Zeroth-order phase transition in the Blume-Emery-Griffiths model without bilinear exchange coupling

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(Received 27 April 2021; revised 15 July 2021; accepted 30 July 2021; published 11 August 2021)

We study the simplified Blume-Emery-Griffiths model without bilinear exchange coupling both in the microcanonical ensemble and in the canonical ensemble. This model can exhibit a zeroth-order phase transition in the microcanonical ensemble accompanied by a finite entropy jump. However, this singularity in entropy cannot be observed in the canonical ensemble, which illustrates the ensemble inequivalence. Moreover, the global phase diagram of this model is given in both ensembles.

DOI: 10.1103/PhysRevE.104.024114

I. INTRODUCTION

Phase transitions (PTs) are quite common in nature, such as the freezing of water near 0 °C under one standard atmosphere. A PT is the phenomenon that the macroscopic properties of a thermodynamic system change drastically as the parameters of the system (such as the energy and temperature) are varied [1–4]. PTs can be theoretically described by the nonanalyticities in the functions characterizing thermodynamic quantities. Moreover, the classification of PTs also relies on the degree of nonanalyticity in thermodynamic quantities. For instance, the type of PT of an isolated system is characterized by the discontinuity in the derivatives of its entropy s with respect to the energy ε [5]. Thus, a first-order PT in the microcanonical ensemble is usually accompanied by a temperature singularity (jump, cusp, or divergence) based on the usual thermodynamic relation

$$\frac{\partial s}{\partial \varepsilon} = \frac{1}{T}. \tag{1}$$

And a singularity in the specific heat capacity C emerges during a microcanonical second-order PT since $\partial^2 s/\partial \varepsilon^2 = -T^{-2}C^{-1}$. Singularities in temperature and specific heat at transition points have been extensively reported in previous literature [6–27].

Compared with the first-order and higher-order PTs, the zeroth-order PTs are much less studied. In the microcanonical ensemble, a transition with a discontinuity in the entropy s itself is of zeroth order. In most cases, the zeroth-order PTs are studied in the black-hole systems [28–39]. The zeroth-order PT in a common spin system was presented by us very recently [40]. By assuming the dynamics of the spin system is defined by its local flipping, we have shown that the spin system with mean-field interactions can exhibit the zeroth-order PT due to the ergodicity breaking [40]. Whether an ergodic spin system which is not restricted to the local-dynamics assumption can exhibit PTs of zeroth order has not been clear up to now. In this paper we are going to illustrate that the Blume-Emery-Griffiths (BEG) model can exhibit the microcanonical zeroth-order PT without the local-dynamics assumption.

The BEG model was introduced to study the superfluid PT and phase separation in the He^3-He^4 mixture [41]. This spin model has become a paradigmatic model and its thermodynamic properties have been extensively studied in many different parameter ranges [6–10,42]. In this paper, we study a simplified version of the BEG model by ignoring its bilinear exchange coupling. The BEG with this simple parameter set can exhibit a microcanonical zeroth-order PT and show very complex phase diagrams which are different in the canonical and microcanonical ensembles.

The paper is arranged as follows. In the next section, the simplified BEG model and its exact canonical solution are briefly described. In Sec. III, the microcanonical solution to this model is presented in detail. The microcanonical zeroth-order PT exhibited by this model is analyzed in Sec. IV, and the microcanonical phase diagram is also given in this section together with the corresponding canonical phase diagram. Finally, our summary is given in the last section.

II. THE SIMPLIFIED BEG MODEL AND ITS CANONICAL SOLUTION

The Hamiltonian of the BEG model describes N identical particles of spin 1 with long-range interactions [8–10]:

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

where S_i represents the spin located at the ith lattice site and can only take one of the values $\{-1, 0, 1\}$. The coupling Δ is the crystal-field interaction controlling the energy difference between the nonmagnetic ($S = 0$) and magnetic ($S = \pm 1$) states. J and K are the bilinear exchange interaction and the biquadratic coupling, respectively, and they are both long-range interactions [14–25,43]. By adopting the prescription of Kac *et al.*, J and K are rescaled by $1/N$ in order to ensure the extensive property of the energy [44]. In this paper, we drop the second term by setting $J = 0$, which means the crystal-field interaction and the biquadratic interaction are much

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stronger than the bilinear exchange interaction. As mentioned in the Introduction, this simplified BEG model without the bilinear exchange coupling can show some prominent properties of the long-range interacting systems at thermodynamic equilibrium such as ensemble inequivalence and nonadditivity of energy [43]. Without loss of generality, the Boltzmann constant k_B and K are set to be unity.

Our simplified BEG model can be solved in both canonical and microcanonical ensembles, and one can easily obtain the analytical descriptions of the equilibrium distribution functions in the thermodynamic limit with the help of the canonical partition function

$$Z(\beta) = \sum_{\{S_i\}} e^{-\beta H} = \sum_{\{S_i\}} e^{-\beta\Delta\sum_{i=1}^{N} S_i^2 + \frac{\beta K}{2N}(\sum_{i=1}^{N} S_i^2)^2}, \tag{3}$$

where $\beta = (k_B T)^{-1}$ is the inverse temperature. Using the Hubbard-Stratonovich transformation [45]

$$e^{ba^2} = \sqrt{\frac{b}{\pi}} \int_{-\infty}^{+\infty} \exp(-by^2 + 2aby)dy, \tag{4}$$

the partition function of our model can be rewritten as

$$Z(\beta) = \sqrt{\frac{\beta KN}{2\pi}} \int_{-\infty}^{\infty} \sum_{\{S_i\}} e^{-\frac{\beta KN}{2}y^2 - \beta(\Delta - Ky)Nq} dy, \tag{5}$$

where $q = \sum_i S_i^2/N$ is the quadrupole moment per particle. Note that the Hubbard-Stratonovich transformation should be utilized twice to solve the ordinary BEG model with bilinear exchange coupling, and hence, the partition function is expressed by a double integral [8–10]. By dropping the bilinear exchange term, our simplified BEG model becomes much easier to solve.

After summing over all the spin configuration $\{S_i\}$, the partition function is given by

$$\begin{aligned} Z(\beta) &= \sqrt{\frac{\beta KN}{2\pi}} \int_{-\infty}^{\infty} e^{-N\{\frac{\beta K y^2}{2} - \ln[1+2e^{\beta(Ky-\Delta)}]\}} dy \\ &\equiv \int_{-\infty}^{\infty} \exp[-N\beta \widetilde{f}(\beta, y)]dy, \end{aligned} \tag{6}$$

where $\widetilde{f}(\beta, y)$ is an analytic function of β and y. As an example, we plot $\widetilde{f}(\beta, y)$ as a function of y for two different values of Δ in Fig. 1. Given β (or temperature), the equilibrium state of our system corresponds to the absolute minimum of $\widetilde{f}(\beta, y)$ according to the saddle-point analysis, and the value of y corresponds to the equilibrium quadrupole moment per particle q. Figure 1 shows that the system experiences a canonical first-order transition with increasing β (or decreasing temperature) in both cases ($\Delta = 0.55$ and 0.64).

Using the saddle-point analysis, the integration in Eq. (6) can be calculated in terms of y, and the energy per particle of the system ε can be deduced from the partition function by using the canonical relation $\varepsilon = -\frac{1}{N}\partial \ln Z/\partial\beta$. The canonical free energy per particle is given by

$$f(\beta) = \min_y \widetilde{f}(\beta, y) \tag{7}$$

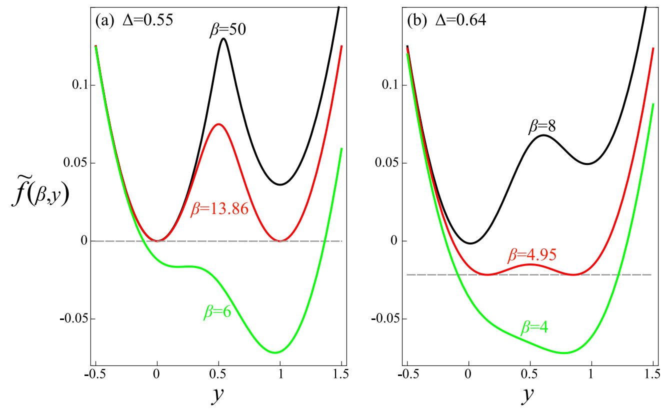

FIG. 1. The function $\widetilde{f}(\beta, y)$ for different Δ and β. A canonical first-order PT occurs at $\beta = 13.86$ (a) or $\beta = 4.95$ (b)

in the thermodynamic limit $N \to \infty$. And the canonical entropy is given by using the conventional expression

$$s(\varepsilon) = \min_\beta \max_y [\beta\varepsilon - \beta\widetilde{f}(\beta, y)]. \tag{8}$$

The canonical results of the energy and entropy of our model are displayed in Fig. 3 in comparison with their corresponding microcanonical quantities.

III. MICROCANONICAL APPROACH

The microcanonical entropy per spin $s(\varepsilon)$, as a function of the energy per spin ε, can be obtained directly by utilizing the saddle-point method given in Refs. [46,47]. The saddle-point method shows that

$$s(\varepsilon) = \max_y \min_\beta [\beta\varepsilon - \beta\widetilde{f}(\beta, y)]. \tag{9}$$

By comparing the expression of the microcanonical entropy given in Eq. (9) with the conventional expression of the canonical entropy [Eq. (8)], it can be seen that these two entropies can be different in different ensembles. However, to gain a better understanding on the origin of the entropy jump during the microcanonical zeroth-order PT, we switch to the conventional microcanonical approach. Note that both methods (the saddle-point method and the conventional microcanonical method presented below) are equivalent.

Suppose there are N_+ up spins, N_- down spins, and N_0 spins taking the value $S = 0$ in the system. Thus, $N_+ + N_- + N_0 = N$. The magnetization and the quadrupole moment become $M = \sum_{i=1}^{N} S_i = N_+ - N_-$ and $Q = \sum_{i=1}^{N} S_i^2 = N_+ + N_-$, respectively, and the number of microstates is

$$\Omega = \frac{N!}{N_+!N_-!N_0!}. \tag{10}$$

Hence, the energy per spin ε and the entropy per spin $s = \frac{1}{N}\ln\Omega$ can be written as

$$\varepsilon = \Delta q - \frac{K}{2}q^2, \tag{11}$$

$$\begin{aligned} s(\varepsilon, m) = -\big[&(1-q)\ln(1-q) + \tfrac{1}{2}(q+m)\ln(q+m) \\ &+ \tfrac{1}{2}(q-m)\ln(q-m) - q\ln 2\big] \end{aligned} \tag{12}$$

in the thermodynamic limit ($N \to \infty$), where $m = M/N$ and $q = Q/N$. q can be obtained by solving Eq. (11) for any given

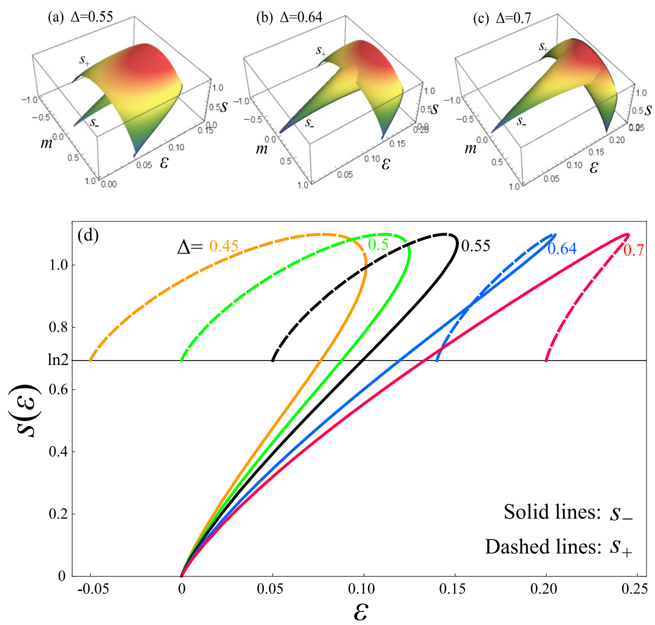

FIG. 2. The microcanonical entropy per spin $s_m(\varepsilon, m)$ as a function of energy per spin ε and magnetization m (a)–(c). (d) $s(\varepsilon)$ as a function of ε for different Δ. Solid and dashed lines represent s_- and s_+, respectively.

energy ε:

$$q_{\pm} = \frac{\Delta}{K} \pm \sqrt{\frac{\Delta^2}{K^2} - \frac{2\varepsilon}{K}}. \tag{13}$$

Since $q_{\pm}$ must be real, the expression under the square root should not be less than 0. Meanwhile, $q_{\pm}$ must lie in the interval [0,1], $0 \leqslant q_{\pm} \leqslant 1$. Therefore, the range of variation of the energy should be $\varepsilon_c \leqslant \varepsilon \leqslant \varepsilon_{\max}$ for q_+ and $0 \leqslant \varepsilon \leqslant \varepsilon_{\max}$ for q_-, where $\varepsilon_c = \Delta - \frac{K}{2}$ and $\varepsilon_{\max} = \frac{\Delta^2}{2K}$.

$s_{\pm}(\varepsilon, m)$ can be obtained for any given Δ by substituting Eq. (13) into Eq. (12), which is shown in Figs. 2(a)–2(c). The global maximum of $s_{\pm}$ locates at $m = 0$ because $\frac{\partial s}{\partial m}|_{m=0} = 0$ and $\frac{\partial^2 s}{\partial m^2}|_{m=0} = -1/q < 0$, which can be seen in Figs. 2(a)–2(c). The entropy for a given energy is obtained by maximizing $s_{\pm}(\varepsilon, m)$ with respect to the magnetization m. Thus, $s_{\pm}(\varepsilon) = \max_m s_{\pm}(\varepsilon, m) = s_{\pm}(\varepsilon, 0)$ and the spontaneous magnetic moment of this system is 0, which indicates that the system stays in the paramagnetic phase. From Fig. 2(d), it can be seen that the microcanonical entropy s is not a univalent function of the energy ε due to the nonuniqueness of the solutions of Eq. (11). The minimal value of s_+ locates at $\varepsilon = \varepsilon_c$, and $s_+(\varepsilon_c) = \ln 2$ owing to the equivalence of $+1$ and -1 states of spin at the lowest energy level.

By looking at the most probable state as determined by the maximum of the entropy, the equilibrium entropy is given by

$$s(\varepsilon) = \max\{s_+(\varepsilon), s_-(\varepsilon)\}. \tag{14}$$

This equation is valid if our model is ergodic. By specifying the model is restricted to the local microcanonical dynamics, the ergodicity can be broken [43,48]. As mentioned in the Introduction, we would like to show an example with an ergodic spin system which is not restricted to the local microcanonical dynamics. Thus, Eq. (14) is true by definition.

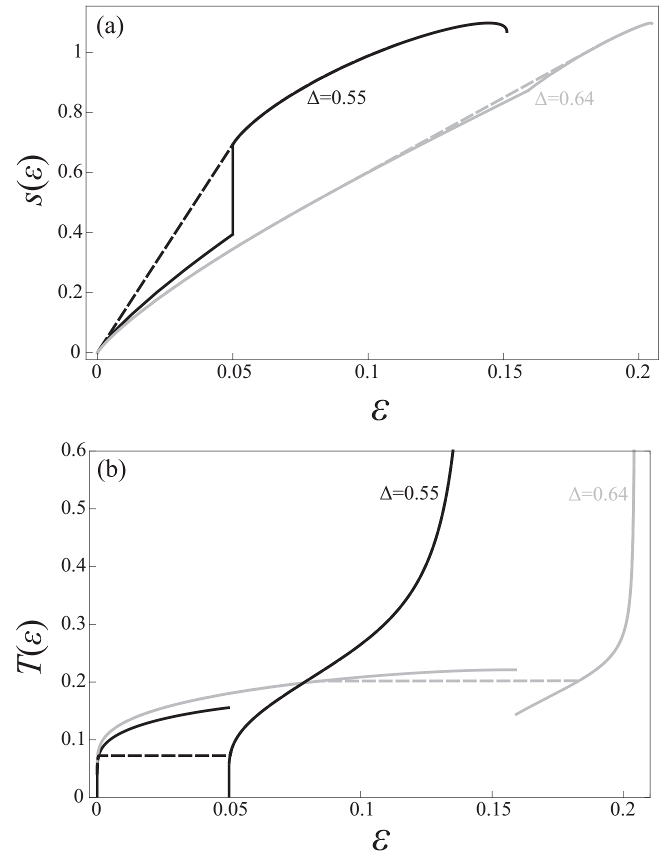

FIG. 3. Entropy (a) and temperature (b) as functions of energy for the microcanonical (solid line) and canonical (dashed line) ensembles.

Using Eqs. (12)–(14), we calculate the microcanonical entropy of our simplified BEG model in the thermodynamic limit ($N \to \infty$) and show the results in Fig. 3(a) together with the corresponding canonical entropy. In this figure, we show the entropy functions for two typical cases, $\Delta = 0.55$ and $\Delta = 0.64$. From Fig. 3(a), a finite entropy jump can be observed at $\varepsilon = \varepsilon_c = 0.05$ for $\Delta = 0.55$ in the microcanonical ensemble. This entropy jump is caused by the switching between these two branches ($+$ and $-$) of the microcanonical entropy [see Fig. 2(a) and 2(d)]. The appearance of a nonconcave point on the microcanonical entropy curve at $\varepsilon \simeq 0.159$ for $\Delta = 0.64$ relies on the same reason [see Figs. 2(b) and 2(d)]. Note that nonconcave regions in microcanonical entropy appear in the presence of PTs, while the corresponding canonical entropy applies to the concave envelope of the microcanonical entropy. Based on the usual thermodynamic relation given in Eq. (1), the microcanonical temperature T may not monotonically increase with the energy ε when the the microcanonical entropy s is nonconcave, as shown in Fig. 3(b).

IV. PHASE TRANSITION AND PHASE DIAGRAM

For the microcanonical case, the energy ε is the control variable. For $\Delta = 0.64$, a transition with the continuous

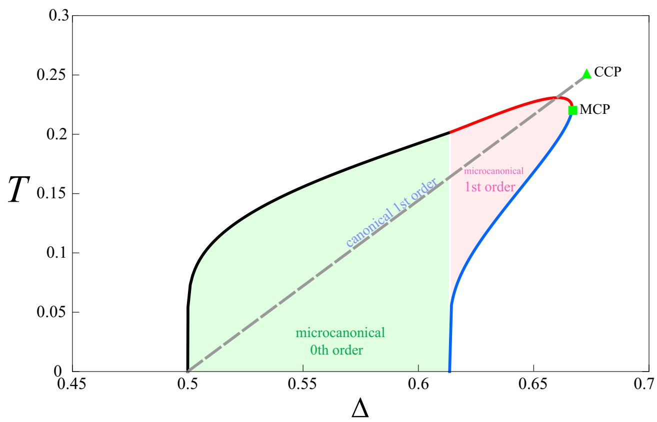

FIG. 4. The microcanonical and canonical (Δ, T) phase diagram. The tinted areas are not accessible in the microcanonical ensemble.

entropy s but a discontinuity in the temperature T is of first order (see the gray solid lines in Fig. 3). On the contrary, for the case of $\Delta = 0.55$, the microcanonical entropy s exhibits a finite jump at the transition point $\varepsilon = 0.05$ which implies a zeroth-order PT. The specific energy of the zeroth-order transition is $\varepsilon_c = \Delta - \frac{K}{2}$, and the entropy jump can be understood by calculating the Boltzmann entropy via the microcanonical approach as we have already illustrated in Sec. III. Note that, the microcanonical temperature T also shows a jump at the zeroth-order PT point and T drops to zero immediately after the transition.

In the canonical ensemble, the temperature T (or the inverse temperature β) is the control variable and the energy per spin ε is deduced from the partition function Z by using the canonical relation $N\varepsilon = -\partial \ln Z(\beta)/\partial\beta$. From the caloric curves (T-ε curves) indicated by dashed lines in Fig. 3(b), the PTs are of first order for both cases ($\Delta = 0.55$ and $\Delta = 0.64$) accompanied by latent heats. This can also be verified by checking the $\widetilde{f}(\beta, y)$ function shown in Fig. 1.

The (Δ, T) phase diagrams in both the microcanonical ensemble and the canonical ensemble are shown in Fig. 4. These two phase diagrams illustrate the ensemble inequivalence quite clearly. Both the zeroth-order PT (the light green area) and the first-order PT (the light pink area) can be found in the microcanonical phase diagram while the system cannot exhibit the zeroth-order PT in the canonical ensemble.

In the microcanonical ensemble, starting from the point of ($\Delta = 0.5$, $T = 0$), the zeroth-order PT changes to first order at the vertical boundary separating the light green area and the light pink area. The vertical boundary is shown as a white vertical line at $\Delta_B \backsimeq 0.6135$ in Fig. 4, and Δ_B is simply obtained by solving $s_+(\Delta, \varepsilon) = s_-(\Delta, \varepsilon) = \ln 2$. The first-order PT ends at a microcanonical critical point (MCP, shown as a green square dot in Fig. 4). At the MCP, both $s_+(\Delta, \varepsilon) = s_-(\Delta, \varepsilon)$ and $\partial s_+(\Delta, \varepsilon)/\partial\varepsilon = \partial s_-(\Delta, \varepsilon)/\partial\varepsilon$ should be satisfied at the same time, which leads to $\{\Delta_{\mathrm{MCP}} = \frac{2}{3} \backsimeq 0.667, T_{\mathrm{MCP}} = \frac{2}{9} \backsimeq 0.222\}$. Both the zeroth-order PT and the first-order PT are characterized by a discontinuity in the temperature. Thus, a transition is represented by two lines in the (Δ, T) phase diagram and these two lines are corresponding to the temperatures at the transition point. For the zeroth-order PT, one transition line is shown as the black solid curve in Fig. 4, and another transition line is the horizontal isothermal line at $T = 0$ since the temperature drops to 0 immediately after the PT. The red and blue solid lines in Fig. 4 correspond to the first-order PT.

In the canonical ensemble, the PT is of first order. The PT line (gray dashed line) is straight, starting from ($\Delta = 0.5, T = 0$) and ending at the canonical critical point (CCP). The CCP is characterized by the vanishing of the first-order, the second-order, and the third-order derivatives of $\widetilde{f}(\beta, y)$ with respect to y. Hence, the CCP is then given by $\{\Delta_{\mathrm{CCP}} = \frac{1}{2} + \frac{1}{4}\ln 2 \backsimeq 0.673, T_{\mathrm{CCP}} = \frac{1}{4} = 0.25, y_{\mathrm{CCP}} = \frac{1}{2}\}$. The MCP (■) and the CCP (▲) are quite close to each other but do not coincide.

V. SUMMARY

In this paper, we theoretically studied the simplified Blume-Emery-Griffiths model without bilinear exchange coupling both in the microcanonical ensemble and in the canonical ensemble. We explored the microcanonical and canonical phase diagrams of this model for the entire parameter range of Δ. Similar to the earlier studies with other choices of parameter ranges, the ensemble inequivalence was also observed within our parameter range. We mainly focused on the microcanonical zeroth-order phase transition accompanied by a unique entropy jump. This model can exhibit the microcanonical zeroth-order phase transition without the nonergodic assumption.

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