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LETTER TO THE EDITOR

The Blume–Emery–Griffiths model on a Bethe lattice: bicritical line and re-entrant behaviour

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Abstract. We analyse the global phase diagram of the Blume–Emery–Griffiths model on a Bethe lattice. As a function of coordination, we describe the main features of a staggered quadrupolar phase, and discuss the re-entrant character of some multicritical lines and phase boundaries. In the limit of infinite coordination, we regain the results of a two-sublattice mean-field calculation.

The Blume–Emery–Griffiths (BEG) model in zero field is given by the Hamiltonian

$$\mathscr{H} = -J\sum_{(ij)} S_i S_j - K\sum_{(ij)} S_i^2 S_j^2 + D\sum_i S_i^2 \tag{1}$$

where $S_i = +1, 0, -1$, for all lattice sites i, and (ij) labels a sum over nearest-neighbour pairs of sites. This model Hamiltonian, which is perhaps the simplest generalisation of the ordinary spin-$\frac{1}{2}$ Ising model, has been used to account for multicritical behaviour displayed by magnetic systems (Blume 1966, Capel 1966), ^{3}He–^{4}He mixtures (Blume *et al* 1971), and ternary fluids (Mukamel and Blume 1974, Furman *et al* 1977). Calculations for the thermodynamic properties of the BEG model usually do not consider two sublattices, and refer to a range of parameters associated with a ferromagnetic ground state. Recent effective-field (Chakraborty 1984, Siqueira and Fittipaldi 1985, Kaneyoshi 1987, Kaneyoshi and Sarmento 1988, Chakraborty 1988, Tucker 1988, 1989) and Bethe approximations (Chakraborty and Morita 1984, 1985, Chakraborty and Tucker 1985, 1986) have failed correctly to identify and describe a staggered quadrupolar (SQ) phase for certain ranges of the model parameters. In this Letter, however, we take advantage of a Cayley tree to formulate the problem as a non-linear discrete mapping whose fixed points and cycles are associated with the thermodynamic phases. We can then describe the main features of the global phase diagram, including the SQ phase.

At zero temperature, for $J > 0$, a straightforward minimisation of the energy of the BEG model with respect to all possible spin arrangements yields the ground-state phase

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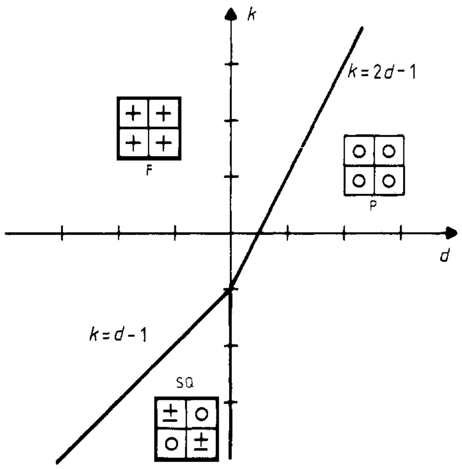

Figure 1. Ground-state phase diagram on the (d, k) plane for the BEG model on bipartite lattices: F, ferromagnetic; P, paramagnetic phase. The insets indicate spin configurations on a square lattice.

diagram shown in figure 1. For a bipartite lattice, it is sufficient to consider the ferromagnetic $(J > 0)$ case. The antiferromagnetic case, $J < 0$, can be mapped into the ferromagnetic problem by changing the signs of the spins on one sublattice, without changing the parameters K and D. In terms of $k = K/J$ and $d = D/zJ$, where z is the coordination of the lattice, the region of the staggered quadrupolar (SQ) phase is given by $k + 1 < d < 0$. In this region we have $m_\alpha = q_\alpha = 0$, for sublattice α, and $m_\beta = 0$ with $q_\beta = 1$, for sublattice β, where $m_\nu = \langle S_i \rangle_\nu$ is the magnetisation and $q_\nu = \langle S_i^2 \rangle_\nu$ is the average quadrupolar moment per spin in sublattice ν. In other words, in the ground state, sublattice α is fully occupied by spins $S_i = 0$, and sublattice β is randomly occupied by spins $S_i = \pm 1$. It is expected that the staggered-order parameter, $(q_\beta - q_\alpha)$, decreases with temperature and vanishes at a critical value defining the SQ–paramagnetic transition. We show, however, that this behaviour is significantly more complex as a function of the coordination z and the parameters of the model.

Kaneyoshi and Sarmento (1988) conjectured the existence of the SQ phase from the peculiar features of the critical curves obtained in their effective-field treatment of the BEG model. Unfortunately, the results depicted in figures 3 and 7 of their paper are not consistent with the calculations for the ground state shown in figure 1 of our paper. A similar failure occurs in the treatment of Chakraborty (1988) for the $D = 0$ case. Tucker (1988) correctly treats the $T = 0$ limit, but does not investigate the possibility of appearance of the SQ phase. The lack of consideration of sublattices in these and similar approaches precludes a more complete treatment of the SQ region of the phase diagram. As a matter of fact, it went unnoticed by some authors that the SQ phase had already been found by Tanaka and Kawabe (1985), in a two-sublattice mean-field approximation supplemented by some Monte Carlo calculations. Wang and Wentworth (1987) have also described this phase in a Monte Carlo simulation of the BEG model on a cubic lattice.

In this Letter we present an exact formulation of the BEG model on a Cayley tree of coordination z as a non-linear discrete two-dimensional mapping. The fixed points and cycles of this mapping, corresponding to the solutions deep in the interior of a very large tree, give the thermodynamic phases of the system on the so-called Bethe lattice. In particular, in the infinite coordination limit, for $z \to \infty$, $J \to 0$, $K \to 0$, with zJ and zK fixed, we regain the well known mean-field solutions (Blume *et al* 1971, Tanaka and Kawabe 1985). A similar calculation on a Cayley tree, for $K = 0$, has been performed by de Oliveira and Salinas (1985).

Consider a Cayley tree of n generations. Let $Z_n^{(+)}$, $Z_n^{(0)}$ and $Z_n^{(-)}$ be the partial partition functions of the BEG model on this tree, with the central spin (nth generation) fixed at the values $+1, 0$, and -1, respectively. We then write the recursion relations

$$Z_{n+1}^{(\pm)} = e^{-\beta D}(e^{\pm\beta J+\beta K} Z_n^{(+)} + Z_n^{(0)} + e^{\mp\beta J+\beta K} Z_n^{(-)})^{z-1} \qquad (2a)$$

and

$$Z_{n+1}^{(0)} = (Z_n^{(+)} + Z_n^{(0)} + Z_n^{(-)})^{z-1} \qquad (2b)$$

between the partial partition functions of trees with $n+1$ and n generations. Defining the dipolar moment, m_n, and the quadrupolar moment, q_n, per spin, in the nth generation

$$m_n, q_n = (Z_n^{(+)} \mp Z_n^{(-)})/(Z_n^{(+)} + Z_n^{(0)} + Z_n^{(-)}) \qquad (3)$$

we can use (2a) and (2b) to write the two-dimensional mapping

$$m_{n+1} = (R_n - Q_n)/(R_n + 1 + Q_n) \qquad (4a)$$

$$q_{n+1} = (R_n + Q_n)/(R_n + 1 + Q_n) \qquad (4b)$$

where the functions $R_n = R(m_n, q_n)$ and $Q_n = Q(m_n, q_n)$ are given by

$$R(m, q), Q(m, q) = e^{-d/t}\{1 - q + e^{k/zt}[q \cosh(1/zt) \pm m \sinh(1/zt)]\}^{z-1} \qquad (5)$$

with $t = (\beta z J)^{-1}$, and $\beta = (k_B T)^{-1}$, where T is the temperature.

Given some boundary conditions, the iterations of the mapping lead to stable fixed points, associated with the thermodynamic phases on the Bethe lattice. It is straightforward to see that at the paramagnetic (P) phase there is a simple stable fixed point, $m^* = 0, q^* \neq 0$. At the ferromagnetic (F) phase, there is also a simple fixed point, $\pm m^* \neq 0, q^* \neq 0$. At the SQ phase, however, there is a two-cycle fixed point, $m^* = 0$, and $q^* = q_1^*, q_2^*$, with $q_1^* \neq q_2^*$ (the value of q^* oscillates between the values q_1^* and q_2^*). From a linear analysis of stability of these fixed points, we can find the critical surfaces in the (k, d, t) space. Overlaps between regions of stability, for distinct boundary conditions, indicate the possibility of phase coexistence and the presence of a first-order surface. In this case, the analysis of stability has to be supplemented by a calculation of the free energy on the Bethe lattice.

For $k < -1$, the limits of stability of the P phase correspond to the F–P and the SQ–P critical surfaces in the (k, d, t) space. In the P phase, q^* is given by

$$q^* = 2R(0, q^*)/(2R(0, q^*) + 1). \qquad (6)$$

With the new variables $x = \exp(k/zt)\cosh(1/zt)$, $y = \exp(k/zt)\sinh(1/zt)$, and $u = \exp(-d/t)$, the F–P critical surface is given by

$$y = (1 - q^* + q^* x)/(z - 1)q^* \qquad (7)$$

where q^* comes from (6), while the SQ–P critical surface is given by

$$1 - q^* + q^* x = -(z - 1)q^*(1 - q^*)(x - 1) \qquad (8)$$

supplemented by (6). The intersection of these surfaces leads to a bicritical line given by the equations

$$x = \tfrac{1}{2}\{y(z - 2) + 1 - [y^2 z^2 + 1 - 2y(z - 2)]^{1/2}\} \qquad (9)$$

and

$$1/u = 2y(x + y)^{z-1}/(1 (- x - y). \qquad (10)$$

The projections of this line on the (d, t) and the (d, k) planes are drawn in figure 2 for

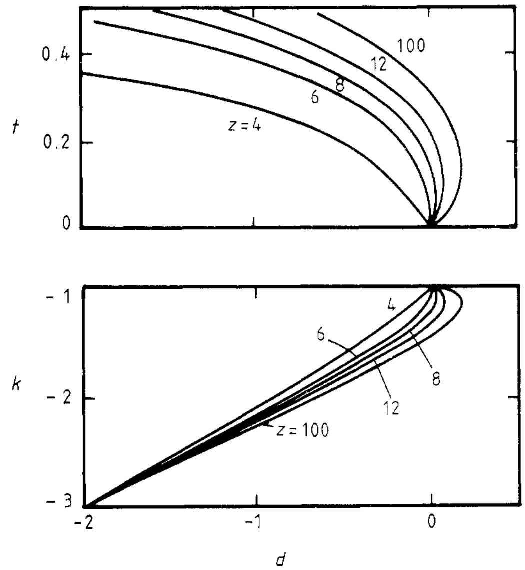

Figure 2. Projections of the bicritical line of the BEG model on (a) the (d, t), and (b) the (d, k), planes for several values of the coordination z. The results for $z = 100$ correspond to the mean-field limit.

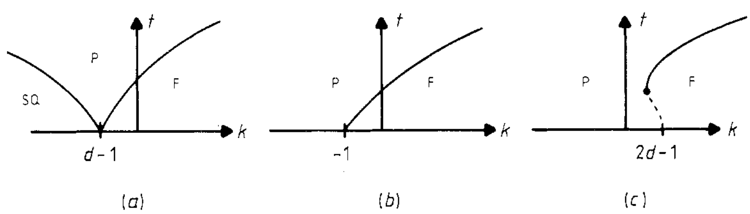

Figure 3. Schematic sections of the global phase diagram of the BEG model on the (k, t) plane for $z = 3$ and (a) $d < 0$, (b) $d = 0$, and (c) $d > 0$. Continuous and first-order transitions are indicated by full and broken curves respectively. In part (c) there is a tricritical point along the F–P phase boundary.

several values of the coordination z. There are no finite temperature solutions for $z \leqslant 3$. The bicritical line clearly displays a re-entrant behaviour in the $d > 0$ region for large enough values of z (in fact, for $z \geqslant 7$).

We have also performed some numerical calculations to investigate the location of the F–P and SQ–P critical surfaces. As illustrated in figures (3)–(5), it is possible to find three qualitative distinct situations, depending on the coordination of the lattice.

(i) For $z = 3$, the bicritical line is given by $t = 0$, and $k = d - 1$. For $d < 0$, the SQ–P and F–P critical surfaces join along this line (see figure 3(a)). At finite temperatures, there is, therefore, no transition between the SQ and F phases. For $d = 0$, there is only a smooth critical line between the paramagnetic and the ferromagnetic phases in the (t, k) plane. For $d > 0$, as shown in figure 3(c), the F–P critical surface is bounded by a tricritical line, below which there is a first-order surface.

(ii) For $4 \leqslant z \leqslant 6$, and $d < 0$, the SQ–P and F–P critical surfaces meet at a bicritical line (figure 4(a)). There is a coexistence surface, indicated by the broken line, bounded by a bicritical line and, at $t = 0$, by the $k = d - 1$ line. Although the bicritical line is not re-entrant, the SQ phase displays a bulge into the $d > 0$ region. For $d = 0$, the bicritical

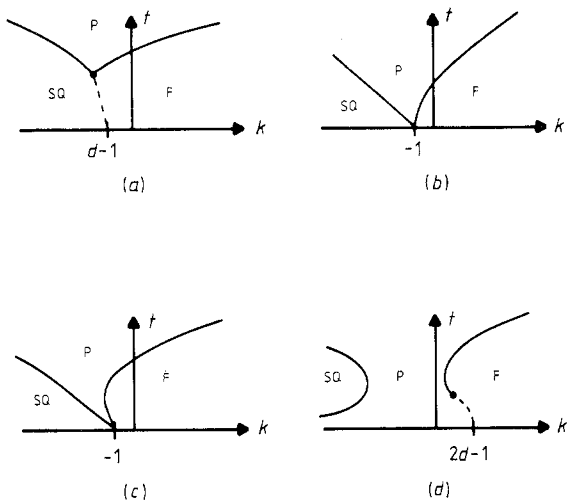

Figure 4. Schematic sections of the global phase diagram of the BEG model on the (k, t) plane for (a) $z = 4, 5, 6$ and $d < 0$, (b) $z = 4$ and $d = 0$, (c) $z = 5, 6$ and $d = 0$, and (d) $z = 4, 5, 6$ and $d > 0$. Continuous and first-order transitions are indicated by full and broken curves respectively. For $d < 0$, there is a bicritical point and a coexistence line between the SQ and F phases. For $d = 0$, the bicritical point collapses at $t = 0$. For $d > 0$, the paramagnetic phase extends down to $t = 0$.

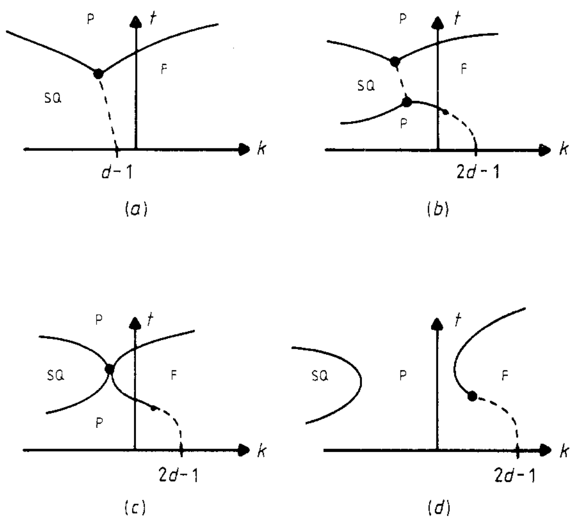

Figure 5. Schematic sections of the global phase diagram of the BEG model on the (k, t) plane for $z \geqslant 7$ and (a) $d \leqslant 0$, (b) $0 < d < d_z$, (c) $d = d_z$, and (d) $d > d_z$. Continuous and first-order transitions are indicated by full and broken curves respectively. For $0 < d < d_z$, there is a coexistence line of SQ and F phases between two bicritical points (which collapse at a special point, for $d = d_z$). This illustrates the re-entrance of the bicritical line in the (k, d, t) space.

line collapses as $t = 0$, as shown in figures 4(b) and 4(c) (the F–P line displays a re-entrance for $z = 5, 6$). These results are in qualitative agreement with the occurrence of re-entrant and 'normal' F–P lines on the cubic and square lattices, respectively, in the Monte Carlo simulations for the BEG model (de Alcântara Bonfim and Obcemea 1986, Wang and Wentworth 1987), although it should be noticed that these simulations do not predict a SQ phase for $d = 0$. Finally, for $d > 0$, our calculations indicate ferromagnetic and SQ regions separated by a paramagnetic phase (figure 4(d)).

(iii) For $z \geqslant 7$, as illustrated in figures 5(a)–(d), the bicritical line itself displays a re-entrant behaviour. For $0 < d < d_z$ where, given the coordination z, d_z is the maximum value of d for which there is still a bicritical line, the phase diagram in the (t, k) plane displays two bicritical points, defining a coexistence line, and a tricritical point, along the F–P critical line.

It is interesting to remark that, in the infinite coordination limit ($z \to \infty$, with k, t, and d, fixed), we regain the results of the two-sublattice mean-field calculation of Tanaka and Kawabe (1985). In this mean-field limit, the F–P and SQ–P critical surfaces are, respectively, given by the simple expressions

$$1/t = 1 + \tfrac{1}{2}\exp(-k + d/t) \tag{11}$$

and

$$t/k = -q^*(1 - q^*) \tag{12}$$

where

$$1/q^* = 1 + \tfrac{1}{2}\exp(-q^*k/t + d/t). \tag{13}$$

The bicritical line is given by

$$t = (k + 1/k) \tag{14}$$

with

$$d/(1 + k) = 1 + (1/k)\ln[-2/(k + 1)]. \tag{15}$$

In conclusion, the formulation of the problem on a Cayley tree as a discrete mapping is quite convenient for investigating the global phase diagram of the BEG model. The possible splitting of the lattice into distinct sublattices comes naturally from the iterations of the mapping. To make contact with Monte Carlo simulations, we show the effect of the coordination of the tree on the re-entrant character of the bicritical line and of the borders of the ordered regions. Unlike previous calculations, we are able correctly to describe the main features of the staggered quadrupolar phase.

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