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COMMENT

Mean-field phase diagram of the spin-1 Ising ferromagnet in a Gaussian random crystal field

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Abstract. We consider the mean-field version of a spin-1 Ising ferromagnet in a random crystal field described by a Gaussian probability distribution. Depending on the width of the Gaussian, we obtain a rich phase diagram, with critical and coexistence lines and some multicritical points. At low temperatures, our numerical results are supported by some analytic asymptotic expansions. We also calculate the ground state for a suitable two-valued delta-function distribution to compare with the results for the Gaussian case.

We consider the mean-field version of a spin-1 Ising ferromagnet in a random crystal field, described by the Hamiltonian

$$H = -\frac{J}{2N}\left(\sum_{i=1}^{N} S_i\right)^2 + \sum_{i=1}^{N} D_i S_i^2 \tag{1}$$

where $J > 0$, $S_i = \pm 1$, 0, and D_i are independent, identically distributed random variables, given by a Gaussian probability distribution,

$$P(D_i) = \frac{1}{(2\pi)^{1/2}\sigma_0} \exp\left(-\frac{(D_i - D)^2}{2\sigma_0^2}\right). \tag{2}$$

Using a Gaussian identity and the law of large numbers, we write a general expression for a free-energy functional, from which it is possible to investigate all the details of the $D/J - k_B T/J$ phase diagram for different values of the width parameter $\sigma = \sigma_0/J$. At low temperatures, the numerical calculations are supplemented by the results of some analytic asymptotic expansions.

It is well known that the spin-1 Ising ferromagnet in a uniform crystal field displays a tricritical point separating lines of first- and second-order phase transitions in the D–T plane [1]. As shown by calculations using delta-function distributions [2–4], randomness in the crystal field introduces several new features in the mean-field phase diagrams of this model. For example, Benyoussef *et al* [2], and the present authors [3], considered a random crystal field given by the distribution

$$P(D_i) = p\delta(D_i - D) + (1-p)\delta(D_i). \tag{3}$$

In the D–T phase diagram, there is still a tricritical point for $p \leqslant 1$, which turns into a pair of critical and double critical end-points as p decreases, and finally disappears for $p < \frac{8}{9}$. In fact, we have shown that, for any dilution, two distinct ferromagnetic phases are present at sufficiently low temperatures, the system remaining ordered for arbitrarily large values of D. Another form of delta-function distribution, including a mixture of two crystal fields, has also been studied by Boccara *et al* [4].

Using a Gaussian identity, the partition function associated with the mean-field Hamiltonian (1) is given by

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

where $\beta=(k_{\mathrm{B}}T)^{-1}$, and

$$g(T,\{D_i\};m)=\tfrac{1}{2}Jm^2-\frac{1}{N\beta}\sum_{i=1}^{N}\ln(2\,\mathrm{e}^{-\beta D_i}\cosh(\beta Jm)+1). \tag{5}$$

In the thermodynamic limit, we can use the law of large numbers to write the free-energy functional

$$g(T,\{D_i\};m)=\tfrac{1}{2}Jm^2-\frac{1}{\beta}E\{\ln(2\,\mathrm{e}^{-\beta D_i}\cosh(\beta Jm)+1)\} \tag{6}$$

where the expectation value $E\{\ldots\}$ is taken with respect to some arbitrary probability distribution $P(D_i)$. In the case of the Gaussian distribution, given by (2), the functional g depends on the temperature T, the parameters D and σ_0 of the probability distribution, and the variable m associated with the magnetisation per spin. The extrema of the functional yield the equation of state,

$$m=\sinh\left(\frac{m}{t}\right)E\left\{\left[\cosh\left(\frac{m}{t}\right)+\frac{1}{2}\exp\left(\frac{d_i}{t}\right)\right]^{-1}\right\} \tag{7}$$

where we use the notation $t=(\beta J)^{-1}$ and $d_i=D_i/J$. It should be remarked that expressions for the free energy and the magnetisation obtained for distinct particular distributions in previous publications can all be deduced from these general expressions. Conditions for the location of the critical line and the tricritical point can also be written in a general form from an expansion of the free-energy functional in powers of m [5]. We thus have

$$\frac{1}{J}g(m)=g_0+Am^2+Bm^4+Cm^6+\ldots \tag{8}$$

where

$$A=\frac{1}{2}-\frac{1}{t}E\left\{\left[2+\exp\left(\frac{d_i}{t}\right)\right]^{-1}\right\} \tag{9}$$

and

$$B=\frac{1}{12t^3}E\left\{\frac{4-\exp(d_i/t)}{[2+\exp(d_i/t)]^2}\right\}. \tag{10}$$

The critical line is given by $A=0$, with $B>0$. The tricritical point is given by $A=B=0$, with $C>0$.

In the particular case of the Gaussian distribution, given by (2), the free-energy functional, $g(m)$, may be written as

$$\frac{1}{J}g(m)=\tfrac{1}{2}m^2-\frac{t}{\sigma(2\pi)^{1/2}}\int_{-\infty}^{+\infty}\exp\left(-\frac{(x-d)^2}{2\sigma^2}\right)\ln\left(2\exp\left(-\frac{x}{t}\right)\cosh\left(\frac{m}{t}\right)+1\right)\mathrm{d}x \tag{11}$$

where $d=D/J$, and $\sigma=\sigma_0/J$. The equation of state is given by

$$m=\frac{1}{\sigma(2\pi)^{1/2}}\sinh\left(\frac{m}{t}\right)\int_{-\infty}^{+\infty}\frac{\exp[-(x-d)^2/2\sigma^2]}{\cosh(m/t)+\frac{1}{2}\exp(x/t)}\,\mathrm{d}x. \tag{12}$$

At the ground state, for $T=0$, (12) may be written as

$$m=\frac{1}{2}\left[1-\operatorname{erf}\left(\frac{d-m}{\sigma\sqrt{2}}\right)\right] \tag{13}$$

where $\operatorname{erf}(x)$ is the standard error function. If we rewrite this expression in the form

$$\operatorname{erf}(x)=2\sqrt{2}\sigma x-2(d-\tfrac{1}{2}) \tag{14}$$

where $x=(m-d)/(\sigma\sqrt{2})$, it is easy to see that there may be three distinct solutions for small enough values of σ. We then use (11) and (13) to write the limiting form of the free energy

$$\frac{1}{J}g(m)=m(d-\tfrac{1}{2}m)-\frac{\sigma}{(2\pi)^{1/2}}\exp\left(-\frac{(m-d)^2}{2\sigma^2}\right) \tag{15}$$

and choose the solution m associated with the absolute minimum of g. As in the case of the delta-function distributions, we have the possibility of a transition between two ferromagnetic phases. For $\sigma>(2\pi)^{-1/2}$, as (14) displays a unique solution for any value of d, a single ferromagnetic phase will be present in the d–t phase diagram. For $\sigma<(2\pi)^{-1/2}$, however, two distinct ferromagnetic phases coexist at $t=0$ and $d=0.5$.

At low temperatures ($t\to 0$), the form of the integrals in (11) and (12) is particularly suitable for a straightforward application of the well known Sommerfeld asymptotic

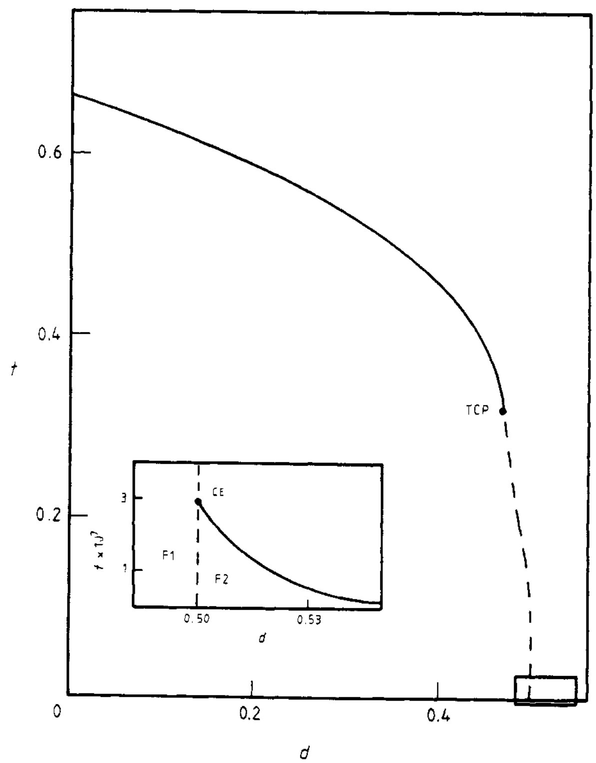

Figure 1. A typical d–t phase diagram for $\sigma<0.202\ldots$ (with numerical results for $\sigma=0.1$). Full curves are second-order boundaries. Broken curves are coexistence curves. The inset shows a critical end-point (CE) and the coexistence line of two distinct ferromagnetic phases.

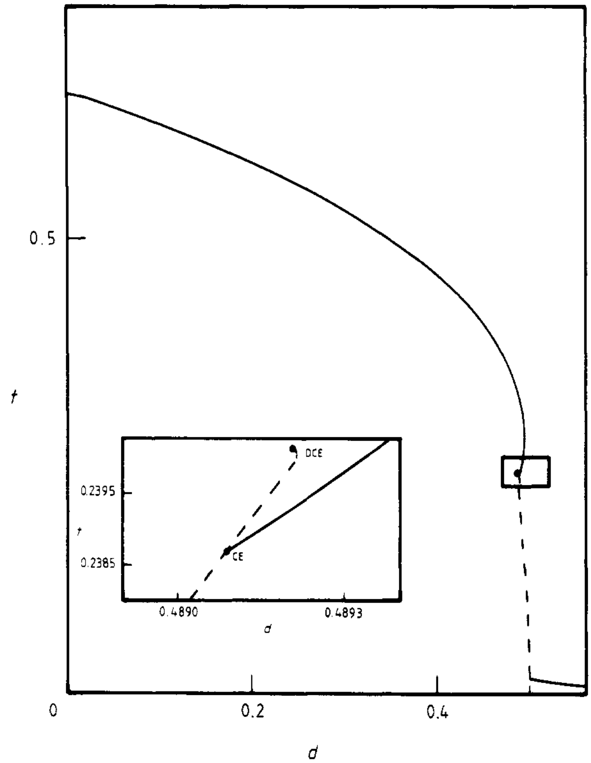

Figure 2. A typical d–t phase diagram for $0.202\ldots < \sigma < 0.229\ldots$ (with numerical results for $\sigma = 0.22$). The inset shows a critical end point (CE) and a double critical end point (DCE).

expansion technique [6]. The expression of the critical line, given by $A = 0$, from (8) and (9), with a Gaussian expectation value, can be written in the asymptotic form

$$t = \frac{1}{2}\left\{1 - \operatorname{erf}\left(\frac{d}{\sigma\sqrt{2}}\right) + \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{d^2}{2\sigma^2}\right)\right.$$
$$\left.\times\left[(\ln 2)\frac{t}{\sigma} + \frac{d}{2\sigma}\left((\ln 2)^2 + \frac{\pi^2}{3}\right)\left(\frac{t}{\sigma}\right)^2 + \ldots\right]\right\} \tag{16}$$

which shows that $d \to \infty$ for $t \to 0$. The asymptotic forms of the magnetisation and the free-energy functional are respectively given by

$$m = \frac{1}{2}\left[1 + \operatorname{erf}\left(\frac{m-d}{\sigma\sqrt{2}}\right)\right] + \frac{\pi^{3/2}(d-m)}{6\sqrt{2}\sigma}\exp\left(-\frac{(m-d)^2}{2\sigma^2}\right)\left(\frac{t}{\sigma}\right)^2 + \ldots \tag{17a}$$

and

$$\frac{1}{J}g(m) = \tfrac{1}{2}m^2 - \tfrac{1}{2}(m-d)\left[1 + \operatorname{erf}\left(\frac{m-d}{\sigma\sqrt{2}}\right)\right] - \frac{\sigma}{(2\pi)^{1/2}}$$
$$\times\exp\left(-\frac{(m-d)^2}{2\sigma^2}\right)\left[1 + \frac{\pi^2}{6}\left(\frac{t}{\sigma}\right)^2 + \ldots\right]. \tag{17b}$$

These asymptotic forms are particularly useful to check the numerical results at low temperatures, where precise calculations become hard to perform.

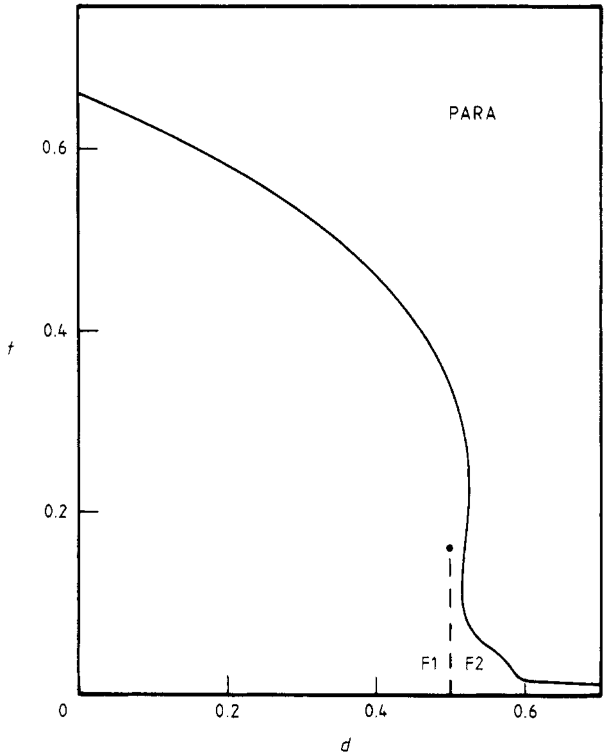

Figure 3. A typical d–t phase diagram for $0.229\ldots < \sigma < (2\pi)^{-1/2}$ (with numerical results for $\sigma = 0.3$). The broken curve represents the coexistence between two distinct ferromagnetic phases.

To obtain the global phase diagrams, the Gaussian integrations were performed numerically. Figures 1–3 display typical phase diagrams, depending on the ratio, σ, between the width of the Gaussian distribution, σ_0, and the exchange parameter, J.

(i) For $\sigma = \sigma_0/J < 0.202\ldots$, the tricritical point of the pure system is still present, but there are two ferromagnetic phases at low temperatures (figure 1).

(ii) For $0.202\ldots < \sigma < 0.229\ldots$, the tricritical point disappears, giving rise to a critical and a double critical end-point (figure 2).

(iii) For $0.229\ldots < \sigma \leqslant (2\pi)^{-1/2}$, the para-ferromagnetic transition becomes second order at all temperatures, but the two ferromagnetic phases are still present at low temperatures (figure 3). As naive numerical integrations may lead to large distortions at low temperatures, the asymptotic expansions become extremely useful to obtain the line of first-order transitions in this figure.

(iv) Finally, for $\sigma > (2\pi)^{-1/2}$, there exists a single ferromagnetic phase which remains stable up to arbitrarily large values of d.

It is interesting to consider a new delta-function distribution, given by

$$p(D_i) = \tfrac{1}{2}\delta[D_i - (D + \sigma_0)] + \tfrac{1}{2}\delta[D_i - (D - \sigma_0)] \tag{18}$$

to compare with the results for the Gaussian distribution of (2). At $T = 0$, this new distribution yields the following results.

(i) For $\sigma \leqslant 0.25$, a fully ordered phase ($m = 1$) coexists with the paramagnetic phase at $d = 0.5$.

(ii) For $0.25<\sigma<0.75$, two ferromagnetic phases ($m=1$ and $m=\frac{1}{2}$) coexist at $d=0.75-\sigma$, and the system becomes paramagnetic for $d\geqslant 0.25+\sigma$.

(iii) For $\sigma\geqslant 0.75$, a ferromagnetic phase ($m=\frac{1}{2}$) coexists with a paramagnetic phase at $d=0.25+\sigma$. In this case it is not difficult to explain the existence of two ferromagnetic phases. Half of the system, with crystalline field $D+\sigma_0$, disorders before the other half, with a smaller crystalline field, $D-\sigma_0$. For sufficiently large σ_0, one half of the system is disordered even at $D=0$, and therefore a single ferromagnetic phase is present. It is interesting that these features also appear in the case of the Gaussian distribution. On the other hand, for the Gaussian distribution, the stability of the ordered phase up to arbitrarily large values of D is to be expected due to the tail of the Gaussian curve for negative values of D_i, which guarantees that part of the system remains ordered for any D.

In conclusion, the spin-1 Ising ferromagnet in a Gaussian random crystal field displays a rich phase diagram, with new phases, critical and coexistence lines and some multicritical points. It remains to be checked whether these features are not artifacts of a mean-field calculation.

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