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Phase diagrams for the simple-cubic Ising lattice with re-entrant ferromagnetism

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Abstract. Using the finite-cluster approximation and renormalization technique we study the spin-$\frac{1}{2}$ Ising model for a simple-cubic lattice with nearest-neighbour random interactions. We consider nearest-neighbour ferromagnetic exchange interactions J with concentration $1-p$ and exchange interactions αJ ($|\alpha| \leqslant 1$) with concentration p. The phase diagrams were obtained for this model. They show re-entrant behaviour in certain ranges of the concentration p and different α.

1. Introduction

The critical properties of spin-$\frac{1}{2}$ Ising models with nearest-neighbour random exchange interactions have been studied in recent years. These studies have considered antiferromagnetic impurities, i.e. models with competing interactions and thus frustration. Using two different approximate methods the square lattice ($z = 4$) Ising model was studied by Benayad *et al* (1988). Similar results for the honeycomb lattice ($z = 3$) were obtained by Tóth and Tóthová (1991). Using the stochastic lattice model (Handrich 1969), phase diagrams for $z = 3$, 4, 6 lattices with a fixed concentration $p = 0.5$ were studied by Bobák and Jaščur (1990). The common result of previous papers is that the phase diagrams predict the existence of re-entrant behaviour, i.e. two-phase transitions at finite temperatures, in certain ranges of the concentration p and different α.

The purpose of this paper is to show that re-entrant behaviour exists also for the simple-cubic lattice ($z = 6$), which has not been confirmed previously (Bobák and Jaščur 1990).

We shall study this problem using two different approximate methods. The first method is the finite-cluster approximation based on an extension of Callen's identity and on the introduction of differential operators into the exact identity for a cluster of one or two neighbouring spins (Honmura and Kaneyoshi 1979, Bobák and Jaščur 1986). The second method is similar to phenomenological renormalization based on the comparison of systems of different finite sizes (Nightigale 1976, Indekeu *et al* 1982).

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2. The theory and results

We consider the ferromagnetic simple-cubic lattice with the reduced Hamiltonian

$$\beta H = -\sum_{(i,j)} t_{ij} s_i s_j \qquad t_{ij} = \beta J_{ij} \qquad \beta = (k_B T)^{-1} \tag{1}$$

where $s_i = \pm 1$, J_{ij} is the exchange interaction between spins at sites i and j, and the summation runs over all neighbouring pairs. The reduced nearest-neighbour interactions t_{ij} are assumed to be independent random variables with the distribution (Wolff and Zittartz 1985)

$$P(t_{ij}) = p\delta(t_{ij} - t) + (1-p)\delta(t_{ij} - \alpha t) \tag{2}$$

where $t = \beta J$, $|\alpha| \leqslant 1$ and $0 \leqslant p \leqslant 1$. Thus, if $\alpha > 0$, all interactions are ferromagnetic and there is no frustration; if $\alpha = 0$, we have a bond-diluted model; if $\alpha < 0$, some interactions are antiferromagnetic and there is frustration.

2.1. One-spin cluster approximation

We consider a particular spin s_i; then the thermal average according to Callen's (1963) identity gives

$$\langle s_i \rangle = \langle \tanh h_i \rangle$$

where $h_i = \sum_{j=1}^{z} t_{ij} s_j$ and z is the coordination number.

Using the differential operator method (Honmura and Kaneyoshi 1979), averaging the last equation over the random interactions (2) (denoted by $\langle \ldots \rangle_c$) and neglecting correlations we obtain

$$m = (A + mB)^z \tanh x|_{x=0} \tag{3}$$

where

$$A = p\cosh(t\mathrm{D}_x) + (1-p)\cosh(\alpha t \mathrm{D}_x) \qquad B = p\sinh(t\mathrm{D}_x) + (1-p)\sinh(\alpha t \mathrm{D}_x)$$

$m = \langle\langle s_i \rangle\rangle_c$ is the average magnetization and $\mathrm{D}_x = \partial/\partial x$ is the differential operator.

Close to the critical temperature T_c where the magnetization $m \to 0$, we can linearize (3). Then the critical temperature lines are determined by the equation

$$1 = zA^{z-1}B \tanh x|_{x=0}.$$

For the simple-cubic lattice ($z = 6$) we obtain

$$1 = \tfrac{3}{16} \sum_{n=1}^{21} a_n \tanh(d_n t_c) \qquad t_c = \frac{J}{k_B T_c}. \tag{4}$$

The coefficients a_n depend on p, and the coefficients d_n depend on α only. They are given in appendix 1. The phase diagrams in the p–t_c^{-1} plane, for different values of α, calculated from equation (4), are represented in figure 1. In accordance with these calculations there is re-entrant behaviour for the ranges $0 > \alpha > -0.2$, $-0.2 > \alpha > -0.24$ and $-\frac{1}{3} > \alpha > -0.45$.

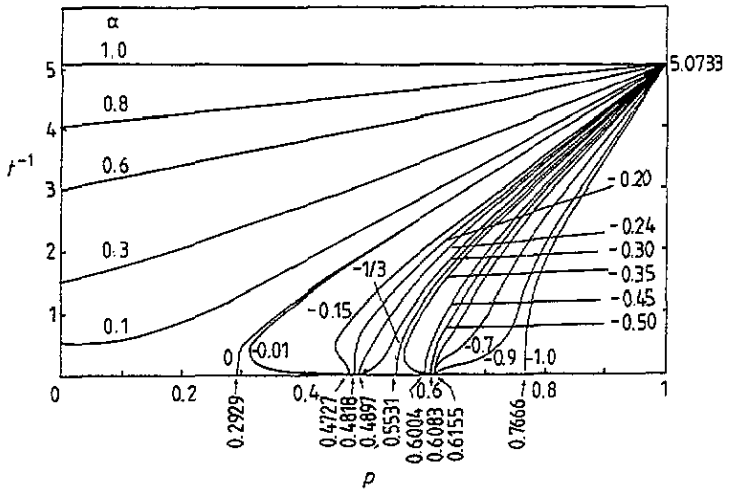

Figure 1. Phase diagrams obtained from the one-spin cluster approximation.

2.2. Two-spin cluster approximation

Previous calculations can be extended to the two-spin cluster approximation (see, e.g., Bobák *et al* (1989), and references therein). We have

$$\tfrac{1}{2}\langle s_i + s_j\rangle = \left\langle \frac{\sinh(h_i + h_j)}{\cosh(h_i + h_j) + \exp(-2t_{ij})\cosh(h_i - h_j)} \right\rangle \tag{5}$$

where

$$h_i = \sum_{k(\neq i,j)}^{z-1} t_{ik}s_k \qquad h_j = \sum_{l(\neq i,j)}^{z-1} t_{jl}s_l.$$

We can take the configurational average of equation (5) using distributions analogous to (2) for t_{ik} and t_{jl}. Within the framework of the differential operator method it is convenient to make the coordinate transformations (Mockovčiak 1991)

$$x = u + v \qquad y = u - v$$

and

$$\mathrm{D}_u = \mathrm{D}_x + \mathrm{D}_y = \frac{\partial}{\partial u} \qquad \mathrm{D}_v = \mathrm{D}_x - \mathrm{D}_y = \frac{\partial}{\partial v}.$$

Then, neglecting correlations, we have

$$\tfrac{1}{2}\langle\langle s_i + s_j\rangle\rangle_c \equiv m = (A + mB)^{z-1}(C + mD)^{z-1} f_c(u,v)|_{u=0,v=0} \tag{6}$$

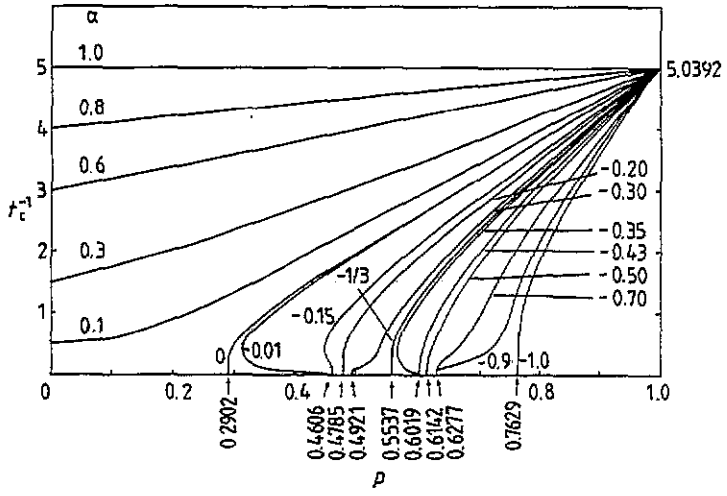

Figure 2. Phase diagrams obtained from the two-spin cluster approximation.

where

$$A = p\cosh(tD_u) + (1-p)\cosh(\alpha t D_u) \qquad B = p\sinh(tD_u) + (1-p)\sinh(\alpha t D_u)$$
$$C = p\cosh(tD_v) + (1-p)\cosh(\alpha t D_v) \qquad D = p\sinh(tD_v) + (1-p)\sinh(\alpha t D_v)$$
$$f_c(u,v) = p\sinh(u+v)/[\cosh(u+v) + \exp(-2t)\cosh(u-v)]$$
$$+ (1-p)\sinh(u+v)/[\cosh(u+v) + \exp(-2\alpha t)\cosh(u-v)]. \quad (7)$$

We again need the critical temperature equation only, so that we can linearize (6). It follows that

$$1 = 2(z-1)A^{z-2}BC^{z-1}f_c(u,v)|_{u=0,v=0}$$
$$= 2(z-1)A^{z-1}C^{z-2}Df_c(u,v)|_{u=0,v=0}.$$

For the simple-cubic lattice ($z = 6$), by performing very tedious calculations, we obtain

$$1 = \tfrac{5}{128}\sum_{n=1}^{18}\sum_{m=1}^{18} b_n c_m f_c^*(e_n t_c, e_m t_c) \quad (8)$$

where

$$f_c^*(u,v) = \tfrac{1}{2}[f_c(u,v) + f_c(u,-v)]$$

and the function $f_c(u,v)$ is given in (7). The coefficients b_n and c_m depend on p, and the coefficients e_n depend on α only. They are given in appendix 2.

The phase diagrams in the p–t_c^{-1} plane for different values of α, calculated from equation (8), are represented in figure 2. In accordance with these calculations there is re-entrant behaviour for the ranges $0 > \alpha > -0.18$, $-0.2 > \alpha > -0.23$ and $-\frac{1}{3} > \alpha > -0.43$.

2.3. *Phenomenological renormalization approximation*

We can apply the renormalization group technique in the framework of the phenomenological renormalization to our problem (Benayad *et al* 1988). Using the one-spin result (4) and the two-spin cluster result (8), we obtain the recursion relation

$$3\sum_{n=1}^{21} a_n \tanh(d_n t_c) = \tfrac{5}{8}\sum_{k=1}^{18}\sum_{l=1}^{18} b_k c_l f_c^*(e_k t_c, e_l t_c) \tag{9}$$

where the coefficients a_n and d_n and the coefficients b_k, c_l and e_k are given in appendix 1 and appendix 2, respectively.

The phase diagrams in the p–t_c^{-1} plane for different values of α, calculated from equation (9), are represented in figure 3. In accordance with our calculations there is re-entrant behaviour for the ranges $0 > \alpha > -0.07$, $-0.14 > \alpha > -0.17$, $-0.2 > \alpha > -0.25$ and $-\frac{1}{3} > \alpha > -0.78$.

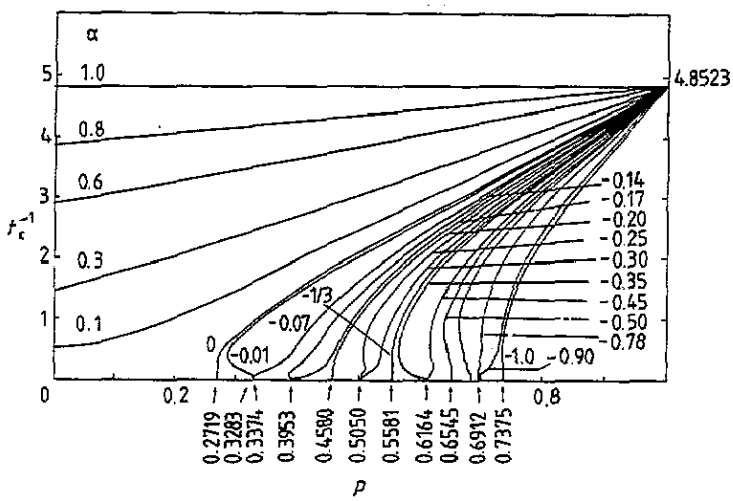

Figure 3. Phase diagrams obtained from the phenomenological renormalization approximation.

3. Discussion

The phase diagrams for all three cases show that, for non-frustrated models $\alpha > 0$, there is always just one phase transition at a finite critical temperature $T_c(p, \alpha) = (J/k_B)t_c^{-1}(p, \alpha) > 0$ from the disordered phase to the ordered ferromagnetic phase. At $\alpha = 0$ we have the bond-diluted model, which at zero temperature exhibits a transition at the percolation threshold p^*. For frustrated models $\alpha < 0$, and for certain ranges of α we have re-entrant behaviour, where two critical temperatures occur. We can see some kind of regularity in the ranges of re-entrant behaviour.

Two important characteristics of the phase diagrams, namely the reduced critical temperatures t_c^{-1} (for $p = 1$, ordered phase) and the percolation thresholds p^* ($\alpha = 0$, 'bond problem'), for our approximations are shown in table 1. No exact value for any 3D lattice is known. So, numerical values were obtained by the series expansion (SE) method (Sykes and Essam 1964). The critical value t_c^{-1} was taken from the work of Domb (1974). In randomly diluted magnetic systems ('site problem') for the simple-cubic lattice, within the framework of the one-spin cluster and two-spin cluster approximations only, the same values for percolation thresholds were obtained (Bobák and Karaba (1987), and references therein). It seems that finite-cluster approximations do not distinguish between the 'bond problem' and the 'site problem'. Also, as distinguished from the $z = 3$ and $z = 4$ lattices (Benayad *et al* 1988, Tóth and Tóthová 1991), numerical values for percolation thresholds 'decrease' in our case ($z = 6$) towards the SE value (from the one-cluster to the renormalization approximation). We should also mention that the phenomenological renormalization approximation substantially improves our solutions towards the SE value.

Table 1. Values of the critical temperature and the percolation threshold.

Physical quantity	One-spin cluster	Two-spin cluster	Renormalization	SE
t_c^{-1}	5.0733	5.0392	4.8523	4.5108
p^*	0.2929	0.2902	0.2719	0.247

This problem within the framework of the two-spin cluster approximation and for only the concentration $p = 0.5$ was studied by Bobák and Jaščur (1990). Re-entrant behaviour was not obtained in this special case.

In our more general approach the existence of re-entrant behaviour in disordered systems with a simple-cubic lattice was confirmed. The purpose of this paper was not to obtain very precise numerical results but to determine the quantitative features of the model.

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Appendix 1

The coefficients in equation (4) are given explicitly below.

The a coefficients are as follows:

$a_1 = p^6$; $a_2 = (1-p)^6$; $a_3 = 6p^5(1-p)$; $a_4 = 4p^5(1-p)$; $a_5 = 6p(1-p)^5$; $a_6 = -4p(1-p)^5$; $a_7 = 15p^4(1-p)^2$; $a_8 = 5p^4(1-p)^2$; $a_9 = 15p^2(1-p)^4$;

$a_{10} = -5p^2(1-p)^4$; $a_{11} = 20p^9(1-p)^3$; $a_{12} = 4p^6 + 20p^4(1-p)^2$; $a_{13} = 4(1-p)^6 + 20p^2(1-p)^4$; $a_{14} = 20p^5(1-p) + 40p^3(1-p)^3$; $a_{15} = 20p^3(1-p)^3 + 10p^5(1-p)$; $a_{16} = 40p^3(1-p)^3 + 20p(1-p)^5$; $a_{17} = -20p^3(1-p)^3 - 10p(1-p)^5$; $a_{18} = 40p^4(1-p)^2 + 40p^2(1-p)^4$; $a_{19} = 5p^6 + 40p^4(1-p)^2 + 30p^2(1-p)^4$;

$a_{20} = 30p^4(1-p)^2 + 40p^2(1-p)^4 + 5(1-p)^6$; $a_{21} = 20p^5(1-p) + 60p^3(1-p)^3 + 20p(1-p)^5$.

The d coefficients are as follows:

$d_1 = 6$; $d_2 = 6\alpha$; $d_3 = 5+\alpha$; $d_4 = 5-\alpha$; $d_5 = 1+5\alpha$; $d_6 = 1-5\alpha$; $d_7 = 4+2\alpha$; $d_8 = 4-2\alpha$; $d_9 = 2+4\alpha$;

$d_{10} = 2-4\alpha$; $d_{11} = 3+3\alpha$; $d_{12} = 4$; $d_{13} = 4\alpha$; $d_{14} = 3+\alpha$; $d_{15} = 3-\alpha$; $d_{16} = 1+3\alpha$; $d_{17} = 1-3\alpha$; $d_{18} = 2+2\alpha$; $d_{19} = 2$;

$d_{20} = 2\alpha$; $d_{21} = 1+\alpha$.

Appendix 2

The coefficients in equation (8) are given explicitly below.

The e coefficients are as follows:

$e_1 = 5$; $e_2 = 5\alpha$; $e_3 = 4+\alpha$; $e_4 = 4-\alpha$; $e_5 = 1+4\alpha$; $e_6 = 1-4\alpha$; $e_7 = 3+2\alpha$; $e_8 = 3-2\alpha$; $e_9 = 2+3\alpha$;

$e_{10} = 2-3\alpha$; $e_{11} = 3$; $e_{12} = 3\alpha$; $e_{13} = 2+\alpha$; $e_{14} = 2-\alpha$; $e_{15} = 1+2\alpha$; $e_{16} = 1-2\alpha$; $e_{17} = 1$; $e_{18} = \alpha$.

The b coefficients are as follows:

$b_1 = p^5$; $b_2 = (1-p)^5$; $b_3 = 5p^4(1-p)$; $b_4 = 3p^4(1-p)$; $b_5 = 5p(1-p)^4$; $b_6 = -3p(1-p)^4$; $b_7 = 10p^3(1-p)^2$; $b_8 = 2p^3(1-p)^2$; $b_9 = 10p^2(1-p)^3$;

$b_{10} = -2p^2(1-p)^3$; $b_{11} = 3p^5 + 12p^3(1-p)^2$; $b_{12} = 3(1-p)^5 + 12p^2(1-p)^3$; $b_{13} = 12p^4(1-p) + 18p^2(1-p)^3$; $b_{14} = 4p^4(1-p) + 6p^2(1-p)^3$; $b_{15} = 12p(1-p)^4 + 18p^3(1-p)^2$; $b_{16} = -4p(1-p)^4 - 6p^3(1-p)^2$; $b_{17} = 2p^5 + 6p(1-p)^4 + 12p^3(1-p)^2$; $b_{18} = 2(1-p)^5 + 6p^4(1-p) + 12p^2(1-p)^3$.

The c coefficients are as follows:

$c_1 = p^5$; $c_2 = (1-p)^5$; $c_3 = 5p^4(1-p) = c_4$; $c_5 = 5p(1-p)^4 = c_6$; $c_7 = 10p^3(1-p)^2 = c_8$; $c_9 = 10p^2(1-p)^3 = c_{10}$;

$c_{11} = 5p^5 + 20p^3(1-p)^2$; $c_{12} = 5(1-p)^5 + 20p^2(1-p)^3$; $c_{13} = 20p^4(1-p) + 30p^2(1-p)^3 = c_{14}$; $c_{15} = 20p(1-p)^4 + 30p^3(1-p)^2 = c_{16}$; $c_{17} = 10p^5 + 30p(1-p)^4 + 60p^3(1-p)^2$; $c_{18} = 10(1-p)^5 + 30p^4(1-p) + 60p^2(1-p)^3$.

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