Microscopic dynamics of a phase transition: equilibrium vs out-of-equilibrium regime

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We present for the first time to the nuclear physics community the Hamiltonian Mean Field (HMF) model. The model can be solved analytically in the canonical ensemble and shows a second-order phase transition in the thermodynamic limit. Numerical microcanonical simulations show interesting features in the out-of-equilibrium regime: in particular the model has a negative specific heat. The potential relevance for nuclear multifragmentation is discussed.

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1. INTRODUCTION

In the last years there has been a lot of interest in the nuclear physics community for multifragmentation reactions and for the study of liquid-gas phase transition in finite systems such as nuclei. It is still a debated question whether nuclear multifragmentation is an equilibrium type of transition, and if it is first or second-order. With the scope of adding new useful arguments to this debate, we present for the first time to the nuclear physics community the Hamiltonian Mean Field (HMF) model, a system of classical spins coupled through long-range attractive forces. HMF can be solved analytically in the canonical ensemble and shows a second-order phase transition in the thermodynamic limit. Moreover HMF has the double advantage of allowing a microcanonical and dynamical approach to explore the dynamics of a phase transition in a finite system. We believe that, in the same spirit of the Ising model, introduced many years ago, but still studied with extreme interest in statistical mechanics, the HMF model, though its dynamics is probably less complex than that one of a real system, can become a tool of primary importance to extract information on the microscopic dynamics of a second-order phase transition.

In this paper we discuss the equilibrium and out-of-equilibrium properties of the model, focusing our attention on the importance of the relaxation to equilibrium and on the possible discrepancies between different ensembles. In this respect the model can be extremely useful also for the nuclear multifragmentation phase transition. In particular in section 3, we show how misleading information on the order of a phase transition can

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Figure 1. Equilibrium microcanonical simulations for N=500 (open squares) in comparison with the theoretical predictions (full curves). The numerical results are averaged over several runs. The small discrepancies around the critical point ($U_c = 0.75$) and in the high energy region are due to finite-size effects.

be obtained from a specific heat analysis [13] if the system is not perfectly equilibrated.

2. HMF: THE CANONICAL ENSEMBLE

The Hamiltonian Mean Field (HMF) model was introduced by Ruffo [16] in 1994 and has been since then intensively studied both analytically and numerically [17–21]. The Hamiltonian of the model describes a system of N fully-coupled particles moving on the unitary circle, where the particles are characterized by the angles $\theta_i$ and the conjugate momenta $p_i$. It reads:

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

being $K$ and $V$ the kinetic and potential energy. If one considers a spin vector associated to each particle $m_i \equiv [\cos \theta_i, \sin \theta_i]$, the Hamiltonian then describes a linear chain of N classical fully-coupled spins, similarly to the XY model, and we can define a total magnetization vector $M \equiv [M_x, M_y] = \frac{1}{N} \sum_{i=1}^{N} m_i$. A very important feature of the HMF model is that it presents an analytical solution in the canonical ensemble. The solution has been worked out by Antoni and Ruffo, by means of the Hubbard-Stratonovich method.
to perform the integration over the angles \[16\]. The system behaves as a ferromagnet at low energy and shows a second-order phase transition at the critical energy density \(U_c = 0.75 (U = E/N \text{ where } E \text{ is the total energy})\), corresponding to a critical temperature \(T_c = 0.5 \text{(} U = E/N \text{)}\). If the sign of the interaction is inverted, one gets an antiferromagnetic behavior: this case has been studied in detail in refs \[16,20,22\]. The theoretical caloric curve reads:

\[
U = \frac{E}{N} = \frac{\partial (\beta F)}{\partial \beta} = \frac{1}{(2 \beta)} + \frac{1}{2} \left(1 - M^2\right),
\]

(2)

where \(\beta = 1/kT\) is the inverse of the temperature (the Boltzmann constant \(k\) is set to be equal to 1). The canonical caloric curve is shown in fig.1 (a) as a full curve: it increases almost continuously with energy, but has a discontinuity at the critical point. The modulus of the total magnetization, \(M\), shown as full curve in fig.1(b), is close to one for very low energy and decreases to zero by increasing the energy. It is equal to zero for \(U \geq U_c\). It has been shown that the phase-transition in the HMF model is a second-order one with mean field critical exponents \(\beta = 1/2, \alpha = 0 \text{ } [16,18]\). It is very intriguing the fact that, though HMF was not constructed to describe a nucleus, its caloric curve turns out to be very similar to the one measured by the ALADIN group[1] and more recently by other experimental collaborations[2,3,5] for nuclear systems.

3. HMF: THE MICROCanonical ENSEMBLE

In this section we discuss the microcanonical numerical simulations and we compare with the equilibrium canonical solution. The Hamilton equations of motion for the \(N\) particles are

\[
\dot{\theta}_i = p_i , \quad \dot{p}_i = -\sin(\theta_i)M_x + \cos(\theta_i)M_y , \quad i = 1, ..., N ,
\]

(3)

and can be solved numerically for different sizes of the system. In this way HMF allows a dynamical microcanonical approach, perfect to explore the dynamics of a phase transition in a finite system. The equations of motion were integrated by means of a 4th order simplicial algorithm [23] with a time step \(\delta t = 0.2\) and a relative error in the total conserved energy smaller than \(\Delta E/E = 10^{-5}\). More details can be found in Refs [17,18].

3.1. Equilibrium Results

In this paper we consider a system with \(N = 500\), a number of particles of the same order of the typical number of nucleons in a nuclear multifragmentation reaction. We start the system out-of-equilibrium, in the so-called “water bag”, i.e. by putting all rotators at \(q_i = 0\) and giving an initial velocity according to a constant probability distribution function of finite width centered around zero [16,17]. We remind the reader that, though the interaction in HMF is not explicitly constructed to model a nuclear system, such a far-off-equilibrium initial condition is a good way to simulate the strong off-equilibrium conditions present in a hot and compressed nuclear system before multifragmentation.

We follow the dynamics of HMF up to a final time \(t = 2 \cdot 10^6\) and we show in fig.1 the final results of the numerical integration. The numerical results were integrated also on several different runs. Such long integration times are necessary because, when out-of-equilibrium initial conditions are used, the system equilibration can be very slow. This is
especially evident close to the critical point, where the presence of quasi-stationary (long living) non-equilibrium states (QSS) [17,18] has been revealed. The temperature, the total magnetization, the kinetic fluctuations and the specific heat per particle are reported as a function of the energy density as open squares and compared to the theoretical predictions (full curves). The temperature is computed from the average kinetic energy per particle $T = 2 \langle K \rangle /N$, where the symbol $\langle \rangle$ stands for time averages. The kinetic energy fluctuations $\Sigma$, obtained from the scaled variance of the kinetic energy $\Sigma = \sqrt{\frac{\langle K^2 \rangle - \langle K \rangle^2}{N}}$, are compared to the theoretical prediction in the microcanonical ensemble. The latter is given by the formula $\Sigma = \frac{T}{\sqrt{2}} \sqrt{1 - [1 - 2M(\frac{dM}{dT})]^{-1}}$ [18]. Finally, in panel (d), we compute the specific heat per particle at constant volume in the microcanonical ensemble using the formula proposed for the first time by Lebowitz, Percus and Verlet [24]:

$$C_V = \frac{1}{2} \left[ 1 - 2 \left( \frac{\Sigma}{T} \right)^2 \right]^{-1}.$$  

(4)

In general, the numerical microcanonical caloric curve and the magnetization obtained at very long times agree quite well with the canonical predictions, apart from small finite-size effects located mainly around the critical point and in the supercritical region, the homogeneous phase. In the latter, the magnetization, due to the fact that $N=500$, is not
Figure 3. Non-equilibrium microcanonical simulations N=500 (open circles) in comparison with the theoretical predictions (full curves). The integration was stopped at time $t = 3000$ and the results averaged over several runs. Compare also with figs. 2, 4 and see text for further details.

exactly zero and assumes a finite value, i.e. $M \sim 1/\sqrt{N}$. This has visible consequences on the temperature, according to formula (2) and thus also on the kinetic energy fluctuations and the specific heat. We note that the microcanonical specific heat at equilibrium is always positive and agrees with the theoretical formula (reported as a solid line). In conclusions the canonical ensemble and the microcanonical simulations at equilibrium are in good agreement. The equivalence of different ensembles in the thermodynamic limit is also supported by recent analytical results in the microcanonical ensemble [21].

3.2. Out-of-Equilibrium results

In the previous subsection we have presented the microcanonical numerical results obtained in the equilibrium regime. In the present one we study the process of relaxation to equilibrium and we show that HMF has a very rich dynamics.

In fig.2 we report the time evolution of the temperature for different energies, and we study how it relaxes to the canonical value, represented by dashed straight lines. Though for $U=0.8,0.4$ the equilibrium temperature is almost reached already at a time $t = 3000$, close to the critical point, and in particular for the energy $U=0.7$, we have to wait for much longer times (for a time $t > 5 \cdot 10^5$). In fact, before the relaxation to the canonical value, there is a well defined plateau, where the temperature assumes a constant value
Comparison of specific heat formulas

Evolution towards relaxation

U = 0.6 N = 500

Figure 4. We show, for a typical event, the time evolution of the specific heat per particle at constant volume $C_V$ for $N = 500$ and $U = 0.6$. $C_V$ assumes negative values in the non-equilibrium regime (up to time $t \sim 3000$). The dashed straight line gives the equilibrium value.

smaller than the canonical prediction. The same behavior appears in a whole energy region $0.5 < U \leq U_c$ and, as shown in ref. [19,27], it corresponds to the presence of Quasi-Stationary States (QSS). The plateaus are longer the greater the system size, and in the $N \to \infty$ the system does not relax to the standard canonical equilibrium, remaining forever in the QSS [27]. The QSS represent a different dynamical equilibrium for non-extensive systems, and according to an intriguing scenario recently proposed by Tsallis [28], the reason could be the inversion of the time limit with the size limit, an inversion which is implicit in our numerical simulations.

In fig.3 we report the same quantities shown in fig.1, now calculated for a very short time, i.e. at $t = 3000$ instead of $t = 2 \cdot 10^6$. For this time, average variables, such as $T$ and $M$, have almost reached the canonical equilibrium for a large range of initial energies $U$, see panel (a) and (b). There are, however, relevant differences with respect to the equilibrium values in the region $0.5 < U \leq U_c$, in correspondence to the presence of the QSS, where the caloric curve $T(U)$ shows a backbending typical of a first-order phase transition, see in particular the magnification reported in the inset of panel (a). On the other hand, fluctuations are affected by non-equilibrium effects in the whole spectrum of energy. In fig.3(c) the kinetic energy fluctuations are bigger than the equilibrium ones. As a consequence, see eq.4, the specific heat per particle reported in fig.3(d) assumes negative values and the behavior of $C_V$ versus $U$ thus obtained is similar to the one found in nuclear multifragmentation data, see fig.4 of ref.[13]. In particular the authors
of ref.\[13\] claim that such a negative branch in the heat capacity is a direct evidence of a first-order phase transition. Here we have a practical example that also a system with a second-order phase transition can show a negative specific heat and a backbending in the caloric curve, due to the non perfect equilibration. This effect increases with the size of the system and becomes stable in the limit $N \to \infty$ \[26,27\]. This dynamical effect that simulates a first-order phase transition can be somehow explained by the presence of superdiffusion and Lévy walks in the out-of-equilibrium regime \[19\], that implies the coexistence of a liquid (clustered particles) and a gas (free particles) phase \[26\]. It is interesting to investigate the relaxation of the specific heat to the equilibrium value. In fig.4 we report $C_V$, calculated by means of eq. \[4\] versus time for the case $U=0.6$. $C_V$ is negative in the out-of-equilibrium regime, in correspondence of QSS, and converges very slowly to the equilibrium value. It is therefore necessary to wait for very long times, longer than for the temperature thermalization, to have also the thermalization of specific heat to positive values. A more complete study of the specific heat in HMF is in preparation \[26\]. We notice in conclusions that the slow relaxation around the critical point persist notwithstanding the strong chaocity found for the microscopic dynamics and reported in our previous work \[17,18,20\]. The reason for that is not completely understood, though it has been found that the Lyapunov exponent is proportional to the kinetic fluctuations and some heuristic conjectures have been proposed \[27\].

4. CONCLUSIONS

We have presented equilibrium and out-of equilibrium microcanonical simulations of HMF, a simple system of interacting spins. Though the model is not explicitly built to describe nuclear system, we think it can give interesting information for the multifragmentation phase transition. In fact, HMF can be solved in the canonical ensemble and has a second-order phase transition in the thermodynamic limit. Moreover, the advantage with respect to Ising, lattice gas models and percolation, is that HMF allows a dynamical microcanonical approach to the study of phase transitions in a finite system. HMF has a very rich dynamical behavior in a transient out-of-equilibrium regime whose timescale depends on the energy and on the size of the system. When the microcanonical simulations are started in an out-of-equilibrium initial state, for example in a “water bag”, we find the appearance of quasi-stationary-states. In correspondence we have a caloric curve with a well defined backbending and negative specific heat. These indications of a first-order phase transition, at variance with the second-order phase transition predicted in the thermodynamic limit, are effects of the non-equilibrium. Certainly the non-equilibrium features of the model are strictly linked to the long-range nature of the interaction, however the general validity of these results is not completely clear and further work in this direction is needed.

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