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

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(March 22, 2022)

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.

PACS numbers: 05.20.Gg, 05.70.Fh, 64.60.-i

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); (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 [3]. 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) [4] or condition (ii) only [5]. Similar anomalies are also present for systems with a finite number of particles, e.g., for nuclear multifragmentation [6], as well as for atomic clusters [7]. In all these cases, preliminary results suggest that ensemble inequivalence can be observed in proximity of a canonically first order phase transition [8, 9].

In this article, 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 [10]. The novelty of the present model consists in the presence of a tunable coupling $A$ that allows 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 ($CP_1$) occurring 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 homogeneous 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 homogeneous one $HP$ 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 [11].

Our results demonstrate that, irrespectively of the nature of the phases involved in the transition, the micro-

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canonical negative specific heat regime can be well reproduced even within the canonical ensemble. Once not only the absolute minima of the Helmholtz free energy are taken in 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 $K = \sum_{i=1}^{N} \left( \frac{p_{i}^2}{2} + \frac{p_{i}^2}{2} \right)$ is the kinetic energy and the potential energy reads as

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

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 momenta. 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 $[13]$. In this case, as shown in $[5]$, a second order phase transition appears, both in the microcanonical and 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 non zero values of $A$, the two spatial directions are coupled. Previous investigations were limited to the value $A = 1$ 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 $[14]$ 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 $[13]$.

Due to the long-range nature of the interactions, the collective behaviour of the particles can be described in terms of the following mean-field vectors: $\bar{M}_z = (\langle \cos(z) \rangle_N, \langle \sin(z) \rangle_N) = M_z (\cos(\phi_z), \sin(\phi_z))$ where $\phi_z \in [0,\pi/2]$ and $z = x$ or $y$; $\bar{P}_z = (\langle \cos(z) \rangle_N, \langle \sin(z) \rangle_N) = P_z (\cos(\psi_z), \sin(\psi_z))$ 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 $[14]$). Therefore, the potential energy can be rewritten, in the mean-field limit $N \rightarrow \infty$, as $V_A = [2 + A - 2M^2 - AP^2]/2$.

For $U \approx 0$ (or equivalently at low temperature), the system described by model $[14]$ is in the CP$_1$, particles have all the same location in a single point-like 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 $A > A_2 \approx 3.5$, 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 $[14]$ can be derived analytically within the canonical ensemble following the approach of Ref. $[5]$. In particular, the Helmholtz free energy reads as

$$F(M,P,T,A) = T(M^2 + P^2) - \ln[\int G(M,P,A)]$$

with $G = \int_0^{2\pi} \int_0^\infty (M + \sqrt{2AP} \cos(s)) \exp(M \cos(s)) ds$, 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 $P \rightarrow -P$ symmetry of $F$, we can limit our analysis to the $P \geq 0$ half-plane. The transition lines, obtained by considering the absolute minima of $F$, are reported as solid lines in Fig. $[14]$.
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): $0 \leq A \leq A_1 = 2/5$ - in this case one observes a continuous transition from a $CP_1$ to a $HP$, the critical line is located at $T_M = 1/2 \left( U_M = 3/2 + A \right)$. 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 (grey 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 b clustered phase $CP_2$, which ends up in the $HP$ due to a continuous transition. The critical line associated to this last transition is $T_P = A/4 \left( U_P = 3A/4 + 1 \right)$. (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.

Let us now concentrate on first order phase transitions, in particular we will compare microcanonical results obtained via molecular dynamics simulations with canonical results. Outside the grey area in Fig. 1(b) the microcanonical and canonical results coincide everywhere, but inside such 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 Fig. 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. Let us first consider the case $A = 1$ for $1/2 \leq T \leq 0.551$, that 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 to a metastable $HP$ state. Exactly at the same temperature also two symmetric saddles appear in the $(M,P)$-plane inbetween 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 $T = T_M \approx 0.54$ the $CP_1$ and $HP$ minima 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 energy and temperature 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 to 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. 2 as dashed lines. A similar behaviour 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 to 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 to 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 $P$ semi-plane. For $T > T_P \approx 0.95$ 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 $T \approx 0.965$). For higher temperatures the $CP_2$'s approach symmetrically the origin, where a saddle (not involved in the first order transition) is present corresponding to the $HP$ unstable phase. At $T = T_M \approx 1$ 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)).

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

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 behaviour of a $N$-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 to the existence of a spinodal region for the canonical solutions. For energy values within this region microcanonically stable states corresponds 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]).

The MPIPKS Institute in Dresden is acknowledged for providing computational facilities and F. Chauvet and H. Scherrer for their advice. We thank J. Barré, F. Bouchet, P.-H. Chavanis, T. Dauxois and D. Mukamel for useful discussions. This work is part of the MURST-COFIN00 research project “Chaos and localization in classical and quantum mechanics”.

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