PHYSICAL REVIEW B VOLUME 44, NUMBER 2 1 JULY 1991-II

Mixed-spin Ising model on the Bethe lattice

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(Received 12 September 1990; revised manuscript received 15 January 1991)

We obtain the phase diagram of a ferromagnetic mixed Ising system, consisting of spin-$\frac{1}{2}$ and spin-S variables, on a Bethe lattice of coordination number z, with nearest-neighbor exchange interactions and single-ion terms. The problem is formulated as a discrete nonlinear map. There is a tricritical point for S integer and $z \geq 5$. In the infinite-coordination-number limit, we regain the results of an exact calculation for a Curie-Weiss version of the model.

I. INTRODUCTION

We consider a ferromagnetic mixed-spin Ising model, given by the Hamiltonian

$$H=-J\sum_{(i,j)} s_i\sigma_j + D\sum_i s_i^2 \ , \tag{1.1}$$

where the first sum is over nearest-neighbor sites on different sublattices, $s_i = S, S-1, \ldots, -S$, for all sites i belonging to sublattice A, and $\sigma_i = \pm 1$, for j belonging to B. In two dimensions, for three-fold-coordinated lattices, a simple decimation can be used to reduce the problem to an exactly solvable spin-$\frac{1}{2}$ Ising model.[1,2] The temperature ($t=k_BT/J$) versus anisotropy ($d=D/J$) phase diagram displays a simple λ line of second-order phase transitions. For lattices of higher coordination numbers, however, including square and cubic lattices, recent mean-field calculations indicate a much richer phase diagram, with the possible existence of a tricritical point.[3,4] In particular, the model with $S=1$, with only two parameters in the even space, may be simpler than other systems which are known to display a rich multicritical behavior.[5] To verify the main features of these phase diagrams, we have decided to undertake a more detailed investigation of some versions of this model. It should be remarked that the study of mixed-spin systems is relevant for the consideration of the behavior of ferrimagnetic compounds.

In Sec. II the statistical problem is formulated as a discrete nonlinear map on a Cayley tree. The spin variables s_i and σ_j are associated with sites on successive generations of the tree. The stable fixed points of the map, corresponding to solutions on the Bethe lattice, give the thermodynamic phases of the physical model.[5] From an analysis of the stability of these fixed points, supplemented by a Maxwell construction, we obtain all the features of the phase diagrams for arbitrary values of the lattice coordination number, z, and the spin S. For $z=3$, the results can be compared to the exact solutions. For half-integer values of S, the t-d phase diagrams display a λ line bordered by two asymptotes for very large and very small values of d. The phase diagrams are qualitatively different for integer values of S. In particular, there is a tricritical point for $S=1$ and $z \geq 5$ (which does not include a square lattice, in disagreement with a recent approximate calculation[4]).

In Sec. III we perform some exact calculations for a Curie-Weiss or mean-field version of the mixed-spin Ising Hamiltonian. From an expression for the free energy, we obtain the phase diagrams for integer as well as half-integer values of S. The mean-field equations of state correspond to the limit of infinite coordination number of the solutions on the Bethe lattice.[5]

II. SOLUTION ON THE BETHE LATTICE

Let us consider the mixed-spin model on a Cayley tree of coordination number $z=r+1$. The spin variables σ and s are associated with sites belonging to successive generations of the tree (see Fig. 1). Let us call $Z_n(s)$ the partition function of the mixed-spin model on a tree of n generations with spin s on the top site, and $W_n(\sigma)$ the

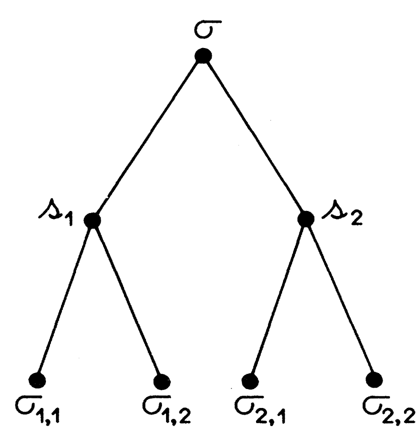

FIG. 1. Three generations of a Cayley tree of coordination number 3 ($r=2$) with a σ spin on top.

partition function for a tree with n generations and a spin $\sigma=\pm 1$ on the top site. Assuming interactions between nearest-neighbor spins, it is easy to write the recursion relations

$$Z_{n+1}(s)=e^{-ds^2/t}[e^{s/t}W_n(+)+e^{-s/t}W_n(-)]^r \quad (2.1)$$

and

$$W_{n+1}(\sigma)=\left[\sum_{s=-S,\ldots,S} e^{\sigma s/t}Z_n(s)\right]^r . \quad (2.2)$$

Introducing the notation

$$W_n(\sigma)=\exp(A_n+B_n\sigma) ,$$

and defining $m_n=\tanh B_n$, it is straightforward to rewrite Eqs. (2.1) and (2.2) as a second-order recursion relation,

$$m_{n+2}=\tanh[r\tanh^{-1}(M_1/M_2)] , \quad (2.3)$$

where

$$M_1=2\sum_s e^{-ds^2/t}\cosh^r(s/t) \times\sinh(s/t)[1-m_n^2\tanh^2(s/t)]^{r/2} \times\sinh\{r\tanh^{-1}[m_n\tanh(s/t)]\} \quad (2.4)$$

and

$$M_2=\eta+2\sum_s e^{-ds^2/t}\cosh^{r+1}(s/t) \times[1-m_n^2\tanh^2(s/t)]^{r/2} \times\cosh\{r\tanh^{-1}[m_n\tanh(s/t)]\} , \quad (2.5)$$

with $\eta=1$ for integer S and $\eta=0$ for half-integer S. In these expressions, and throughout this section, the sums are over $s=1,2,\ldots,S$ for integer S, and over $s=\frac{1}{2},\frac{3}{2},\ldots,S$ for half-integer S.

Given a set of boundary conditions, the fixed points of Eq. (2.3), $m_{n+2}=m_n=m^*$, correspond to the equation of state on the so-called Bethe lattice. From an expansion of the right-hand side of Eq. (2.3) about the trivial fixed point, $m^*=0$, we obtain the paramagnetic limit of stability,

$$\sum_s e^{-ds^2/t}\cosh^{r+1}(s/t)[r^2\tanh^2(s/t)-1]=\tfrac{1}{2} \quad (2.6)$$

for integer S, and

$$\sum_s e^{-ds^2/t}\cosh^{r+1}(s/t)[r^2\tanh^2(s/t)-1]=0 \quad (2.7)$$

for half-integer S. Equations (2.6) and (2.7), which are drawn in the phase diagrams of Fig. 2 for $S=1$ and Fig. 3 for $S=\frac{3}{2}$, give the paramagnetic critical line when there is no possibility of overlapping between the regions of ferromagnetic and paramagnetic fixed points.

In the d-t phase diagram, for integer S, the stability border of the paramagnetic region comes from $d=r+1$ at $t=0$, being asymptotically limited by $r\tanh(S/t)=1$.

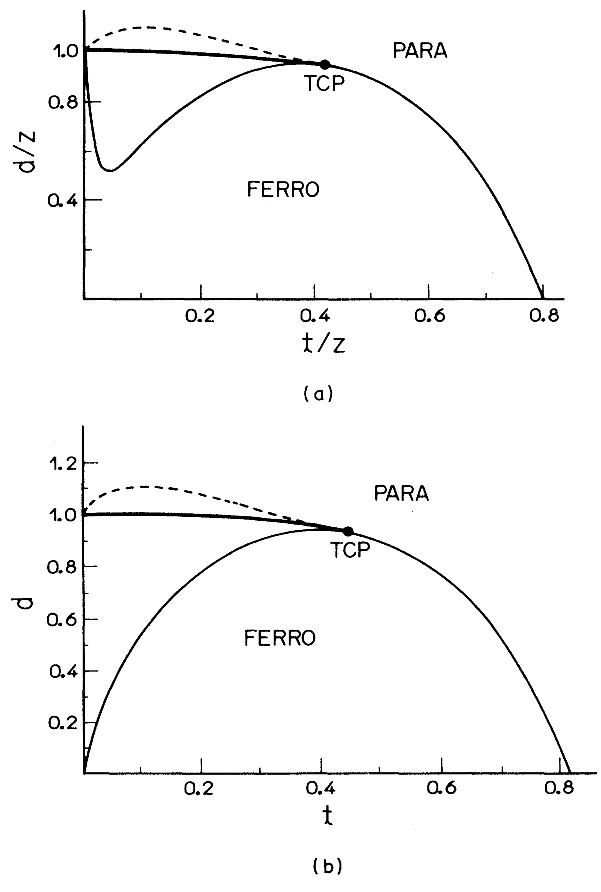

FIG. 2. (a) Phase diagram in the d/z vs t/z plane for $S=1$ and $z=50$. TCP is a tricritical point. The heavy line represents the first-order transition. The dashed line is the upper limit of stability of the ferromagnetic fixed point. The paramagnetic line, given by Eq. (2.6), is represented by the light solid curve. This is a typical phase diagram for an S integer and $z>4$. (b) Phase diagram for $S=1$ in the limit of infinite coordination number. The notation is the same as in Fig. 2(a). These results also come from the Curie-Weiss version of the model.

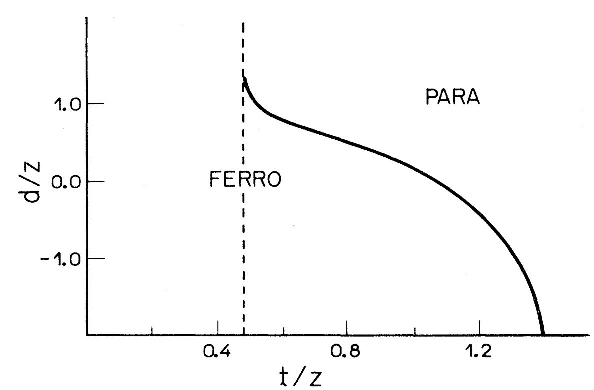

FIG. 3. Typical phase diagram for half-integer S. The solid line represents the paramagnetic border. The dashed line is one of the asymptotes. This figure is drawn for $S=\frac{3}{2}$ and $z=20$.

As shown in Fig. 2, for large r, the stability line is depressed with a pronounced minimum approaching the origin as r increases. In the infinite-coordination-number limit, $r \to \infty$ and $J \to 0$, with Jr fixed, as shown in Sec. III, we finally regain the Curie-Weiss phase diagram for integer S. The equation of state leads to the possible existence of a tricritical point whose location is given by Eq. (2.6) supplemented by the condition

$$\sum_s e^{-ds^2/t} \cosh^{r+1}(s/t) \tanh^2[(r-2)r^2 \tanh^2(s/t) - 5r - 2] = 0 \ . \tag{2.8}$$

For the typical case $S=1$, some calculations can be performed explicitly. From Eq. (2.6), the line of stability of the paramagnetic fixed point is given by

$$d = t \ln\{[r^2 \tanh^2(1/t) - 1] \cosh^{r+1}(1/t)\} \ . \tag{2.9}$$

From Eqs. (2.6) and (2.8), we obtain the tricritical temperature,

$$1/t = \tanh^{-1}\left[\frac{1}{r}\left[\frac{5r+2}{r-2}\right]^{1/2}\right] \ . \tag{2.10}$$

A simple inspection shows that there is no tricritical point for $r<4$, in agreement with the results of the exact calculations for threefold-coordinated lattices in two dimensions.[2] However, it should be pointed out that our Bethe-lattice calculation indicates that there is no tricritical point for the square lattice ($r=3$), in disagreement with recently reported approximate calculations.[4]

For $r \geq 4$, below the tricritical temperature, there is a region of stability of both paramagnetic and ferromagnetic fixed points. The border of stability of the ferromagnetic fixed point is calculated numerically. As we have not calculated an analytic expression for the free energy, we can use a Maxwell construction to locate the first-order thermodynamic border. It is easier to work with the "field" D and the expectation value of s^2, $Q = \langle s^2 \rangle$, as the conjugate thermodynamic variables to be considered. From an equal-area construction for the isotherm Q versus D, we have obtained the heavy line drawn in Fig. 2. In the limit of the infinite coordination number, this procedure reproduces the results for the Curie-Weiss model in Sec. III.

For half-integer S, the stability border of the paramagnetic region is asymptotically limited by the curves $r \tanh(1/2t) = 1$ and $r \tanh(S/t) = 1$. As indicated in Fig. 3, where we show the critical line for $S = \frac{3}{2}$ and $z = 20$, there is no tricritical point. In the infinite-coordination-number limit we obtain the Curie-Weiss results of the following section.

III. EXACT SOLUTION OF THE CURIE-WEISS VERSION OF THE MODEL

The Curie-Weiss version of the mixed-spin model is given by the Hamiltonian

$$H = -(2J/N) \sum_{i \in A} \sum_{j \in B} s_i \sigma_j + D \sum_{i \in A} s_i^2 \ , \tag{3.1}$$

where a spin variable s_i, belonging to sublattice A, interacts with all the spins variables σ_j belonging to sublattice B. As there are $N/2$ spins on each sublattice, we use a factor 2 in the exchange term to give the same ground-state energy as from Eq. (1.1).

The partition function is written as

$$Z = \sum_{\{\sigma\}} \sum_{\{s\}} \exp(-H/K_B T) \ , \tag{3.2}$$

where the sums are over all spin configurations. Performing the first sum over the configurations $\{s\}$, we have

$$Z = \sum_{\{\sigma\}} \left[\sum_S \exp\left[(2J/Nk_B T) \sum_{j \in B} \sigma_j s - Ds^2/k_B T\right]\right]^{N/2} \ , \tag{3.3}$$

where $s = -S, -S+1, \ldots, S-1, S$. Defining a new variable, $m = (2/N) \sum_{j \in B} \sigma_j$, it is easy to rewrite this expression as

$$Z = \sum_m \frac{(N/2)!}{[(N/4)(1-m)]![(N/4)(1+m)!} \times \left[\sum_s \exp(ms/t - ds^2/t)\right]^{N/2} \ , \tag{3.4}$$

where $m = -1, -1+2/N, -1+4/N, \ldots, +1$.

In the thermodynamic limit $N \to \infty$ we have

$$Z = (N/2) \int_{-1}^{+1} dm \, \exp[-(N/2t) g(t,d;m)] \tag{3.5}$$

and

$$\lim_{N \to \infty} [-(2t/N) \ln Z] = g(t,d;m_0) \ , \tag{3.6}$$

where the free energy $g(t,d;m_0)$ corresponds to the minimum of the functional

$$g(t,d;m) = -t \ln 2 + t \int_0^m dm \tanh^{-1} m - t \ln\left[\sum_s \exp(ms/t - ds^2/t)\right] \ . \tag{3.7}$$

The equation of state given by

$$m = \tanh\left[\frac{\sum_s (s/t) \exp(ms/t - ds^2/t)}{\sum_s \exp(ms/t - ds^2/t)}\right] \ , \tag{3.8}$$

displays qualitatively different features for integer and half-integer values of S. Let us consider the typical cases $S=1$ and $\frac{3}{2}$.

For $S=1$, we have $s = -1, 0, +1$. Equation (3.7) is then written as

$$g(t,d;m) = -t \ln 2 + t \int_0^m dm \tanh^{-1} m - t \ln[1 + 2e^{-d/t} \cosh(m/t)] \ , \tag{3.9}$$

from which we have the equation of state

$$m = \tanh\left[\frac{(2/t)e^{-d/t}\sinh(m/t)}{1+2e^{-d/t}\cosh(m/t)}\right] . \tag{3.10}$$

From this equation, we find an expression for the critical line,

$$d = t\ln[2(1-t^2)/t^2] . \tag{3.11}$$

It should be noted that Eq. (3.11) is the limit of Eq. (2.9) for $r \to \infty$, $J \to 0$, with rJ fixed, and with d and t scaled to d/r and t/r, respectively. The tricritical point (TCP) is given by $t_{\mathrm{TCP}} = \sqrt{5}/5$ and $d_{\mathrm{TCP}} = (3\sqrt{5}\ln 2)/5$. Below the tricritical temperature there is a region of coexistence of phases. The border of stability of the ferromagnetic phase is obtained from Eq. (3.10). As we have an explicit expression for the free energy, it is easy to obtain the line of first-order transitions. Also, we have used this form of the free energy to check the Maxwell construction of the preceding section. At $T=0$, from the minima of Eq. (3.9), we have (i) for $0<d<1$, $m=1$ and $g=-1+d$; (ii) for $d>0$, $m=0$ and $g=0$. This leads to a first-order transition at $t=0$ and $d=1$, as shown in Fig. (2b). The same general features of the d-t phase diagram are also obtained for all other integer values of the spin S.

For $S=\frac{3}{2}$, we have the expression

$$g(t,d;m) = -2t\ln 2 + t\int_0^m dm\, \tanh^{-1}m + (d/4t) - \ln[e^{-2d/t}\cosh(3m/2t) + \cosh(m/2t)] \tag{3.12}$$

and

$$m = \tanh\left[\frac{(3/t)e^{-2d/t}\sinh(3m/2t) + (1/t)\sinh(m/2t)}{e^{-2d/t}\cosh(3m/2t) + \cosh(m/2t)}\right] . \tag{3.13}$$

The critical line is given by

$$d = (t/2)\ln[(9-4t^2)/(4t^2-1)] , \tag{3.14}$$

without the existence of a tricritical point. The minima of Eq. (3.12), at $T=0$, yield (i) $m=1$ and $g=d/4-\frac{1}{2}$, for $d>\frac{1}{2}$; (ii) $m=1$ and $g=9d/4-\frac{3}{2}$, for $d<\frac{1}{2}$. As there is no overlap between regions of different phases, the first-order transition is limited to the point $t=0$ with $d=\frac{1}{2}$.

IV. CONCLUSIONS

Along the lines of a previous work for the spin-1 BEG model,[5] we have formulated a mixed-spin Hamiltonian on a Cayley tree as a discrete nonlinear-mapping problem. The stable fixed points of the map are associated with the thermodynamic solutions on a Bethe lattice. For half-integer values of S, the d-t phase diagrams display a simple λ line with an asymptotic behavior corresponding to the spin-$\frac{1}{2}$ Ising limits, $s=\pm\frac{1}{2}$ or $s=\pm S$, for $d\to\infty$. For integer values of S, the phase diagrams are qualitatively different, with a tricritical point for lattices of coordination numbers $z\geq 5$ (at the ground state, for large enough values of the anisotropy d, the spins are in the state $s=0$). Although exact for the Bethe lattice, these results are, at most, another approximation for the physical Bravais lattices. In the limit of infinite coordination number, $z\to\infty$, $J\to 0$, with zJ fixed, we regain the mean-field results of an exact calculation for a Curie-Weiss version of the model.

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