Ferrimagnetic Phases in the Blume-Emery-Griffiths Model: Implications for the Antiferromagnetic Potts Model

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The cluster-variation method is used to study the phase diagram of the Blume-Emery-Griffiths model on a simple cubic lattice. The main attention is paid to the ferrimagnetic phases occurring in a certain range of coupling parameters. A new topology, including three ferrimagnetic phases, is obtained in the vicinity of the line in parameter space where the model reduces to the antiferromagnetic three-state Potts model. The results imply the existence of three phase transitions in the antiferromagnetic Potts model.

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The spin-1 Ising model with both bilinear and biquadratic nearest-neighbor interactions, the Blume-Emery-Griffiths (BEG) model, was initially proposed in order to describe phase separation and superfluid ordering in ^{3}He-^{4}He mixtures [1]. Later the model was used to describe the properties of multicomponent fluids [2], microemulsions [3], semiconductor alloys [4], and electronic conduction models [5].

The Hamiltonian of the BEG model is

$$\mathcal{H} = -J\sum_{\langle ij\rangle} s_i s_j - K\sum_{\langle ij\rangle} s_i^2 s_j^2 + \Delta\sum_i s_i^2, \qquad (1)$$

where $s_i = 0, \pm 1$ and $\langle ij\rangle$ indicates summation over nearest-neighbor pairs.

An extensive analysis of the BEG model with $J+K > 0$, $J > 0$ was made by means of mean-field approximations (MFA) [1,2,6,7] and renormalization-group (RG) techniques [8,9]. Exact results for the two-dimensional honeycomb lattice were obtained on a subspace of parameters J, K, and Δ [10–12]. Further, Monte Carlo (MC) simulation for $J+K < 0$ revealed a new, staggered-quadrupolar phase [13–15]. In this phase, $s_i = 0$ on one sublattice and $s_i = \pm 1$ at random on the other.

Recently a very rich phase diagram was obtained for three-dimensional bipartite lattices by the MFA [16], featuring single- and double-reentrancy regions and ferrimagnetic phases for $K < -1$. Though RG studies [17] did not obtain reentrancy and ferrimagnetic phases, it was suggested this was a result of a restricted flow space and the MFA result was assumed to be correct. This assumption was confirmed by Monte Carlo renormalization-group (MCRG) calculations [18].

Here we present results of cluster-variation method (CVM) calculations of the BEG model on a simple cubic (sc) lattice. For $K/J > -3$ our results are qualitatively similar (except for minor details) to those of the MFA [16] and quantitatively close to the MCRG results [18]. Therefore the main attention in our investigation was paid to the occurrence of the ferrimagnetic phases in the vicinity of $K/J = -3$ and $\Delta/J = -12$, where the BEG model reduces to the antiferromagnetic (AF) Potts model and where we obtain a remarkable difference from the MFA result. This particular region was not covered by MC calculations.

The two-sublattice phase of the BEG model can be described by the magnetizations and quadrupolar moments of the sublattices a and b:

$$m_a = \langle s_a\rangle\,,\ m_b = \langle s_b\rangle\,,\ q_a = \langle s_a^2\rangle\,,\ q_b = \langle s_b^2\rangle\,. \qquad (2)$$

The values of these parameters define four phases with different symmetry. These are (1) paramagnetic (P) with $m_a = m_b = 0$, $q_a = q_b$; (2) ferromagnetic (F) with $m_a = m_b \neq 0$, $q_a = q_b$; (3) staggered quadrupolar (SQ) with $m_a = m_b = 0$, $q_a \neq q_b$; and (4) ferrimagnetic (I) with $m_a \neq m_b \neq 0$, $q_a \neq q_b$.

In the following we put $J = 1$, i.e., temperatures and energies are normalized by J, when not stated explicitly. The $J < 0$ case can be mapped on the $J > 0$ case by redefining the spin direction for one sublattice.

The phase diagram was calculated by the CVM in eight-point "cube" approximation. The details of the CVM for the BEG model are given elsewhere [19].

The phase diagram for $K = -3$ is a particular one, since the line $\Delta = -12$ (or, to be precise, its $J < 0$ counterpart) corresponds to the three-state AF Potts model with the Hamiltonian

$$\mathcal{H} = -2J\sum_{\langle ij\rangle} \delta_{s_i s_j}, \qquad (3)$$

and we get the Potts transition at $T_{c1} = 2.535$, which is only 2.4% above the best MC estimation $T_c/J = 2.47 \pm 0.01$ [20]. The ordered phase of this model is sixfold degenerate, and it was suggested [16] that these six phases should be accommodated in the BEG model by the first-order line meeting the twofold degenerate SQ phase and fourfold degenerate I phase. The I phase was readily obtained in the MFA [16] in the region $-13 < \Delta < -12$. Our CVM analysis gives a much more narrow region of existence for the low-temperature ferrimagnetic phase $-12.05 < \Delta < -12$ (Fig. 1) and reveals a new quite odd topology — actually *two* different ferri-

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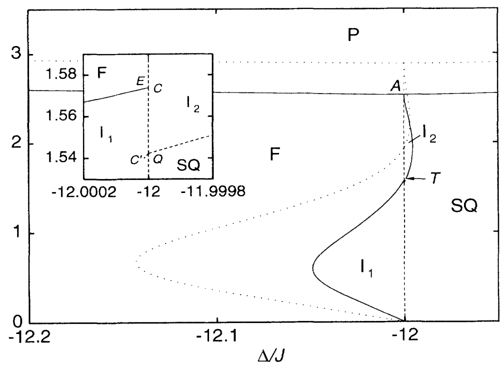

FIG. 1. Calculated (T, Δ) phase diagram of the BEG model at $K/J = -3$. Solid and dashed lines represent the second- and first-order phase transition lines, respectively, obtained by the "cube" approximation of the CVM. The dotted line is the result of CVM "pair" approximation. The special points are critical (C, C'), critical end point (E), multicritical (A), tricritical (T), and quadruple (Q).

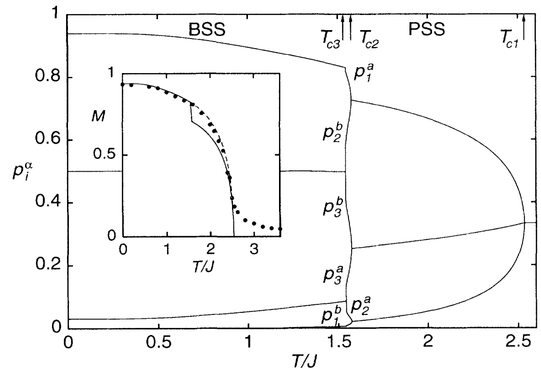

FIG. 2. The temperature dependence of the expectation values for different states of the AF Potts model, corresponding to $K/J = -3$ and $\Delta/J = -12$. Inset: The temperature dependence of the global order parameter [Eq. (5)]. The solid line represent CVM results; the dots, Monte Carlo simulation (Ref. [22]). The dashed line is for the unstable BSS solution in the CVM.

magnetic phases do exist: one (I_1) corresponds to that obtained by MFA and is a result of the instability of the ferromagnetic phase against a two-sublattice ordering, another one (I_2) is caused by the instability of the SQ phase against spontaneous magnetization. Thus, in the higher temperature region $1.574 < T < 2.535$ the sixfold degeneracy is obtained by the coexistence of the twofold F phase and fourfold ferrimagnetic I_2 phase. At lower temperature, $0 < T < 1.543$, the phase diagram is qualitatively similar to the MFA result [16].

The appearance of two ferrimagnetic phases is a rather unexpected result, because it implies the existence of additional phase transitions in the ordered phase of the three-state AF Potts model on the sc lattice. These phase transitions separate regions with different types of ordering, which can be better described by the expectation values p_i^α of the three Potts states $i = 1, 2, 3$ on the two sublattices $\alpha = a$, b instead of magnetizations and quadrupolar moments [Eq. (2)]. The relations between them are

$$p_1^\alpha = \tfrac{1}{2}(q_\alpha - m_\alpha),\ p_2^\alpha = 1 - q_\alpha,\ p_3^\alpha = \tfrac{1}{2}(q_\alpha + m_\alpha). \quad (4)$$

The temperature dependencies of the expectation values p_i^α for the AF Potts model, obtained by our CVM calculations, are presented in Fig. 2.

A simplified description of the sixfold low-temperature ordered phase corresponds to $p_1^a \simeq 1$, $p_2^a = p_3^a \simeq 0$, $p_1^b \simeq 0$, and $p_2^b = p_3^b \simeq 0.5$ and its three cyclic permutations of Potts state indices and two permutations of lattice indices. In addition, each phase is infinitely degenerate since, e.g., states $i = 2$ and 3 are randomly distributed on the b sublattice yielding a finite zero-temperature entropy per site: $s = \frac{1}{2}\ln 2$. After Grest and Banavar [21] we call this phase the broken-sublattice-symmetry (BSS) phase. Our CVM result at $T = 0.1$, $p_1^a = 0.94$, $p_2^a = p_3^a = 0.03$, $p_1^b = 0.00$, and $p_2^b = p_3^b = 0.5$, is quite the same as that obtained by MC simulation [20]. Moreover, these values are saturated since they practically do not change down to $T = 0$. The entropy also does not reach the expected value $\frac{1}{2}\ln 2 = 0.3466$, instead saturating at $s = 0.3669$. It was pointed out [22] that the difference from the simplified description is due to the possibility for a Potts state to be on a "wrong" sublattice if nearest neighbors permit that.

In the higher temperature range, just below the second-order Potts transition, the ordered state corresponds to another type of ordering, namely, $p_1^a = p_2^b > \frac{1}{3}$, $p_2^a = p_1^b < p_3^a = p_3^b < \frac{1}{3}$. Here the sets of expectation values for both sublattices are equivalent, except for index permutations, but the sixfold degeneracy is still obtained via six complete permutations of the Potts state indices. We call this phase the permutationally symmetric sublattices (PSS) phase.

The transformation from the PSS ordering to the BSS ordering appears to be rather complicated. In the inset to Fig. 1 we present the details of the phase diagram in the vicinity of this transformation. The critical line between the ferromagnetic and the ferrimagnetic I_1 phases approaches the $\Delta = -12$ line from the left terminating with a critical end point E at $T_{c2} = 1.574$. This point is also a critical point C for the ferrimagnetic phase on the right, though there is no critical line outside the phase separation line $\Delta = -12$ to the right. The origin of this criticality will be discussed later.

At the same time there is another first-order transition on the Potts line at the locus $T_{c3} = 1.543$ of the quadruple point Q with first-order phase boundaries (phase separation lines) spanning both sides of the $\Delta = -12$ line. On the left it terminates with critical point C' inside the ferrimagnetic phase I_1, while on the right it transforms at the tricritical point T to the second-order critical line between the SQ and I_2 phases above $T = 1.589$. The two types of sixfold degenerate ordered structures take place above T_{c2} and below T_{c3}. The structure of the three-state AF Potts model between these temperatures is even more complicated. Actually all six p_i^α happen to be different in this region. One could say that the second-order transition breaks up the permutational symmetry between sublattices a and b, while the first-order transition establishes the symmetry between two of the three Potts states.

The ordered phase at $T_{c3} < T < T_{c2}$ should be 12 times degenerate, because of the sixfold permutational symmetry of the Potts states and the twofold symmetry of the sublattices. The coexistence of the two fourfold ferrimagnetic phases does not provide this degeneracy. Indeed, during further investigations we have found a third ferrimagnetic phase, I_3, coexisting with the other two on the line $\Delta = -12$ in this narrow temperature range. This phase does not appear in the phase diagram outside the multiphase line at $K = -3$, but it emerges at $K < -3$ in a narrow range of Δ. The above-mentioned critical point C at T_{c2} from the right appears to be a critical point of the phase separation line between I_3 and I_2 phases. This means that the $\Delta = -12$ line is a three-phase coexistence line below T_{c2} and a two-phase line above. In the three-dimensional (K, Δ, T) phase diagram the line $\Delta = -12$, $K = -3$ is the intersection of three first-order surfaces of coexistence between phases I_1, I_2, and I_3. The surface between I_2 and I_3 is terminated from above by the isolated critical line with the critical end point C at $\Delta = -12$, $K = -3$, and $T = T_{c2}$.

To our knowledge, this is the first observation of several phase transitions in the three-state AF Potts model. In such a case, the applicability and accuracy of the CVM for this highly degenerate model are the key questions. The applicability of the CVM for degenerate systems has been proven for a number of models, the most relevant one being the BEG model on the honeycomb lattice [19]. Our calculations for the BEG model on the sc lattice near $K = -1$, when compared to the MC data [14], also confirm the good accuracy of the CVM. However, the MC calculations for the three-state AF Potts model [20], though giving values of T_c and expectations of the Potts states at low temperatures very close to ours, make no hint of the additional phase transitions at intermediate temperature. It is possible that these transitions do not manifest themselves during the MC simulation. To support this suggestion we present in Fig. 3 the results of the specific heat versus temperature obtained in our calculations, together with the MC results [20]. The anomaly at T_{c2} and T_{c3} is very small and is not expected to be seen in MC results due to statistical uncertainty. In our case the anomaly just fits in between two successive MC points.

We present below an indirect argument in favor of our results. We have applied the simplest approximation of

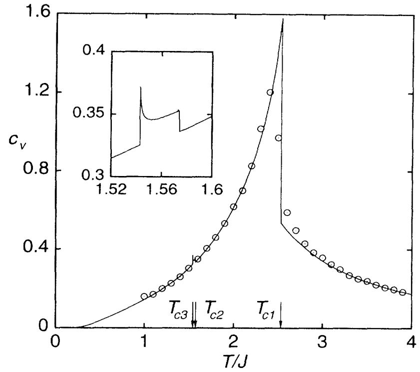

FIG. 3. The temperature dependence of the specific heat for the AF Potts model on the sc lattice. The line represents CVM results; the circles, Monte Carlo simulation (Ref. [20]).

the CVM series, the two-point cluster approximation, to calculate the phase diagram for $K = -3$ near $\Delta = -12$. The result is presented in Fig. 1. One can see that it gives a higher T_{c1} and a much wider I_1 phase in the (T, Δ) diagram. At the same time, the I_2 phase shrinks but still is clearly observable. Thus, the change in the ordering mode for the AF Potts model still takes place in this approximation. Note that the MFA, being a one-point cluster approximation, gives an even wider I_1 phase, higher T_{c1}, and no I_2 phase. According to common experience, the accuracy of the CVM increases with enlarging the basic cluster. So we expect the phase diagram of the eight-point approximation to be much closer to the exact one than that of the two-point approximation and even more than that of the MFA. Thus, in the limit of an infinite cluster (which is equivalent to the exact result) we expect the I_1 phase to shrink a little and the I_2 phase to become even larger, thereby decreasing the transition temperatures T_{c2} and T_{c3}.

It should be mentioned that the ordering of the 3D AF Potts model on the sc lattice has been a controversial subject for some time. From a rescaling argument Berker and Kadanoff [23] suggested the possibility of a low-temperature phase with no true ordering, but with algebraically decaying correlations. In contrast, Banavar, Grest, and Jasnow [22] obtained an ordered low-temperature phase by means of MC simulation and presented the temperature dependence of the "global" order parameter, which in our notations could be defined as

$$M = \frac{1}{2}\left\{|p_1^a - p_1^b| + |p_2^a - p_2^b| + |p_3^a - p_3^b|\right\} . \qquad (5)$$

The temperature dependence of this order parameter obtained in Ref. [22] is presented in the inset to Fig. 2 together with our CVM results for the same parameter. The MC points and CVM line coincide at lower temperatures, where the BSS phase is predicted by the CVM. For $T_{c2} < T < T_{c1}$ the line corresponding to the PSS phase lies well below the MC data. It is interesting to find that the CVM calculation of $M(T)$ for the BSS phase in this temperature range (shown by the dashed line) nearly coincides with the MC points. However, this phase has higher free energy than the PSS phase and is not even stable in CVM. The MFA gives a stable solution for the BSS phase everywhere below T_{c1} in agreement with Refs. [16,24]. We argue that this discrepancy between the MC and CVM results could be a result of a finite-size effect on the MC results. A "tail" like that above T_{c1} could be present as well above T_{c2}, thus "smoothing out" the drop of M between T_{c3} and T_{c2}.

A more sophisticated two-component order parameter was introduced in the MC calculation by Ono [25]. The BSS phase was clearly present below $T \simeq 1$, but fluctuations of the order parameter make it hard to distinguish the stable phase at intermediate temperature. The fluctuation area of the components of this order parameter in the two-dimensional plot at $T = 2.35$ covers the loci of order parameters of both the BSS and PSS phases.

In summary, the phase diagram of the BEG model on the simple cubic lattice was calculated by means of the CVM. Near the locus $K/J = -3$, $\Delta/J = -12$, where the BEG model reduces to the three-state AF Potts model, we unexpectedly obtain two ferrimagnetic phases, one on each side of the line $\Delta/J = -12$, instead of the single phase predicted by the MFA. A third ferrimagnetic phase emerges at $K/J < -3$. This implies the existence of additional phase transitions in the ordered phase of the three-state AF Potts model. Actually we have found two additional transitions of the first and second order. These transitions control the changes in the ordering regime of the three states on the two sublattices.

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