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COMMENT

Comment on the mean-field phase diagram of the spin-1 Ising model in a random crystal field

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Abstract. We show the existence of additional ferromagnetic phases and transition lines in the mean-field calculations of Benyoussef and collaborators for the phase diagram of a spin-1 Ising model in a random crystal field Δ_i with probability distribution $P(\Delta_i) = p\delta(\Delta_i - \Delta) + (1-p)\delta(\Delta_i)$.

The mean-field solution of the random uniaxial crystal-field spin-1 Ising model, described by the Hamiltonian

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

where $S_i = -1, 0, +1$, for all sites i, has been discussed by Benyoussef *et al* (1987) for a random distribution of the crystal field, given by

$$P(\Delta_i) = p\delta(\Delta_i - \Delta) + (1-p)\delta(\Delta_i). \tag{2}$$

According to Benyoussef and collaborators, this model presents three kinds of phase diagram.

(i) Type 1 displays a single critical line in the T–Δ plane.

(ii) Type 2 presents first- and second-order transition lines with a critical and a double critical end point.

(iii) Finally, the type 3 phase diagram shows first- and second-order lines meeting at a tri-critical point.

The different types of phase diagram correspond to different ranges of concentrations: $p < \frac{8}{9}$, $\frac{8}{9} \leqslant p < 0.926$ and $0.926 \leqslant p \leqslant 1$, respectively.

The existence of two distinct ferromagnetic phases was, however, overlooked in the mean-field calculations of Benyoussef and collaborators. As shown in figures 1 and 2, a coexistence line separating these two ferromagnetic phases is present, at low temperatures, in the three types of phase diagram and for all values of the concentration p, except at $p = 1$ (which is the pure Blume–Capel case). Also, one of the ferromagnetic phases, which we call ferromagnetic phase 2, is stable at low temperatures, for arbitrarily large values of Δ and at any concentration $p < 1$, not only for $p < \frac{8}{9}$ (type 1 phase diagram), as argued by Benyoussef and collaborators. These phase diagrams can be obtained numerically from the mean-field expression for the free energy. At $T = 0$, the

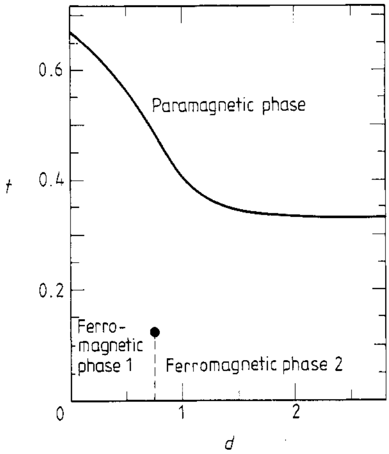

Figure 1. A typical (d, t) phase diagram for a situation of type 1 (with $p = 0.5$): ———, second-order boundary; – – –, line which ends at a critical point, indicating the coexistence of two distinct ferromagnetic phases.

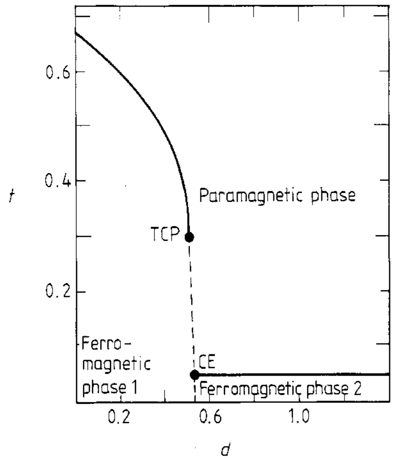

Figure 2. A typical (d, t) phase diagram for a situation of type 3 (with $p = 0.927$): ———, second-order boundaries; – – –, first-order boundaries; TCP, tri-critical point; CE, critical end point.

existence of the two ferromagnetic phases and the stability of ferromagnetic phase 2 can be verified analytically.

Using a Gaussian identity, the partition function corresponding to the infinite-range Hamiltonian

$$\mathcal{H} = -\frac{J}{2N}\sum_{i,j=1}^{N} S_i S_j + \sum_{i=1}^{N} \Delta_i S_j^2 \tag{3}$$

can be written as

$$Z = \left(\frac{N\beta J}{2\pi}\right)^{1/2} \int_{-\infty}^{+\infty} \exp[-N\beta g(T, p, \{\Delta_i\}; m)]\,\mathrm{d}m \tag{4}$$

where $\beta = (k_B T)^{-1}$. In the thermodynamic limit, we can use the law of large numbers, with the probability distribution given by equation (2), to write the free-energy functional

$$\begin{aligned} g(T, p, \Delta; m) = {} & \tfrac{1}{2}Jm^2 - (p/\beta)\ln[2\cosh(\beta Jm) + \exp(\beta\Delta)] \\ & - [(1-p)/\beta]\ln[2\cosh(\beta Jm) + 1] + p\Delta \end{aligned} \tag{5}$$

which is identical with the mean-field free energy of Benyoussef and collaborators. The extrema of this functional lead to the equation of state

$$\begin{aligned} m = {} & 2p\sinh(m/t)[2\cosh(m/t) + \exp(d/t)]^{-1} \\ & + 2(1-p)\sinh(m/t)[2\cosh(m/t) + 1]^{-1} \end{aligned} \tag{6}$$

where $t = (\beta J)^{-1}$ and $d = \Delta/J$.

Given t, p and d, the physical solutions of equation (6) should correspond to the absolute minima of the free-energy functional. First, let us consider the (ferromagnetic) ground state. If we define a step function $\theta(x)$ such that $\theta(x > 0) = 1$ and $\theta(x < 0) = 0$, equations (5) and (6), for $T = 0$, can be written as

$$(1/J)g(t=0,p,d;m_0) = \tfrac{1}{2}m_0^2 - p(m_0-d)\theta(m_0-d) - (1-p)m_0 \qquad (7)$$

and

$$m_0 \equiv m(t=0,p,d) = 1 - p\theta(d-m_0). \qquad (8)$$

The ferromagnetic solutions of equation (8), which minimise the free-energy functional given by equation (7), can be written as

$$m_0 = 1 - p\theta(d - 1 + \tfrac{1}{2}p). \qquad (9)$$

Ferromagnetic phase 1, with $m_1 = 1$, is therefore stable for $0 \leqslant d < 1 - \frac{1}{2}p$, and ferromagnetic phase 2, with $m_2 = 1 - p$, is stable for $d > 1 - \frac{1}{2}p$, for all concentrations. At $T = 0$, the paramagnetic phase is stable only for $p = 1$ (and $d \geqslant \frac{1}{2}$). The 'tail' of the critical lines, which went unnoticed by Benyoussef *et al* in phase diagrams of types 2 and 3, may be obtained by rewriting their expressions for the critical lines in the form

$$t_c = 2p/[2 + \exp(d/t)] + \tfrac{2}{3}(1-p). \qquad (10)$$

For large d, the critical temperature tends asymptotically to $\frac{2}{3}(1-p)$, for all values of the concentration p, except at $p = 1$; only at $p = 1$ does equation (10) yield $t_c = 0$. As expected, the 'tail' is absent in the phase diagram of the pure Blume–Capel model (Blume *et al* 1971). It remains to be shown whether these features of the phase diagrams are still present in a calculation taking into account the spin fluctuations.

References

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