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Mean-field theory of the spin-1 Ising model with a random crystal field

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Abstract. A spin-1 Ising model with a random crystal field Δ_i has been studied within the mean-field approximation. For the particular two-valued distribution $P(\Delta_i) = \frac{1}{2}\{\delta[\Delta_i - \Delta(1+\alpha)] + \delta[\Delta_i - \Delta(1-\alpha)]\}$, depending upon the value of α, three types of diagram have been found in the (Δ, T) plane.

The regular spin-1 Ising model with a crystal field exhibits a tricritical point, at which the phase transition changes from second to first order, when the value of the anisotropy constant Δ takes a critical value Δ_t (Blume *et al* 1971). In a previous investigation (Benyoussef *et al* 1987), general expressions needed for evaluating the phase diagram of a spin-1 Ising model with a random crystal field have been obtained within the mean-field approximation.

In this paper we study, via the mean-field approximation, the influence of crystal-field disorder on the phase transition in the spin-1 Ising system on a regular lattice described by the following Hamiltonian:

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

where $J > 0$, $S_i = -1, 0, +1$. The first sum runs over all pairs of nearest neighbours and Δ_i is a random crystal field distributed according to the law

$$P(\Delta_i) = \tfrac{1}{2}\{\delta[\Delta_i - \Delta(1+\alpha)] + \delta[\Delta_i - \Delta(1-\alpha)]\} \tag{2}$$

where $\alpha \geqslant 0$.

In a recent paper, Kaneyoshi (1988) has studied this problem using the differential operator technique, but his conclusions were limited to second-order phase transitions and left aside both possible first-order transitions and the possible existence of new phases.

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In fact, we shall see that the last possibility is realised within the mean-field approximation. The mean-field equation of state is easy to obtain. It is given by

$$m = \int \frac{2e^{-\Delta_i/T}\sinh(zJm/T)}{2e^{-\Delta_i/T}\cosh(zJm/T)+1} P(\Delta_i)\,d(\Delta_i)$$

and, after integration over the distribution of Δ_i,

$$m = \sinh(m/t)\left(\frac{1}{2\cosh(m/t)+e^{[d(1+\alpha)/t]}} + \frac{1}{2\cosh(m/t)+e^{[d(1-\alpha)/t]}}\right) \qquad (3)$$

where m is the magnetisation, $t = T/zJ$ the reduced temperature, z the number of nearest neighbours and $d = \Delta/zJ$ the reduced crystal field.

In general, an additional equation that gives the mean value of S^2 should be added to (3), however, within the mean-field approximation; this mean value does not appear in (3) and, therefore, it is not necessary for constructing the phase diagram.

The free energy per spin is given by

$$F = \frac{zJm^2}{2} + T\int \ln\left(1 - \frac{2\cosh(zJm/T)}{2\cosh(zJm/T)+e^{\Delta_i/T}}\right) P(\Delta_i)\,d(\Delta_i)$$

and, here again, after integration over the distribution of Δ_i the reduced free energy is

$$f = F/zJ = \tfrac{1}{2}m^2 - \tfrac{1}{2}t[[\ln\{2\cosh(m/t)+e^{[d(1+\alpha)/t]}\} + \ln\{2\cosh(m/t)+e^{[d(1-\alpha)/t]}\}]] + d. \qquad (4)$$

In order to determine the transition lines we have investigated the behaviour of different solutions for m that minimise the free energy (4). In the neighbourhood of the second-order transition line, m is small and, expanding the right-hand side of the equation of state, we have

$$m = am + bm^3 + cm^5 + \ldots$$

with

$$a = (1/t)(X+Y) \qquad b = (1/t^3)[X(\tfrac{1}{6}-X) + Y(\tfrac{1}{6}-Y)]$$
$$c = (1/t^5)\{X[\tfrac{1}{120} - X(\tfrac{1}{4}-X)] + Y[\tfrac{1}{120} - Y(\tfrac{1}{4}-Y)]\}$$

where

$$X = 1/\{2+e^{[d(1+\alpha)/t]}\} \qquad Y = 1/\{2+e^{[d(1-\alpha)/t]}\}.$$

The second-order phase transition line is determined by putting $a = 1$ and $b < 0$. The tricritical point corresponds to $a = 1$, $b = 0$ and $c < 0$.

The study of the phase diagram in the (t, d) plane yields three different situations depending on the value of α. To classify them we shall proceed as follows. Let us first discuss the ground-state phase diagram in the (α, d) plane for the particular distribution (2) (figure 1).

For $T = 0$ and $\alpha \geqslant 0$, equation (3) has three solutions: $m = 0$ (paramagnetic phase); $m = \frac{1}{2}$ (partly ordered phase); and $m = 1$ (ordered phase). The energies of all possible solutions can easily be calculated. By comparing these energies, the type of the ground state is then determined and we see from figure 1 that three cases can be distinguished.

(i) For $0 \leqslant \alpha < \frac{1}{2}$ a first-order transition between the $m = 1$ phase and the $m = 0$ phase occurs at $d = \frac{1}{2}$.

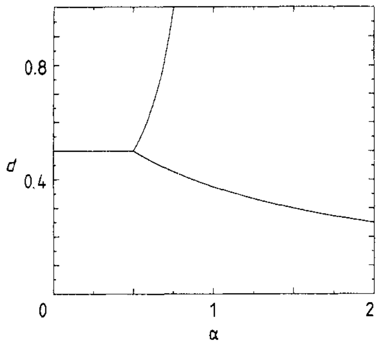

Figure 1. The ground-state phase diagram for the two-valued distribution of the anisotropy constant.

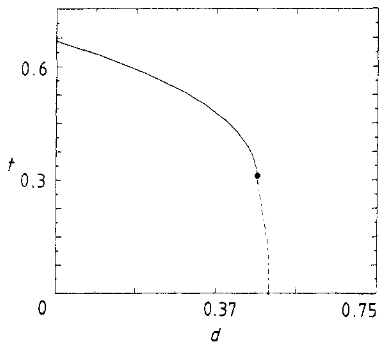

Figure 2. A typical phase diagram in the (d, t) plane obtained for $0 \leqslant \alpha < \frac{1}{2}$. The numerical results presented were obtained for $\alpha = \frac{1}{4}$.

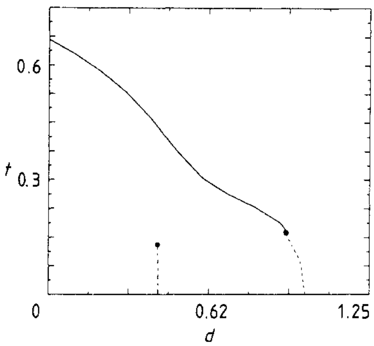

Figure 3. As figure 2 but for $\frac{1}{2} \leqslant \alpha < 1$. The results presented are for $\alpha = \frac{3}{4}$.

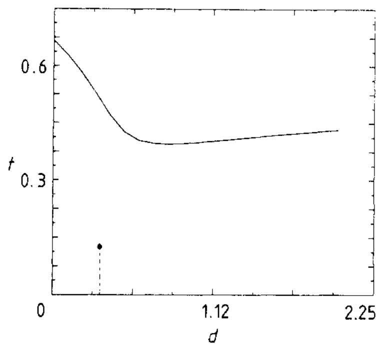

Figure 4. As figure 2 but for $\alpha \geqslant 1$. The results presented are for $\alpha = \frac{5}{4}$.

(ii) For $\frac{1}{2} \leqslant \alpha < 1$ two first-order transitions between the $m = 1$ phase and the $m = \frac{1}{2}$ phase and between the $m = \frac{1}{2}$ phase and the $m = 0$ phase occur respectively at $d = 3/4(1 + \alpha)$ and $d = 1/4(1 - \alpha)$.

(iii) For $\alpha \geqslant 1$ a first-order transition between the $m = 1$ phase and the $m = \frac{1}{2}$ phase occurs at $d = 3/4(1 + \alpha)$.

For $T \neq 0$, the phase diagram in the (d, t) plane for different values of α was determined numerically. The result is the following. There are two special values of α, $\alpha = \frac{1}{2}$ and $\alpha = 1$, which divide the interval $[0, \infty[$ into three sub-intervals where three topologically different types of phase diagram occur.

Type 1 ($0 \leqslant \alpha < \frac{1}{2}$): the diagram contains second-order and first-order lines which meet at the tricritical point (figure 2).

Type 2 ($\frac{1}{2} \leqslant \alpha < 1$): in this case, a new ordered phase ($m = \frac{1}{2}$, the partly ordered phase) appears in the interval $3/4(1 + \alpha) \leqslant d \leqslant 1/4(1 - \alpha)$. In this phase the magnetisation is smaller than that of the $m = 1$ phase at $0 \leqslant d \leqslant 3/4(1 + \alpha)$. The two ordered phases $m = \frac{1}{2}$ and $m = 1$ are separated, at low temperatures by a first-order line starting at $d = 3/4(1 + \alpha)$ at $T = 0$. The first-order line separating the two ordered phases terminates at a fluid-like critical point (see figure 3).

Type 3 ($\alpha \geqslant 1$): the system does not exhibit a tricritical behaviour but we have a first-order transition line separating the two ordered phases (figure 4). The same situation occurs for the $s = \frac{1}{2}$ Ising model in an external random field (Kaufman *et al* 1986).

In conclusion, the spin-1 Ising model with crystal-field disorder exhibits a variety of phase transitions together with a number of multicritical points.

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