

Rotators with Long-Range Interactions: Connection with the Mean-Field Approximation

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We analyze the equilibrium properties of a chain of ferromagnetically coupled rotators which interact through a force that decays as $r^{-\alpha}$ where r is the interparticle distance and $\alpha \geq 0$. By integrating the equations of motion we obtain the microcanonical time averages of both the magnetization and the kinetic energy. We detect three different regimes depending on whether α belongs to the intervals $[0, 1)$, $(1, 2)$, or $(2, \infty)$. For $0 < \alpha < 1$, the microcanonical averages agree, after a scaling, with those obtained in the canonical ensemble for the mean-field case ($\alpha = 0$). This correspondence offers a mathematically tractable way of dealing with systems governed by slowly decaying long-range interactions.

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One of the most important questions in statistical mechanics refers to the connection between dynamics and thermodynamics: To what extent does a suitable ensemble average allow one to predict the time average of a physical observable performed by our instruments in the laboratory? Or, in other words, what are the mechanical specifications of those systems to which the results of statistical physics can be applied? Within this context, while ergodicity and mixing have been analyzed intensively in the literature, there is another important point which has not received the same degree of attention, that is, the possibility of defining a thermodynamically suitable energy function. In fact, for systems governed by sufficiently long-range interactions decaying as $r^{-\alpha}$ with the interparticle distance r , there results a *nonextensive* Hamiltonian; i.e., the energy per particle diverges in the thermodynamic limit $N \rightarrow \infty$ [1,2]. Gravitational ($\alpha = 1$, $d = 3$) and monopole-dipole ($\alpha = 2$, $d = 3$) interactions are only two well known instances among many others. Furthermore, such forces are particularly interesting since they can lead to equilibrium behaviors different from those observed in short-range systems and even give place to phase transitions otherwise absent, even in the $d = 1$ case.

Our aim here is to investigate how to deal with systems governed by long-range interactions by analyzing a simple but rich prototype with adjustable α . The main goal of this Letter is to show that the mean-field limit ($\alpha = 0$) is able to describe the thermodynamics in the whole range $0 < \alpha < 1$. The model consists in a one-dimensional chain of N interacting rotators with periodic boundary conditions. Each rotator moves on the unit circle, and therefore it is fully described by the angle $-\pi < \theta_i \leq \pi$ and its conjugate momentum p_i (with $i = 1, \dots, N$). The dynamics of the chain is governed by the following Hamiltonian:

$$H = \frac{1}{2} \sum_i p_i^2 + \frac{1}{2} \sum_{i \neq j} \frac{1 - \cos(\theta_i - \theta_j)}{r_{ij}^\alpha} \equiv K + U, \quad (1)$$

where, without loss of generality, we have chosen unitary moments of inertia for all the particles. Here r_{ij} measures the minimal distance between rotators i and j along the chain. The Hamiltonian (1) describes a classical inertial XY ferromagnet. K and U denote the kinetic and potential energies, respectively. The equations of motion ruling this dynamical system are

$$\dot{\theta}_i = p_i, \quad (2)$$

$$\dot{p}_i = - \sum_{j \neq i} \sin(\theta_i - \theta_j) / r_{ij}^\alpha. \quad (3)$$

We associate with each particle a spin vector

$$\mathbf{m}_i = (\cos \theta_i, \sin \theta_i) \quad (4)$$

and define the total magnetization of the system as

$$\mathbf{M} = \frac{1}{N} \sum_i \mathbf{m}_i. \quad (5)$$

The long-time behavior of \mathbf{M} determines whether the system orders ($\mathbf{M} \neq 0$) or not ($\mathbf{M} = 0$).

We also introduce a time dependent temperature $T(t)$ as $T(t) = (2/N) \langle K \rangle(t)$, where $\langle \dots \rangle$ denotes a time average performed over the time interval $(0, t)$. By calculating the long-time behavior of T as a function of the total energy of the system one gets the *caloric curve* T vs E/N from which the specific heat function is extracted.

Note that the $\alpha \rightarrow \infty$ limit yields the first-neighbor case while $\alpha = 0$ represents the mean-field version. The later case has a correspondence with the model known in the literature as Hamiltonian mean-field (HMF) XY, provided the potential energy (thus the strength of the interactions) is scaled by the number of particles N , i.e.,

in the HMF model $U = \frac{1}{2N} \sum_{i \neq j} [1 - \cos(\theta_i - \theta_j)]$. The HMF model has received special attention during the last years, and very interesting results have been obtained for both its equilibrium and nonequilibrium properties [3–5]. This model can be solved analytically within the canonical ensemble formalism [3]. It is found that there is a critical specific energy at which the system suffers a phase transition separating a paramagnetic high energy phase (with $\mathbf{M} = 0$) from a ferromagnetic low energy one (with $\mathbf{M} \neq 0$). More precisely, $E/N = T/2 + (1 - \mathbf{M}^2)/2$, with $|\mathbf{M}| = yT$ where y is the value maximizing $-y^2 T/2 + \ln I_0(y)$, I_0 being the modified Bessel function of order 0. For $E/N > 3/4$ ($T > 1/2$) the only solution is $y = 0$, while below the critical energy the null solution becomes unstable and a new stable solution appears, giving place to a second order phase transition. On the opposite limit of first-neighbor interactions ($\alpha \rightarrow \infty$), when $U = \sum_i [1 - \cos(\theta_{i+1} - \theta_i)]$, one does not observe an order-disorder thermodynamical transition [6]. In this case, $E/N = T/2 + 1 - I_1(1/T)/I_0(1/T)$, where I_n stands for the modified Bessel function of order n . The dynamics generated by the Hamiltonian (1) has been analyzed before [7]. In the limit $N \rightarrow \infty$ and for energies above a critical value, the maximal Lyapunov exponent was shown to vanish for $0 \leq \alpha < 1$, while it tends to a finite value otherwise.

For arbitrary values of α we have integrated numerically the set of equations of motion (2) and (3) using a fourth order symplectic method [8] with a fixed time step selected so as to keep the energy constant within an error $\Delta E/E$ of order 10^{-4} . Initial configurations ($t = 0$) were chosen as follows: all the angles were set to zero and the momenta were chosen at random from the uniform distribution with zero mean value. Next, all the momenta were scaled in order to attain the desired total energy E . We varied the size of the systems from $N = 100$ to 1600 in order to analyze finite size effects [9]. Once a transient elapsed (that depends both on the size of the system and on the total energy E), we computed the time averages of both the magnetization and the kinetic energy looking for their asymptotic behavior.

We start considering the region $0 \leq \alpha < 1$. Systems characterized by values of α within that interval do not have a well defined Hamiltonian in the sense that, in the thermodynamics limit $N \rightarrow \infty$, the potential energy diverges. One of the goals of this work is to establish precisely a connection between our microcanonical temporal averages obtained for α inside that range and those obtained theoretically by averaging in the canonical ensemble the HMF model [3].

Figure 1a displays the modulus of the magnetization $|\mathbf{M}|$ as a function of the energy per particle E/N for $\alpha = 0.5$ and different system sizes. We observe that the system undergoes a phase transition from a ferromagnetic low energy phase with $\mathbf{M} \neq 0$ to a

paramagnetic high energy phase where $\mathbf{M} = 0$. As expected, the critical specific energy diverges as N increases, due to the lack of *extensivity* of the system. In Fig. 1b we present the same results but now with the specific energy scaled by a factor \tilde{N} that depends both on the system size N and on α . To understand the origin of this scaling, let us stress that the lack of extensivity in the range $0 \leq \alpha \leq 1$ emerges as a consequence of the divergence of the specific potential energy upper bound in

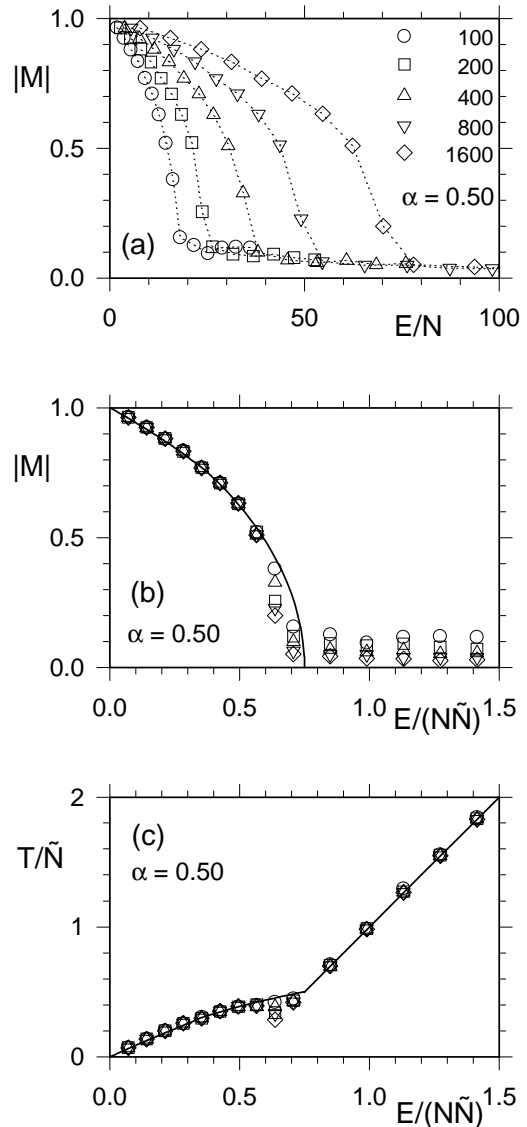


FIG. 1. (a) Modulus of the magnetization, $|\mathbf{M}|$, as a function of the specific energy E/N ; (b) $|\mathbf{M}|$ as a function of the scaled specific energy $E/(N\tilde{N})$; (c) scaled temperature T/\tilde{N} as a function of $E/(N\tilde{N})$. The symbols correspond to numerical simulations in the microcanonical ensemble for $\alpha = 0.5$ and different system sizes indicated on the figure. Each symbol corresponds to an average of different initial conditions (typically 10). The solid lines correspond to the theoretical equilibrium predictions for the HMF model (for which $\tilde{N} = 1$, since the HMF Hamiltonian is already N scaled).

(1). \tilde{N} is nothing else than twice the value of this upper bound:

$$\tilde{N} \equiv 2 \sum_{r=1}^{N/2} \frac{1}{r^\alpha} \approx 2 \int_{1/2}^{N/2} dr r^{-\alpha} = 2^\alpha \frac{N^{1-\alpha} - 1}{1 - \alpha}, \quad (6)$$

For $N \rightarrow \infty$, \tilde{N} behaves as

$$\tilde{N}(\alpha) \sim \begin{cases} 2^\alpha \frac{1}{1-\alpha} N^{1-\alpha} & \text{for } 0 \leq \alpha < 1, \\ 2 \ln N & \text{for } \alpha = 1, \\ \Theta(\alpha) \frac{1}{\alpha-1} & \text{for } \alpha > 1, \end{cases} \quad (7)$$

where $\Theta(\alpha)$ is a function of α which, for $\alpha \rightarrow \infty$ goes to $2(\alpha - 1)$. Note that all the curves for different N collapse into a unique one, despite small discrepancies around the critical value. Similar \tilde{N} -scaling collapse was already observed for magnetic systems [10,11] and also for systems governed by interactions of the Lennard-Jones type [12]. In all these cases, although the α -dependent prefactor in (7) is model dependent, the behavior of \tilde{N} with N is invariant.

Figure 1c plots T/\tilde{N} vs the scaled specific energy $E/(N\tilde{N})$ (caloric curve) also for $\alpha = 0.5$ and the same system sizes considered in Figs. 1a and 1b. Here again the \tilde{N} scaling leads to data collapse. It is worth stressing here that around the critical energy this plot depends strongly on the equilibration transient, the size of the system, and the initial configuration adopted. Our results within this parameter range seem to indicate the existence of a first order phase transition, with the high energy phase coexisting with the ordered one. An analogous behavior, already reported for the HMF model [4], where the transition is second order, was believed to be a purely microcanonical result reflecting the existence of long living quasistationary nonequilibrium states whose lifetimes increase with N . This also seems to be the case for any $0 \leq \alpha < 1$ since the discrepancy around the transition for fixed energy and fixed size is attenuated by averaging over larger time intervals.

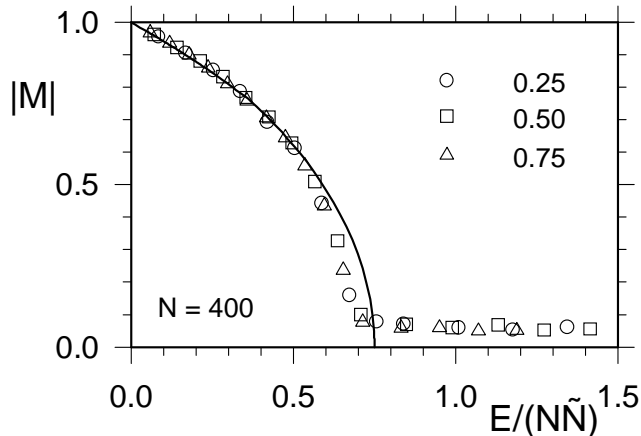


FIG. 2. $|M|$ as a function of $E/(N\tilde{N})$. The symbols correspond to numerical simulations in the microcanonical ensemble for $\alpha = 0.25, 0.5$, and 0.75 , all for $N = 400$. The solid line corresponds to the theoretical results for the HMF model.

Figure 2 exhibits $|M|$ vs $E/(N\tilde{N})$ for $\alpha = 0.25, 0.5$, and 0.75 , all for $N = 400$. Observe that the curves agree with a unique one. The same collapse is also detected for the caloric curve (not shown). Let us recall the main motivation of this Letter, namely, the possible relation between statistical and temporal averages for systems for which one cannot *a priori* define an extensive energy, such as the case we are considering now. In Fig. 2 we have also included the plot (solid line) of the theoretical predictions of the equilibrium values obtained, by means of the canonical ensemble formalism, in the HMF version ($\alpha = 0$ with N -scaled potential energy) [3]. What we now observe is that not only different size and different α curves, with $0 \leq \alpha < 1$, collapse into a unique one, but they collapse precisely to the mathematically tractable extensive mean-field limit. A similar collapse had already been found for the Ising ferromagnet submitted to a Monte Carlo process [10] but this is, as much as we know, the first time this effect can be confirmed in a conservative model with deterministic dynamics. Since slowly

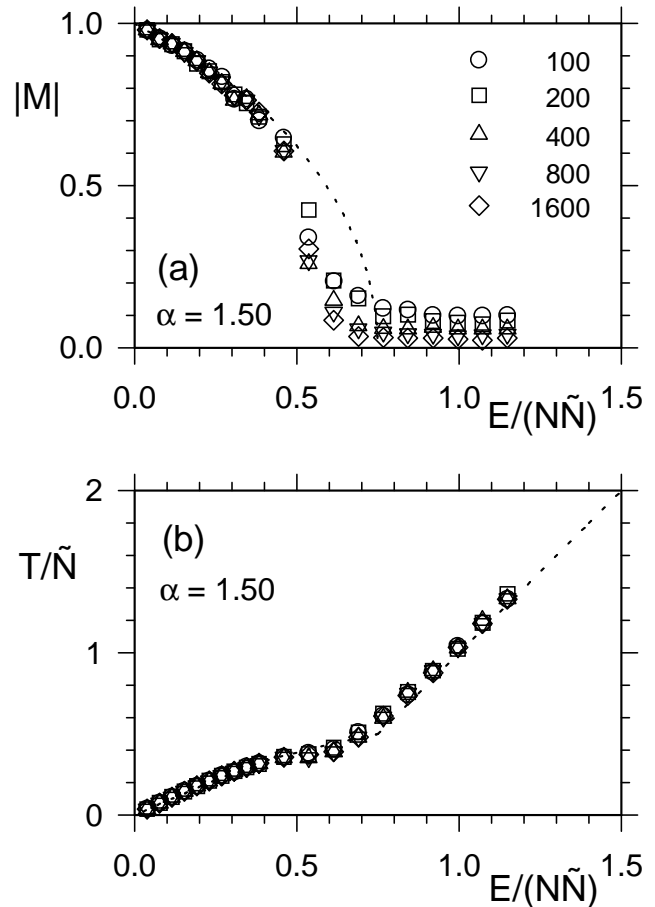


FIG. 3. (a) $|M|$ as a function of $E/(N\tilde{N})$; (b) scaled temperature T/\tilde{N} as a function of $E/(N\tilde{N})$. The symbols correspond to numerical simulations in the microcanonical ensemble for $\alpha = 1.5$ and different system sizes. For comparison, the dotted line corresponds to the theoretical equilibrium predictions of the HMF model.

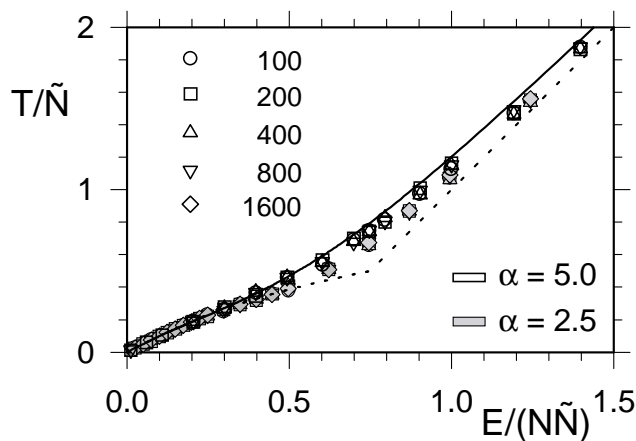


FIG. 4. Scaled temperature T/\tilde{N} as a function of $E/(N\tilde{N})$. The symbols correspond to numerical simulations in the micro-canonical ensemble for $\alpha = 2.5$ (gray), 5.0 (white), and different system sizes indicated on the figure. The dashed and solid lines correspond to the theoretical results for the HMF ($\tilde{N} = 1$) and the $\alpha \rightarrow \infty$ ($\tilde{N} = 2$) limits, respectively.

decaying long-range interacting systems are ubiquitous in nature, our results, if valid for all those systems such that $\alpha < d$, reveal a simple way of calculating quantities at the equilibrium.

Next we briefly describe what happens for $1 < \alpha < 2$. There exists still an order-disorder transition, as can be observed in Figs. 3a and 3b for the particular case $\alpha = 1.5$, but with a sensitive dependence on the value of α . Contrary to the previous case where the critical energy (above which the magnetization falls down to zero as N increases) remains independent on α although slightly smaller than the theoretical prediction, here as the value of α approaches 2, the critical energy decreases until a finite value which can be nonzero [13].

Finally, we analyze the region $\alpha > 2$. Here, as expected, the system behaves similarly as in the first-neighbor limit; i.e., it never does order since for any finite energy the magnetization goes down to zero as $N \rightarrow \infty$. In Fig. 4 we plot T/\tilde{N} vs $E/(N\tilde{N})$ obtained numerically (symbols) for $\alpha = 2.5$ and 5.0 , together with the theoretical values for both the limit $\alpha \rightarrow \infty$ [6] (solid line) and the HMF model [3] (dashed line). We see how the numerical results approach those of the $\alpha \rightarrow \infty$ limit.

To summarize, we have studied the equilibrium behavior of a one-dimensional conservative system of interacting particles as a function of the range of the interactions α . By integrating numerically the equations of motion we have found three different classes of systems. For $0 \leq \alpha < 1$ the systems undergo a second order phase transition, and the measured quantities (e.g., the critical energy) when suitably scaled *do not depend* on the value

of α . For $1 < \alpha < 2$ the systems undergo also a second order phase transition but, unlike the previous case, the critical energy and the magnetization curve depend sensitively on the range of the interactions α . Finally, for $\alpha > 2$ the systems adopt the first-neighbor behavior where there is no order at finite temperature for $N \rightarrow \infty$.

It is also worth noting that the \tilde{N} scaling performed over the results produced by Hamiltonian (1) leads to the same results as those produced by an artificial “extensive” Hamiltonian constructed with \tilde{N} -scaled potential energies generalizing the HMF approximation. For a correspondence between both treatments when looking at dynamical aspects, time should be $\tilde{N}^{1/2}$ scaled.

Probably the nontrivial data collapse here reported for $0 \leq \alpha < 1$ can be extended to $0 \leq \alpha < d$ for an arbitrary dimension d , being [from the generalization of (6) to d dimensions] $\tilde{N} \sim \frac{1}{1-\alpha/d}(N^{1-\alpha/d} - 1)$. If true, our findings reveal a simple way of calculating macroscopic quantities at the equilibrium when long-range interactions are involved.

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