Blume-Emery-Griffiths Model on the Square Lattice with Repulsive Biquadratic Coupling

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Abstract

Using a real-space renormalization group procedure with no adjustable parameters, we investigate the Blume-Emery-Griffiths model on the square lattice. The formalism respects sublattice symmetry, allowing the study of both signs of $K$, the biquadratic exchange coupling. Our results for $K > 0$ are compared with other renormalization group calculations and with exact results, in order to assess the magnitude of the errors introduced by our approximate calculation. The quantitative agreement is excellent; values for critical parameters differ, in some cases, by less than 1% from exact ones. For $K < 0$, our results lead to a rich phase diagram, with antiquadrupolar and ferromagnetic ordered phases. Contrarily to Monte Carlo simulations, these two phases meet only at zero temperature. Both antiquadrupolar-disordered and ferromagnetic-disordered transitions are found to be continuous and no ferrimagnetic phase is found.

Key words: Blume-Emery-Griffiths model; phase diagrams; renormalization group.

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1 Introduction

The most general spin-1 Ising model with up-down symmetry is the Blume-Emery-Griffiths (BEG) model, which Hamiltonian reads:

$$\mathcal{H} = -J \sum_{<i,j>} S_i S_j - K \sum_{<i,j>} S_i^2 S_j^2 + \Delta \sum_i S_i^2,$$

(1)

where the first two sums are over all nearest-neighbor pairs on a lattice, the last one is over all sites and $S_i = \pm 1$, 0 \[1, 2\]. This model was originally introduced to study phase separation and superfluidity in $^3$He-$^4$He mixtures [1]. Later it has been applied to describe properties of multicomponent fluids [3], microemulsions [1], semiconductor alloys [5], and electronic conduction models [6].

From the theoretical point of view, the BEG model was extensively studied for positive biquadratic exchange ($K > 0$). Its phase diagram is well understood: it exhibits two disordered phases and a ferromagnetic phase. The transition between them can be a continuous or a first order one, with the presence of an ordinary tricritical line, an isolated critical line, and a line of critical end points [2].

Recently, attention has been drawn to the repulsive biquadratic ($K < 0$) model. In this case, sublattice symmetry may be broken and the possible phases are classified according to the values of $M_A \equiv \langle S_i \rangle_A$, $M_B \equiv \langle S_i \rangle_B$, $Q_A \equiv \langle S_i^2 \rangle_A$, and $Q_B \equiv \langle S_i^2 \rangle_B$, where the subscripts $A$ and $B$ refer to the two sublattices of a bipartite lattice (which we limit ourselves in this work). A mean-field solution, firstly proposed by M. Tanaka and T. Kawabe [7] and later extended by W. Houston and A. N. Berker [8], leads to a rich phase diagram, with two new ordered phases: antiquadrupolar ($M_A = M_B = 0$, $Q_A \neq Q_B$) and ferrimagnetic ($0 \neq M_A \neq M_B \neq 0$ and $Q_A \neq Q_B$). Moreover, the ($J$, $K$, $\Delta$) phase diagram shows a variety of multicritical points, such as critical end points, bicritical, tetracritical, etc. [4, 8]. However, results obtained using mean-field approaches are expected to hold only at high dimensions; in what concerns the BEG model, discrepancies have been found between
results obtained by the cluster-variational method \cite{10} and by Monte Carlo simulation \cite{11}: both predict more than one ferrimagnetic phase for the three-dimensional model while the mean-field approach \cite{8} detects just one ferrimagnetic phase. In two dimensions, previous studies \cite{7, 11, 12} found no ferrimagnetic phase, although they disagree in what concerns the shape of the boundary between the ferromagnetic and the antquadrupolar phases. While in Ref. \cite{7} it is found that there is a first order transition between these two phases, the results of Refs. \cite{11, 12} suggest that the phases meet only at zero temperature and that the antquadrupolar-disordered (AD) and ferromagnetic-disordered (FD) transitions are continuous.

Since the question is not yet settled, an independent calculation is desirable. In order to address these questions, we apply a real-space renormalization group (RG) procedure to study the BEG model on the square lattice. Our formalism allows the study of both attractive ($K > 0$) and repulsive ($K < 0$) biquadratic interaction. Although the former is now well understood, we also present our results for this case: comparing them with more precise or with exact results, we can infer the errors introduced by the approximate procedure we use.

Before we carry on with a brief explanation of the formalism, let us review some of the exact information and symmetries associated with the model:

(i) on bipartite lattices, the antiferromagnetic model ($J < 0$) can be mapped onto the ferromagnetic one ($J > 0$) by flipping every spin on one sub-lattice. So, we can restrict ourselves to the ferromagnetic case without loss of generality;

(ii) $\Delta \ll -1$: in this region, those configurations with $S_i = \pm 1$ dominate the ensemble averages and the spin-1/2 Ising model is reobtained;

(iii) $\Delta \gg 1$, $J$ and $K$ finite: all spins are in the zero state and both $M$ and $Q$ are zero;

(iv) $\Delta \gg 1$ and $2(J + K) \sim \Delta$; either the configuration with all spins $S_i = 0$ or
the configuration with all spins $S_i = +1$ (or, equivalently, $S_i = -1$) is the ground state. Their energies are $E/N(\{S_i = 0\}) = 0$ and $E/N(\{S_i = \pm 1\}) = 2(J + K) - \Delta$; so, there is a first order transition at $2(J + K) = \Delta \gg 1$;

(v) **Griffiths symmetry:** at $J = 0$ we can define a new variable for each site $i$, $t_i = 2S_i^2 - 1$. The Hamiltonian is then transformed into (apart from additive constant terms):

$$
\mathcal{H} = -J_G \sum_{<i,j>} t_i t_j + H_G \sum_i t_i, \quad t_i = \pm 1,
$$

with $J_G = K/4$ and $H_G = K + \frac{1}{8}(\ln 2 - \Delta)$ (on the square lattice). For $K > 0$ ($K < 0$), this is the ferromagnetic (antiferromagnetic) spin-$1/2$ Ising model on a uniform magnetic field. Thus, in an exact renormalization group procedure, one expects to obtain $(J = 0, \ K = 1.763, \ \Delta = 4.219)$ and $(J = 0, \ K = -1.763, \ \Delta = -2.832)$ as critical fixed points for the ferromagnetic and antiferromagnetic model on the square lattice, respectively.

(vi) **Three-state Potts model:** for $K = 3J$ and $\Delta = 8J$, the BEG Hamiltonian reduces to the ferromagnetic three-state Potts model [2]. On the other hand, $K = -3J$ and $\Delta = -8J$ is equivalent to the antiferromagnetic three-state Potts model [8]. The exact location of the ferromagnetic model fixed point would be $(J = 0.5025, \ K = 1.5076, \ \Delta = 4.0202)$, while the corresponding fixed point for the antiferromagnetic model is at $(J = \infty, \ K = \infty, \ \Delta = \infty)$ [8].

We expect a reliable RG procedure to respect, at least in an approximate way, these symmetries, which are not a priori incorporated in the formalism we apply in this work.

The remaining of the paper is organized as follows. In Section 2 we explain the RG formalism, in Section 3 we present the results, for both $K < 0$ and $K > 0$, and finally in Section 4 we briefly review the results obtained in this article.
2 Formalism

As is usual in small-cell RG approaches, we approximate the Bravais lattice (in our case, the square lattice) by an appropriate hierarchical lattice. As long as the symmetries of the ground-states are preserved, no spurious results are introduced. In the present work, this requires a cell which respects sub-lattice symmetry, in order to get the correct behavior for $K < 0$. We note that the results obtained are exact on the chosen hierarchical lattice but only approximate on the Bravais lattice; in particular, one does not expect to obtain results as precise as those achieved using Monte Carlo simulations or conformal invariance arguments (although the precision obtained in the present work is excellent). More generally, it is known that two-dimensional real-space RG procedures yield more accurate results than their three-dimensional counterpart (see, for instance, [14] and references therein).

We are here mainly interested in qualitative features of the phase diagram, like, for instance, the presence of distinct phases and universality classes.

The cell chosen (see Figure 1) has been used with success in many studies of antiferromagnetic systems ([15, 16] and references therein). We then impose that the correlation function between the two terminal sites of the original and renormalized graphs are preserved [17]:

$$\exp(-\beta H_{12}) = Tr \exp(-\beta H_{123456}),$$

where $Tr$ means a partial trace over the internal sites of the cell (those marked with 3, 4, 5 and 6 in Figure 1). We rewrite the Hamiltonian as a sum of “bond” terms (from now on, the factor $-\beta$ will be absorbed into the interaction parameters):

$$H_{12} = -J S_1 S_2 - K' S_1^2 S_2^2 + \frac{A'}{4} (S_1^2 + S_2^2) + G',$$

and:

$$H_{123456} = -J(2S_1 S_3 + S_1 S_4 + S_3 S_6 + S_3 S_5 + S_4 S_6 + S_2 S_5 + 2S_2 S_6)$$
\[-K(2S_1^2S_3^2 + S_1^2S_4^2 + S_3^2S_6^2 + S_3^2S_2^2 + S_1^2S_6^2 + S_2^2S_8^2 + 2S_2^2S_6^2) + \frac{\Delta}{4}(3S_1^2 + 4S_3^2 + 2S_4^2 + 2S_6^2 + 4S_6^2 + 3S_2^2),\]

(4)

where primed quantities are renormalized parameters and $G'$ is necessary to redefine the zero of energy.

Note that this way to write the cell Hamiltonian is equivalent to attribute weights to the sites in the one-site (crystal-field $\Delta$) interaction, according to their coordination number. This is necessary for finite lattices to approximate correctly the infinite lattice behavior (see, for instance, [16]).

In this way, we obtain the RG relations between original and renormalized parameters:

\[J' = J'(J, K, \Delta); \quad K' = K'(J, K, \Delta); \quad \Delta' = \Delta'(J, K, \Delta).\]

(5)

The critical points are then evaluated as non-trivial fixed points of the above relations and critical indices are obtained linearizing the equations around these fixed points.

As we shall see later, some of the symmetries of the model are exactly reproduced by our procedure and some are reproduced to a very good approximation.

## 3 Results

### 3.1 Positive K

For positive biquadratic interaction, the phase diagram is qualitatively similar to the one found in [2] (see Figure 2). One exception is the $OGF_2$ line, which is not a straight line in our treatment; this means that the Griffiths symmetry is not exactly respected (see item (i) in the first section). We show in Figure 3 the exact curve (dotted line), slightly above the curve found in our work (full line): note that the discrepancy is very small. It is easy to show that the Griffiths symmetry is not
respected due to surface sites i.e., those sites at the boundary of the cell which have less than 4 first neighbors. So, we expect that the discrepancy will diminish as bigger cells are used. Nevertheless, even with the small cells used, the agreement is very good, as Figure 3 shows. In particular, the fixed point $G$ in Table I is within 2% of the exact value. It is worthy to stress that, contrarily to some RG procedures, we do not impose this symmetry \textit{a priori}.

Another model which is not exactly recovered in our formulation is the three-state ferromagnetic Potts model. Nevertheless, the corresponding fixed-point, $P$ in Table I, differs by less than 0.1% from the exact value.

In Table I we compare our evaluation of the fixed points with exact or previous results. As for $G$ and $P$, the agreement is a remarkable one, taking into account the size of the cells used. Let us mention that our evaluation of the critical exponents are not as precise as for the critical points but are in qualitative agreement with expected results. In particular, we can correctly describe first-order phase transitions associated with a discontinuity in $Q$, like the one cited at (iv) in the Introduction. In order to detect discontinuities in $M$ a study of odd interactions is necessary; since we can determine the order of the transitions for $K < 0$ from general arguments, we limited ourselves to even interactions.

Finally, let us mention that the symmetries (i) to (iv) in the Introduction are exactly respected by our treatment.

### 3.2 Negative K

For this case, competition between bilinear ($J$) and biquadratic ($K$) couplings takes place and, as a result, a new phase is present in two dimensions, namely the antiquadrupolar phase. Early works do not agree in what concerns the boundary (if any) between this phase and the ferromagnetic one. Our results suggest that these phases meet only at zero temperature and, as expected, that the FD and AD transitions
are continuous.

Initially, let us comment on the Griffiths symmetry (see item (v) in the Introduction). For $J = 0$ and $K < 0$, we reobtain the antiferromagnetic Ising model in the presence of a uniform field. The phase diagram of this model is known [10]: it presents an antiferromagnetic ordered phase and a paramagnetic phase. The critical temperature between these two phases diminishes as the field is increased, reaching zero for a critical field $H_C = 4 \mid J \mid$ (on the square lattice). The universality class for finite field transitions is the same as for the zero-field Ising model, i.e. the flux along the boundary between the antiquadrupolar and the disordered phases is towards the zero-field fixed point. So, in an exact RG formalism one expects to obtain a fixed point at $(J = 0, K = -1.763, \Delta = -2.832)$, which is stable along the phase boundary. Our results are depicted in Figure 4; the exact result is shown as a dark circle while our evaluation of the fixed point ($A^*$) is represented by a dark square. Note that the shape of the boundary is qualitatively correct, while the location of the fixed point is different from the expected result. Again this discrepancy is related to surface sites and one expects $A^*$ to approach the exact result as the size of the cell grows. However, we obtain the correct behavior in what regards universality class, i.e. the fixed point is stable along the boundary (in fact, as we will comment later, it is stable along the surface which separates the disordered and antiquadrupolar phases; this surface is present for $J > 0$ as well).

For $J < 0.4407$ the only ordered phase is the antiquadrupolar one, while for $J \geq 0.4407$ a ferromagnetic ordered phase is present. The attractor of the AD transition surface is the fixed point $(J^*, K^*, \Delta^*) = (0, -3.23, -2.03)$; as discussed above, this is not the exact result but it correctly represents the antiquadrupolar phase, in the sense that it belongs to the $J = 0$ plane; moreover, its eigenvalues show that the AD transition is a continuous one (a first-order transition is indicated by $\lambda = b^d$, where $\lambda$ is the eigenvalue associated with the field conjugated to the order
parameter, $b$ is the scaling parameter and $d$ is the dimension of the system [18]. This is the correct result, since this transition is in the same universality class of the zero-field Ising model. On the other hand, the FD boundary is attracted to the $C$ fixed point (see Table I), which represents the spin-1/2 Ising model. Our procedure obtains this transition as a continuous one, as well.

In Figure 5 we show sections of constant $K/J < 0$. In (a) the behavior is representative of small values of $|K/J|$: the transition is always continuous, except for the zero-temperature fixed point. Note that no reentrant behavior is obtained, contrarily to the mean-field result (MF); our result is supported by the Monte Carlo calculation of Reference [7] (not depicted in Figure 5a). In (b) the $K/J = -2$ section is shown; as discussed above, two ordered phases are present, namely the ferromagnetic and antiquadrupolar phases. The AD and FD transitions are both continuous and their boundaries meet at zero temperature, where the transition is first order. For smaller values of $K/J$ the antiquadrupolar phase bulges out but the qualitative behavior is the same as for $K/J = -2$. Since for $K/J = -3$ and $\Delta/J = -2$ the antiferromagnetic three-state Potts model on the square lattice is reobtained and this model does not order at finite temperatures, no phase transition should be detected along this line: this is consistent with our results but not with the Monte Carlo result (MC).

We also compare, in Figure 5b, our results with Monte Carlo and mean-field calculations. The difference with respect to the latter is expected but notice that the Monte Carlo calculation predicts a first-order transition between the two ordered phases for $K/J = -2$. This is in contradiction with our results; bearing in mind the connection with the antiferromagnetic three-state Potts model, the present approach yields the correct qualitative behavior (taking into account that the phase diagram for $K/J = -3$ presents the same overall qualitative features as for $K/J = -2$).
4 Summary

We apply a real-space RG procedure to study the BEG model. Our results for \( K > 0 \) are in excellent qualitative and quantitative agreement with previous works. For \( K < 0 \), the phase diagram is qualitatively different from mean field results; since these correctly describe high-dimensional systems, while our work is on the square lattice, this difference is expected. Some discrepancy is found with Monte Carlo results, in what concerns the existence of a first order transition between antiquadrupolar and ferromagnetic phases; our results do not predict this transition, which is consistent with the lack of an ordered phase at finite temperatures for the antiferromagnetic three-state Potts model on the square lattice.

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Table Caption

**Table I:** Fixed points obtained in the present work (middle column) and exact results (right column: those with a subscript \( p \) are not exact but refer to the RG calculation of [2]).

Figure Captions

**Figure 1:** Construction of a hierarchical lattice adequate to simulate the square lattice. Numbers 1 and 1' and 2 and 2' denote terminal spins while 3, 4, 5, and 6 denote internal spins. (a): original lattice, with parameters \( J, K, \) and \( \Delta \); (b) cell obtained from collapsing the terminal sites: it is essential that collapsed sites 1 and 1’ (as well as 2 and 2’) belong to the same sub-lattice; (c) renormalized lattice, with renormalized parameters \( J', K', \) and \( \Delta' \).

**Figure 2:** Phase diagram for \( K > 0 \). Wavy lines denote smooth continuation of surfaces. Full lines denote continuous transitions and dotted lines denote first-order transitions (except the line \( PL \), which is a line of critical end points). \( T_0P \) is an ordinary tricritical line and \( GP \) is an isolated critical line. \( T \) is the attractor of tricritical transitions, \( P \) is the three-state ferromagnetic Potts model, and \( G \) is the Griffiths fixed-point (see text).

**Figure 3:** \( J = 0 \) section of the phase diagram for positive \( K \), showing the Ising fixed point (black circle); our evaluation of this point is indistinguishable from
the exact location (see Table 1). The broken line is the exact result and the full curve represents the present approximation; note that they are indistinguishable just below and above the $G$ fixed point.

**Figure 4:** $J = 0$ portion of the phase-diagram for negative $K$. $A^*$ is the fixed-point obtained in the present approximation, which should be compared to the exact one (dark circle). The flux along the boundary is towards $A^*$.

**Figure 5:** Phase diagram for constant and negative $K/J$. Full (broken) lines represent continuous (first-order) transitions and $f$, $d$ and $i$ stands for the ferromagnetic, antiquadrupolar, and ferrimagnetic ordered phases respectively. (a) : $K/J = -1$: the behavior is representative of small values of $K/J$. (b) : $K/J = -2$: we compare our results ($RG$) with mean-field ($MF$) and Monte Carlo ($MC$) calculations. In the latter, filled (empty) circles denote continuous (first-order) phase transitions.
Table I:

| Fixed Point | Our results \((J^*, K^*, \Delta^*)\) | Exact or previous result |
|-------------|---------------------------------|--------------------------|
| \(C\)       | \((0.4407, -0.0831, -\infty)\) | \((0.4407, K^*, -\infty)\) |
| \(G\)       | \((0, 1.795, 4.217)\)           | \((0, 1.763, 4.219)\)    |
| \(L\)       | \((0.4407, \infty, 2K^* + 0.957)\) | \((0.4407, \infty, 2K^* + 1.078)\) |
| \(T\)       | \((1.470, 0.0529, 2.903)\)       | \((1.139, 0.9944, 4.245)_p\) |
| \(P\)       | \((0.5025, 1.508, 4.020)\)       | \((0.5025, 1.508, 4.020)\) |
| \(Fe\)      | \((\infty, \ln 2 - J^*, -\infty)\) | \((\infty, K^*, -\infty)\) |
| \(F_2\)     | \((0, \infty, 2K^* + \ln 2)\)   | \((0, \infty, 2K^* + \ln 2)\) |
| \(Pa_+\)    | \((0, 0, -\infty)\)             | \((0, 0, -\infty)\)      |
| \(Pa_-\)    | \((0, 0, \infty)\)              | \((0, 0, \infty)\)       |