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Phase diagrams of the spin-1 Ising Blume-Emery-Griffiths model: Monte Carlo simulations

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The Monte Carlo simulation technique is used to study the phase diagrams of a two-dimensional spin-1 Ising model with bilinear and biquadratic nearest-neighbor pair interactions and a single-ion potential. A staggered quadrupolar phase appears at low temperatures with the competing bilinear and biquadratic interactions. The phase boundary line of the staggered quadrupolar phase and that of the ferromagnetic phase are extremely close to each other at low temperatures. An argument is used to distinguish the most probable phase diagram from the several possible ones based on the Monte Carlo data.

The spin-1 Ising model with bilinear and biquadratic nearest-neighbor pair interactions and a single-ion potential is known as the Blume-Emery-Griffiths (BEG) model.[1] The model with vanishing biquadratic interactions is called the Blume-Capel model.[2] Both have been studied extensively[3-9] because of the fundamental interest in the tricritical phenomena of physical systems such as ^{3}He-^{4}He mixtures, multicomponent fluids, metamagnets, and ternary alloys.

The Hamiltonian of the BEG model is

$$H=D\sum_i s_i^2-J\sum_{\langle i,j\rangle} s_i s_j-K\sum_{\langle i,j\rangle} s_i^2 s_j^2 \quad (J>0) \ , \tag{1}$$

where each s_i can take the values 1, 0, -1. The mean-field approximation has been used for investigations of the phase diagrams. Qualitatively correct results have generally been found but with some exceptions. More sophisticated methods have been used to provide the correct pictures, especially for the two-dimensional lattices. All the treatments have essentially been confined to the parameter space with $J+K>0$ (with $J>0$).

In the region of $J+K<0$, a new ordered phase occurs at low temperatures which we name the staggered quadrupolar phase. Recently, the mean-field approximation[9] has been used to describe the phase diagram including this region. Certain Monte Carlo simulation pictures have also been shown.[9]

In this paper we present the major results of the phase diagram of the BEG model ($J>0$) in a plane square lattice with interaction parameters including the region $J+K<0$. The results have been obtained by the Monte Carlo simulation technique.

The standard Metropolis "importance sampling" method is used with a vectorized program running on the Cyber 205. The size of the lattice has been chosen from 10×10 up to 200×200 in the simulations. To locate the phase transition points, we have analyzed the data of the order parameters and the susceptibilities. The energy and specific-heat data have also been produced, but the peak of the specific heat is often overshadowed by the Schottky anomaly associated with the anisotropy of the system. We have also adopted the fourth-order cumulant method to locate the critical temperature more accurately. The critical exponents are estimated with finite size scaling and appropriate extrapolations.

In Fig. 1 the phase diagram in the $(T/J,K/J)$ plane is shown near $K/J=-1$. The solid lines represent the second-order phase-transition boundaries and the dashed lines the first-order phase-transition boundaries. Data of high statistical accuracy have been used to locate the phase boundary. In this plot the error bounds are about twice the thickness of the line drawn. The phase boundaries are labeled by the single-ion potential parameter in units of J.

To discuss the phase diagram, first we take $D=0$. It is a second-order phase-transition boundary separating the ferromagnetically ordered phase and the paramagnetic (disordered) phase. As the value of K/J approaches -1 the critical temperature approaches zero *linearly* given by

$$T_c=3.8J(1+K/J) \ . \tag{2}$$

The accuracy of the coefficient 3.8 is well within 1%. There is no ordering for $K/J<-1$ in contrast with the results of solving the model on the Bethe lattice.[7] There is

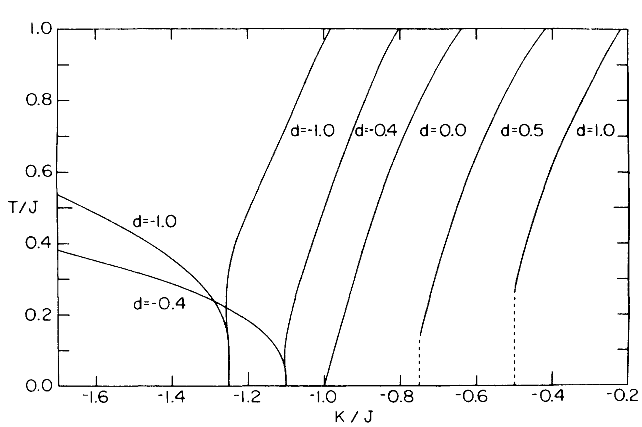

FIG. 1. Phase diagram of the BEG model near $K/J=1$. Solid lines represent the second-order phase boundaries and dashed lines, the first-order phase boundaries. The phase boundary lines are labeled by the values of $d=D/J$.

no first-order phase transition as speculated by Siqueira and Fittipaldi.[5] At $K=0$, the model is reduced to the spin-1 Ising model with only the bilinear pair interaction and $T_c/J=1.69$ which agrees with the results of the series expansion analysis[10] ($T_c/J=1.693$). As K approaches $+\infty$, the model is then equivalent to the spin-$\frac{1}{2}$ model.

In the cases with $D>0$, a second-order phase-transition line joins with a first-order phase-transition line at the tricritical point. At $T=0$, the ferromagnetic phase and a phase with $s_i=0$ at every site become coexisting at

$$K/J=D/(2J)-1 \ . \tag{3}$$

The tricritical points are located as the hysteresis starts to disappear.[11] In the region of K/J close to -1, the tricritical point is located at

$$T_t=0.3D \ , \tag{4}$$

with the value of K/J extremely close to the value given by Eq. (3). The tricritical exponent β has been estimated using the finite-size scaling method. The tricritical behavior dominates as the tricritical point is approached. We obtain

$$\beta_t=0.04\pm0.01 \ , \tag{5}$$

in agreement with the earlier work of Landau and Swendsen.[12]

For $D<0$, a new ordered phase occurs in the region of $K/J<-1$. It is a staggered quadrupolar ordered phase with two interpenetrating superlattices; one sublattice has $s_i=0$ at every site and the other sublattice has sites occupied randomly by $s_i=1$ or -1. The ordering is similar to that of the hard-core lattice gas,[13] but in such interpretation, there are two types of atoms in the present case.

The ordering parameter can be designated as

$$Q=\frac{2}{N}\left(\sum_{f\in A}s_f^2-\sum_{g\in B}s_g^2\right) \ , \tag{6}$$

where N is the total number of sites of the lattice and the two sublattices are labeled by A and B. The phase transition can be located at the peak of the susceptibility,

$$X_Q=N(\langle Q^2\rangle-\langle Q\rangle^2)/k_BT \ . \tag{7}$$

The critical exponents β and γ are found to assume the two-dimensional Ising values ($\beta=0.125$ and $\gamma=1.75$) as expected. The critical temperature curves for $D/J=-1.0$ and $D/J=-0.4$ are plotted in Fig. 1.

At $T=0$ the staggered quadrupolar phase and the ferromagnetic phase are separated at

$$K=-J+D/4 \ . \tag{8}$$

For $K>-J+D/4$ the system is ordered ferromagnetically. The phase transitions from the ferromagnetic phase to the disordered phase and from the staggered quadrupolar phase to the disordered phase are both of second order. In Fig. 1 the phase diagram shows that the two second-order phase boundary lines approach and become extremely close to each other at low temperatures. Using only the Monte Carlo data some possible pictures can be produced and some can be eliminated but no definite final answer can be reached. In the following we first discuss the pictures of the phase diagram based on the Monte Carlo data and then use an argument to obtain the most likely picture.

Assuming that the two phase boundary lines meet at a finite temperature, a possible picture indicated by the Monte Carlo data, the two ordered phases (ferromagnetic and staggered quadrupolar) will then be separated by a phase boundary line which is either second order (picture A) or first order (picture B) observed in the mean-field approximation.[9] A careful examination of the critical exponents ruled out picture A. It is argued that in picture A three second-order lines meet at a tricritical point, and the exponent β should then be a factor of 3 smaller. The tricritical behavior has been observed dominating near the tricritical point in many models studied. The fact that the estimated critical exponent β stays always in the range of 0.1 and 0.15 along the boundary line indicates that where the three phase boundary lines meet is unlikely to be a tricritical point.

However, the second-order phase-transition behavior observed can not eliminate the possibility of picture B. Recently,[14] in the study of the three-dimensional three-state Potts model and the two-dimensional q-state Potts models with q equal to 5 and 6, such "pseudocritical" phenomena have been observed with no regular first-order transition features detected, even though it is known that the phase transition are of first order for these models, especially for the two-dimensional models for which exact solutions exist.[15] The phase transitions of these models are named as "weak first-order phase transition." At the transition, the discontinuity of the order parameter is small and is superposed by a second-order-like power-law behavior. In the Monte Carlo study of the present model, the observations of the apparent coexistence of the two ordered phases in the plots of the spin configurations at the boundary line and the fact that the system can stay in either of the ordered phases for a long period of time compared to the time it takes the system to change from one phase to the other phase (with some second-order-like fluctuations) seem to support picture B. Because of the statistical fluctuations and finite-size effects in the Monte Carlo simulations, it is a difficult problem to distinguish the order of the phase transition.

An argument, however, rejects picture B and presents the more probable picture of the two second-order phase boundary lines meeting at zero temperature.

The argument follows from observing the finite field behavior of the system and considering the zero-field limit. Adding an external magnetic field to the system yields the Zeeman energy term $-\sum s_i$ in the Hamiltonian. At low temperatures if $\beta h\gg1$, the possibility of $s_i=-1$ is very small. Thus in such limit, $s_i^2=s_i$ and the Hamiltonian becomes

$$H=-(-D+h)\sum_i s_i-(J+K)\sum_{\langle i,j\rangle}s_is_j \ . \tag{9}$$

Expressing the Hamiltonian in terms of $t_i=s_i-\frac{1}{2}$,

$$H=-[h-D-(J+K)z/2]\sum_i t_i-(J+K)\sum_{\langle i,j\rangle}t_it_j+\text{const} \ , \tag{10}$$

with $t_i = \pm \frac{1}{2}$ and $z = 4$ for the plan square lattice.

For $J+K<0$, the situation we are considering, Eq. (10) can be interpreted as an Ising antiferromagnet with nearest-neighbor coupling in an external field. The phase transition is known as second order.[16]

This implies that the phase transition of the staggered quadrupolar phase at low temperature is of second order with a field applied, and the field can be of arbitrarily small value as long as the temperature is sufficiently low (i.e., $\beta h \gg 1$).

According to the picture B (mean-field approximation) a finite portion of the boundary line of the staggered quadrupolar phase is of first order. When an external field is applied to the system, the region of the first-order transition becomes smaller but it should still appear for sufficiently small field. As discussed above, at sufficiently low temperatures ($\beta h \gg 1$) the phase transition should be of second order. This means that in picture B the phase boundary of the staggered quadrupolar phase in the presence of a small field consists of at least a part of second order at sufficiently low temperatures and a part of first order at higher temperatures. In fact at high temperatures the transition of the quadrupolar phase to the disordered phase is observed as second order in the present simulation and other approximations. Thus two tricritical points would appear on the phase boundary. It is a rather rare feature. However, as mentioned previously, the tricritical exponent β is three times smaller than the second-order value and normally dominates near the tricritical point (as observed in the case of $D>0$ of the present BEG model). The observed critical exponent β along the phase boundary line of the staggered quadrupolar phase always shows the second-order value within the statistical uncertainty in the current Monte Carlo simulations. The opposition of both picture A and picture B leads us to propose that most probable phase diagram with the phase boundary lines of the staggered quadrupolar phase and the ferromagnetic phase meet at zero temperature in the cases of $D<0$, and both are of second order.

In conclusion, a phase diagram which includes the staggered quadrupolar phase for the BEG model has been presented. The most likely picture is that for $D<0$ the staggered quadrupolar phase and the ferromagnetic phase are separated by a disordered phase and the second-order phase boundary lines of the two ordered phases meet only at zero temperature. It is different from the mean-field picture.[9]

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