Magnetization process of a disordered phase in a mixed-bond spin-1 Ising ferromagnet

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The magnetization process of a disordered phase (or the $S_i^z=0$ state) in a mixed-bond spin-1 Ising ferromagnet on a honeycomb lattice is investigated by use of the effective-field theory with correlations. We find that it exhibits a characteristic phenomenon similar to, but with an important difference from, that of the standard Blume-Capel model.

I. INTRODUCTION

In the past few decades the magnetic properties of binary random-substitutional alloys have been intensively investigated from bond and site perspectives. The bond model considers all lattice sites to be equivalent, but the interaction energy between each pair of adjacent sites is randomly assigned one set of possible values. In the site model the lattice sites are randomly occupied by two different species of magnetic ions, and the interaction between two ions is determined entirely by the species of these ions. However, most works have not discussed the effects of negative crystal-field interactions on the magnetic properties.

On the other hand, the spin-1 Ising model with a negative crystal-field interaction is described by the following Hamiltonian:

$$H=-\sum_{(i,j)}J_{ij}S_i^zS_j^z+D\sum_i(S_i^z)^2\ , \tag{1}$$

where the first summation runs over all pairs of nearest neighbors and J_{ij} and D ($D>0$) are respectively the exchange interaction and the crystal-field parameter. The model Hamiltonian, which is often called the Blume-Capel model,[1,2] has been studied in some detail, using a variety of methods.[1-8] It is well known in the system that there exists a tricritical point in the phase diagram at which the phase transition changes from second order to first order, when the crystal-field interaction takes on a large negative value.

The purpose of this work is to investigate the effects of crystal-field interaction on transition temperature and the magnetization process in a mixed-bond Ising ferromagnet by the use of the effective-field theory with correlations (EFT).[3] Accordingly, the exchange interaction J_{ij} in (1) is assumed to be randomly distributed by an independent probability distribution function $p(J_{ij})$. In Sec. II, we briefly present the basic framework of the EFT in a honeycomb lattice. In Sec. III, a phase diagram of the mixed-bond Ising ferromagnet with a coordination number $z=3$ is obtained for zero field. A disordered phase (or the $S_i^z=0$ state) is found in a concentration region of mixed bonds, when the value of D becomes large. In Sec. IV, the magnetization process in the disordered phase is examined. We find some interesting phenomena for the field dependences of magnetization and quadrupolar moment in the disordered phase.

II. FORMULATION

We consider a mixed-bond ferromagnetic Ising system in a honeycomb lattice. The Hamiltonian is given by

$$H=-\sum_{(i,j)}J_{ij}S_i^zS_j^z+D\sum_i(S_i^z)^2-H\sum_i S_i^z\ , \tag{2}$$

where H is the applied magnetic field and S_i^z can take the values, ±1 and 0. D is taken to be positive.

As discussed in the previous work,[3] within the EFT, the averaged magnetization for the honeycomb lattice with $z=3$ is given by

$$\begin{aligned}m&=\langle\langle S_i^z\rangle\rangle_r\\&=[q\langle\cosh(J_{ij}\nabla)\rangle_r+m\langle\sinh(J_{ij}\nabla)\rangle_r\\&\quad+1-q]^3F(x+h)|_{x=0}\end{aligned} \tag{3}$$

with

$$F(x)=\frac{2\sinh(\beta x)}{2\cosh(\beta x)+\exp(\beta D)}\ , \tag{4}$$

where $\beta=1/k_BT$, $h=\beta H$, and $\nabla=\partial/\partial x$ is the differential operator. $\langle\cdots\rangle_r$ denotes the random-bond average for $p(J_{ij})$. The parameter q is defined by $q=\langle\langle(S_i^z)^2\rangle\rangle_r$. The quadrupolar moment is given by

$$\begin{aligned}q&=[q\langle\cosh(J_{ij}\nabla)\rangle_r+m\langle\sinh(J_{ij}\nabla)\rangle_r\\&\quad+1-q]^3G(x+h)|_{x=0}\end{aligned} \tag{5}$$

with

$$G(x)=\frac{2\cosh(\beta x)}{2\cosh(\beta x)+\exp(\beta D)} . \quad (6)$$

By expanding the right-hand side of (3) and (5), they can be described as

$$m = A_1(q)+3A_2(q)m+3A_3(q)m^2+A_4(q)m^3 , \quad (7)$$

$$q = B_1(q)+3B_2(q)m+3B_3(q)m^2+B_4(q)m^3 , \quad (8)$$

with

$$\begin{aligned} A_1(q)&=q^3K_1+3q^2(1-q)K_2+3q(1-q)^2K_3 \\ &\quad +(1-q)^3K_4 , \\ A_2(q)&=q^2K_5+2q(1-q)K_6+(1-q)^2K_7 , \\ A_3(q)&=qK_8+(1-q)K_9 , \\ A_4(q)&=K_{10} , \end{aligned} \quad (9)$$

where $B_i(q)$ $(i=1-4)$ can be given by replacing the coefficients K_i in (9) with L_i $(i=1-10)$. The coefficients K_i $(i=1-10)$ and L_i $(i=1-10)$ are given in the Appendix. For $H=0$, we can easily prove that $A_1(q)$, $A_3(q)$, $B_2(q)$, and $B_4(q)$ reduce to zero, by using that $\phi_{\text{even}}(\nabla)F(x)|_{x=0}=0$ and $\phi_{\text{odd}}(\nabla)G(x)|_{x=0}=0$, which is valid for any even and odd functions $\phi(\nabla)$.

For $H=0$, as discussed in the previous work,[3] in the vicinity of the second-order phase transition line, the averaged magnetization can be given by

$$m^2=\frac{1-a}{b} . \quad (10)$$

The second-order transition line can be determined by

$$a=1 \quad (11)$$

in the expression (10). In the vicinity of the second-order phase transition line, the right-hand side of (10) must be positive. If this is not the case, the transition is of the first order, and hence the point at which

$$a=1 \text{ and } b=0 \quad (12)$$

is the tricritical point. Here, the expressions of a and b for the present system can be easily derived by using the previous framework.[3]

III. PHASE DIAGRAM FOR $H=0$

For the latter discussions, let us show a phase diagram for the mixed-bond ferromagnetic Ising ferromagnet where the probability distribution function $p(J_{ij})$ is given by

$$p(J_{ij})=p\delta(J_{ij}-J_1)+(1-p)\delta(J_{ij}-J_2) . \quad (13)$$

We assume that $J_1>J_2>0$ without loss of generality and introduce a parameter

$$\alpha=\frac{J_2}{J_1} . \quad (14)$$

By solving the relations (11) and (12) numerically, the phase diagram of the system with $z=3$ and $\alpha=0.5$ is depicted in Fig. 1, changing the value of D. For the system with $p=1.0$ (or the standard Blume-Capel model), it is well known that the transition temperature at $D=0$ is given by, within the EFT,

$$\frac{k_BT_c}{J_1}=1.5191 \quad (15)$$

and the tricritical point is obtained at the values $(k_BT_t=0.68J_1$ and $D_t=1.42J_1)$. These values can be compared with those obtained from other approximate methods (see Tables I and II in Ref. 6). Furthermore, from the energetic point of view, at $T=0$ K the system at $p=1.0$ may exhibit two equivalent ferromagnetic ground states $(S_i^z=\pm1)$ for $D/J_1<1.5$ and one ground state $(S_i^z=0)$ for $D/J_1>1.5$.

Since $J_2=0.5J_1$, the transition temperature T_c and the tricritical value D_t for the system with $p=0$ in Fig. 1 should be given by the half values of T_c and D_t at $p=1.0$. The system at $p=0$ is in the $S_i^z=0$ state, when the value of D becomes larger than $D=0.75J_1$. In fact, the figure shows that the conditions are really satisfied. For the curves with $D=0.8J_1$ and J_1, there are no solutions satisfying the conditions (11) and (12) in the regions near $p=0.0$; it means that $T_c=0$ in the region and the ground state is the $S_i^z=0$ state.

In Fig. 1 the solid circles denote the tricritical point. The dashed line parts express the first-order phase transition, below which the system may be in the $S_i^z=0$ state. In the figure, for the curve with $D=0.0$ (or $D=0.5J$) the effect of mixed bond on the phase diagram exhibits a weak downward curvature instead of the linear interpolation (dot-dashed curve) between $p=1$ and $p=0$. This is

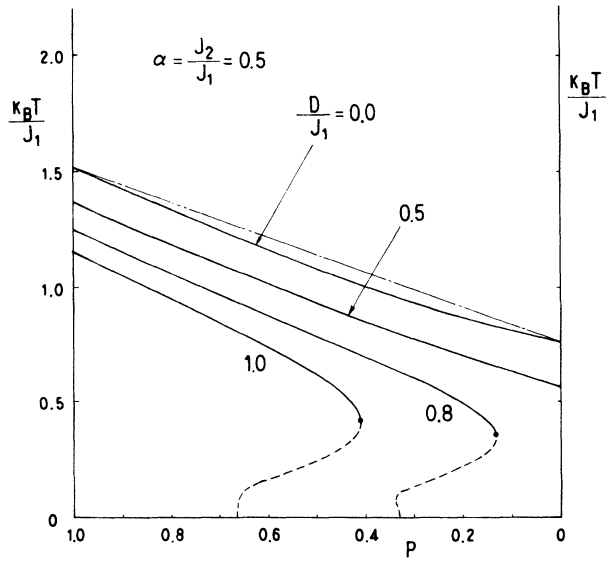

FIG. 1. The change of T_c vs p for the mixed-bond spin-1 Ising ferromagnet with $z=3$ and $\alpha=0.5$, when the value of D is changed. The solid circles and dashed lines express the tricritical points and the first-order transition, respectively.

consistent with some general discussions of phase diagram for quenched random-bond systems with $D=0$;[9,10] the phase diagram should show a weak downward curvature.[11]

IV. MAGNETIZATION PROCESS

As shown in Fig. 1, when the value of D takes a large value, the transition temperature reduces to zero in the region of p near $p=0$ (see the curves of $D=0.8J_1$ and $D=J_1$). In order to examine the physical content of the disordered phases, the magnetization process is examined in this section, especially by solving the coupled equations (7) and (8) numerically for the systems with $p=0$ and $p=0.2$.

Figure 2(a) shows the magnetization process for the system with $p=0.0$, $D=J_1$, and $\alpha=0.5$. As noted in Sec. III, the system is in the $S_i^z=0$ state at $T=0$ K, since $D=J_1$ is larger than the critical value $D=0.75J_1$. As is seen from the figure, m at $k_BT=0.05J_1$ expresses a first-order transition at a critical field H_c ($H_c\cong 0.25J_1$) from $m=q=0$ to $m=q=1$. The gap width Δm where the value of m becomes discontinuous at $H_c/J_1=h^*$ decreases with the increases of T. In Fig. 2(b), the thermal variations of Δm and h^* for the system are also depicted. Δm decreases rapidly to zero, when the value of T becomes larger than $k_BT=0.15J_1$. By contrast, the value of h^* is nearly fixed at $h^*\cong 0.25$. These behaviors are very similar to those usually found in metamagnets. The same phenomena can be also obtained for the system with $p=1.0$ (or the standard Blume-Capel model), when the value of D becomes larger than $D=1.5J_1$.

On the other hand, the magnetization process of the system with $p=0.2$, $\alpha=0.5$, and $D=J_1$ (being also in the $S_i^z=0$ state) is shown in Fig. 3(a), changing the value of T. At $k_BT=0.05J_1$, the magnetization (or the quadrupolar moment) changes discontinuously from $m=0$ (or $q=0$) to $m=1$ (or $q=1$) at the critical field h^* ($h^*\cong 0.06$). In contrast to Fig. 2(a), the critical field h^* exhibiting the discontinuity of m clearly depends on the value of T as well as p. In Fig. 3(b), the variation of h^* versus p is depicted at the fixed temperature $k_BT=0.05J_1$. As is seen from the figure, the value of h^* rapidly reduces to zero, when the value of p increases from $p=0.0$.

Comparing Fig. 3(a) with Fig. 2(a), we find that the magnetization process in the $S_i^z=0$ state (or the disordered phase) of the mixed-bond Ising ferromagnet is different from that for $p=0$ (or $p=1$). In order to show the difference more clearly, the thermal variations of Δm and h^* for the system with $p=0.2$, $\alpha=0.5$, and $D=J_1$ are depicted in Fig. 4. Δm also decreases rapidly to zero, when the value of T becomes larger than $k_BT=0.15J_1$. However, the behavior of h^* in the system is completely different from that of Fig. 2(b); For the value of T larger than $k_BT=0.2J_1$, h^* takes the constant value ($h^*\cong 0.13$). With decreasing T, on the other hand, h^*

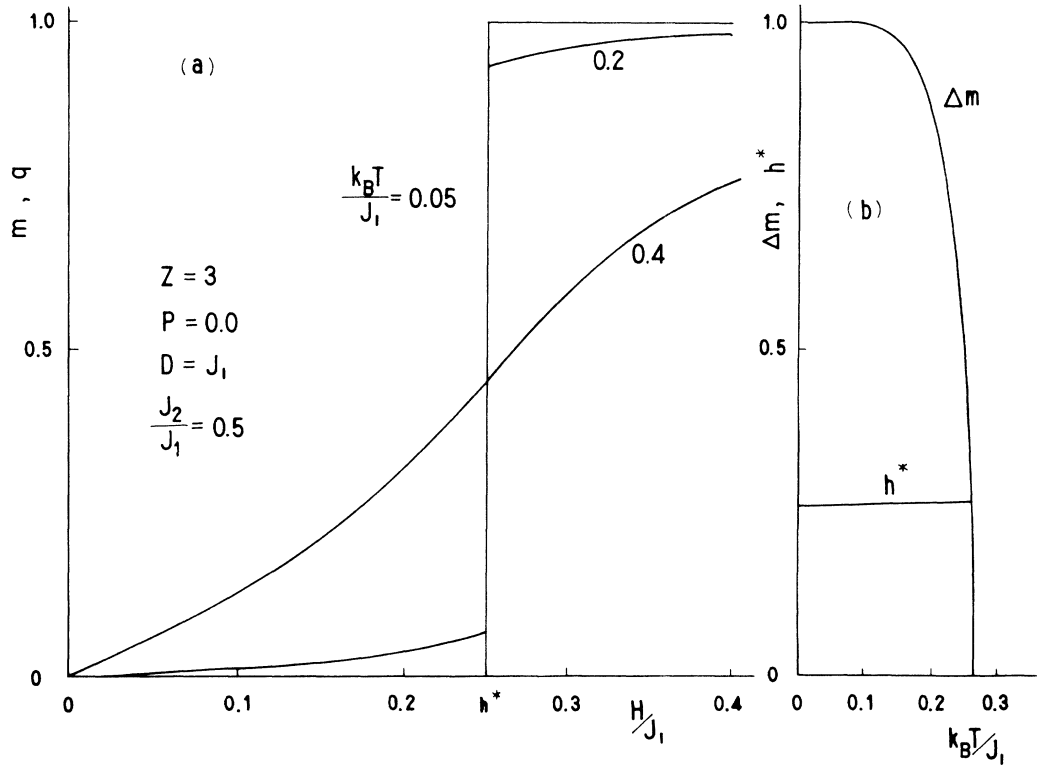

FIG. 2. (a) Magnetization processes in the $S_i^z=0$ state of the system with $p=0$, $\alpha=0.5$, and $D=J_1$, when T is changed as $k_BT=0.05J_1$, $0.2J_1$, and $0.4J_1$. (b) Temperature dependence of h^* and Δm at the point where magnetization exhibits a discontinuity.

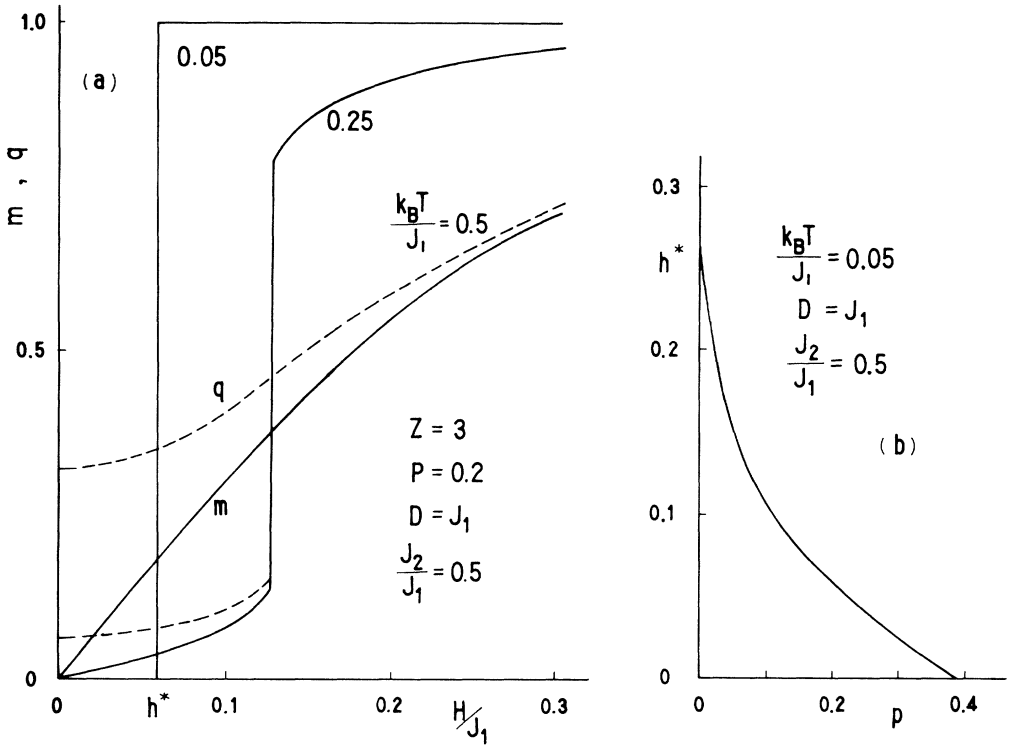

FIG. 3. (a) Magnetization processes in the disordered phase (the region with $T_c=0$ in Fig. 1) of the system with $p=0.2$, $\alpha=0.5$, and $D=J_1$, when T is changed as $k_BT=0.05J_1$, $0.25J_1$, and $0.5J_1$. The dashed lines express the field dependences of q. (b) The change of h^* vs p for the system of Fig. 3(a) at a fixed temperature $k_BT=0.05J_1$.

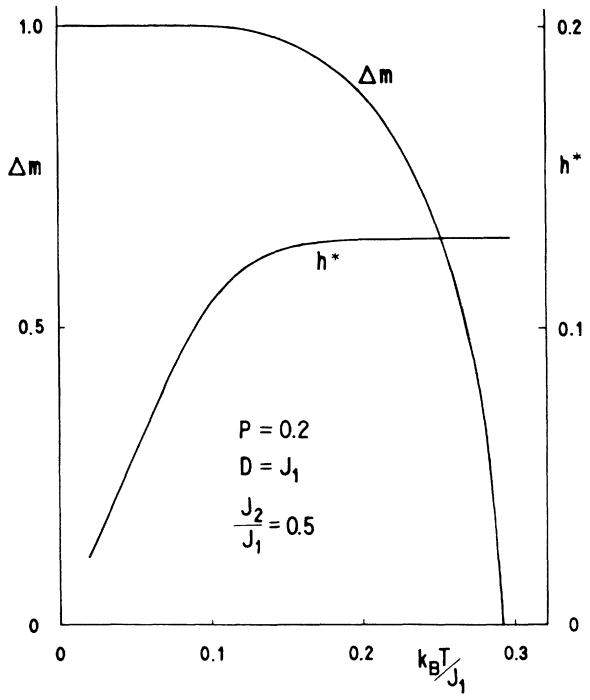

FIG. 4. The temperature dependences of Δm and h^* for the system with $p=0.2$, $\alpha=0.5$, and $D=J_1$.

decreases almost linearly with T in the region $(0.02J_1 < k_BT < 0.08J_1)$. When T becomes smaller than $0.02J_1$, it is difficult to determine the value of h^* because of the large numerical errors, although it seems to go to zero at $T=0$ K. Thus, the magnetization process in the disordered phase of the mixed-bond spin-1 Ising ferromagnet with $p=0.2$ exhibits a characteristic behavior. As is seen from Figs. 3(a) and 4, it is different from that of $p=0.0$ (or $p=1.0$) shown in Fig. 2.

V. CONCLUSIONS

In this work, we have examined the magnetization process of a disordered phase in a mixed-bond spin-1 Ising ferromagnet with the use of the effective-field theory with correlations. We find that it exhibits characteristic phenomena similar to, but with an important difference from, that of the Blume-Capel model for $p=0.0$ and $p=1.0$, as shown in Figs. 2, 3, and 4. As far as we know, such behaviors have not been discussed, although the results in Fig. 2 are very similar to those usually found in metamagnets.

In this work, the effective-field theory with correlations has been applied to the present problem. It is based on the decoupling approximation, namely

$$\langle S_j^z (S_k^z)^2 \ldots S_l^z \rangle \cong \langle S_j^z \rangle \langle (S_k^z)^2 \rangle \ldots \langle S_l^z \rangle$$

for $j \neq k \neq \ldots = l$, which appears in the expression of an

exact Ising spin identity.[3,6] Because of this fact, the present framework essentially corresponds to the approximation of Zernike theory in the spin-$\frac{1}{2}$ Ising model.[12] Very recently, Kaneyoshi[13] has developed a new theory of spin-1 Ising systems in which the multispin correlation functions can be exactly treated when the concept of correlated effective-field introduced by Lines[14] is applied. Comparing the results of both theories, the present framework gives reasonable results to the Blume-Capel model and is superior to the standard mean-field theory.

Finally, for crystalline alloys there is surprisingly little experimental data to compare with the present results. We hope that this work will stimulate further experimental and theoretical work on the magnetic properties of alloys.

APPENDIX

The coefficients K_i $(i=1-10)$ in (9) are given by

$$
\begin{aligned}
K_1&=[\langle\cosh(J_{ij}\nabla)\rangle_r]^3F(x+h)|_{x=0}\ ,\\
K_2&=[\langle\cosh(J_{ij}\nabla)\rangle_r]^2F(x+h)|_{x=0}\ ,\\
K_3&=\langle\cosh(J_{ij}\nabla)\rangle_rF(x+h)|_{x=0}\ ,\\
K_4&=F(h)\ ,\\
K_5&=\langle\sinh(J_{ij}\nabla)\rangle_r[\langle\cosh(J_{ij}\nabla)\rangle_r]^2F(x+h)|_{x=0}\ ,\\
K_6&=\langle\sinh(J_{ij}\nabla)\rangle_r\langle\cosh(J_{ij}\nabla)\rangle_rF(x+h)|_{x=0}\ ,\\
K_7&=\langle\sinh(J_{ij}\nabla)\rangle_rF(x+h)|_{x=0}\ ,\\
K_8&=[\langle\sinh(J_{ij\nabla})\rangle_r]^2\langle\cosh(J_{ij}\nabla)\rangle_rF(x+h)|_{x=0}\ ,\\
K_9&=[\langle\sinh(J_{ij}\nabla)\rangle_r]^2F(x+h)|_{x=0}\ ,\\
K_{10}&=[\langle\sinh(J_{ij}\nabla)\rangle_r]^3F(x+h)|_{x=0}\ ,
\end{aligned}
\tag{A1}
$$

with

$$
\begin{aligned}
\langle\cosh(J_{ij}\nabla)\rangle_r&=p\cosh(J_1\nabla)+(1-p)\cosh(J_2\nabla)\\
\langle\sinh(J_{ij}\nabla)\rangle_r&=p\sinh(J_1\nabla)+(1-p)\sinh(J_2\nabla)\ ,
\end{aligned}
\tag{A2}
$$

where the coefficients can be easily calculated by using a mathematical relation $e^{\alpha\nabla}f(x)=f(x+\alpha)$.

The coefficients L_i $(i=1-10)$ in B_i are given by replacing the function $F(x)$ in (A1) with the function $G(x)$.

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