Rapisarda 18 seem to indicate also the divergence of the lifetime with $N$, encouraging Tsallis’ interpretation. Furthermore, it is possible to prepare states on the metastable branch which have initially a Maxwellian momentum distribution and those states are observed to relax to equilibrium pretty fast. It seems that the “water bag” condition, which corresponds to an initial truncation of the tails, is a necessary one for obtaining a divergence of the relaxation time.

V. CONCLUSIONS AND PERSPECTIVES

Let us summarize what we have found. The microcanonical solution of the Hamiltonian Mean Field model is here obtained with Legendre transform techniques, which avoid state counting. The entropy is computed using a min-max procedure and the energy-temperature relation is derived analytically. The equilibrium states are shown to coincide with the canonical ones in the thermodynamic limit. This result is not obvious since, due to the long-range interparticle coupling, ensemble equivalence might have been violated. Besides the equilibrium solutions, other states are found, corresponding to the metastable homogeneous configurations lying below the critical energy. The study of their relaxation time to equilibrium exhibits a divergence proportional to the number of particles, meaning that in the thermodynamic limit the trajectory in the phase-space remains indefinitely trapped in a non-equilibrium region (something similar to so-called “mechanical” initial states for the Fermi-Pasta-Ulam model in Ref. 12). Further investigations are necessary to understand the relevance of the metastable states for other more realistic long-range forces, beginning with the very interesting extension of the HMF proposed by Tsallis and co-workers 20,21, whose canonical solution has been recently obtained in Ref. 24. These results could be relevant for the physics of self-gravitating systems and for nuclear dynamics, where long-range forces play a distinctive role.

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FIG. 1. The entropy $S$ as a function of $U$ (upper graph) and the corresponding energy temperature relation (lower graph). The equilibrium values of $S$ and $T$ vs. $U$ is plotted as a solid line, both above (HP) and below (CP) the critical energy $U_c = 3/4$. These same quantities, evaluated for the metastable homogeneous phase $MS_{HP}$, are represented by dashed lines. The inset in the upper graph zooms in the energy range where the phase transition occurs. The vertical dotted line indicates the critical energy $U_c$.

FIG. 2. Average relaxation time $t_{\text{av,relax}}$ for an initial $MS_{HP}$ configuration as a function of $N$ for several values of $U$ with $\sigma = 0.9$. The upper solid line indicates the slope of the linear $N$ dependence for comparison.