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First- and second-order clustering transitions for a system with infinite-range attractive interaction

M. Antoni,[1] S. Ruffo,[2,3,*] and A. Torcini,[1,2]
[1] *UMR-CNRS 6171, Université d'Aix-Marseille III, Avenue de l'Escadrille Normandie-Niemen, 13397 Marseille Cedex 20, France*
[2] *Dipartimento di Energetica "Sergio Stecco," Universitá di Firenze, Via S. Marta 3, 50139 Firenze, Italy*
[3] *ENS-Lyon, Laboratoire de Physique, 46 Allée d'Italie, Lyon Cedex, France*

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We consider a Hamiltonian system made of N classical particles moving in two dimensions, coupled via an *infinite-range interaction* gauged by a parameter A. This system shows a low energy phase with most of the particles trapped in a unique cluster. At higher energy it exhibits a transition towards a homogenous phase. For sufficiently strong coupling A, an intermediate phase characterized by two clusters appears. Depending on the value of A, the observed transitions can be either second or first order in the canonical ensemble. In the latter case, microcanonical results differ dramatically from canonical ones. However, a canonical analysis, extended to metastable and unstable states, is able to describe the microcanonical equilibrium phase. In particular, a microcanonical negative specific heat regime is observed in the proximity of the transition whenever it is canonically discontinuous. In this regime, *microcanonically stable* states are shown to correspond to *saddles* of the Helmholtz free energy, located inside the spinodal region.

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It is well known that thermodynamic quantities derived within different statistical ensembles should coincide in the thermodynamic limit. However, this statement is valid only if the interaction among the particles satisfies two conditions: (i) the pairwise interaction potential is integrable (i.e., it decays faster than $1/r^d$, where d is the space dimension); and (ii) the potential energy per particle is bounded from below [1]. Whenever one of these conditions is violated, ensemble inequivalence and thermodynamical instabilities can occur. An extreme situation is represented by the gravitational potential for which neither condition is satisfied. Indeed, for gravitating systems the usual laws of equilibrium thermodynamics are expected not to hold: one of the most striking anomalies is related to the negative values taken by the specific heat [2–4]. Discrepancies between results obtained in the microcanonical and canonical ensembles, with an associated negative specific heat regime, have been observed in the thermodynamic limit for several systems with attractive potentials violating either condition (i) [5–7] or condition (ii) only [8,9]. Similar anomalies are also present for systems with a finite number of particles, e.g., for nuclear multifragmentation [10], as well as for atomic clusters [11]. In all these cases, preliminary results suggest that ensemble inequivalence can be observed in proximity of a canonically first-order phase transition [6,12,13].

In this paper we aim at better clarifying the origin of such inequivalence by considering a generalization of a previously studied N-body classical Hamiltonian system with infinite-range attractive interactions [5]. The novelty of the present model consists in the presence of a tunable coupling A that allows us to change the nature and the order of the transitions. These are investigated analytically within the canonical ensemble and numerically via microcanonical molecular dynamics simulations. This system shows three different phases: a clustered phase (CP_1) occuring at low internal energy U (temperature T), with most of the particles trapped in a unique cluster, a second clustered phase (CP_2), exhibiting two clusters, at intermediate energy (temperature) and sufficiently strong coupling A, and a homogenous phase (HP), with particles uniformly distributed, at high values of U (T). The canonical equilibrium solutions are computed from the lowest-lying extrema of the Helmholtz free energy and reveal that the system undergoes either first- or second-order transitions, depending on the value of the coupling constant A. In particular, we have focused our attention on first-order transitions separating the ordered phase CP_1 and the HP and between the two clustered phases. In both cases canonical and microcanonical equilibrium predictions differ dramatically near the transition, revealing a negative specific heat regime within the microcanonical ensemble. No discrepancy between microcanonical and canonical results appear at continuous phase transitions, at least for what concerns the temperature-energy equilibrium relation [14].

Irrespectively of the nature of the phases involved in the transition, the microcanonical negative specific heat regime can be well reproduced even within the canonical ensemble if not only the absolute minima of the Helmholtz free energy are taken into account, but also the relative extrema corresponding to canonically metastable and unstable states.

The model we consider is a classical N-body Hamiltonian system defined on a two-dimensional periodic cell. The interparticle potential is infinite ranged and all the particles are identical with unitary mass. The Hamiltonian of the model is $H_A = K + V_A$ where $K = \sum_{i=1}^{N}[(p_{x,i}^2 + p_{y,i}^2)/2]$ is the kinetic energy and the potential energy reads as

$$V_A = \frac{1}{2N}\sum_{i,j=1}^{N}[2 + A - \cos(x_i - x_j) - \cos(y_i - y_j) - A\cos(x_i - x_j)\cos(y_i - y_j)] \quad (1)$$

with $(x_i, y_i) \in]-\pi:\pi]\times]-\pi:\pi]$ representing the coordinates of the i particle and $(p_{x,i}, p_{y,i})$ the conjugated mo-

*Also at INFM and INFN, Firenze, Italy.

menta. For $A=0$, the two spatial directions x and y are uncoupled and the Hamiltonian reduces to the sum of two independent one-dimensional mean-field models [15]. In this case, as shown in [15], a second-order phase transition appears, both in the microcanonical and in the canonical ensemble, connecting a single clustered phase (CP_1), at sufficiently low specific energy $U=H/N$ to a homogeneous phase (HP) at high energy. For nonzero values of A, the two spatial directions are coupled. Previous investigations were limited to the value $A=1$ [5] and a transition was also observed from a CP_1 to a HP phase. This transition is first order in the canonical ensemble, while microcanonical simulations are compatible with a continuous transition associated with a negative specific heat regime. Both for $A=0$ and $A=1$, at low energies, all particles are trapped in a cluster, while, for sufficiently high energies, they are uniformly distributed in the cell.

In order to better investigate the origin of ensemble inequivalence within a unique framework, we have introduced model (1) which allows, by continuously varying parameter A, to pass from a situation where the microcanonical and canonical results coincide ($A=0$) to a situation where the two ensembles disagree over a finite energy range near the transition. As we will show, this model is indeed richer than expected because it reveals also more complicated transitions than those previously studied in [5,15].

Due to the long-range nature of the interactions, the collective behavior of the particles can be described in terms of the following mean-field vectors: $\vec{M}_z=(\langle\cos(z)\rangle_N,\langle\sin(z)\rangle_N)=M_z(\cos(\phi_z),\sin(\phi_z))$ where $\phi_z\in[0,\pi/2]$ and $z=x$ or y; $\vec{P}_z=(\langle\cos(z)\rangle_N,\langle\sin(z)\rangle_N)=P_z(\cos(\psi_z),\sin(\psi_z))$ where $\psi_z\in[0,\pi/2]$ and $z=x\pm y$. The average over all the particles is indicated by $\langle\ldots\rangle_N$. It can be shown that on average $M_x\approx M_y\approx M$ and $P_{x+y}\approx P_{x-y}\approx P$ (for more details see [5]). Therefore, the potential energy can be rewritten, in the mean-field limit $N\to\infty$, as $V_A=[2+A-2M^2-AP^2]/2$.

For $U\approx 0$ (or equivalently at low temperature), the system described by model (1) is in the CP_1, particles have all the same location in a single pointlike cluster, and $M\approx P\approx 1$, whereas at large enough energy (temperature) the system is in the HP and $M\approx P=O(1/\sqrt{N})$. For sufficiently high values of $A>A_2\sim 3.5$, a third intermediate phase CP_2, exhibiting two clusters, appears. In this phase, due to the symmetric location of the two clusters $M\sim O(1/\sqrt{N})$ and $P\sim O(1)$.

In the mean-field limit, the equilibrium properties of model (1) can be derived analytically within the canonical ensemble following the approach of Ref. [5]. In particular, the Helmholtz free energy reads as

$$\frac{F(M,P;T,A)}{T}=T(M^2+P^2)-\ln[T\,G(M,P;A)] \qquad (2)$$

with $G=\int_0^{2\pi}I_0[M+\sqrt{2A}P\,\cos(s)]\exp[M\cos(s)]ds$, where I_0 is the modified Bessel function of zero order. Since we are interested also in metastable and unstable states we will not restrict ourselves to the study of the lowest-lying minima of F, but we will keep track of all the other extrema. Due to the $P\to -P$ symmetry of F, we can limit our analysis to the $P\geqslant 0$ half-plane. The transition lines, obtained by considering the absolute minima of F, are reported as solid lines in Fig. 1. The minima can be easily associated with the three observed phases, since HP will correspond to $M=P=0$, CP_1 to $|M|>0$, $|P|>0$, and CP_2 to $M=0$ and $|P|>0$.

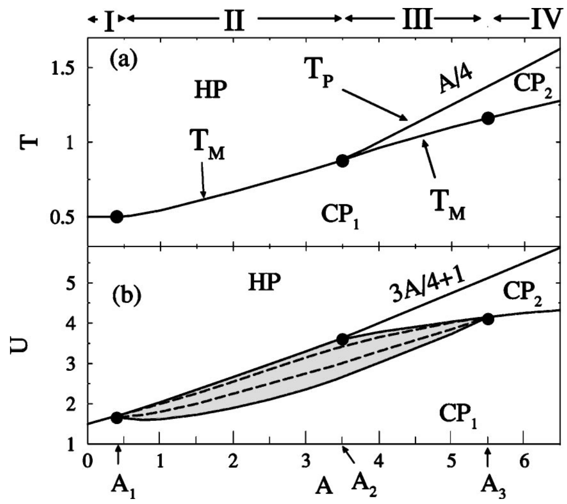

FIG. 1. Phase diagrams of model (1) reporting the transition temperatures versus the coupling parameter A (a) and the corresponding specific energy $U=H/N$ versus A (b). The solid lines indicate the canonical transition lines and the dots the points where the nature of the transitions change. A_1, A_2, and A_3 are the threshold coupling constants that determine the transition scenario I $\to$IV displayed above the graphs. The gray shaded area in (b) indicates the domain where two phases coexist. Inside this area, the dashed curves are the two spinodal lines.

Let us describe the observed phase transitions within the canonical ensemble with the help of Fig. 1: the line referred to as T_M in the inset (a) indicates the transition temperatures where M vanishes and where the phase CP_1 looses its stability, while the line T_P is where $P\to 0$ and the CP_2 leaves place to the HP. The phase diagram U versus A reported in the inset (b) gives clearer hints for what concerns first-order transitions, indicating the corresponding energy jumps (latent heats). Depending on the value of A, four different scenarios can be distinguished. (I): $[0\leqslant A\leqslant A_1=2/5]$—in this case one observes a continuous transition from a CP_1 to a HP; the critical line is located at $T_M=1/2$ $(U_M=3/2+A)$. Along this line, at $A_1=2/5$, there is a tricritical point: here the transition becomes discontinuous. (II): $[A_1<A<A_2\approx 3.5]$—the transition between CP_1 and HP is first order in all this range of parameters with a finite energy jump [gray shaded area in Fig. 1(b)]. (III): $[A_2<A<A_3\approx 5.7]$—in this region the third phase begins to play a role and two successive transitions are observed: first CP_1 disappears at T_M via a first-order transition that gives rise to the biclustered phase CP_2, which ends up in the HP due to a continuous transition. The critical line associated with this last transition is $T_P=A/4$ $(U_P=3A/4+1)$. (IV): $[A>A_3]$—finally, region (IV) differs from region (III) just for the nature of the transition connecting the two clustered phases that becomes second order.

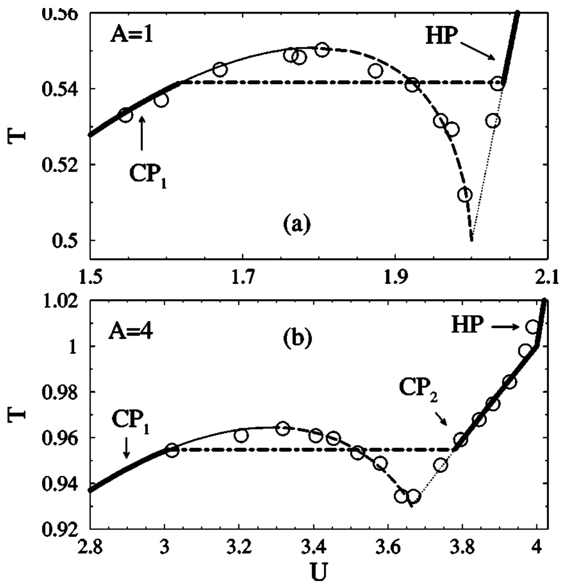

FIG. 2. Temperature-energy relation in the coexistence region for $A=1$ (a) and $A=4$ (b). Lines indicate canonical analytical results, while circles correspond to microcanonical simulations. Solid thick lines are equilibrium results, solid thin lines metastable states, and dashed thin lines unstable states. The straight dot-dashed thick line is the Maxwell construction. (a) refers to a canonical first-order transition from CP_1 to HP, (b) to a canonical discontinuous transition connecting the two clustered phases. In (b) the canonical and microcanonical second-order transition at $U\approx 4$ is also shown. The microcanonical results have been obtained via molecular dynamics simulations of model (1) with $N=5000$ particles [16].

Let us now concentrate on first-order phase transitions; in particular we will compare microcanonical results obtained via molecular dynamics simulations [16] with canonical results. Outside the gray area in Fig. 1(b) the microcanical and canonical results coincide everywhere, but inside such a region strong discrepancies are observed. This can be clearly seen in Fig. 2, where T is plotted as a function of U near the discontinuous transition for two different values of A (namely, $A=1$ and $A=4$). Within the canonical ensemble, first-order phase transitions occur at a given temperature and the coexistence region is bridged with a horizontal line [$T=T_M$ in Fig. 2(a) and $T=T_P$ in 2(b)], according to the Maxwell construction.

However, this region is accessible via microcanonical simulations and the corresponding equilibrium results are shown as circles in Fig. 2. Within this region these results disagree with the canonical ones, the transition is now continuous, and a negative specific heat region appears. It is remarkable that both in the transition connecting the clustered phase CP_1 to the HP as well as in that connecting the two clustered phases the essential features of the transition are the same.

We will now show that the microcanonical results can be obtained even within the canonical ensemble by considering also the relative minima and the saddles of F. A schematic sketch of the relevant extrema of F in the (M,P) plane close to the two transitions discussed above is reported in Fig. 3.

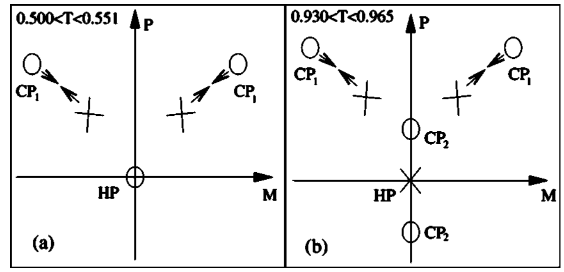

FIG. 3. Schematic representation of the extrema of the free energy for a fixed temperature in the intervals reported in the figures for $A=1$ (a) and $A=4$ (b). Circles denote the positions of the minima, while the crosses represent the saddles. The motion of the extrema for increasing temperatures is indicated by the arrows.

Let us first consider the case $A=1$ for $1/2\leqslant T\leqslant 0.551$, which is reported in Fig. 3(a). For $T<1/2$ the free energy has a unique minimum corresponding to the CP_1 phase, while at $T=1/2$ a second relative minimum emerges at $M=P=0$ associated with a metastable HP state. Exactly at the same temperature also two symmetric saddles appear in the (M,P) plane in between the CP_1 and the HP minima. For increasing temperature the depth of the CP_1 minimum decreases while that of the HP minimum increases and, simultaneously, the saddles and the CP_1 minima approach each other. At $T=T_M\simeq 0.54$ the CP_1 and HP mimima reach exactly the same depth and this singles out the canonical transition temperature. At $T=0.551$ the saddles and the CP_1 minima finally merge and disappear. If the energies and temperatures denoting these unstable and metastable states are reported in a graph together with the equilibrium solutions, one observes that they connect continuously the CP_1 equilibria to the HP ones (see Fig. 2). Moreover, as shown again in Fig. 2(a), the microcanonical results essentially coincide with the metastable and unstable canonical solutions in the coexistence region. In particular, the negative specific heat regime is associated with the saddles bridging the metastable minima. The limits of existence of these unstable states are typically referred to as spinodals and are reported in Fig. 1 as dashed lines [17]. A similar behavior is observed for the CP_1 to CP_2 transition, in this case for $T<0.93$ the unique minimum of F is again associated with the CP_1 and at $T=0.93$ two symmetric minima appear on the $M=0$ axis with $|P|\neq 0$, and these metastable states are clearly associated with the CP_2. Also two saddle points appear in the F profile separating the CP_1 minima from the metastable CP_2 minimum in the positive P semiplane. For $T>T_P\simeq 0.95$ the CP_2 minima become the stable ones. For increasing temperatures the CP_1 minima and the saddles approach each other and finally vanish at the spinodal (located at $T\simeq 0.965$). For higher temperatures the CP_2's approach the origin symmetrically where a saddle (not involved in the first-order transition) is present, corresponding to the HP unstable phase. At $T=T_M\simeq 1$ the two minima merge with the saddle at the origin, giving rise to a unique minimum for F corresponding to a stable HP. This second transition is clearly continuous. Also in this case, the microcanonical continuous transition is well reproduced by the metastable and unstable states involved in the discontinuous transition [see Fig. 2(b)].

In conclusion, we have shown that a study of the absolute and relative extrema of the Helmholtz free energy is sufficient to provide a complete microcanonical and canonical description of the equilibrium behavior of an N-body Hamiltonian with infinite-range attractive interaction. Depending on the value of the tuning parameter A canonically first- or second-order transitions are observed. The comparison of the canonical results with the microcanonical ones shows that ensemble inequivalence occurs in proximity of canonically discontinuous transitions. Irrespective of the phases involved in the transitions a negative specific heat regime has been observed. In particular, this regime is always associated with the existence of a spinodal region for the canonical solutions. For energy values within this region microcanonically stable states correspond to saddles of the free energy. We have validated this scenario by considering two different discontinuous transitions connecting the one cluster phase either to the homogeneous one or to the two cluster phase.

We believe that the results reported in this article are not limited to systems with infinite-range interactions, but they should be applicable also to systems with power-law decaying potentials (as shown in [18]) and to finite systems with short-ranged forces (see [12]).

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