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Position-space renormalization-group investigation of the spin-3/2 Blume–Emery–Griffiths model with repulsive biquadratic coupling

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Abstract

Phase transitions of a four-component lattice gas or spin-3/2 Blume–Emery–Griffiths model, with a single-ion uniaxial anisotropy and nearest-neighbour pair interactions, both bilinear and biquadratic, are investigated for two-dimensional lattices using an approximate renormalization-group approach of the Migdal–Kadanoff type. The set of fixed points and flows provide the characteristic phase diagrams, in the case of repulsive biquadratic interaction, featuring four ordered phases including high-entropy ferrimagnetic and staggered quadrupolar phases. Successive phase transitions and multicritical points are also found.

1. Introduction

The Blume–Emery–Griffiths (BEG) model [1], which is the most general spin-1 Ising model with nearest-neighbour interactions, both bilinear and biquadratic, in which a crystal field is included, was originally investigated in the context of superfluidity and phase separation in helium mixtures [1]. It is the basic lattice gas model for all of the physical systems characterized by three different local states at each lattice site, and has since been widely used in describing a variety of physical phenomena, ranging from solid–liquid gas mixtures [2], through multicomponent fluid and liquid-crystal mixtures [2], to the phase changes in microemulsions [3].

Most of the recent works on the phase transitions of the BEG model have been devoted to the case of repulsive biquadratic interaction, relevant to ordering in semiconductor alloys [4] and electron conduction models [5], because it may be expected to give a rich phase diagram due to the competition of interactions. In this case, a very rich phase diagram was obtained for three-dimensional lattices by using the mean-field approximation (MFA) [6], featuring single and double re-entrancy regions and ferrimagnetic phases.

This model can also be generalized to describe the BEG model by inclusion of higher spin values. A spin-3/2 BEG model, in which each spin variable can take four different values, is probably the simplest extension of the general spin-1 Ising model, which can exhibit a variety of multicritical phenomena accompanied with the onset of first- and second-order transitions.

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The spin-3/2 BEG model, with dipolar and quadrupolar exchange interactions, was initially introduced [7] in connection with experimental results on successive phase transitions in some rare-earth compounds such as $DyVO_4$, and its phase diagram was determined within the MFA. A modified version of the spin-3/2 model, including an octupolar exchange term, was later introduced [8] to describe tricritical properties in ternary fluid mixtures; this was also solved within the MFA. Recently, the spin-3/2 BEG model with bilinear (J) and biquadratic (K) nearest-neighbour interactions and a single-ion uniaxial crystal-field anisotropy (Δ) has been studied with the use both of the MFA and Monte Carlo (MC) simulations [9], an effective-field theory based on the differential operator technique [10], and by means of a position-space renormalization-group (PSRG) calculation [11].

It has been shown that the spin-3/2 BEG model exhibits various phase transitions of first and higher order against the temperature. In particular, as long as the biquadratic interaction is ferromagnetic ($K > 0$) there occurs, at a higher temperature, a second-order transition line separating the paramagnetic phase from two distinct ferromagnetic phases. At lower temperature, these ordered phases are separated by a first-order transition line, in the region of negative values of Δ. On the other hand, when repulsive biquadratic ($K < 0$) interaction and $\Delta = 0$ are considered, where two sublattice structures must be introduced, the results for the K-dependent part of the phase diagram present a paramagnetic phase also separated by a second-order transition line from the ferromagnetic phases characterized by equal values of the sublattice magnetizations, but large and small quadrupolar momenta. Within this ordered region lies a ferrimagnetic phase, distinguished by unequal sublattice magnetizations and sublattice symmetry breaking, separated by a second-order transition line from the region of equal sublattice magnetizations.

Previous studies undertaken within the spin-3/2 BEG model have only considered some portions of the phase diagram. By contrast, in the research reported here, the global phase diagram of the model is studied in considerable detail using a PSRG technique based on the Migdal–Kadanoff (MK) [12, 13] recursion relations, obtained by employing the transformation of variables under a length scaling. We complete an earlier renormalization-group study [11] and present the major results for the phase diagram of the BEG model for a two-dimensional ($d = 2$) square lattice with repulsive biquadratic interactions. It has been shown that such a spin system is still rich enough to exhibit phase diagrams of considerable richness, including four ordered phases among which there are high-entropy ferrimagnetic and staggered quadrupolar orderings. The set of fixed points and flows provide the complete characteristic phase diagrams. On the basis of the topology of the PSRG flows linking the various fixed points, first we determine the unified global phase diagram in (J, K, Δ) space, with supplementary representative cross sections of constant K/J, temperature $1/J$ and chemical potential Δ/J, which will be used later for comparison with the results obtained from other treatments carried out for this model. Then, local analysis for the recursion relations near the fixed points gives all of the critical exponents.

An outline of the paper is as follows. After defining the model and describing the approximate recursion relations embodying the renormalization group in section 2, we discuss the global phase diagram and some features of the fixed-point structure in section 3. Section 4 contains our conclusions.

2. Model and method

We study the spin-3/2 BEG model described by the following reduced Hamiltonian:

$$-\beta H = J \sum_{\langle ij \rangle} S_i S_j + K \sum_{\langle ij \rangle} S_i^2 S_j^2 + \Delta \sum_i S_i^2 \tag{1}$$

where the spins S_i located at site i on a discrete lattice can take the values $\pm 3/2$ and $\pm 1/2$, and the first two summations run over all nearest-neighbour spins. The terms on the right-hand side describe, respectively, the bilinear exchange, biquadratic exchange, and crystal-field interactions. We restrict this study to $J > 0$ (since we are interested in the ferromagnetic case) and $K < 0$ (so sublattice order parameters must be introduced).

In order to obtain self-consistent recursion relations, the adding of a new coupling

$$+ C \sum_{\langle ij \rangle} (S_i S_j^3 + S_i^3 S_j) + F \sum_{\langle ij \rangle} S_i^3 S_j^3 \qquad (2)$$

to the Hamiltonian must be considered. Here we will not be concerned about the physical origin of these couplings, and we will treat them as parameters in the calculations.

The different phases of the BEG model can be characterized by two order parameters, corresponding to the magnetizations and quadrupolar moments of the two sublattices a and b:

$$m_a = \langle S_a \rangle \qquad m_b = \langle S_b \rangle \qquad q_a = \langle S_a^2 \rangle \qquad q_b = \langle S_b^2 \rangle$$

where $\langle \cdots \rangle$ denotes the thermal average.

The values of these parameters define six phases with different symmetries. These are:

(1) two paramagnetic phases labelled $P_{3/2}$ and $P_{1/2}$ distinguished by $m_a = m_b = 0$ with $q_a = q_b > 5/4$, and $q_a = q_b < 5/4$, respectively;
(2) two ferromagnetic phases referred to as $F_{3/2}$ and $F_{1/2}$ characterized, respectively, by $m_a = m_b \neq 0$ with $q_a = q_b > 5/4$, and $q_a = q_b < 5/4$;
(3) a staggered quadrupolar (SQ) phase which has $m_a = m_b = 0$ and $q_a \neq q_b$; and
(4) a ferrimagnetic (FR) phase distinguished by non-zero magnetizations and sublattice symmetry breaking ($m_a \neq m_b \neq 0$ and $q_a \neq q_b$).

For a more reliable qualitative understanding of features of the phase transitions of the model, we apply a MK renormalization-group method, which combines decimation and bond shifting. In what follows we specialize to the 'series–parallel' method in which a one-dimensional (exact) decimation is first used to combine bonds in series and then bond shifting accomplishes the parallel combination of bonds. The main advantage of this scheme is its simplicity. One can very easily obtain approximate recursion relations and find the fixed points and the critical exponents. In this scheme it is also possible to compute non-universal quantities like the critical temperature or the free energy as a function of the temperature. Nonetheless, it has several shortcomings:

(1) It should be clear from the way in which it was carried out for this spin problem that the MK method does not conserve the dimensionality of the parameter space, and may miss certain features of the phase diagram owing to the restricted flow space in which the renormalization must of necessity be carried out. Therefore, it should be stressed that a complete description of the phase transitions requires consideration of an enlarged parameter space for a d-dimensional lattice, which involves lengthy calculations and a large amount of computation.
(2) It turns out that the MK method considers only the interactions among the spins of a finite cluster, neglecting the effect of the surrounding spins and thus underestimating the interactions among the spins, which leads to a lower value of the critical temperature. If larger clusters are used, further-neighbour and multispin couplings are generated, and allowance for these in an extended parameter space leads to a quite satisfactory results even with moderate-sized clusters.

Provided that such limitations are understood, the MK renormalization-group method can be an extremely valuable one in many situations requiring a direct approach. It is tractable in all space dimensionalities; therefore we shall give the recursion relations for a d-dimensional hypercubic spin-3/2 BEG model after briefly describing the method.

We choose the length-rescaling factor b as an odd integer so as to preserve, under scaling, the possible sublattice-symmetry-breaking character of the system. In the present study we use $b = 3$ and consider a one-dimensional chain of four spins S_1, S_2, S_3, and S_4 coupled by the interactions J, K, Δ, C, and F. The reduced Hamiltonian of this four-spin cluster reads

$$\begin{aligned} -\beta H = {} & J(S_1S_2 + S_2S_3 + S_3S_4) + K(S_1^2S_2^2 + S_2^2S_3^2 + S_3^2S_4^2) + \frac{\Delta}{2d}(S_1^2 + 2S_2^2 + 2S_3^2 + S_4^2) \\ & + C(S_1S_2^3 + S_1^3S_2 + S_2S_3^3 + S_2^3S_3 + S_3S_4^3 + S_3^3S_4) + F(S_1^3S_2^3 + S_2^3S_3^3 + S_3^3S_4^3). \end{aligned} \tag{3}$$

The coefficient in the crystal-field term takes into account the coordination of the sites 1, 2, 3, and 4 in the d-dimensional hypercubic lattice. The rescaling transformation involves taking the trace over spins S_2 and S_3, which generates the transformed reduced Hamiltonian of the system; after series combination this gives

$$-\beta\tilde{H} = \tilde{J}S_1S_4 + \tilde{K}S_1^2S_4^2 + \frac{\tilde{\Delta}}{2d}(S_1^2 + S_4^2) + \tilde{C}(S_1S_4^3 + S_1^3S_4) + \tilde{F}S_1^3S_4^3 \tag{4}$$

where $\tilde{J}$, $\tilde{K}$, $\tilde{\Delta}$, $\tilde{C}$, and $\tilde{F}$ are the scaled one-dimensional interactions, resulting from the series combination, given as functions of J, K, Δ, C, and F.

Since we are interested in the scalings of J, K, and Δ only, we may use here the unnormalized Boltzmann probability $\mathcal{P} = \exp(-\beta H)$.

Maintaining the same form of $\mathcal{P}$ under scaling, we have for the series combination of three bonds by decimating the two intermediate spins

$$\exp(-\beta\tilde{H}(S_1, S_4)) = \mathrm{Tr}_{S_2,S_3}\left[\prod_{i=1,j=i+1}^{3} \exp(-\beta H(S_i, S_j))\right]. \tag{5}$$

Equation (5) and the bond-shifting process yield the finally renormalized couplings J', K', Δ', C', and F' of the transformed system as functions of the original ones. They are simply

$$\begin{aligned} J' &= b^{d-1}\tilde{J}(J, K, \Delta, C, F) \\ K' &= b^{d-1}\tilde{K}(J, K, \Delta, C, F) \\ \Delta' &= b^{d-1}\tilde{\Delta}(J, K, \Delta, C, F) \\ C' &= b^{d-1}\tilde{C}(J, K, \Delta, C, F) \\ F' &= b^{d-1}\tilde{F}(J, K, \Delta, C, F). \end{aligned}$$

In translationally invariant systems, one is at a critical point when the interaction parameters after rescaling are the same as those before, which is known as the fixed point. This is because the correlation length has gone to infinity and so the system is invariant under a change in the length scale. Thus, in terms of the renormalization-group scheme, all phases and all phase transitions are derived from the global study of PSRG flows in Hamiltonian space, which are governed by the fixed points. The various fixed points of the transformation have been determined and classified according to their relative stability and connectivity. For repulsive biquadratic ($K < 0$) interactions we find a total of 14 different fixed points underlying the structure of the system, yielding critical (second-order) phase boundaries and multicritical points. Amongst them there are six trivial fixed points which correspond, respectively, to the six different phases. Two of them, namely $(0, -\infty, +\infty, 0, 0)$ and $(+\infty, -\infty, +\infty, -\infty, -\infty)$, are completely stable and characterize, respectively, the staggered quadrupolar and ferrimagnetic phases, whereas eight distinct non-trivial fixed points are unstable and provide the second-order phase transitions in our phase diagram. The coordinates of the various fixed points and the phase transitions that they characterize are given in table 1. It is worth noting that none of the fixed points listed in table 1 fulfils the Nienhuis and Nauenberg conditions [14] for seeing first-order transitions in the PSRG approach.

Table 1. Coordinates and classification of the fixed points underlying the phase diagram of the spin-3/2 BEG model in two dimensions with repulsive biquadratic coupling.

Fixed points	Coordinates $(J^*, K^*, \Delta^*, C^*, F^*)$	Type
$P_{3/2}$	$(0, 0, +\infty, 0, 0)$	Sink for ($m_a = m_b = 0$ and $q_a = q_b > 5/4$) phase
$P_{1/2}$	$(0, 0, -\infty, 0, 0)$	Sink for ($m_a = m_b = 0$ and $q_a = q_b < 5/4$) phase
$F_{3/2}$	$(+\infty, -\infty, +\infty, -\infty, +\infty)$	Sink for ($m_a = m_b \neq 0$ and $q_a = q_b > 5/4$) phase
$F_{1/2}$	$(+\infty, -\infty, -\infty, -\infty, +\infty)$	Sink for ($m_a = m_b \neq 0$ and $q_a = q_b < 5/4$) phase
SQ	$(0, -\infty, +\infty, 0, 0)$	Sink for ($m_a = m_b = 0$ and $q_a \neq q_b$) phase
FR	$(+\infty, -\infty, +\infty, -\infty, -\infty)$	Sink for ($m_a \neq m_b$ and $q_a \neq q_b$) phase
M_1	$(0, -0.8696, 3.0563, 0, 0)$	Critical surface
M_2	$(0, -0.8695, 5.6398, 0, 0)$	Critical surface
M_3	$(0, -0.7218, 3.6090, 0, 0)$	Critical line
Z	$(0.2706, -\infty, +\infty, -0.6015, 0.4812)$	Critical surface
$C_{3/2}$	$(0.0050, -0.0216, +\infty, -0.020, 0.0802)$	Critical surface
$C_{1/2}$	$(3.653, -0.0215, -\infty, -1.622, 0.7206)$	Critical surface
$I_{3/2}$	$(+\infty, -\infty, +\infty, -\infty, -0.0885)$	Critical surface
$I_{1/2}$	$(+\infty, 0.515, -2.5798, -\infty, -0.5170)$	Critical surface

Critical (higher-order) renormalization-group exponents y_i, associated with the non-trivial fixed points and listed in table 2, are defined by

$$\lambda_i = b^{y_i} \tag{6}$$

where λ_i denotes an eigenvalue of the recursion relations linearized at the appropriate fixed points whose domain is the locus of the transition in question, and $b = 3$ is the rescaling factor of the renormalization-group transformation. The eigenvalues λ_i give the critical exponents

Table 2. Critical exponents of the higher-order fixed points.

	Eigenvalue exponents		
Fixed points	y_J	y_K	y_Δ
M_1	2.457	0.765	0
M_2	2.457	0.765	0
M_3	2.249	1.145	0
Z	3.0	2.249	1.145
$C_{1/2}$	3.0	2.249	1.145
$C_{3/2}$	3.0	2.252	1.146
$I_{1/2}$	3.0	3.0	2.562
$I_{3/2}$	3.0	3.0	0

and the direction of flow around the fixed point. Unlike the eigenvalues λ_i, the eigenvalue exponents y_i are transformation independent (i.e., independent of b). For a particular λ_i greater than 1, the fixed point is unstable with respect to perturbations in the direction of the corresponding eigenvector. The non-universal character in the PSRG is governed by the presence of marginal fixed points whose eigenvalues must be equal to 1. This is not fulfilled for any of the fixed points in table 2.

3. Results and discussion

As previously discussed [15], the MK type of recursion relations are eminently suited to providing insight into the qualitative properties of the spin-1 BEG model. Here, we make use of this approximation to determine the phase diagram of the spin-3/2 BEG model, with single-site and nearest-neighbour interactions. The main attention in our investigation was focused on the case of repulsive biquadratic ($K < 0$) interaction, where the staggered quadrupolar and ferrimagnetic phases are particularly of interest, and where we obtain a remarkable difference from the MFA results.

Before discussing the general situation, let us consider the particular case corresponding to the invariant subspace $J = C = F = 0$. Following Griffiths symmetry [16] for the spin-1 BEG model, we note here that the system in this case reduces to an antiferromagnetic spin-1/2 Ising model in an external magnetic field.

Defining a new variable τ_i at each site i by $\tau_i = S_i^2 - 5/4$, and substituting into (1), one obtains the equivalent Hamiltonian

$$-\beta H = J_\tau \sum_{\langle ij \rangle} \tau_i \tau_j + h_\tau \sum_i \tau_i \tag{7}$$

with $\tau_i = \pm 1$ and the new interaction constants are related to the original ones by

$$J_\tau = K < 0$$
$$h_\tau = \Delta + \frac{5}{4} z K$$

where z is the number of nearest neighbours of a site (four in our square lattice).

This is the spin-1/2 Ising model in a magnetic field h_τ. The MK recursion relations for this model have only three non-trivial fixed points, namely M_1, M_2, and M_3, of coordinates $(-0.869, 3.056)$, $(-0.869, 5.639)$, and $(-0.721, 3.609)$, respectively. The first and the second fixed points characterize the critical transition line separating the distinct domains which are the regions of attraction of the three phase sinks SQ, $P_{3/2}$, and $P_{1/2}$, respectively, of coordinates $(-\infty, +\infty)$, $(0, +\infty)$, and $(0, -\infty)$, whereas the last fixed point describes the coexistence of the three different phases, and characterizes the antiferromagnetic transition in zero field.

We now come back to the general situation for the BEG model. On iterating the renormalization-group recursion relations, several interesting results emerge from our study. For repulsive biquadratic coupling, first we obtain the complete set of fixed points for the recursion relations in a five-dimensional parameter space and study the connectivity of the renormalization-group flows linking them. Second, we determine the unified global phase diagram of the BEG model in the space of the three parameters (J, K, Δ), displayed in figure 1, in which the locations of the various phase sinks have been indicated. This picture holds irrespective of the space dimensionality d, since the results are qualitatively similar for $d \geqslant 2$. Therefore, in the following we will be concerned almost entirely with the two-dimensional ($d = 2$) square lattice, though the same recursion relations can be applied in other dimensions as well.

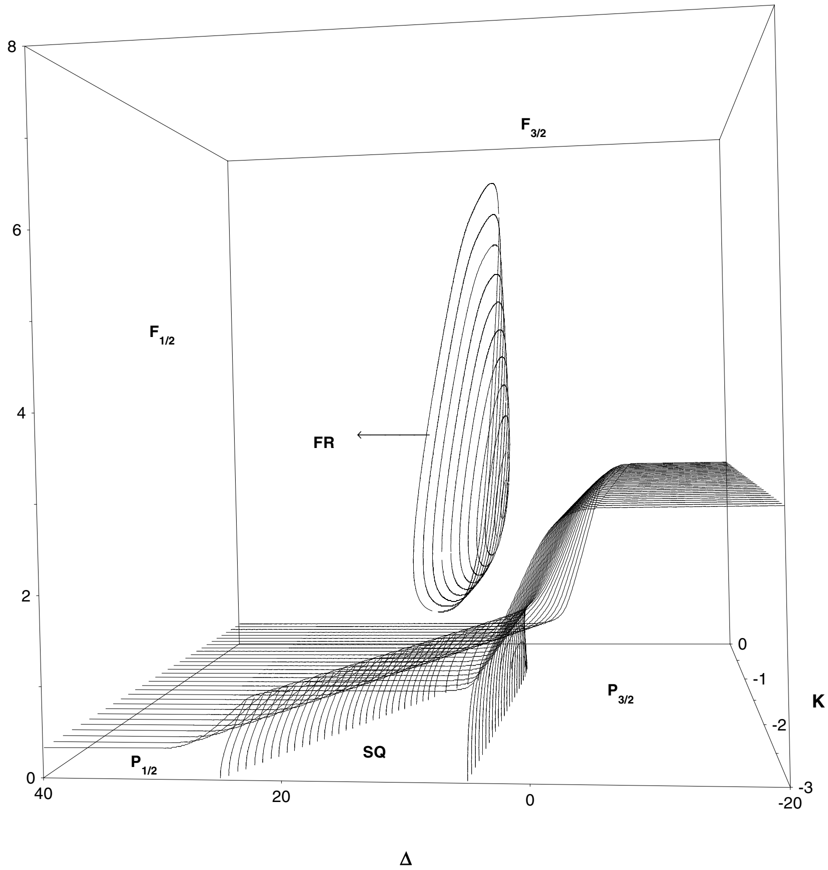
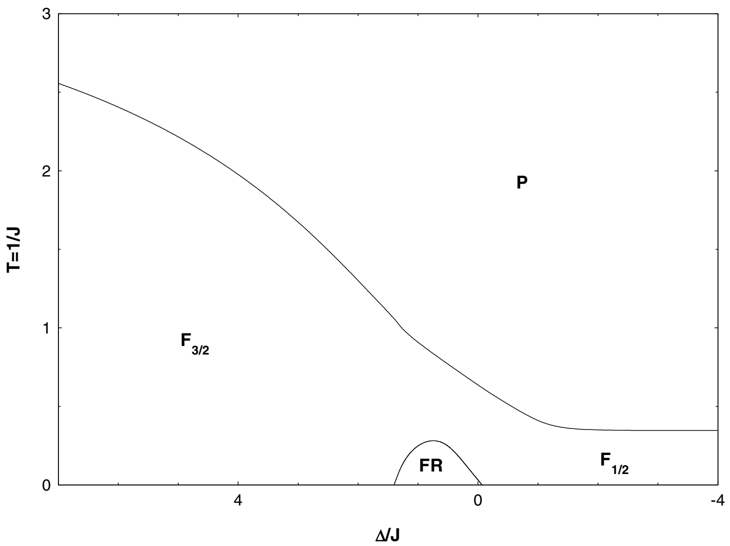


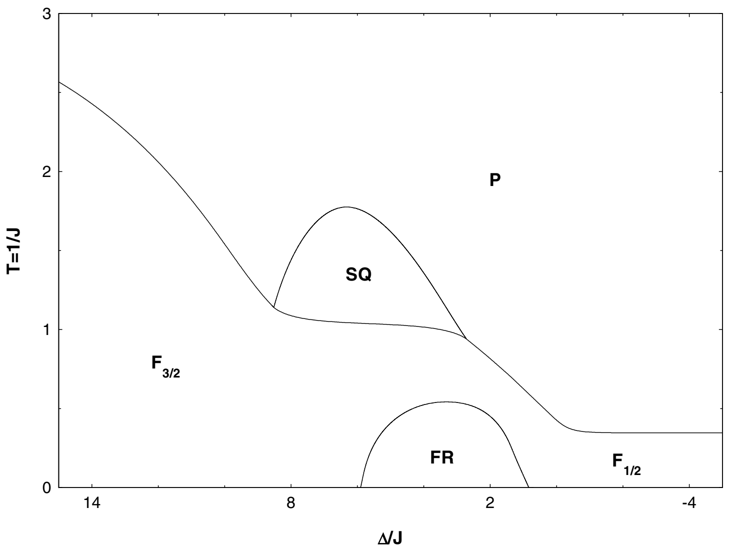
Figure 1. The spin-3/2 BEG phase diagram, in the (J, K, Δ) space, obtained by the Migdal–Kadanoff renormalization-group treatment, for repulsive biquadratic ($K < 0$) interaction.

The volume ($J > 0, K < 0$) under study is divided by transition surfaces into six regions. Two of them are occupied by the paramagnetic phases $P_{3/2}$ and $P_{1/2}$. In the remaining regions, four ordered phases among which two ferromagnetic phases referred to as $F_{3/2}$ and $F_{1/2}$, together with staggered quadrupolar (SQ) and ferrimagnetic (FR) phases, are found. We observe also seven important boundary surfaces of critical (second-order) phase transitions. The ferromagnetic ($F_{3/2}$) phase is separated from the paramagnetic ($P_{3/2}$), staggered quadrupolar (SQ), and ferrimagnetic (FR) phases by three critical transition surfaces characterized, respectively, by the fixed points $C_{3/2}$, Z, and $I_{3/2}$, whereas the fixed points $C_{1/2}$ and $I_{1/2}$ describe two additional second-order transition surfaces separating the ferromagnetic ($F_{1/2}$) phase from both the paramagnetic ($P_{1/2}$) and ferrimagnetic (FR) phases, respectively. On the other hand, at a higher temperature, the SQ phase is separated from the two distinct paramagnetic phases by two critical surfaces controlled by the fixed points M_1 and M_2, which have in common a critical line represented by the fixed point M_3, where the three phases coexist. This line is the locus of points where a second-order transition line meets two second-order transition lines. A point of this kind will be called a multicritical point.

Representative cross sections of constant K/J, extended to negative values, in terms of temperature $1/J$ and chemical potential Δ/J, are shown in figures 2(a) and 2(b). They



(a)



(b)

Figure 2. The representative phase diagrams obtained from the global position-space renormalization-group method, for K/J values of (a) -0.6 and (b) -1.5.

exhibit the two additional ordered phases which have sublattice symmetry breaking. Moreover, according to the values of the ratio K/J, and as the temperature is lowered at fixed Δ/J, there occurs a single or successive phase transitions which are of second order.

For values $-1 < K/J < -1/4$ (figure 2(a)), the ferrimagnetic phase lies, at low temperature, within the ferromagnetic phase, and three separate second-order transitions are found. There are transitions from the paramagnetic to a ferromagnetic phase, from the ferromagnetic to a ferrimagnetic phase and from the ferrimagnetic back to a ferromagnetic phase. One should note also no re-entrance occurring in the PSRG phase diagram, contrasting with previous MFA results where a pronounced re-entrance is observed in the interval $-1/3 < K/J < -1.73$. We note here that the shape of the resulting phase boundary is in agreement with that of the MC simulations [9].

For values of $K/J < -1$ (figure 2(b)), the staggered quadrupolar phase occurs at high temperatures, whereas, at finite temperature, this phase is always separated from the ferrimagnetic one by a ferromagnetic phase. Thus, as the temperature is lowered at fixed Δ/J in the region $3 < \Delta/J < 6$, there occur phase transitions successively between the paramagnetic, staggered quadrupolar, ferromagnetic, and ferrimagnetic phases. All of the corresponding phase boundaries are of second order.

One should also notice that, unlike in previous studies on the spin-1 BEG model, where the ferrimagnetic phase has never appeared at all temperatures when using recursion relations of the MK type, here, on increasing the spin values to $S = 3/2$, the method that we have used shows a stable fixed point characterizing the ferrimagnetic phase over a large region at low temperature. On the other hand, while the staggered quadrupolar phase appears at low temperature for the spin-1 BEG model, in the spin-3/2 model this phase is completely stable at high temperature and separated from the ferrimagnetic one by a ferromagnetic phase, whereas the MFA phase diagram for the spin-1 BEG model [6] exhibits phase transitions between the SQ and FR phases which can be first order, second order, or tricritical.

4. Conclusions

We have determined the critical properties of the square-lattice spin-3/2 BEG model, with repulsive biquadratic interaction, by using the Migdal–Kadanoff method of decimation followed by bond shifting. Treatments are provided for a discrete value of the length rescaling factor b. In particular, we have computed the phase boundaries which separate the disordered domain from any of the four distinct ordered domains. We have located eight unstable fixed points characterizing the various phase transitions, with their global connectivity and local critical exponents. The global phase diagram in (J, K, Δ) space (with $J > 0$ and $K < 0$) is found to have seven important boundary surfaces of critical phase transitions between paramagnetic, ferromagnetic, staggered quadrupolar, and ferrimagnetic phases.

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