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Phase diagrams for two- and three-dimensional Ising models with fluctuating exchange integrals

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Abstract. The Ising ferromagnet with fluctuating exchange integrals has been investigated using the two-spin cluster approximation. The phase diagrams were obtained for both two- and three-dimensional systems. They show a re-entrant behaviour only for a square lattice. It is argued that this behaviour is expected in disordered systems where one has competition between ferromagnetic and antiferromagnetic interactions in a certain range of the concentration of the bond mixture.

1. Introduction

During the last 20 years a considerable amount of theoretical and experimental work has been dedicated to the analysis of the magnetic properties of structurally disordered systems (see, e.g., Kaneyoshi 1984). Theoretically, there exist a great number of sophisticated techniques for discussing disordered magnets. For instance, in a series of papers, pure and diluted Ising ferromagnets with random exchange parameters have been investigated using the one-spin cluster approximation (Kaneyoshi *et al* 1984, Kaneyoshi 1985, Mielnicki *et al* 1990). In all these papers the fluctuations of the exchange integrals were considered only for the square lattice. The common result is that the phase diagrams predict the existence of re-entrant magnetism, i.e. two-phase transitions, and the range where re-entrant behaviour occurs is considerably reduced with increase in the calculation accuracy.

The purpose of this paper is to show that the existence of a re-entrant ferromagnetic phase is not a general characteristic of all lattices in which the fluctuations of the exchange integrals are present. For this reason we have evaluated phase diagrams for both two- and three-dimensional systems using the two-spin cluster method (Bobák and Jaščur 1986) which is superior to the one-spin cluster approximation. The two-spin cluster method is able to discern between lattices of the same coordination number but of different dimensions (e.g. plane triangular and simple cubic); it is known that the one-spin cluster method fails in recovering this type of result (Tomczak *et al* 1987).

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2. The theory

The Hamiltonian for a disordered Ising ferromagnet is

$$H = -\sum_{(i,j)} J_{ij} s_i s_j \tag{1}$$

where $s_i = \pm 1$, J_{ij} are the uncorrelated random exchange integrals and the summation runs over all neighbouring pairs. To describe the structural disorder in a simple way, we shall use the stochastic lattice model (Handrich 1969), in which the structural disorder is replaced by the fluctuation ΔJ_{ij} from the mean exchange J in a crystalline lattice, namely

$$J_{ij} = J + \Delta J_{ij}. \tag{2}$$

According to Bóbak and Jaščur (1986), we can obtain an exact equation for a pair of neighbouring spins as follows:

$$\tfrac{1}{2}\langle s_i + s_j \rangle = \langle [\sinh(h_i + h_j)]/[\cosh(h_i + h_j) + \exp(-2t_{ij})\cosh(h_i - h_j)] \rangle \tag{3}$$

where $t_{ij} = \beta J_{ij}$, $\beta = (k_B T)^{-1}$ and

$$h_i = \sum_{k=1}^{z-1} t_{ik} s_k \qquad h_j = \sum_{l=1}^{z-1} t_{jl} s_l$$

with the terms $k = j$ and $l = i$ excluded from summations over k and l respectively. The angular brackets $\langle \ldots \rangle$ indicate a thermal average defined as

$$\langle A \rangle = \mathrm{Tr}\,[A \exp(-\beta H)]/\mathrm{Tr}[\exp(-\beta H)].$$

Here, in order to write the exact identity (3) in a form which is particularly amenable to approximation, the differential operator method will be used. In this method the following identity is used:

$$\exp(\lambda D_x + \gamma D_y + \delta D_z) f(x, y, z) = f(x + \lambda, y + \gamma, z + \delta) \tag{4}$$

where

$$D_x = \partial/\partial x \qquad D_y = \partial/\partial y \qquad D_z = \partial/\partial z$$

are the differential operators. Applying these operators to (3), one obtains

$$\tfrac{1}{2}\langle s_i + s_j \rangle = \exp(-2t_{ij} D_z) \left\langle \prod_{k=1}^{z-1} A_{ik} \prod_{l=1}^{z-1} B_{jl} \right\rangle f(x, y, z) \Big|_{x=0,\, y=0,\, z=0} \tag{5}$$

where

$$A_{ik} = \cosh[t_{ik}(D_x + D_y)] + s_k \sinh[t_{ik}(D_x + D_y)]$$
$$B_{jl} = \cosh[t_{jl}(D_x - D_y)] + s_l \sinh[t_{jl}(D_x - D_y)]$$

and

$$f(x, y, z) = (\sinh x)/(\cosh x + \exp z \cosh y).$$

For deriving equation (5) from equation (3), we have used the following relation:

$$\exp(a s_k) = \cosh a + s_k \sinh a. \tag{6}$$

Equation (5) is an expression for a particular configuration of exchange integrals, and hence it is necessary to take an average over all possible configurations. However, it is clear that, if we try to treat exactly all the spin–spin correlations present in equation (5), the problem becomes unmanageable. Therefore, let us take an approximation

$$\langle s_i s_j \dots s_k \rangle \simeq \langle s_i \rangle \langle s_j \rangle \dots \langle s_k \rangle. \tag{7}$$

This approximation neglects correlations between different spins but takes relations such as $\langle s_i^2 \rangle = 1$ exactly into account. Now applying the approximation (7) in equation (5), the configurational average (denoted by $\langle \dots \rangle_c$) of (5) can be found. In the case of exchange interactions being given by independent random variables, equation (5), upon performing the configurational average, reduces to

$$m = \langle \exp(-2t_{ij}\mathrm{D}_z \rangle_c [\langle\langle A_{ik} \rangle\rangle_c \langle\langle B_{jl} \rangle\rangle_c]^{z-1} f(x, y, z) \Big|_{\substack{x=0\\y=0\\z=0}} \tag{8}$$

where $m = \langle\langle s_i \rangle\rangle_c$ is the average magnetization.

For further calculations the Handrich–Kaneyoshi approximation (see, e.g., Kaneyoshi 1984) will be used, according to which we have

$$\langle (\Delta J_{ij})^{2n} \rangle_c \simeq [\langle (\Delta J_{ij})^2 \rangle_c]^n \qquad \langle (\Delta J_{ij})^{2n+1} \rangle_c \simeq 0 \tag{9}$$

where n is an integer. By means of relation (2) and the approximation (9), the configurational averages are then given by

$$\langle \cosh[t_{ik}(\mathrm{D}_x \pm \mathrm{D}_y)] \rangle_c \simeq \cosh[t\,\Delta(\mathrm{D}_x \pm \mathrm{D}_y)] \cosh[t(\mathrm{D}_x \pm \mathrm{D}_y)] \tag{10}$$

$$\langle \sin[t_{ik}(\mathrm{D}_x \pm \mathrm{D}_y)] \rangle_c \simeq \cosh[t\Delta(\mathrm{D}_x \pm \mathrm{D}_y)] \sinh[t(\mathrm{D}_x \pm \mathrm{D}_y)] \tag{11}$$

$$\langle \exp(-2t_{ij}\mathrm{D}_z \rangle_c \simeq \exp(-2t\mathrm{D}_z) \cosh(2t\Delta\mathrm{D}_z) \tag{12}$$

where

$$\Delta^2 = \langle (\Delta J_{ij})^2 \rangle_c / J^2$$

represents the mean square deviation in the distribution of the random exchange integrals. The results (10)–(12) can also be obtained by using a distribution function $P(J_{ij})$ of the exchange integrals in the form

$$P(J_{ij}) = \tfrac{1}{2}\{\delta[J_{ij} - J(1 + \Delta)] + \delta[J_{ij} - J(1 - \Delta)]\}. \tag{13}$$

We are now interested in the phase boundary of the model. Close to the critical temperature, where the magnetization is small, we can linearize equation (8), and then the second-order critical line is determined by the equation

$$1 = [(z-1)/2^{2(z-1)}] \sinh(2t_c\mathrm{D}_x) [\cosh(2t_c\Delta\mathrm{D}_x) + \cosh(2t_c\Delta\mathrm{D}_y)]^{z-1}$$
$$\times [\cosh(2t_c\mathrm{D}_x) + \cosh(2t_c\mathrm{D}_y)]^{z-2} g(x, y) \Big|_{\substack{x=0\\y=0}} \tag{14}$$

where

$$g(x, y) = 2\langle \exp(-2t_{ij}\mathrm{D}_z \rangle_c f(x, y, z)|_{z=0}$$

and $t_c = J/k_\mathrm{B}T_c$. In obtaining (14) we have made use of the fact that $g(x, y) = -g(-x, -y)$ and therefore only odd differential operator functions make non-zero contributions.

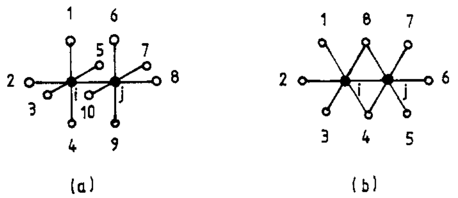

Figure 1. Two-spin cluster on the lattices with coordination number $z = 6$: (*a*) simple cubic lattice; (*b*) plane triangular lattice.

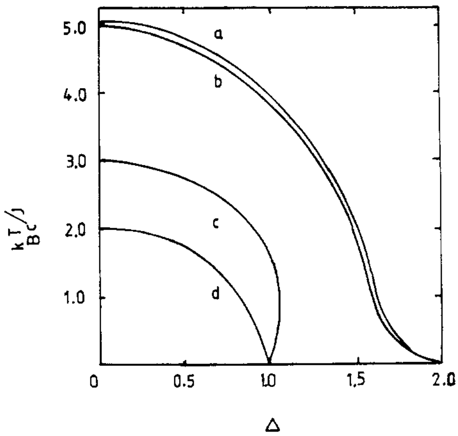

Figure 2. Phase diagrams in the (T, Δ) space for different crystallographic lattices: curve a, simple cubic lattice; curve b, triangular lattice; curve c, square lattice; curve d, honeycomb lattice.

By performing a tedious but straightforward calculation, the right-hand side of equation (14) can be expressed as a sum of the functions $g(x, y)$ with appropriate arguments x and y. For instance, for the honeycomb lattice ($z = 3$), we have

$$\begin{aligned} 1 = (1/2^6)\{ & g[4t_c(1+\Delta), 0] + g[4t_c(1-\Delta), 0] + 2g[4t_c, 4t_c\Delta] \\ & + 4g[4t_c, 0] + 8g[2t_c, 2t_c] + 4g[2t_c(2+\Delta), 2t_c\Delta] \\ & + 4g[2t_c(2-\Delta), 2t_c\Delta] + 2g[2t_c(1+2\Delta), 2t_c] \\ & + 2g[2t_c(1-2\Delta), 2t_c] + 2g[2t_c, 2t_c(1+2\Delta)] \\ & + 2g[2t_c, 2t_c(1-2\Delta)] + 4g[2t_c(1+\Delta), 2t_c(1+\Delta)] \\ & + 4g[2t_c(1+\Delta), 2t_c(1-\Delta)] + 4g[2t_c(1-\Delta), 2t_c(1+\Delta)] \\ & + 4g[2t_c(1-\Delta), 2t_c(1-\Delta)]\}. \end{aligned} \qquad (15)$$

It should be noted here that equation (14) is the general equation for the critical temperature of a disordered Ising ferromagnet valid for any lattice with the coordination number z, except the plane triangular lattice. In particular, for the crystal case of $\Delta = 0$, one finds that the t_c^{-1}-values are equal to 1.9870, 3.0250 and 5.0392 for honeycomb ($z = 3$), square ($z = 4$) and simple cubic ($z = 6$) lattices, respectively.

Now, on the basis of equation (5), we shall consider the plane triangular lattice with coordination number $z = 6$. In the plane triangular lattice which is of the same coordination number as the simple cubic, each of the two central sites belonging to the cluster has, besides another central site, only three nearest neighbours of its own, and in addition two nearest neighbours shared with the central site (the latter are marked by 4 and 8 in figure 1(*b*)). On the other hand, in the cubic lattice, each of two central sites belonging to the cluster has, besides another central site, five nearest neighbours of its own (figure 1(*a*)). Using the same approximations as above, this leads immediately to the following equation for the critical temperature of the disordered ferromagnetic triangular lattice:

$$1 = (1/2^{10})[\cosh(2t_c\Delta D_x) + \cosh(2t_c\Delta D_y)]^5[2\sinh(10t_c D_x) + 12\sinh(6t_c D_x) + 10\sinh(2t_c D_x) + 9\sinh(8t_c D_x)\cosh(2t_c D_y) + 6\sinh(6t_c D_x)\cosh(4t_c D_y) + 21\sinh(4t_c D_x)\cosh(2t_c D_y) + 6\sinh(2t_c D_x)\cosh(4t_c D_y) + \sinh(4t_c D_x)\cosh(6t_c D_y)]g(x, y)\Big|_{\substack{x=0\\y=0}}. \qquad (16)$$

It should be noted also that, for $\Delta = 0$, from equation (16) we get $t_c^{-1} = 4.9504$ which is different from the value of t_c^{-1} for the simple cubic lattice.

We are now in a position to examine the phase diagrams for both two- and three-dimensional disordered magnetic systems. The numerical results are given in the next section.

3. Numerical results and discussion

By solving equations (14) and (16) numerically, the critical lines in the (T, Δ)-space are plotted in figure 2 for honeycomb, square, simple cubic and triangular lattices.

As can be seen from this figure, for the square lattice only there is a Δ-range $(1 < \Delta < 1.1224)$ where two critical temperatures occur, which corresponds to the re-entrant phenomenon. It should be noted here that, for $\Delta > 1$, one bond in (13) becomes negative; thus some interactions are antiferromagnetic, so that the effect of frustration may appear in the system. For the honeycomb lattice $\Delta < 1$, all interactions are ferromagnetic; hence no frustration of the lattice appears. As a result, only one value of critical temperature exists for a given value of Δ.

On the other hand, the phase diagrams for plane triangular and simple cubic lattices do not exhibit the re-entrant behaviour even for $\Delta > 1$. This can be understood by comparing our results with those obtained within the two-spin cluster approximation by Benayad *et al* (1988) for the square lattice. First of all it should be mentioned that the concentration p of the bond mixture in the above paper corresponds to the value of 0.5 in our considerations and that the parameter α is related to our parameter Δ by the equation

$$\alpha = (1 - \Delta)/(1 + \Delta).$$

Further, as shown by Benayad *et al* (1988), there is the re-entrant behaviour for the range $0.429 < p < 0.597$ and $\alpha < 0$. Our Δ-range $(1 < \Delta < 1.1224)$ for a square lattice corresponds to $-0.058 \leqslant \alpha < 0$ and $p = 0.5$ which is in agreement with the results of the cited paper. Hence, the random fluctuations of the exchange interactions, leading to the appearance of ferromagnetic and antiferromagnetic bonds with the same concentration, may cause the re-entrant magnetism phenomenon in the square lattice. However, as seen from our calculations, competition between ferromagnetic and antiferromagnetic couplings with $p = 0.5$ does not lead to re-entrant behaviour for both triangular and simple cubic lattices, and the disorder may only lower the transition temperature.

Therefore, for lattices with coordination number $z > 4$ the effect of frustration is diminished in comparison with that of the square lattice. We believe that re-entrant phenomena are also possible in the lattices with $z > 4$, but the concentrations of the ferromagnetic and antiferromagnetic bonds must be different.

Finally, it is worth mentioning that the Δ-range with re-entrant magnetism obtained for the square lattice in the present paper ($1 < \Delta < 1.1224$) is somewhat larger than that obtained by Mielnicki *et al* (1990) ($1 < \Delta < 1.1218$) from the one-spin cluster method in the framework of the first-order Matsudaira (1973) approximation. As the t_c^{-1}-values for the perfect crystal case resulting from the one- and two-spin cluster approximations are 3.0898 and 3.0250, respectively, this result is in contradiction with the conclusion of Mielnicki *et al* (1990) that the range of Δ where re-entrant magnetism exists strongly reduces with increase in the calculation accuracy, The disagreement arises probably because, besides neglecting the correlations between next-nearest neighbours, the present treatment based on the approximation (7) also neglects (except for the honeycomb lattice) the correlations between nearest neighbours. It can therefore be concluded that correlations between nearest neighbours have—at least within the framework of the two-spin cluster approximation—a major effect on the range of Δ where re-entrant magnetism exists.

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