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Upper Bounds on the Critical Temperature for the Two-Dimensional Blume–Emery–Griffiths Model

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We obtain rigorous upper bounds for the critical temperature associated with second-order phase transitions of the two-dimensional spin-1 BEG model for real values of K and D coupling constants and for $J \geqslant 0$. We use some correlation equalities and inequalities to show the exponential decay of the two-point function characterizing the disordered phase.

KEY WORDS: Classical spin model; BEG model; phase transitions; critical temperature; correlation inequalities.

1. INTRODUCTION

In this paper we obtain exponential decay of spin–spin correlation functions (and consequently an upper bound for the critical temperature) for the two-dimensional spin-1 Blume–Emery–Griffiths (BEG) model for real values of K and D coupling constants and for $J \geqslant 0$.

This model[1] has played an important role in the study of tricritical points. In its most general form the model is described in a d-dimensional lattice Λ by the Hamiltonian

$$-H_\Lambda = J \sum_{\|i-j\|=1} S_i S_j + K \sum_{\|i-j\|=1} S_i^2 S_j^2 + D \sum_{i\in\Lambda} S_i^2 + h_3 \sum_{\|i-j\|=1} S_i S_j (S_i + S_j) + h \sum_{i\in\Lambda} S_i \tag{1}$$

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Each spin S_i occupies a site at a square lattice, taking values 0, ± 1, and interacting with a nearest-neighbor interaction. Coupling constants are interpreted as follows: h stands for the magnetic field and D for the crystal field (or single-ion anisotropy) strength, J is the bilinear (or dipolar) interaction, K is the quadrupolar interaction, and h_3 is a third-order spin interaction. The BEG model (1) is the most general model with three states and nearest-neighbor interaction on undirected bonds. For $h_3 = K = 0$ the model reduces to the Blume–Capel model[2, 3] whose mean-field solution for $h = 0$ shows a tricritical point. For $h = J = h_3 = 0$ the model maps into a spin-1/2 model[4]. Another spin-1/2 Ising model version is obtained in the limit of $D \to +\infty$ (or $K \to +\infty$), when the state $S_i = 0$ is suppressed. For $K = 3J$, $D = -2zJ$ (z is the coordination number), and $h = h_3 = 0$, one gets a 3-state Potts model with coupling $2J$.[5]

The most important version of the model, connected with the phase separation of helium mixtures, is obtained for $h_3 = 0$ and was first studied by mean-field techniques by the authors who named the model.[1] The Hamiltonian (1) was also studied in connection with ternary mixtures[6] and lattice-gas models.[7] Also, spin-3/2 extensions of the BEG model have been considered.[8–10] More recently, a mean-field solution of the general spin Blume–Capel model was presented[11] where it is shown that for any value of the spin a multiphase point is found at $T = 0$ from which different ordered phases spread out when the temperature is increased, terminating at an isolated critical point.

More sophisticated methods than mean-field approximation have been used to study the BEG and the Blume–Capel models. High- and low-temperature series expansions have been derived for the Blume–Capel model.[12, 13] Monte Carlo studies have been reported[14, 15] for the spin-1 model and also for the spin-3/2 model.[10] Within the real space renormalization group many studies have been considered for the Blume–Capel model[16, 17] and for more general model.[5, 18–20] The values of the exponents for the tricritical points obtained by those different methods can be found in Tables IV–VI of ref. 21.

We now discuss three recent works on the spin-1 BEG model, where $h = h_3 = 0$, $J \geqslant 0$, and K, D are real numbers. Mean-field results have shown a rich phase diagram.[22] Three ordered phases, namely the ferromagnetic, the ferrimagnetic, and the antiquadrupolar phases, occur and are separated by first- and continuous second-order transition lines. A multitude of multicritical points is present in the phase diagram as well as phase reentrances. A renormalization study for the same model[23] in $d = 2$ and $d = 3.05$ dimensions differs from the mean-field results in two aspects. The ferrimagnetic phase is not present and there is no reentrance phenomenon. On the other hand, a more recent prefaced renormalization group calculation[24] shows that in two dimensions a ferrimagnetic phase and a disordered–ferromagnetic–disordered reentrance structure do not occur but are present in three dimensions. In ref. 25 a Monte Carlo renormalization group technique has been applied to the three-dimensional system for values of $K/J = -0.5$ and -1.5. For these ratio values this Monte Carlo study agrees with the mean-field results concerning the presence of a ferrimagnetic phase (when $K/J = -1.5$) and reentrances. Further Monte Carlo simulations[26, 27] indicate that the disordered–ferromagnetic–disordered reentrance structure occurs in three but not in two dimensions.

Now we make a brief review of the literature on upper bounds on the critical temperature. For Ising and multicomponent spin systems, upper bounds for the critical temperature have been obtained by showing exponential decay for the two-spin correlation function for temperatures $T > T_{c,\,\text{upper}}$.[28–30] Using correlation identities and Griffiths and Newman inequalities, beyond mean-field upper bounds were obtained for the spin-1/2 Ising model.[31] Improved bounds obtained from simple methods (as in ref. 31) have been systematically obtained in recent years.[32, 33]

In the present work, we adapt the methods of ref. 31 to the BEG model, where $h = h_3 = 0$, $J \geqslant 0$, and K, D are real numbers. Based on correlation identities and on the positivity of correlations (see Proposition A1 in the appendix), an iteration procedure implies exponential decay of the two-spin correlation function. This procedure is similar to the one in ref. 29 and 31, the difference being that we do not recover the two-point function after the iteration starts. It can be generalized, in principle, to any model for which Griffiths' first inequality holds. As far as we know, ours is the first rigorous study of the ferromagnetic–disordered phase boundaries of the BEG model in a two-dimensional lattice for K and D as negative as one wishes as long as J is not too large ($J \geqslant 0$).

In the following section we will prove Theorem 1, which is the mathematical tool used to obtain the upper bounds. We make use of two correlation inequalities, proven in the appendix. One of them is a generalization of Griffiths' first inequality for the BEG model with $J \geqslant 0$, K and D real, and the other one gives upper bounds for correlations containing even powers of spin variables. The methods used to prove Theorem 1 can in principle be generalized for any model for which Griffiths' first inequality holds. In Section 3 we discuss the obtained phase diagrams for $K/J = 0$, -1.0, -1.5, -3.0, -3.5 in the $1/(zJ)$ versus $-D/(zJ)$ plane. In our case the coordination number is $z = 4$. We discuss the general behavior of the phase diagrams for any value of K/J ranging from positive to negative values and present figures showing our curves together with the mean-field phase diagrams from ref. 22 for the five above-mentioned values of K/J. Finally in Section 4 we make some concluding remarks.

2. RIGOROUS RESULTS

Let Λ stand for the 2-dimensional lattice volume $[-L, L] \times [-L, L] \cap Z^2$. Given any $\Gamma \subset \Lambda$, we define the following Hamiltonian in Γ:

$$-H_\Gamma = J \sum_{\|i-j\|=1} S_i S_j + K \sum_{\|i-j\|=1} S_i^2 S_j^2 + D \sum_{i \in \Gamma} S_i^2 \tag{2}$$

where $i, j \in \Gamma$. Coupling constants K and D are real-valued, while $J \geqslant 0$. The spin variables assume the values $S_i = 0, \pm 1$. When $\Gamma = \Lambda$, we obtain the Hamiltonian for the two-dimensional Blume–Emery–Griffiths (BEG) model with free boundary conditions, which will be assumed in the sequel. Expected values are defined by

$$\langle \cdot \rangle_\Gamma \equiv \frac{\sum_{\{S\}} \cdot e^{-H_\Gamma}}{Z_\Gamma}$$

where the sum is over all spin configurations in Γ. Here Z_Γ is the normalization factor, given by

$$Z_\Gamma \equiv \sum_{\{S\}} e^{-H_\Gamma}$$

We will prove that:

Theorem 1. (a) Given $J \geqslant 0$, K such that $e^K \cosh J - 1 \geqslant 0$ and $D \in \mathbb{R}$, there exist positive functions $C_1 = C_1(J, K, D)$ and $m_1 = m_1(J, K, D)$ (independent of x and y) such that

$$\langle S_x S_y \rangle_\Lambda \leqslant C_1 e^{-m_1 \|x-y\|} \tag{3}$$

whenever

$$\frac{2e^{D+3K} \sinh 3J}{1 + 2e^D} < 1 \tag{4}$$

and $\|x - y\| \geqslant 3$.

(b) If $e^K \cosh J - 1 < 0$, the same statement holds (with new functions C_2 and m_2) whenever

$$\frac{2e^D}{1 + 2e^{D+3K}} \left[3e^K \sinh J + e^{3K} \left(\frac{\sinh 3J}{4} - \frac{3 \sinh J}{4} \right) \right] < 1 \tag{5}$$

To prove Theorem 1, we need Lemmas 1 and 2 stated below. To prove them, we need some definitions and simple identities.

Given $\Gamma \subset \Lambda$ and $i \in \Gamma$, we define:

Definition 1. N_i is defined as $N_i \equiv \{j \in \Gamma \backslash \|j-i\| = 1\}$, and z_i as the number of sites $j \in N_i$.

Definition 2. Given $i \in \Gamma$, we define $\Gamma_i \equiv \Gamma \backslash \{i\}$.

Definition 3. The energy of the spin at site i (with respect to the set Γ) is defined as

$$-H_i \equiv J \sum_{\|j-i\|=1} S_i S_j + K \sum_{\|j-i\|=1} S_i^2 S_j^2 + DS_i^2$$

where the sums are restricted to $j \in \Gamma$.

Definition 4. Let $M = \{m_j\}_{j \in \Lambda}$ be a multiindex, where each m_j is integer-valued. M is even (odd) if $\sum m_j$ is even (odd). We define

$$S^M = \prod_{i \in \Lambda} S_i^{m_i}$$

S^M is even (odd) if M is even (odd).

Using that $S_i^{2n} = S_i^2$ and that $S_i^{2n+1} = S_i$ for $n = 1, 2,...$ and defining the functions $A(J, K) = A$ and $B(J, K) = B$ as $A \equiv e^K \sinh J$ and $B \equiv (e^K \cosh J - 1)$, it is simple to verify the following identities:

$$\exp(JS_iS_j + KS_i^2S_j^2) = 1 + AS_iS_j + BS_i^2S_j^2 \tag{6}$$

$$e^{-H_i} = e^{DS_i^2} \prod_{\{j \backslash \|j-i\|=1\}} (1 + AS_iS_j + BS_i^2S_j^2) \tag{7}$$

$$\sum_{S_i=0,\pm 1} e^{-H_i} = 1 + 2e^D \left(1 + \sum_M C_M S^M\right) \tag{8}$$

$$\sum_{S_i=0,\pm 1} S_i e^{-H_i} = 2e^D \sum_N C_N S^N \tag{9}$$

The sum appearing in (8) is over all even multiindexes M supported on the set N_i, for which $m_i = 1$ or 2, while the sum in (9) is over all odd multiindexes N obeying the same restriction $n_i = 1$ or 2. The coefficients $C_M = C_M(J, K)$ (same for C_N) are products of integer powers of the functions $A(J, K)$ and $B(J, K)$. Their explicit form depends on the number of nearest neighbors of the spin variable S_i, which will be integrated out [see Eq. (A1) in appendix].

Lemma 1. Given $\Gamma \subset \Lambda$, $i \in \Gamma$, and the Hamiltonian (2), we have:

(a) For $J \geqslant 0$, $D \in \mathbb{R}$, and K such that $e^K \cosh J - 1 \geqslant 0$

$$\frac{Z_{\Gamma_i}}{Z_\Gamma} \leqslant \frac{1}{1+2e^D} \tag{10}$$

(b) For $J \geqslant 0$, $D \in \mathbb{R}$, and K such that $e^K \cosh J - 1 < 0$

$$\frac{Z_{\Gamma_i}}{Z_\Gamma} \leqslant \frac{1}{1+2e^{D+z_i K}} \tag{11}$$

Proof. To prove the lemma when $e^K \cosh J - 1 \geqslant 0$, we use identities (6) and (8) to develop the partition function Z_Γ as follows:

$$\begin{aligned} Z_\Gamma &= \sum_{\{S\}} e^{-H_\Gamma} = \sum_{\{S\}}{}' \left(\sum_{S_i} e^{-H_i} \right) e^{-H_{\Gamma_i}} \\ &= \sum_{\{S\}}{}' \left(1 + e^D \sum_{S_i = \pm 1} \prod_{\|j-i\|=1} e^{(JS_iS_j + KS_i^2S_j^2)} \right) e^{-H_{\Gamma_i}} \\ &= \sum_{\{S\}}{}' \left[1 + 2e^D \left(1 + \sum_M C_M S^M \right) \right] e^{-H_{\Gamma_i}} \end{aligned}$$

where the sums $\sum'$ are over spin variables S_k, $k \in \Gamma_i$, and the products are over $j \in \Gamma$, $\|j-i\| = 1$. The inequality (10) becomes clear if we observe that each coefficient C_M is nonnegative whenever $e^K \cosh J - 1 \geqslant 0$ and that each sum

$$\sum_{\{S\}}{}' S^M e^{-H_{\Gamma_i}}$$

is also nonnegative, by Proposition A1 (see the appendix).

On the other hand, if $e^K \cosh J - 1 < 0$, we develop the partition function as follows:

$$\begin{aligned} Z_\Gamma &= \sum_{\{S\}} e^{-H_\Gamma} = \sum_{\{S\}}{}' \left(\sum_{S_i} e^{-H_i} \right) e^{-H_{\Gamma_i}} \\ &= \sum_{\{S\}}{}' \left(1 + e^D \left(\prod_{\|j-i\|=1} e^{KS_j^2} \right) \sum_{S_i = \pm 1} \prod_{\|j-i\|=1} e^{JS_iS_j} \right) e^{-H_{\Gamma_i}} \\ &= \sum_{\{S\}}{}' \left\{ 1 + 2e^D \left(\prod_{\|j-i\|=1} e^{KS_j^2} \right) \left[1 + \sum_M C_M(J,0) S^M \right] \right\} e^{-H_{\Gamma_i}} \\ &\geqslant (1 + 2e^{(D+z_i K)}) \sum_{\{S\}}{}' e^{-H_{\Gamma_i}} \end{aligned}$$

In the fourth equality, we have used identities (6) (with $K=0$) and (8) (with D replaced by $D+\sum KS_j^2$). The inequality follows from Proposition A1 (see the appendix), using that $C_M(J,0)\geqslant 0$ and that $K<0$ when $e^K\cosh J-1<0$. ∎

Remark. The upper bound for the ratio of partition functions can be improved. Defining $K^*\equiv -\log(\cosh J)$ and $C_M^*\equiv C_M(J,K^*)$, we rewrite the above expansion, pulling out the exponent $K-K^*$, with coefficients C_M^*. The new upper bound is

$$\frac{Z_{\Gamma_i}}{Z_\Gamma}\leqslant\frac{1}{1+2e^D(1+\min\{B,0\})^{z_i}}$$

Lemma 2. Let $\mathscr{M}$ be an even multiindex supported on a set $P\subset\Gamma$ for which $n_k\leqslant 3$ for all $k\in P$. Suppose that i and $x\in\Gamma\backslash P$, that $\|i-x\|\geqslant 2$, and that $z_i\leqslant 3$. Then there exists an even multiindex $\mathscr{N}$, supported on a set $Q\subset P\cup N_i$, and a site $j\in(P\cup N_i)\backslash Q$, $n_j\leqslant 3$, such that

$$\langle S_iS^{\mathscr{M}}S_x\rangle_\Gamma\leqslant C(J,K,D)\langle S_jS^{\mathscr{N}}S_x\rangle_{\Gamma_i} \tag{12}$$

where the coefficient $C(J,K,D)$ is given by (4) for $e^K\cosh J-1\geqslant 0$ and by (5) for $e^K\cosh J-1<0$.

Proof. Using identity (9), we obtain that

$$\langle S_iS^{\mathscr{M}}S_x\rangle_\Gamma=\frac{Z_{\Gamma_i}}{Z_\Gamma}\sum_N 2e^DC_N\langle S^NS^{\mathscr{M}}S_x\rangle_{\Gamma_i}$$

where the multiindexes N have their support on the set N_i (see Definition 1). From Proposition A1 in the appendix, we know that correlations $\langle S^NS^{\mathscr{M}}S_x\rangle_{\Gamma_i}$ are nonnegative. Let $\langle S^{N_{\max}}S^{\mathscr{M}}S_x\rangle_{\Gamma_i}$ be the maximum among all of them. By symmetry, $S^{N_{\max}}S^{\mathscr{M}}$ must be odd, otherwise the correlation function $\langle S^{N_{\max}}S^{\mathscr{M}}S_x\rangle_{\Gamma_i}$ is identically zero. Therefore, there exists $j\in P\cup N_i$, a set $Q\subset P\cup N_i\backslash\{j\}$, and an even multiindex $\mathscr{N}$, supported on Q, such that

$$\langle S^{N_{\max}}S^{\mathscr{M}}S_x\rangle_{\Gamma_i}=\langle S_jS^{\mathscr{M}}S_x\rangle_{\Gamma_i}$$

As remarked earlier, the coefficients C_N are nonnegative whenever $B=e^K\cosh J-1\geqslant 0$. Under this condition, we get the upper bound

$$\langle S_iS^{\mathscr{M}}S_x\rangle_\Gamma\leqslant\left(\frac{Z_{\Gamma_i}}{Z_\Gamma}\sum_N 2e^DC_N\right)\langle S_jS^{\mathscr{N}}S_x\rangle_{\Gamma_i}$$

where

$$\sum_N C_N = \begin{cases} A & \text{if } z_i = 1 \\ 2A + 2AB & \text{if } z_i = 2 \\ 3A + 6AB + 3AB^2 + A^3 & \text{if } z_i = 3 \end{cases}$$

It is simple to verify that $3A + 6AB + 3AB^2 + A^3 = e^{3K} \sinh 3J$ and that it is the largest possible value for the sum $\sum C_N$. Therefore, after using inequality (10), we obtain

$$\langle S_i S^{\cdot\mathscr{U}} S_x \rangle_\Gamma \leqslant \left(\frac{2e^{D+3K} \sinh 3J}{1 + 2e^D} \right) \langle S_j S^{\cdot\mathscr{V}} S_x \rangle_{\Gamma_i} \tag{13}$$

On the other hand, if $e^K \cosh J - 1 < 0$, some coefficients C_N will be negative. In what follows, we argue how to get the bound (12) when $z_i = 3$. Similar steps can be done for $z_i = 1$ and $z_i = 2$. From Eq. (A1) (see the appendix), we observe that the sum multiplying the coefficient AB, which is negative, has six parcels. Three of them will be skipped because they give a negative contribution for the coefficient. The other three will be appended to the sum of the AB^2 coefficient (with three parcels, too), generating terms like

$$AB^2 \langle S_j^2 S_k^2 S_l S^{\cdot\mathscr{U}} S_x \rangle_{\Gamma_i} - A\, |B|\, \langle S_k^2 S_l S^{\cdot\mathscr{U}} S_x \rangle_{\Gamma_i}$$

Using inequality (A3) and that $|B| \leqslant 1$, it is easy to see that terms like the one above are negative. Therefore, we get the upper bound

$$\langle S_i S^{\cdot\mathscr{U}} S_x \rangle_\Gamma \leqslant \left(\frac{Z_{\Gamma_i}}{Z_\Gamma} 2e^D \sum_N \max\{C_N, 0\} \right) \langle S_j S^{\cdot\mathscr{V}} S_x \rangle_{\Gamma_i}$$

where the sum $\sum \max\{C_N, 0)$ is bounded above by $3A + A^3$. For the other cases we obtain

$$\sum_N \max\{C_N, 0\} \leqslant \begin{cases} A & \text{if } z_i = 1 \\ 2A & \text{if } z_i = 2 \end{cases}$$

It is clear that $3A + A^3$ is the largest possible value for the above bounds, and that

$$3A + A^3 = 3e^K \sinh J + e^{3K} \left(\frac{\sinh 3J}{4} - \frac{3 \sinh J}{4} \right)$$

Using inequality (11), we get the claimed upper bound

$$\langle S_i S^{\cdot\mathscr{U}} S_x \rangle_\Gamma$$
$$\leqslant \frac{2e^D}{1 + 2e^{D+3K}} \left[3e^K \sinh J + e^{3K} \left(\frac{\sinh 3J}{4} - \frac{3 \sinh J}{4} \right) \right] \langle S_j S^{\cdot\mathscr{V}} S_x \rangle_{\Gamma_i} \quad \blacksquare$$

Proof of Theorem 1. Without loss of generality, we assume $y=0$. The proof is by iteration of inequality (12). First, we arrange things in order to apply Lemma 2:

$$\begin{aligned}\langle S_0 S_x\rangle_\Lambda &= \frac{Z_{\Lambda_0}}{Z_\Lambda}\left\langle\left(\sum_{S_0=0,\,\pm 1} S_0 e^{-H_0}\right) S_x\right\rangle_{\Lambda_0}\\ &= \frac{Z_{\Lambda_0}}{Z_\Lambda}\sum_N 2e^D C_N \langle S^N S_x\rangle_{\Lambda_0} \end{aligned}\tag{14}$$

where the sum is over odd multiindexes, as remarked earlier. By Proposition A1, the expected values $\langle S^N S_x\rangle_{\Lambda_0}$ are nonnegative. Let $\langle S^{N_{\max}} S_x\rangle_{\Lambda_0}$ be the largest among the expected values $\langle S^N S_x\rangle_{\Lambda_0}$ appearing in the sum (14). From Lemma 1, it is clear that

$$\frac{Z_{\Lambda_0}}{Z_\Lambda} \leqslant \frac{1}{1+2e^{(D+4\min\{K,0\})}}$$

Taking into account that some coefficients C_N could be negative, it is also clear that

$$\frac{2e^D}{1+2e^{(D+4\min\{K,0\})}}\left(\sum_N \max\{C_B, 0\}\right)\langle S^{N_{\max}} S_x\rangle_{\Lambda_0}$$

is an upper bound for (14).

As in the proof of Lemma 2, $\langle S^{N_{\max}} S_x\rangle_{\Lambda_0}$ must be of the form $\langle S_i S^{\mathscr{M}} S_x\rangle_{\Lambda_0}$ for some $i\in N_0$. Here $\mathscr{M}$ is an even multiindex supported on the set N_0. Therefore, the two-point function is bounded above by

$$\langle S_0 S_x\rangle_\Lambda \leqslant C' \langle S_i S^{\mathscr{M}} S_x\rangle_{\Lambda_0}$$

Now we start the iteration process, working with the correlation $\langle S_i S^{\mathscr{M}} S_x\rangle_{\Lambda_0}$, for which we apply Lemma 2, with $\Gamma=\Lambda_0$. Observe that in this case $z_i=3$ but in general $z_i\leqslant 3$. We apply Lemma 2 a number of times at least equal to $\|x\|-1$, after which it may happen that the site i over which the iteration is done is exactly the site x, not allowing, therefore, the application of Lemma 2. We have

$$\begin{aligned}\langle S_0 S_x\rangle_\Lambda &\leqslant C'(C(J,K,D))^{\|x\|-1}\langle S_j S^{\mathscr{M}} S_x\rangle_\Gamma\\ &\leqslant C'(C(J,K,D))^{-1}(C(J,K,D))^{\|x\|}\end{aligned}$$

which is equal to ·

$$Ce^{-m\|x\|}$$

whenever condition (4) or condition (5) is satisfied. In the above second inequality, we use 1 as an upper bound for the correlation functions. ∎

3. PHASE DIAGRAMS

In this section we show some phase diagrams corresponding to distinct constant-(K/J) cross sections in the temperature, $1/(4J)$, versus the crystal field, $-D/(4J)$, plane. Our curves give upper bound values to the critical temperature associated with a ferromagnetic order–disorder second-order phase transition. For each constant-(K/J) cross section plane $1/(4J)$ versus $-D/(4J)$ we fix the factor $-D/(4J)$. Then we determine numerically the value $1/(4J_o)$ which makes the coefficient given by expression (4) or (5) of Section 2 (depending upon whether $e^K \cosh J - 1 \geqslant 0$ or $e^K \cosh J - 1 < 0$, respectively) equal to one. For values of $1/(4J)$ greater than $1/(4J_o)$ we have that the appropriated coefficient (4) or (5) is strictly less than one. This means exponential decay behavior for the two-point function and characterizes the ferromagnetically disordered phase.[29] Here $1/J_o$ represents an upper bound for the ferromagnetic critical temperature. We also obtain numerically the value c_o such that for $-D/(4J) > c_o$ we have exponential decay for any value of $1/(4J)$. For $K/J = 0$, -1.0, -1.5, -3.0, and -3.5 we have, respectively, $c_o = 0.75000 \pm 0.00005$, 0.26895 ± 0.00005, 0.15748 ± 0.00002, -0.19225 ± 0.00005, and -0.313018 ± 0.000002. For the sake of comparison we show in Figs. 1–5 our ferromagnetic upper bounds (dash-dotted curves) together with the corresponding mean-field (MFA) ones from ref. 22. In the MFA curves dashed and solid lines indicate, respectively, first- and second-order phase

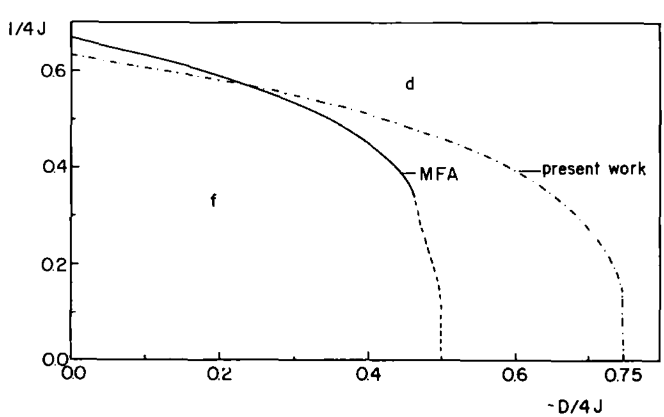

Fig. 1. Phase diagram in the temperature $(1/4J)$ versus the crystal field $(-D/4J)$ plane when $K/J = 0$. Our ferromagnetic upper bounds are represented by the dash-dotted curve. The predicted mean-field phase diagram[22] is also shown with the disordered (d) and ferromagnetic (f) phases. Dashed and solid lines indicate, respectively, first- and second-order phase transitions.

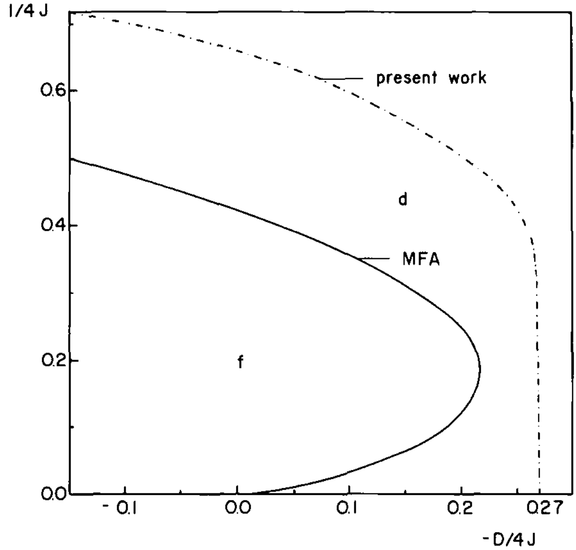

Fig. 2. The same as Fig. 1, except that $K/J = -1.0$.

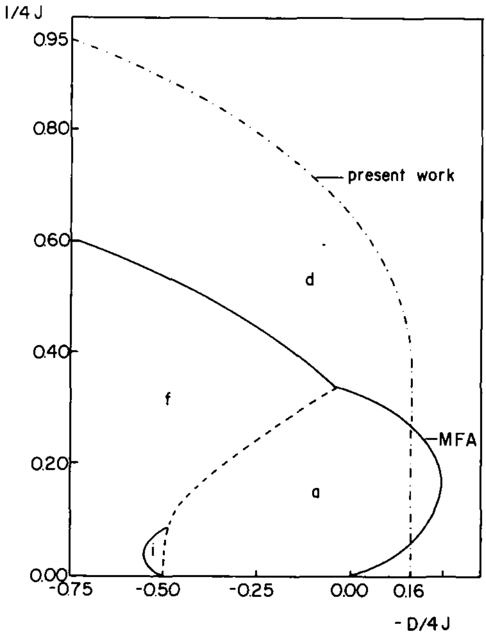

Fig. 3. The same as Fig. 1, except that $K/J = -1.5$ and now the mean-field phase diagram presents also ferrimagnetic (i) and antiquadrupolar (a) phases.

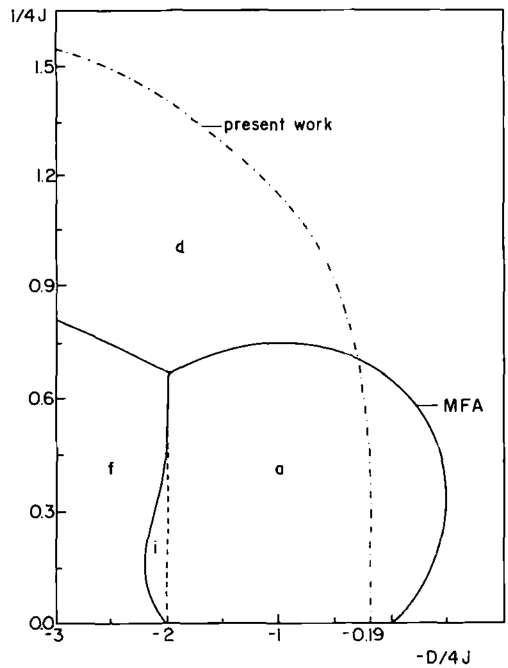

Fig. 4. The same as Fig. 3, except that $K/J = -3.0$.

transition. As each figure shows, curves from the present work fall off sharply toward a zero-temperature point as $-D/(4J)$ approaches the above c_o values from the left.

4. CONCLUDING REMARKS

Our methods are dimension independent. We have applied them to the two-dimensional BEG model. In two dimensions, all the richest aspects of the phase diagrams are present and the calculations are simpler than in higher dimensions.

Although we can conclude that disordered–ferromagnetic–disordered reentrance curves cannot exist in those portions of the phase diagrams where the two-point correlation function decays exponentially, that is not enough if we wish to get a similar conclusion for the disordered–antiquadrupolar–disordered reentrance lines [those boundary phases appear within the mean-field[22] and Monte Carlo renormalization group calculations $(d=3)$[26]]. We believe that one is still left to prove the uniqueness of the Gibbs measure in those regions.

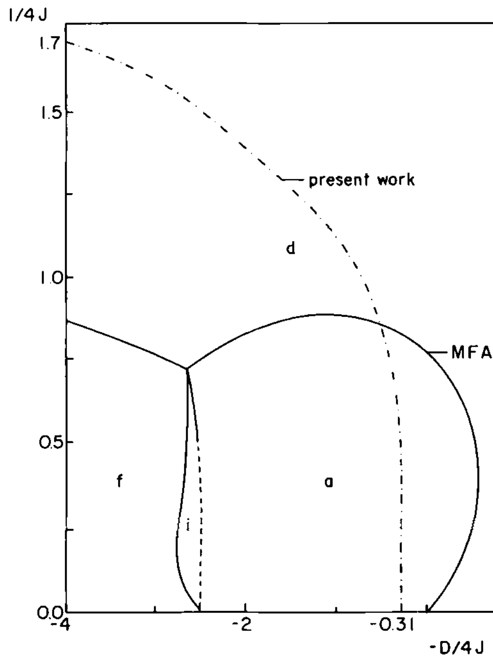

Fig. 5. The same as Fig. 3, except that $K/J = -3.5$.

We intend to develop this approach for the three-dimensional model, where similar questions can be formulated. We also intend to use low-temperature expansions to get lower bounds on the critical temperature. In this way, one could localize the possible parameter values (and therefore low and high temperature portions of the phase diagrams) for which ferromagnetic reentrance curves are prohibited.

Correlation inequalities as proven in the appendix can be generalized for not necessarily ferromagnetic models (see ref. 34, where "comparison inequalities" have been proved). This opens the possibility to apply our methods for disordered systems.

APPENDIX

For the sake of completeness, we obtain the identity (9) for the case $n_i = 3$, with $i = 0$ being the site at the origin. We also enumerate the nearest neighbors of 0 as 1, 2, and 3. Developing the product (7) and integrating over the spin variable S_0, we obtain

$$\sum_{S_0=0,\pm 1} S_0 e^{-H_0}$$
$$= 2e^D \Big[A \sum_i S_i + A^3 S_1 S_2 S_3 + AB(S_1 S_2^2 + S_1 S_3^2 + S_2 S_1^2 + S_2 S_3^2 + S_3 S_1^2 + S_3 S_2^2) + AB^2(S_1^2 S_2^2 S_3 + S_1^2 S_3^2 S_2 + S_2^2 S_3^2 S_1) \Big] \quad \text{(A1)}$$

Griffiths' first inequality, as well as Proposition A2 stated below, can be generalized for even (in each spin variable) perturbations of ferromagnetic models (for a generalization of Griffiths' second inequality, see ref. 34). Here, we prove them for the BEG model (2):

Proposition A1. For any multiindex $M = \{m_i\}_{i\in\Gamma}$, Griffiths' first inequality

$$\langle S^M \rangle_\Gamma \geqslant 0 \quad \text{(A2)}$$

holds for real values of K and D and for $J \geqslant 0$.

Proof. To prove inequality (A2) for real values of K and D, it is sufficient to show that

$$N_\Gamma \equiv \sum_{\{S\}} S^M e^{-H_\Gamma}$$

is nonnegative. We first expand the exponential

$$\exp\left(J \sum_{i,j} S_i S_j \right)$$

in power series. Therefore, N_Γ will be a superposition of terms in the following type:

$$\sum_{\{S\}} S_1^{n_1} \cdots S_k^{n_k} \exp\left(K \sum_{i,j} S_i^2 S_j^2 + D \sum_{i\in\Gamma} S_i^2 \right)$$

whose coefficients are nonnegative, because $J \geqslant 0$. Now, if all exponents $n_1,..., n_k$ are even, then the last sum is clearly nonnegative. On the other hand, if at least one exponent, say n_1, is odd, then by changing the spin variable S_1 to $-S_1$ we conclude that the sum is zero. ∎

Proposition A2. For any given multiindex $M = \{m_j\}_{j\in\Gamma}$ supported on a set $A \subset \Gamma$ and for any $i \notin A$, the following inequality holds:

$$\langle S_i^2 S^M \rangle_\Gamma \leqslant \langle S^M \rangle_\Gamma \quad \text{(A3)}$$

Proof. We have

$$\langle S_i^2 S^M \rangle_\Gamma = \frac{1}{Z_\Gamma}\left(\sum_{\{\{S\}\backslash S_i = +1\}} S^M e^{-H_\Gamma} + \sum_{\{\{S\}\backslash S_i = -1\}} S^M e^{-H_\Gamma} \right)$$

while

$$\langle S^M \rangle_\Gamma = \frac{1}{Z_\Gamma}\left(\sum_{\{\{S\}\backslash S_i = +1\}} S^M e^{-H_\Gamma} + \sum_{\{\{S\}\backslash S_i = -1\}} S^M e^{-H_\Gamma} + \sum_{\{\{S\}\backslash S_i = 0} S^M e^{-H_\Gamma} \right)$$

On the other hand,

$$\sum_{\{\{S\}\backslash S_i = 0\}} S^M e^{-H_\Gamma} = \tfrac{1}{3} \sum_{\{S\}} S^M e^{-H_{\Gamma_i}}$$

By Proposition A1, the last sum is nonnegative. This proves inequality (17). ∎

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