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Comparison of effective-field and mean-field theories for the spin-one Ising model with a random crystal field

T Kaneyoshi† and J Mielnicki‡

† Department of Physics, Nagoya University, 464-01 Nagoya, Japan

‡ Institute of Physics, Polish Academy of Sciences, Al Lotonikow 32, Warsaw, Poland

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Abstract. The phase diagram of the spin-one Ising model with a random crystal field is investigated by the use of the effective-field theory with correlations. The important differences from the results obtained by the standard mean-field theory are indicated. The differences are very similar to those found in the dilution problem of magnetic systems.

1. Introduction

In a series of studies, several authors (Benyoussef *et al* 1987, Carneiro *et al* 1989, Boccara *et al* 1989) have discussed the phase diagrams of the spin-one Ising model with a random crystal field within the framework of the mean-field approximation. On the other hand, Kaneyoshi (1986, 1988) has also studied the same problems by the use of the effective-field theory with correlations (EFT), which is superior to the standard mean-field theory (MFA). The Hamiltonian of the system with a random crystal field is then given by

$$H = -J \sum_{(i,j)} S_i^z S_j^z + \sum_i D_i (S_i^z)^2 \tag{1}$$

where $S_i^z = \pm 1, 0$, and $J > 0$. The first sum runs over all pairs of nearest neighbours and D_i is a random crystal field distributed according to the law

$$P(D_i) = p\delta(D_i - D) + (1 - p)\delta(D_i) \tag{2}$$

or

$$P(D_i) = \tfrac{1}{2}[\delta(D_i - \Delta(1 + d)) + \delta(D_i - \Delta(1 - d))] \tag{3}$$

where $0 \leqslant p \leqslant 1$ and $0 \leqslant d \leqslant 1$.

In this paper, we investigate, via the EFT, the influence of crystal-field disorder on the phase transition in the spin-one Ising system. We find that many previous conclusions based on mean-field theories may not provide any insight into the nature of the phase transition of the system. The situation is very similar to that of diluted alloys, where the MFA predicts that the transition temperature will remain finite until zero concentration is reached, but where sophisticated theories that are better than the MFA predict the transition temperature to reduce to zero below a critical concentration.

In order to clarify the defects of the MFA as applied to these systems, we study in section 2 the transition temperature for the special case of a system in which the probability distribution function $P(D_i)$ is given by (2) and also $D = \infty$. In fact, our conclusion from the EFT predicts the existence of a critical value of p, namely p^*, at which the transition temperature T_c reduces to zero, although the mean-field theories give a finite transition temperature $k_B T_c/zJ = \frac{2}{3}(1-p)$ even in the region $p^* < p < 1$ (z is the coordination number). In section 3, the transition temperature of the system with the probability distribution function (3) and $d = 1$ is also investigated by the use of the EFT. In contrast with the MFA results, we find re-entrant phenomena due to the crystal-field disorder, when the transition temperature is plotted as a function of Δ, and the transition temperature reduces to zero for large values of Δ in accordance with the prediction of section 2.

2. Comparison with the MFA and EFT

According to the mean-field theory of a spin-one Ising model with a random crystal field D_i described by (2) (Benyoussef *et al* 1987), the magnetization m in the vicinity of the second-order transition line is given by

$$m = \bar{a}m + \bar{b}m^3 + \bar{c}m^5 + \dots \tag{4}$$

with

$$\bar{a} = \frac{2}{t}\left(\frac{p}{2+\exp(\delta/t)} + \frac{1-p}{3}\right) \tag{5}$$

$$\bar{b} = \frac{2}{t^3}\left[\frac{p}{2+\exp(\delta/t)}\left(\frac{1}{6} - \frac{1}{2+\exp(\delta/t)}\right) - \frac{(1-p)}{18}\right] \tag{6}$$

$$\bar{c} = \frac{2}{t^5}\left\{\frac{p}{2+\exp(\delta/t)}\left[\frac{1}{120} - \frac{1}{2+\exp(\delta/t)}\left(\frac{1}{4} - \frac{1}{2+\exp(\delta/t)}\right)\right] + \frac{13(1-p)}{1080}\right\} \tag{7}$$

where $t = k_B T/zJ$ and $\delta = D/zJ$.

Let us at first discuss the special case of $D = \infty$ ($\delta = \infty$), in order to clarify the defects of the MFA results. For $D = \infty$, the parameters $\bar{a}$, $\bar{b}$ and $\bar{c}$ reduce to

$$\bar{a} = 2(1-p)/3t \qquad \bar{b} = -(1-p)/9t^3 < 0 \qquad \bar{c} = 13(1-p)/540t^5 > 0. \tag{8}$$

Thus, the transition is of second-order and the transition temperature T_c^{MFA} for $D = \infty$ is determined from $\bar{a} = 1$:

$$k_B T_c^{\mathrm{MFA}}/zJ = \tfrac{2}{3}(1-p). \tag{9}$$

On the other hand, Kaneyoshi (1986) has discussed some general expressions for determining the second-order phase transition line and the tricritical point within the framework of the EFT. In the vicinity of the second-order transition line, the magnetization m can be also expanded in the form (4). According to the theory, the second-order transition line for the honeycomb lattice with $z = 3$ and $D = \infty$ can be obtained from the relation $\bar{a} = 1$:

$$1 = 3(1-p)[q^2K_1 + 2q(1-q)K_2 + (1-q)^2K_3] \tag{10}$$

with

$$\begin{aligned} K_1 &= \cosh^2(J\nabla)\sinh(J\nabla)F_0(x)|_{x=0} = \tfrac{1}{4}(F_0(3J) + F_0(J)) \\ K_2 &= \tfrac{1}{2}F_0(2J) \qquad K_3 = F_0(J) \end{aligned} \tag{11}$$

where $\nabla = \partial/\partial x$ is the differential operator and the function $F_0(x)$ is defined by

$$F_0(x) = 2\sinh(\beta x)/(2\cosh(\beta x) + 1) \tag{12}$$

with $\beta = 1/k_BT$. Here, the parameter $q = \langle (S_i^z)^2 \rangle$ for the system with $z = 3$ and $D = \infty$ can be determined from

$$q = (1-p)[q^3Q_1 + 3q^2(1-q)Q_2 + 3q(1-q)^2Q_3 + (1-q)^3Q_4] \tag{13}$$

with

$$\begin{aligned} Q_1 &= \cosh^3(J\nabla)G_0(x)|_{x=0} = \tfrac{1}{4}(G_0(3J) + 3G_0(J)) \\ Q_2 &= \tfrac{1}{2}(G_0(2J) + G_0(0)) \qquad Q_3 = G_0(J) \qquad Q_4 = G_0(0) \end{aligned} \tag{14}$$

where the function $G_0(x)$ is defined by

$$G_0(x) = 2\cosh(\beta x)/(2\cosh(\beta x) + 1). \tag{15}$$

The functions $F_0(x)$ and $G_0(x)$ can be easily obtained from the functions $F(x)$ and $G(x)$ in Kaneyoshi (1986) by using (2) and taking the limit $D = \infty$.

In figure 1(a) the numerical result of the coupled equations (10) and (13) is plotted as a function of p, as well as the MFA result (9) for $z = 3$. The transition temperature T_c at $p = 0$ for the system with $D = \infty$ is given by

$$k_BT_c/J = 1.5191 \qquad \text{at } p = 0 \tag{16}$$

which is equivalent to that of the honeycomb ($z = 3$) lattice with $p = 1$ and $D = 0$ (Benayad *et al* 1985, Kaneyoshi 1986). In contrast with the MFA result, the result from the EFT decreases monotonically from (16) with increasing p and reduces to zero at the critical value $p^* = 0.484$ ($1 - p^* = 0.5160$). The behaviour is very similar to that usually found in the dilution problem of magnetic atoms; in the dilution problem, the standard MFA gives the transition temperature T_c^{MFA} as

$$k_BT_c^{\mathrm{MFA}}/zJ = \tfrac{2}{3}c \qquad \text{for } D = 0 \tag{17}$$

where c is the concentration of magnetic atoms. On the other hand, a sophisticated theory superior to the MFA normally predicts the existence of a critical concentration c^*, as shown schematically in figure 1(b) (see Stinchcombe 1983). Notice that the critical concentration c^* of the spin-$\frac{1}{2}$ Ising honeycomb lattice obtained by the EFT for the site dilution is given by $c^* = 0.5575$ (Li and Yang 1985). Thus, the similarity between the two cases (the dilution problem and the random crystal field with (2) and $D = \infty$) may indicate that the results obtained from the MFA (Benyoussef *et al* 1987, Boccara *et al* 1989) do not provide any insight into the nature of possible (second-order or first-order) transition lines, especially for a value of p larger than the critical value p^* (except $p = 1$).

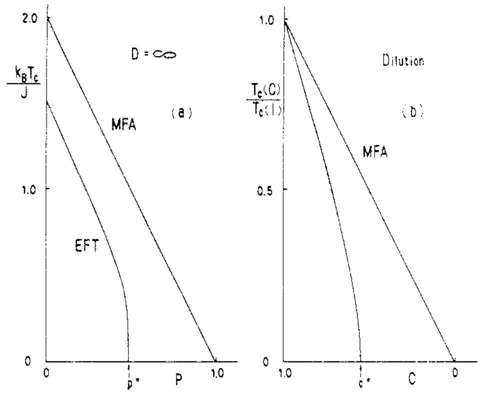

Figure 1. (a) The transition temperature T_c versus p in an Ising honeycomb ($z = 3$) lattice with a random crystal field described by (2) for the case where $D = \infty$. MFA indicates the result (9) from mean-field theory. EFT indicates the solution of coupled equations (10) and (13). The critical value p^* is given by $p^* = 0.484$. (b) A schematic phase diagram of a site-diluted Ising ferromagnet. MFA indicates the mean-field result (17) and c^* is the critical concentration.

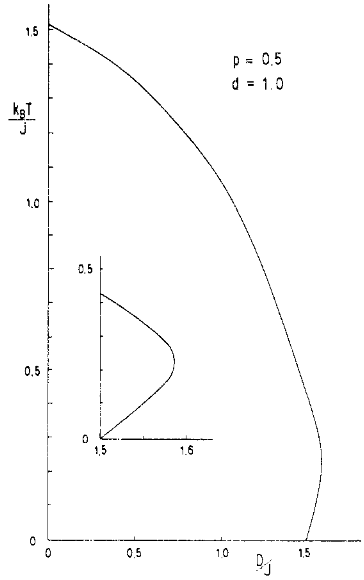

Figure 2. The phase diagram in the (T, D) plane of the spin-one Ising system with crystal-field disorder ($p = 0.5$ and $d = 1$) given by (3).

3. Re-entrant phenomena

Within the framework of the MFA, Boccara *et al* (1989) recently investigated the phase diagrams of the spin-one Ising system with a random crystal field, whose probability distribution function is given by (3). However, the probability distribution function (3) corresponds to the special case of (2), namely with $p = 0.5$ in (2); $p = 0.5$ is smaller than the critical value $1 - p^* = 0.5160$ for the system with $z = 3$ discussed in the previous section, and hence the transition temperature for the system with $z = 3$ and $d = 1$ should reduce to zero for large values of Δ (or D), although their MFA results predict a finite transition temperature for a large value of Δ and a first-order transition line separating the two ordered phases (the $m = 1$ phase and the $m = \frac{1}{2}$ phase).

In order to clarify the above discussions, let us here study the influence of crystal-field disorder on the (T, Δ) phase diagram for the honeycomb lattice ($z = 3$) with a given concentration $p = 0.5$ and a fixed value of d ($d = 1$) by the use of the EFT; the transition temperature of the system with $p = 0.5$ and $d = 1$ can be easily obtained from the coupled equations (5) and (9) in Kaneyoshi (1986) by using (2) and putting $p = 0.5$ and $D = 2\Delta$, as in the previous section. The numerical result is shown in figure 2.

In figure 2, the transition temperature T_c at $\Delta = 0$ ($D = 0$) is given by

$$k_B T_c/J = 1.5191 \qquad \text{for } \Delta = 0 \tag{18}$$

which is also equivalent to the previous result for the pure ($p = 1$) system at $D = 0$ (Benayad *et al* 1985, Kaneyoshi 1986). On increasing the value of D, the transition temperature decreases, and reduces to zero at the value $D = 2\Delta = 1.5J$. A characteristic behaviour due to the crystal-field disorder is found in the figure; the result clearly shows the re-entrant phenomena in the region $1.50 \leqslant D/J \leqslant 1.586$. This is emphasized in the inset of the figure. As discussed in previous work (Benayad *et al* 1985, Kaneyoshi 1986), the pure system with $z = 3$ and $p = 1$ may exhibit tricritical behaviour. The tricritical point can be determined from using the condition $\bar{a} = 1$ and $\bar{b} = 0$ in the expansion (4). In figure 2, however, there is no tricritical point satisfying the condition $\bar{a} = 1$ and $\bar{b} = 0$. As predicted in section 2, the transition temperature of the system with $p = 0.5$ and $d = 1$ reduces to zero for a large value of D. These results are completely different from those obtained from the MFA (Boccara *et al* 1989).

4. Conclusions

In this work we have investigated the effects of crystal-field disorder on the transition temperature (phase diagram) in the spin-one Ising system within the framework of the EFT. The results obtained are very different from those of the MFA. As discussed in section 2, however, the similarity between the two systems (the dilution of magnetic atoms and the present system with $D = \infty$) may indicate that the results obtained from MFA do not provide any reliable information about the phase diagram especially for a value of p in the region $p^* < p < 1$ where the transition temperature goes to zero. In section 3, we have also found that re-entrant phenomena due to the crystal-field disorder are possible.

Finally, it may be worth adding the following physical arguments. In section 2, Np spins among the total number N of spins are in the $S_i^z = 0$ state, because $D = \infty$, and $N(1 - p)$ spins behave as the usual Ising spins with $D = 0$. Therefore, the spins in the $S_i^z = 0$ state simply correspond to the introduction Np of non-magnetic atoms in the system, since they are inactive as regards producing ferromagnetic ordering. Thus, as the number of spins in the $S_i^z = 0$ state increases, the ferromagnetic transition temperature should decrease, and finally reduce to zero at the percolation threshold, just like it does in the standard dilution problem. Thus, the present problem should not be confused with the random anisotropy model where the directions of anisotropy at the various sites are randomly distributed (Chudnovsky *et al* 1986, Fischer 1987, Kaneyoshi 1984).

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