Inequivalence of Ensembles in a System with Long-Range Interactions

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We study the global phase diagram of the infinite-range Blume-Emery-Griffiths model both in the *canonical* and in the *microcanonical* ensembles. The canonical phase diagram shows first-order and continuous transition lines separated by a tricritical point. We find that below the tricritical point, when the canonical transition is first order, the phase diagrams of the two ensembles disagree. In this region the microcanonical ensemble exhibits energy ranges with negative specific heat and temperature jumps at transition energies. These results can be extended to weakly decaying nonintegrable interactions.

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Systems in d dimensions, with a pairwise interaction potential which decays at large distances as $V(r) \sim 1/r^{d+\sigma}$ with $-d \leq \sigma \leq 0$, are referred to as *nonintegrable*, or systems with *long-range* interactions. Such systems have an ill defined thermodynamic limit [1]. This may be correctly restored by applying the Kac prescription [2], within which the potential is rescaled by an appropriate, volume dependent, factor which vanishes in the thermodynamic limit. However, even within this scheme, the energy remains *nonadditive,* i.e., the system cannot be divided into independent macroscopic parts, as is usually the case for short-range interactions. This fact has no dramatic consequences if one is restricted to the *canonical* ensemble, but it produces striking phenomena in the *microcanonical* ensemble. One should, however, recall that the canonical ensemble has no foundation if it cannot be derived from the microcanonical, and this is possible only for additive systems [3]. In the microcanonical ensemble the specific heat may be negative, as was first clearly discussed by Lynden-Bell [4] and Thirring [5]. Indeed, it has been originally observed by Antonov [6] that classical gravitational systems ($\sigma = -2$, $d = 3$) show features of such kind. However, here the physical situation is made more complex by the presence of a singularity of the interaction potential at short distances. For a careful discussion of the statistical mechanics of these systems, see Ref. [7].

In this Letter we consider a simple model for which the main features of the phase diagram can be derived analytically both within the canonical and the microcanonical ensembles. We demonstrate that, in the region where the phase transition in the canonical ensemble is first order, the two ensembles are not equivalent, yielding two distinct phase diagrams. The model we consider is the Blume-Emery-Griffiths (BEG) model with infinite-range interactions ($\sigma = -d$). This is the simplest model known to exhibit both continuous and first-order transition lines. It is defined on a lattice (hence, divergences at short range are removed), where each lattice point i is occupied by a spin-1 variable $S_i = 1, -1, 0$. The Hamiltonian is given by

$$H = \Delta \sum_{i=1}^{N} S_i^2 - \frac{J}{2N}\left(\sum_{i=1}^{N} S_i\right)^2, \qquad (1)$$

where $J > 0$ is a ferromagnetic coupling constant and $\Delta > 0$ controls the energy difference between the magnetic ($S = \pm 1$) and the nonmagnetic ($S = 0$) states. Each spin interacts with every other spin, and the coupling constant J is scaled by $1/N$ make the energy *extensive*. This is just the Kac prescription applied to our model. However, this does not entail *additivity,* in the sense that for a system made of two parts, X and Y, such that $H_{X+Y} = H_X + H_Y + H_{XY}$, the H_{XY} interaction term never becomes negligible in the thermodynamic limit. This property applies to all thermodynamic potentials.

The canonical phase diagram of this model has been studied in the past [8]. At $T = 0$ the model exhibits a ferromagnetic phase for $2\Delta/J < 1$ and a nonmagnetic phase otherwise. The (T, Δ) phase diagram displays a transition line separating the low temperature ferromagnetic phase from the high temperature paramagnetic phase (see Fig. 1).

The transition is first order at high Δ values and becomes continuous at low Δ. The critical (second-order) line is given by

$$\beta J = \frac{1}{2}\, e^{\beta\Delta} + 1, \qquad (2)$$

where $\beta = 1/k_B T$. The two segments of the transition line (high and low Δ) are separated by a tricritical point located at $\Delta/J = \ln(4)/3 \simeq 0.4621$, $\beta J = 3$. The first-order segment of the transition line is obtained numerically by equating the free energies of the ferromagnetic and the paramagnetic states.

We now consider the phase diagram of the BEG model (1) within the microcanonical ensemble. Let N_+, N_-, and N_0 be the number of up, down, and zero spins, respectively, in a given microscopic configuration. Clearly, $N_+ + N_- + N_0 = N$. The energy E of a configuration

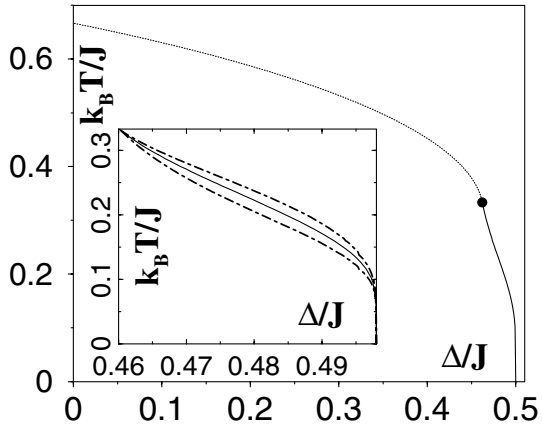

FIG. 1. Transition lines in the canonical ensemble. The critical line (thinner line) ends at the tricritical point (•), where the transition becomes first order (thicker line). The first-order region is zoomed in the inset, where we show again the canonical first-order line (solid line) and the microcanonical transition lines (dot-dashed lines)

is obviously a function only of N_+, N_-, and N_0. It does not depend on the specific spatial distribution of the spin variables. It is given by

$$E = \Delta Q - \frac{J}{2N} M^2, \tag{3}$$

where $Q = \sum_{i=1}^{N} S_i^2 = N_+ + N_-$ is the quadrupole moment and $M = \sum_{i=1}^{N} S_i = N_+ - N_-$ is the magnetization of the configuration. In order to calculate the entropy of a state with energy E we note that the number of microscopic configurations Ω compatible with macroscopic occupation numbers N_+, N_-, and N_0 is

$$\Omega = \frac{N!}{N_+!\, N_-!\, N_0!}. \tag{4}$$

Thus, in the large N limit, the entropy $S = k_B \ln\Omega$ corresponding to these occupation numbers is given by

$$S = -k_B N[(1-q)\ln(1-q) + \tfrac{1}{2}(q+m)\ln(q+m) + \tfrac{1}{2}(q-m)\ln(q-m) - q\ln 2], \tag{5}$$

where $q = Q/N$ and $m = M/N$ are the quadrupole moment and magnetization per site, respectively.

Let $\epsilon = E/\Delta N$ be the energy per site, normalized by Δ. Equation (3) can be written as

$$q = \epsilon + Km^2, \tag{6}$$

where $K = J/2\Delta$. Using this relation, one expresses the entropy per site $s = S/(k_B N)$ as a function of m and ϵ. By maximizing $s(\epsilon, m)$ with respect to m, one obtains both the spontaneous magnetization $m_s(\epsilon)$ and the entropy $s(\epsilon)$ of the system for a given energy. In order to locate the continuous transition line between the paramagnetic and ferromagnetic phases we expand $s(\epsilon, m)$ in powers of m. This expansion takes the form

$$s = s_0 + Am^2 + Bm^4 + O(m^6), \tag{7}$$

where $s_0 \equiv s(\epsilon, m = 0)$ is the entropy at zero magnetization

$$s_0 = -(1-\epsilon)\ln(1-\epsilon) - \epsilon\ln\epsilon + \epsilon\ln 2, \tag{8}$$

and A and B are the expansion coefficients

$$A = -K\ln\frac{\epsilon}{2(1-\epsilon)} - \frac{1}{2\epsilon}, \qquad B = -\frac{K^2}{2\epsilon(1-\epsilon)} + \frac{K}{2\epsilon^2} - \frac{1}{12\epsilon^3}. \tag{9}$$

In the paramagnetic phase both A and B are negative, and the entropy is maximized by $m = 0$. The continuous transition to the ferromagnetic phase takes place at $A = 0$ for $B < 0$. In order to obtain the critical line in the (T, Δ) plane we note that the energy ϵ is related to the temperature by the usual thermodynamic relation

$$\frac{\Delta}{k_B T} = \frac{\partial s}{\partial \epsilon}. \tag{10}$$

By making use of the fact that the magnetization m vanishes on the critical line, one obtains

$$\frac{\Delta}{k_B T} = \ln\frac{2(1-\epsilon)}{\epsilon}. \tag{11}$$

This relation, together with the equation $A = 0$, yields the following expression for the critical line:

$$2\bar{\beta}K = \frac{1}{2}e^{\bar{\beta}} + 1, \tag{12}$$

where $\bar{\beta} \equiv \beta\Delta$. Equivalently, this expression may be written as $\bar{\beta}K = 1/2\epsilon$. The microcanonical critical line thus coincides with the critical line (2) obtained for the canonical ensemble. The tricritical point of the microcanonical ensemble is obtained at $A = B = 0$. By combining these equations with (11), one finds that, at the tricritical point, $\bar{\beta}$ satisfies

$$\frac{1}{8\bar{\beta}^2}\frac{e^{\bar{\beta}} + 2}{e^{\bar{\beta}}} - \frac{1}{4\bar{\beta}} + \frac{1}{12} = 0. \tag{13}$$

Equations (12) and (13) yield a tricritical point at $K \simeq 1.0813$, $\bar{\beta} \simeq 1.3998$. This has to be compared with the canonical tricritical point located at $K = 3/\ln(16) \simeq 1.0820$, $\bar{\beta} = \ln(4) \simeq 1.3995$. It is evident that the two points, although very close to each other, do not coincide and the microcanonical critical line extends beyond the canonical line. In the region between the two tricritical points, the canonical ensemble yields a first-order transition at a higher temperature, while in the microcanonical ensemble the transition is continuous.

To study the microcanonical phase diagram we consider the temperature-energy relation $T(\epsilon)$. This curve has two branches: a high-energy branch (11) corresponding to $m = 0$, and a low-energy branch obtained from (10) using the spontaneous magnetization $m_s(\epsilon)$. At the intersection point of the two branches the two entropies become equal. In Fig. 2 we display the $T(\epsilon)$ curve for increasing values of Δ. For $\Delta/J = \ln(4)/3$, corresponding

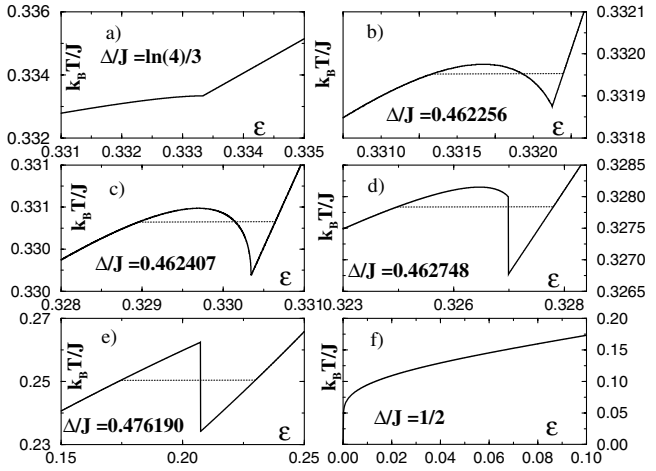

FIG. 2. Temperature versus energy relation in the microcanonical ensemble for different values of Δ. The horizontal line in some of the plots is the Maxwell construction in the canonical ensemble and identifies the canonical first-order transition temperature.

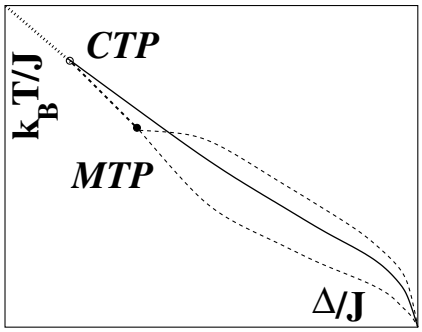

FIG. 3. A schematic representation of the phase diagram, where we expand the region around the canonical (CTP) and the microcanonical (MTP) tricritical points. The second-order line, common to both ensembles, is dotted, the first-order canonical transition line is solid, and the microcanonical transition lines are dashed (with the bold dashed line representing a continuous transition).

to the canonical tricritical point, the lower branch of the curve has a zero slope at the intersection point (Fig. 2a). Thus, the specific heat of the ordered phase diverges at this point. Increasing Δ to the region between the two tricritical points a *negative specific heat* in the microcanonical ensemble first arises ($\partial T/\partial \epsilon < 0$), see Fig. 2b. At the microcanonical tricritical point Δ, the derivative $\partial T/\partial \epsilon$ of the lower branch diverges at the transition point, yielding a vanishing specific heat (Fig. 2c). For larger values of Δ a jump in the temperature appears at the transition energy (Fig. 2d). The lower temperature corresponds to the $m = 0$ solution (11) and the upper one is given by $\exp(\bar{\beta}) = 2(1 - q^*)/\sqrt{(q^*)^2 - (m^*)^2}$, where m^*, q^* are the values of the order parameters of the ferromagnetic state at the transition energy. The negative specific heat branch disappears at larger values of Δ, leaving just a temperature jump (see Fig. 2e). In the $\Delta/J \to 1/2$ limit the low temperature branch, corresponding to $q = m = 1$ in the limit, shrinks to zero and the $m = 0$ branch (11) describes the full energy range (Fig. 2f). In the inset of Fig. 1 we report the transition temperatures in the microcanical ensemble against Δ/J for both the $m = 0$ (lower dot-dashed line) and the $m \neq 0$ solutions (upper dot-dashed line). The lines are drawn starting at the canonical tricritical point. The region between the two tricritical points is too small to be appreciated in the figure. A schematic phase diagram in the first-order region is given in Fig. 3, where we fictitiously expand the region of the tricritical points. Note that the canonical first-order line necessarily crosses the upper microcanonical transition line at some point.

That such unusual effects in the microcanonical ensemble are associated with a first-order phase transition was also suggested in Ref. [9]. Some of these authors discuss mainly short-range interactions, for which such features are produced by finite size effects.

As usual, for mean-field models, one can express the free energy $f(T, m)$ in the canonical ensemble as a function of T and m. The spontaneous magnetization $m_s(T)$, the temperature-energy relation $T(\epsilon)$, and the free energy $f(T)$ may be obtained by minimizing $f(T, m)$ with respect to m and using well-known thermodynamic relations. We now note that the negative specific heat branch of the microcanonical ensemble corresponds to a local *maximum* of the free energy $f(T, m)$ with respect to m.

This result can indeed be derived on quite a general ground. It is easy to show that an extremum of $f(T, m)$ corresponds to an extremum of $s(\epsilon, m)$ with respect to m. Indeed, the free energy $f(T, m)$ may be obtained by minimizing $\tilde{f}(T, \epsilon, m) = \Delta\epsilon - s/\beta$ with respect to ϵ, keeping T and m fixed. This minimization yields the temperature-energy relation (10) which may be multivalued. On the other hand, minimizing $\tilde{f}(T, \epsilon, m)$ with respect to m yields the result that $\partial f(T, m)/\partial m$ and $\partial s(\epsilon, m)/\partial m$ are proportional to each other and thus vanish together. It can be shown [10] by studying the second derivatives that, when the stationary point of $\tilde{f}(T, \epsilon, m)$ with respect to ϵ and m is a saddle point, the resulting entropy exhibits a negative specific heat. As a consequence, we can recover the full microcanonical solution by studying the stationary points of the function $\tilde{f}(T, \epsilon, m)$. However, this function is not typically available for non-mean-field models.

The relevant features of the BEG model with infinite-range couplings persist also for *nonintegrable* interactions. In order to investigate this point, we introduce a generalization of the BEG model given by the Hamiltonian

$$H = \Delta \sum_{i=1}^{N} S_i^2 - \frac{J}{\tilde{N}} \sum_{i>j} \frac{S_i S_j}{r_{ij}^{\alpha}}, \qquad (14)$$

where r_{ij} is the distance on a 1D lattice between spins at sites i and j. The interactions are nonintegrable for $\alpha \leq 1$.

The normalization $\tilde{N} = 2^{\alpha}(N^{1-\alpha} - 1)/(1 - \alpha)$ ensures that the energy is extensive. Models of this type have been previously introduced by other authors, and studied within the canonical ensemble [11]. We apply periodic boundary conditions (pbc), for which the model is more easily tractable, and we then take r_{ij} to be the smallest of the two distances compatible with pbc. The interaction matrix $(r_{ij})^{-\alpha}/\tilde{N}$ can be exactly diagonalized, which allows one to solve model (14) in the canonical ensemble. When appropriately rescaled thermodynamic quantities are chosen, the solution is the same as for the $\alpha = 0$ case (as it happens for the models studied in Ref. [11]). Moreover, using a Fourier representation of Hamiltonian (14) and considering only the long wavelength components, it is possible to obtain an approximate expression for the entropy in the microcanonical ensemble [10]. Maximizing this expression at fixed energy, we find that the $\alpha = 0$ microcanonical solution is also left unchanged. Since both the canonical and the microcanonical solutions are not modified, we conclude that ensemble inequivalence persists for the slowly decreasing case $\alpha < 1$. Details of this analysis will be reported elsewhere [10].

In summary, we have compared the *canonical* with the *microcanonical* solutions of the infinite-range Blume-Emery-Griffiths model. We find that the global phase diagrams are different in the two ensembles. Although they are found to be the same in the domain where the canonical transition is continuous, they differ from each other when the canonical transition is first order. *Negative specific heat* and *temperature jumps* at the transition energy are found in the microcanonical ensemble. These results generalize those of Ref. [5] in the context of a simple model, where, by varying a single parameter, one can observe a variety of possible features of the phase diagram. Moreover, we are able to understand the role played by the constraint of fixing the energy in the microcanonical ensemble, which produces a stabilization of canonically unstable solutions. In the phase coexistence region, the unusual microcanonical thermodynamic properties should result in some peculiar dynamical behavior, as has been observed in studies of a different mean-field model with continuous variables [12]. Our results for the BEG model are not limited to the infinite-range case, but can be extended to weakly decaying *nonintegrable* interactions.

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