Phase Diagram of a Decorated Ising System*

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The phase diagram of a decorated Ising system is obtained on the basis of the equivalent Ising model. It is shown that various phases arise in different regions of the parameter space.

I. INTRODUCTION

The phase diagrams of simple Ising magnets are well known.[1] In an Ising ferromagnet the phase boundary extends along the zero-magnetic-field ($H=0$) axis for temperatures T below the critical value T_c, while in an Ising antiferromagnet the phase boundary intersects the $H=0$ axis at only one point.

The situation is more complicated in a decorated Ising system which was first introduced by Syozi and Nakano[2] as a model of ferrimagnetism. It has been found that in zero magnetic field the decorated Ising systems may exhibit multiple phase transitions.[3] The study on the effect of a nonzero magnetic field in a decorated system would then be more instructive and interesting. It would reveal, among other things, the nature and the occurrence of the various phases. Although the model is not exactly soluble when $H \neq 0$, it turns out that it is possible to draw useful conclusions on the critical behavior and obtain the phase diagram on a schematic basis. We study this problem in the present paper.

II. TRANSFORMATION OF THE MODEL

Consider a bipartite lattice $\mathcal{L}$ of coordination number q with Ising spins located at the N lattice

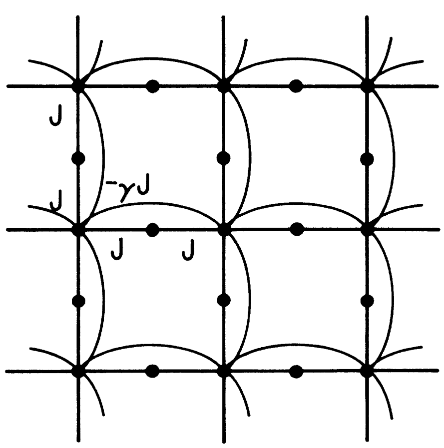

FIG. 1. Decorated Ising lattice on a square lattice ($q=4$).

sites and also on the $\frac{1}{2}qN$ lattice edges as "decorated" spins. Each spin at the lattice sites of $\mathcal{L}$, the site spin, interacts with the q-nearest-site spins with strength $-\gamma J$ and also with the q-nearest decorated spins with strength J. The interaction for a square lattice ($q=4$), for example, is shown in Fig. 1. The Hamiltonian then reads

$$\mathcal{H} = \sum_{\langle ij \rangle} \mathcal{H}_{ij} - mH \sum_i{}' \sigma_i \qquad (1)$$

where m is the magnet moment per spin, σ_i is the spin at the ith lattice site of $\mathcal{L}$, and

$$\mathcal{H}_{ij} = -\gamma J \sigma_i \sigma_j + J\sigma_{ij}(\sigma_i + \sigma_j) - mH\sigma_{ij} \qquad (2)$$

denotes the Hamiltonian of the nearest-neighboring pair $\langle ij \rangle$, including the respective decorated spin σ_{ij}.

The analysis of this model is based on the transformation theory of the Ising models.[4] The idea is to replace the Boltzmann factor involving $\mathcal{H}_{ij}$ by an equivalent one without the decorated spin. Thus we write

$$\sum_{\sigma_{ij}=\pm 1} \exp[\gamma K \sigma_i \sigma_j - K\sigma_{ij}(\sigma_i + \sigma_j) + L\sigma_{ij}] = I \exp[K^* \sigma_i \sigma_j + L'(\sigma_i + \sigma_j)] , \qquad (3)$$

where $K = J/k_B T$, $L = mH/k_B T$. The partition function of the decorated system then becomes

$$Z(\gamma, K, L) = I^{qN/2} Z_{\text{Ising}}(K^*, L^*) \qquad (4)$$

with

$$L^* = qL' + L . \qquad (5)$$

Here $Z_{\text{Ising}}(K^*, L^*)$ is the partition function of an Ising model defined on $\mathcal{L}$ *without* decorated spins. The analytic properties of Z then follow from that of Z_{Ising}.

The solution of (3) is straightforward; we find

$$e^{4K^*} = e^{4\gamma K}[1 + (\sinh 2K/\cosh L)^2] ,$$
$$e^{(4/q)L^*} = e^{(4/q)L} \cosh(2K - L)/\cosh(2K + L) , \qquad (6)$$
$$I^4 = 16 \cosh^2 L \cosh(2K - L)\cosh(2K + L) .$$

It is useful to recall here the phase diagram of a simple Ising system, i.e., that given by $Z_{\text{Ising}}(K^*, L^*)$. As shown in Fig. 2, in the ferromagnetic

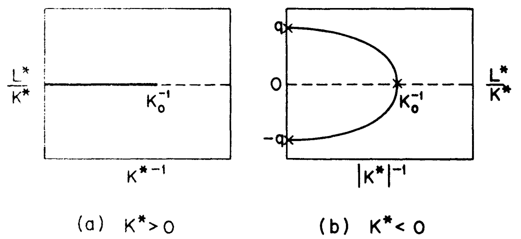

FIG. 2. Phase diagram of simple Ising systems: (a) ferromagnet, (b) antiferromagnet.

case the phase boundary is $L^*=0$, $K^*>K_0$, where[1]

$$\begin{aligned} K_0 &= 0.4407 \quad (\text{square lattice, } q=4) \\ &= 0.2217 \quad (\text{sc lattice, } q=6) \\ &= 0.1575 \quad (\text{bcc lattice, } q=8) . \end{aligned} \tag{7}$$

Across this boundary the first derivative $\partial Z_{\text{Ising}}/\partial L^*$ is discontinuous. In the antiferromagnetic case the phase boundary intersects the $L^*=0$ axis at $K^*=-K_0$. It is also fairly certain that the phase boundary has the two end points[5]

$$K^*=-\infty\,, \quad L^*/K^*=\pm q\ . \tag{8}$$

These three points are denoted by crosses in Fig. 2(b). The phase boundary is shown only schematically in the antiferromagnetic case.

III. PHASE DIAGRAM OF THE DECORATED SYSTEM

The phase diagram of the decorated system in the $(L/K,\ |K|^{-1})$ plane can be derived from that shown in Fig. 2 in conjunction with the transformation (6). We consider the cases $J>0$ and $J<0$ separately.

A. $J>0$ ($K>0$)

The $L^*=0$ axis in Fig. 2 is mapped into the $L=0$ axis and also the curve

$$e^{(4/q)L}=\cosh(2K+L)/\cosh(2K-L)\ , \quad L\neq 0 \tag{9}$$

shown in Fig. 3. The procedure is then to compute K^* along these images. The portion of the image

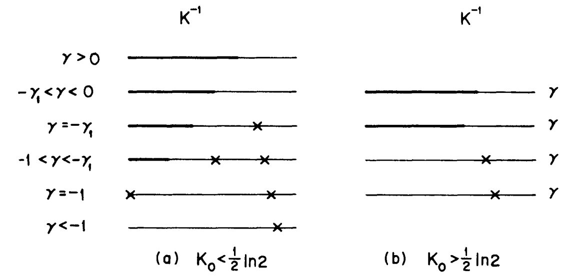

FIG. 4. $L=0$ axis for $K>0$. The heavy line segment denotes a first-order phase boundary and the crosses denote the intersection of a phase boundary.

with $K^*\geq K_0$ and $K^*=-K_0$ are identified as, respectively, a first-order phase boundary and an intersecting point of the phase boundary.

First along the axis $L=0$ we have directly from (6)

$$K^*=\gamma K+\tfrac{1}{2}\ln\cosh 2K\ . \tag{10}$$

Simple analysis then yields the result shown in Fig. 4.[6] Here the heavy line segment denotes the first-order boundary which disappears for $\gamma\leq -1$. The crosses denote the points at which the phase boundary intersects the $L=0$ axis. For $K_0<\frac{1}{2}\ln 2=0.346\,57\ldots$ (the sc and bcc lattices) there are three transition points in the range $-1<\gamma<-\gamma_1$. Here γ_1 is the positive solution of

$$(1+\gamma_1)\ln(1+\gamma_1)+(1-\gamma_1)\ln(1-\gamma_1)=4K_0\,. \tag{11}$$

Thus we find

$$\begin{aligned} \gamma_1 &= 0.8630 \quad \text{sc lattice} \\ &= 0.7485 \quad \text{bcc lattice.} \end{aligned} \tag{12}$$

For $K_0>0.346\,57\ldots$ (the square lattice) at most two transition points occur along $L=0$.

Next along the curve (9) we compute K^* by combining (9) with the first expression in (6). After some algebra the result leads to

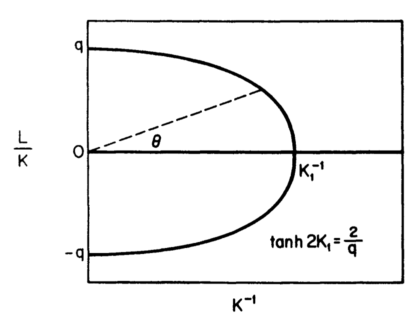

FIG. 3. Image of $L^*=0$ for $K>0$. The equation of the curve is given by (9).

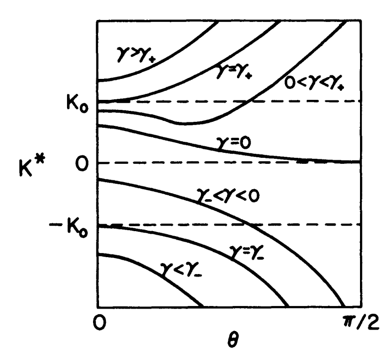

FIG. 5. Plot of $K^*(\gamma,\ \theta)$ given by (13).

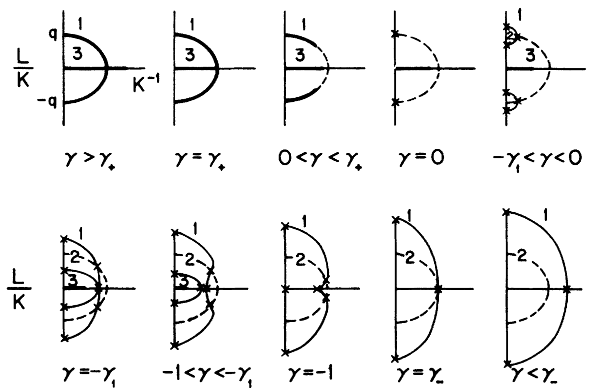

FIG. 6. Phase diagram (schematic) of the decorated system for $J>0$ and $K_0<\frac{1}{2}\ln 2$ (sc and bcc lattices).

$$K^*(\gamma,\theta)=(\gamma+1)\,u(\tan\theta)+(\gamma-1)\,v(\tan\theta) \tag{13}$$

where

$$u(L)=\tfrac{1}{4}\ln\left(\frac{\sinh L}{\sinh(1-2/q)L}\right),\quad v(L)=\tfrac{1}{4}\ln\left(\frac{\sinh(1+2/q)L}{\sinh L}\right)$$

and θ is the angle shown in Fig. 3. Using the inequality $v'(L)>u'(L)>0$, which can be proved by observing that $x\coth x$ is convex and increasing in x, it can be established that $K^*(\gamma,\theta)$ is increasing in θ for $\gamma\geq 1$, decreasing in θ for $\gamma\leq 0$, and $K^*(\gamma,0)$ is decreasing in γ. From these results the dependence of K^* on θ and γ can be easily obtained. The result is exhibited in Fig. 5 where we have defined

$$\gamma_\pm=\frac{\pm 4K_0+\ln(1-4/q^2)}{\ln[(q+2)/(q-2)]} \tag{14}$$

such that $K^*(\gamma_\pm,0)=\pm K_0$. The specific values of $\gamma_\pm$ are computed as

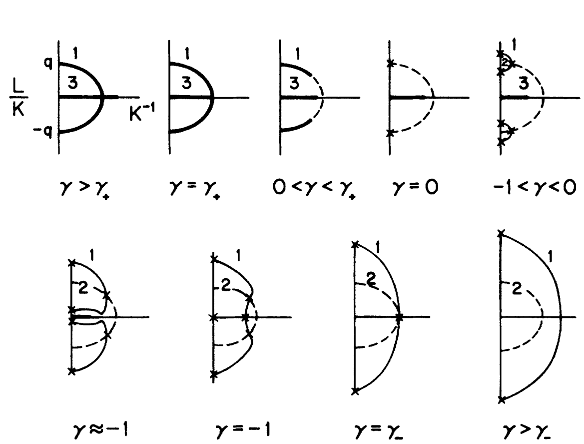

FIG. 7. Phase diagram (schematic) of the decorated system for $J>0$ and $K_0>\frac{1}{2}\ln 2$ (square lattice).

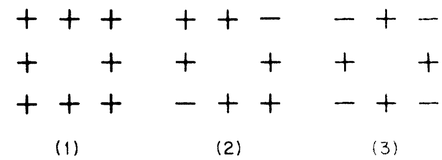

FIG. 8. Three ordered states for $mH>0$: (1) ferromagnetic (or paramagnetic), (2) antiferromagnetic, (3) ferrimagnetic.

$$\begin{aligned} \gamma_+ &= 1.343\,, & \gamma_- &= -1.866 & &\text{square lattice}\,,\\ &= 1.109\,, & &= -1.449 & &\text{sc lattice}\,,\\ &= 1.107\,, & &= -1.359 & &\text{bcc lattice.} \end{aligned} \tag{15}$$

It is observed from Fig. 5 that a first-order boundary extends along the curve (9) completely (for $\gamma\geq\gamma_+$), partially (for $0<\gamma<\gamma_+$), or does not exist ($\gamma\leq 0$). Another phase boundary intersects with (9) for γ in the range $\gamma_-<\gamma<0$. The transition along this boundary will be of the same nature as in a simple Ising antiferromagnet. These features are exhibited in Figs. 6 and 7.

To complete the description of the phase diagram we now map the end points (8). The image points are found to be

$$\begin{aligned} &K=\infty\,,\\ &|L/K|=(1\pm\gamma)q \qquad -1<\gamma<0\,,\\ &\qquad\;\;=(1+\gamma)q\,, \quad \gamma<-1\,. \end{aligned} \tag{16}$$

These points are also denoted by crosses in Figs. 6 and 7. Combining these results with that of Fig. 4, it is now possible to complete the schematic phase diagrams for the decorated system. These diagrams are presented in Figs. 6 and 7 for the cases $K_0<\frac{1}{2}\ln 2$ (sc and bcc lattices) and $K_0>\frac{1}{2}\ln 2$ (square lattice) separately. The curve along which the first-order boundary (the thick curve) extends is given by (9) which does not depend on the value of γ. In both figures the first-order boundary extends far out along the $L=0$ axis for large positive γ so that the system behaves like a simple Ising ferromagnet. For large negative γ (<-1), the phase diagrams are similar to that of a simple

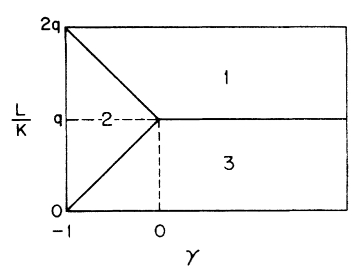

FIG. 9. Ground state for $K>0$, $mH>0$; E_i ($i=1, 2, 3$) is the lowest in the ith region.

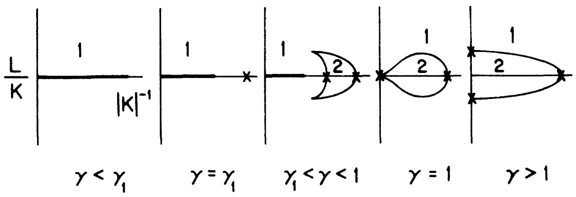

FIG. 10. Phase diagram (schematic) of the decorated system for $J<0$ and $K_0<\frac{1}{2}\ln 2$ (sc and bcc lattices).

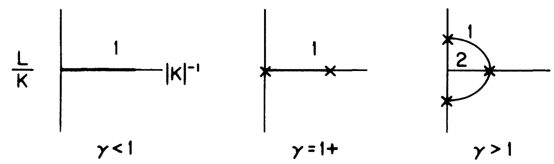

FIG. 11. Phase diagram (schematic) of the decorated system for $J<0$ and $K_0>\frac{1}{2}\ln 2$ (square lattice).

Ising antiferromagnet. While these extreme behaviors are expected, our result leads to the interesting details of the changeover ocurring between these two limits.

The nature of the phases 1, 2, and 3 in Figs. 6 and 7 can be found by examining the ground state energy at $K^{-1}=0$. For $mH>0$ a unit cell of the three ordered states are shown in Fig. 8. Comparing their energies

$$\begin{aligned} E_1 &= N[-\tfrac{1}{2}q\gamma J + qJ - (1+\tfrac{1}{2}q)mH] \,, \\ E_2 &= N[\tfrac{1}{2}q\gamma J - \tfrac{1}{2}qmH] \,, \\ E_3 &= N[-\tfrac{1}{2}q\gamma J - qJ + (1-\tfrac{1}{2}q)mH] \,, \end{aligned} \tag{17}$$

we find the ground state as indicated in Fig. 9 ($E_1<E_2$, E_3 in region 1, etc.). The boundaries in Fig. 9 agree with that in Figs. 6 and 7. It follows then the nature of the various phases in Figs. 6 and 7 are as indicated, i.e., ferromagnetic (or paramagnetic) in region 1, antiferromagnetic in region 2 and ferrimagnetic in region 3.

B. $J<0$ ($K<0$)

The case $J<0$ is simpler because for $K<0$ $L^*=0$ maps only into $L=0$. Furthermore the end points (8) map into

$$\begin{aligned} K &= \infty \,, \\ |L/K| &= (\gamma-1)q \quad \text{for } \gamma>1 \text{ only.} \end{aligned} \tag{18}$$

On the other hand as before three phase transitions occur in zero field when $K_0<0.34657\ldots$ and $\gamma_1<\gamma<1$. The resulting schematic phase diagrams are shown in Figs. 10 and 11. Note that because the mapping of (8) → (18) is valid for $\gamma>1$ only, the shape of the phase diagram is less certain than in the case of $J>0$.

IV. SUMMARY

We have obtained the schematic phase diagram for a decorated Ising system. For $J>0$ and $\gamma>0$ we find ferro- (para-) and ferrimagnetic regions separated by first-order boundaries. The occurrence of a first-order boundary for $H\neq 0$ is reminiscent to the first-order transition found to exist in an Ising model with competing interactions.[7] For $J>0$ and $\gamma<0$, the antiferromagnetic region appears and grows with $|\gamma|$. The detailed behavior is different for two- and three-dimensional models and is shown, respectively, in Figs. 7 and 6. For $J>0$ and $\gamma\leq -1$ the ferrimagnetic region disappear completely and the phase diagram is similar to that of a single Ising antiferromagnetic.

For $J<0$ the first-order boundary occurs only along the $H=0$ axis and for $\gamma\leq 1$. The ferrimagnetic phase does not appear at all and, for $\gamma>1$, the phase diagram is similar to that of a simple Ising antiferromagnet.

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[1]See, for example, M. E. Fisher, Rep. Prog. Phys. **30**, 615 (1967); and Fig. 2, introduced later in this paper.
[2]I. Syozi and H. Nakano, Prog. Theor. Phys. **13**, 69 (1955).
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[6]See H. Nakano, in Ref. 2.
[7]D. P. Landau, Phys. Rev. Lett. **28**, 449 (1972), and the references contained therein.