Phase diagrams of a diluted Ising thin ferromagnetic film in a transverse field

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Phase diagrams for a diluted Ising thin ferromagnetic film in a transverse field are investigated and calculated within the framework of the effective-field theory with correlations. The results show that a lot of interesting properties exist in this system.

From both the experimental and theoretical points of view, the Ising magnetic thin film is very important. It can be taken as a model used to investigate the magnetic size effects and can be regarded as a quasi-two-dimensional system when its thickness is smaller. The magnetic properties of the film will approach those of the corresponding semi-infinite system when its thickness is very big. The semi-infinite system, as we know, is an example by which one can investigate magnetic surface properties, and some especially interesting results were obtained by using different methods.[1–4] Magnetic ordering, for instance, can first appear on the surface as long as the coupling constant between magnetic atoms on the surface is strong enough. For the Ising thin film with a limited thickness, as some authors have discussed,[5,6] its properties are obviously different from those of the corresponding bulk and semi-infinite systems when its thickness is very small. On the other hand, there is a class of magnetic systems which are diluted magnetic alloys. The magnetic atoms on some lattice sites, probably, are randomly replaced by nonmagnetic atoms. Generally speaking, the magnetic properties of the diluted magnetic systems may be obviously different from those of the corresponding pure systems. It has been known that a lot of new physical phenomena can appear in these magnetic systems. Kaneyoshi and his cooperators[2] investigated a semi-infinite system with surface dilution by means of the effective-field theory with correlations. Qing Hong,[7] Benyoussef and his collaborators[8] studied the diluted semi-infinite system using the mean-field theory and renormalization-group method, respectively. Ferchmin and his colleagues[9] have calculated a diluted Ising film and predicted that the surface magnetic phase can appear when the concentration of magnetic atoms on the surface is high enough.

In addition, the transverse Ising model first proposed by de Gennes[10] is of a very significant one. This model has been used to study various systems.[11–13] Recently one of the authors of this paper, Wang and his colleagues[14] have investigated and calculated the magnetic properties and phase diagrams of transverse Ising films. In this paper we consider a diluted Ising film with $s=\frac{1}{2}$ as our model system, with a simple-cubic structure and two (001) free surfaces, in a transverse magnetic field. For the sake of simplicity we assume that the concentration of magnetic atoms of the film and the transverse field on the atomic layers are homogeneous. The film is composed of n atomic layers parallel to the surfaces. The Hamiltonian of the system in the presence of a transverse field can be written as

$$H=-\tfrac{1}{2}\sum_{ij}J_{ij}S_i^zS_j^z\zeta_i\zeta_j-\sum_i F_iS_i^x\zeta_i \tag{1}$$

where the nearest-neighbor coupling constant J_{ij} is equal to J_s if sites i and j are on the surfaces, and to J otherwise; S_i^x and S_i^z are the components of a spin-$\frac{1}{2}$ operator, F_i represent a transverse field on the ith site and the sum extends over all lattice points of the system. ζ_i is the occupation number on the lattice site i, $\zeta_i=1$ if the lattice site i is occupied by a magnetic atom and zero otherwise. According to Eq. (1) and the effective-field approximation with correlations,[15] the average value of any atomic spin in the ith atomic plane parallel to the surfaces is given by

$$\langle a_i^z\rangle=\left\langle\left[\sum_j J_{ij}a_j^z\zeta_j/H_i\right]\tanh(1/4\beta H_i)\right\rangle , \tag{2}$$

where $\langle a_i^z\rangle=2\langle s_i^z\rangle$, $\beta=1/KT$, $\langle\cdots\rangle$ denotes the thermal average, and

$$H_i=\left[(2F_i)^2+\left[\sum_j J_{ij}a_j^z\zeta_j\right]^2\right]^{1/2} . \tag{3}$$

Using the differential operator method, we have

$$\sigma_i=\langle a_i^z\rangle=\left\langle\exp\left[D\sum_j\beta J_{ij}a_j^z\zeta_j\right]\right\rangle G(x)_{x=0} , \tag{4}$$

where $D=\partial/\partial x$ is a differential operator. Considering the transverse field's uniformity, i.e., $F_i=F$, $G_i(x)$ can be expressed as

$$G(x)_i=G(x)=\frac{x}{[4F^2+x^2]^{1/2}}\tanh\{\beta/4[4F^2+x^2]^{1/2}\} . \tag{5}$$

Since magnetic atoms are randomly distributed on lattice sites of the system under consideration, we should further consider the configurational average. The atomic average spin in the ith atomic layer parallel to the surface, thus, can be written as

$$M_i=\langle \zeta_i a_i^z \rangle_r , \tag{6}$$

where $\langle \cdots \rangle_r$ indicates the configurational average.

Using the following approximation,

$$\langle a_i^z a_j^z \cdots a_k^z \rangle = \langle a_i^z \rangle \langle a_j^z \rangle \cdots \langle a_k^z \rangle , \tag{7}$$

$$\langle \zeta_i \zeta_j \cdots \zeta_k \rangle = \langle \zeta_i \rangle \langle \zeta_j \rangle \cdots \langle \zeta_k \rangle , \tag{8}$$

$$\langle\langle \zeta_i a_i^z \rangle\rangle_r = \langle \zeta_i \rangle_r \langle\langle a_i^z \rangle\rangle_r \tag{9}$$

we get

$$M_i = c\prod_j [c\cosh(DJ_{ij}) + M_j \sinh(DJ_{ij}) + (1-c)] G(x)_{x=0} , \tag{10}$$

where $c=\langle \zeta_i \rangle_r$ is the concentration of magnetic atoms in the film. We devote this paper to studying and discussing the critical properties of the film, so only linear terms in the atomic magnetization should be retained when M_i is expanded. As a result, we obtain the following equation:

$$\tilde{A} \begin{bmatrix} M_1 \\ M_2 \\ \vdots \\ M_i \\ \vdots \\ M_{n-1} \\ M_n \end{bmatrix} = 0 . \tag{11}$$

$\tilde{A}$ in Eq. (11) is a $n \times n$ matrix which has nonzero elements as follows:

$$A_{11} = A_{nn} = 4K_1 - 1, \quad A_{12} = A_{nn-1} = K_2 ,$$

$$A_{ii-1} = A_{ii+1} = K_0 , \quad A_{ii} = 4K_0 - 1 \quad (i=2,3,\ldots,n-1) ,$$

where

$$\begin{aligned} K_1 = 4c[&c^4\cosh^3(DJ_s)\sinh(DJ_s)\cosh(DJ) + (1-c)c^3\cosh^3(DJ_s)\sinh(DJ_s) \\ &+3c^3(1-c)\cosh^2(DJ_s)\sinh(DJ_s)\cosh(DJ) + 3(1-c)^2c^2\sinh(DJ_s)\cosh^2(DJ_s) \\ &+3c^2(1-c)^2\cosh(DJ_s)\sinh(DJ_s)\cosh(DJ) + 3c(1-c)^3\cosh(DJ_s)\sinh(DJ_s) \\ &+c(1-c)^3\cosh(DJ)\sinh(DJ_s) + (1-c)^4\sinh(DJ_s)]G(x)_{x=0}, \end{aligned} \tag{12}$$

$$\begin{aligned} K_2 = c[&c^4\sinh(DJ)\cosh^4(DJ_s) + (1-c)^4\sinh(DJ) + 6c^2(1-c)^2\cosh(DJ_s)\sinh(DJ) \\ &+4c^3(1-c)\cosh^3(DJ_s)\sinh(DJ) + 4(1-c)^3c\cosh(DJ_s)\sinh(DJ)]G(x)_{x=0} , \end{aligned} \tag{13}$$

$$\begin{aligned} K_0 = c[&1/2c^5\cosh^4(DJ)\sinh(2DJ) + 5(1-c)^4c\cosh(DJ)\sinh(DJ) \\ &+5c^3(1-c)^2\cosh^2(DJ)\sinh^2(2DJ) + 5(1-c)c^4\sinh(DJ)\cosh^4(DJ) \\ &+5c^2(1-c)^3\sinh(2DJ)\cosh(DJ) + (1-c)^5\sinh(DJ)]G(x)_{x=0} . \end{aligned} \tag{14}$$

The critical properties of the system are determined by

$$|\tilde{A}| = 0 , \tag{15}$$

where $|\tilde{A}|$ represents the determinant of matrix $\tilde{A}$. The relations among the critical temperature (KT_c/J), the concentration of magnetic atoms (c), the transverse field (F), and the surface coupling constants (J_s/J) are, therefore, determined by Eq. (15).

Since the properties of the film approach those of the corresponding semi-infinite system when the film is very thick, we take $n=3$ and 5 here to discuss the critical temperature (KT_c/J) vs the surface coupling constant (J_s/J) for a given concentration and transverse field. For a higher concentration, i.e., $c=0.6$ and a lower concentration, i.e., $c=0.4$, respectively, we present various $KT_c/J - J_s/J$ curves with different values of transverse field in Figs. 1(a) and 1(b). Figure 1(a) corresponds to the film with atomic layer number $n=3$ and the concentration $c=0.4$. The $KT_c/J - J_s/J$ curves for different transverse fields are presented in the figure. The obvious differences from the pure transverse Ising film[14] are for some smaller values of transverse field, with the increase in J_s/J, KT_c/J first increases rapidly and then slowly to the maximum of KT_c/J, after that, it decreases slowly [in the range of Fig. 1(a)]. But for the pure Ising film or transverse Ising film, KT_c/J increases monotonously as J_s/J is increased. For the transverse Ising film with $n=5$, a similar property also exists, but we do not present the corresponding figure here owing to the limitation of space. Figure 1(a) shows that this pattern is held for an ordinary diluted Ising film ($F=0$). In addition, we find that the $KT_c/J - J_s/J$ curves increase monotonously either under the condition of a low concentration (e.g., $c=0.4$) and a strong enough transverse field or under the condition of a weak transverse field (e.g., $F/J=0.3$) and a high enough concentration (e.g., $c=0.6$). This conclusion is from Fig. 1(b). Comparing curve a (or c) with curve b (or d) in Fig. 1(b), we can see that KT_c/J increases more rapidly with the increase in J_s/J for the thinner film. The reason for this point is that the relative importance of the surfaces grows as the film thickness is decreased. In a word, there is no essential difference between the KT_c/J vs J_s/J of the film for a higher concen-

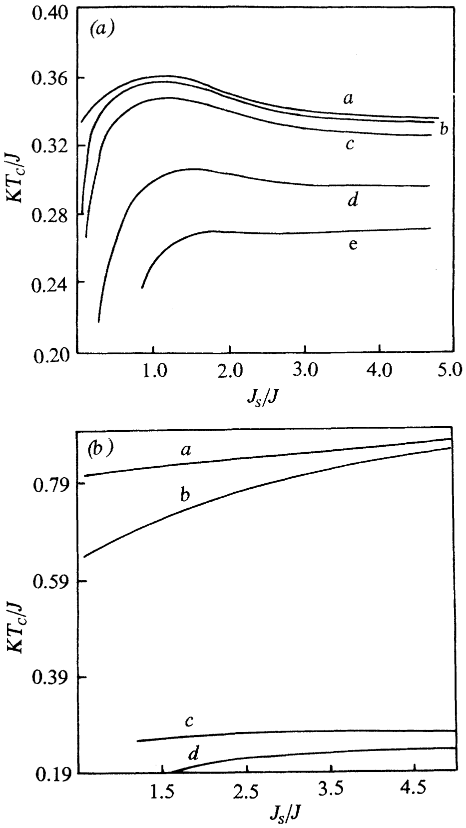

FIG. 1. Critical temperature as a function of surface coupling for different transverse fields and concentrations. (a) For $n=3$ and $c=0.4$, curves a, b, c, d, and e correspond to $F/J=0.0$, 0.1, 0.2, 0.3, and 0.4, respectively. (b) For $c=0.6$ and $F/J=0.3$, curves a and b are related to $n=3$ and 5, respectively; for $c=0.4$, curves c and d correspond to $n=5$ and $F/J=0.75$ and to $n=3$ and $F/J=0.6$, respectively.

tration and those of the pure film. We also calculate and study the curves of the critical temperature (KT_c/J) vs the transverse field (F/J) for various concentrations of magnetic atoms and different coupling constants of the surface. Our results show that for a higher concentration of magnetic atoms (e.g., $c=0.8$) there are no qualitative differences, except quantitative differences, between the $KT_c/J-F/J$ curves of the film and the corresponding curves of the pure transverse Ising film.[14] For a lower concentration of magnetic atoms, however, the qualitative differences appear (see Fig. 2). Figure 2 displays a group of the curves of the critical temperature vs the transverse field for a given concentration ($c=0.4$), the film thickness ($n=3$), and different values of J_s/J. We find that the curves intersect approximately at a point (0.481, 0.274) when $J_s/J>1.20$. It shows that KT_c/J decreases, increases and does not change for $F/J>0.48$, $F/J<0.48$, and $F/J=0.48$, respectively, as J_s/J is enlarged. The similar case also exists for the film with $n=5$.

The relation between the critical temperature and thickness of film, and the relation between the critical temperature and concentration are also very significant.

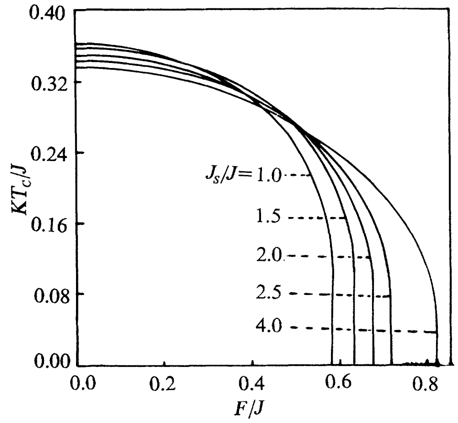

FIG. 2. Critical temperature vs transverse field for $c=0.4$ in the film with $n=3$.

Figure 3 shows KT_c/J vs n (where n is the atomic layer number in the film and represents the thickness of the film). For $c=0.4$ and $F/J=0.5$, the curves a and b correspond to $J_s/J=2.0$ and $J_s/J=1.0$, respectively. These two curves approach to coincidence rapidly with the increase in n. Especially when $n=20$, it can be thought that they approach to the saturation value $KT_c/J=0.485$. This value is also the critical temperature of the corresponding semi-infinite transverse Ising system with the same concentration and in the same transverse field. As compared with curves a and b ($c=0.4$), there is a great quantitative difference between curves a' and b' ($c=0.6$). When n is enlarged, their saturation value is $KT_c/J=0.887$, which is also the critical temperature of the corresponding semi-infinite transverse Ising system under the conditions $F/J=0.5$ and $c=0.6$. From Fig. 3 one can certainly see that the concentration obviously affects KT_c/J. The influence is presented in Fig. 4 where KT_c/J vs c ($n=3$) is shown in some detail. When $F/J=0$ the curve a shows KT_c/J vs c of the ordinary diluted Ising film with $n=3$. Its critical concentration $c=0.321$. When $F/J=0.5$, the critical concentration is $c=0.376$. Figure 4, meanwhile, shows

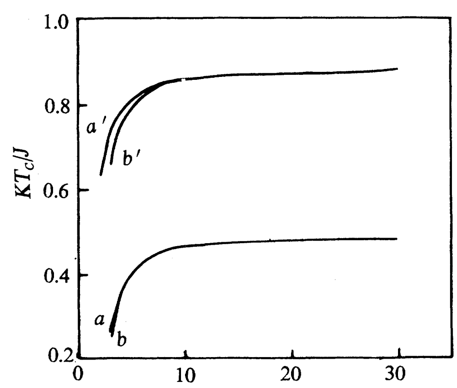

FIG. 3. Critical temperature as a function of the film thickness (n) for $F/J=0.5$: Curve a, $c=0.4$ and $J_s/J=2.0$; curve b, $c=0.4$ and $J_s/J=1.0$; curve a', $c=0.6$ and $J_s/J=2.0$; and curve b', $c=0.6$ and $J_s/J=1.0$.

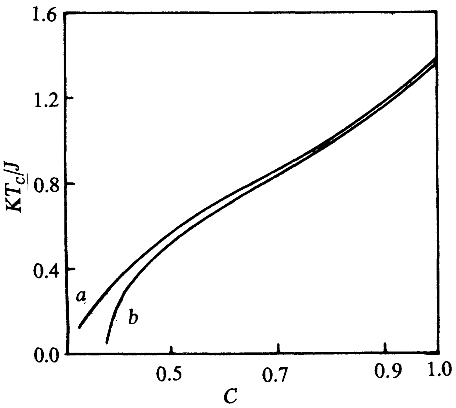

FIG. 4. Critical temperature as a function of concentration (c) for $J_s/J=1.5$ and $n=3$: Curve a, $F/J=0.0$; and curve b, $F/J=0.5$.

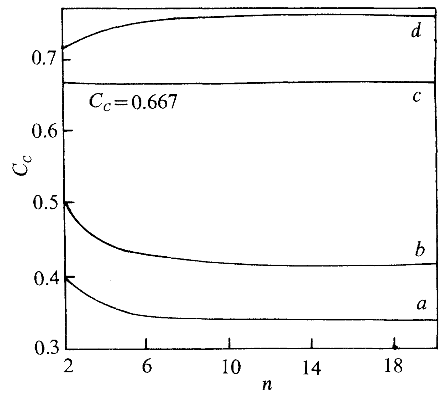

FIG. 5. Critical concentration as a function of the film thickness for $J_s/J=2.0$. Curves a, b, c, and d correspond to $F/J=0.5$, 1.0, 1.78, and 2.0, respectively.

that the transverse field has a greater effect on KT_c/J when the concentration is lower.

Finally, we discuss the critical concentration as a function of the film thickness. In the absence of transverse field the critical concentration decreases as the thickness increases.[16,17] But when the transverse field is applied, and when J_s is greater than J, some new features can appear (see Fig. 5). For a given J_s/J, the critical concentration as a function of n has different patterns because of different transverse fields, i.e., c_c can increase, decrease, or remain unchanged when n is increased. Our calculations show that c_c is unchanged, increases and decreases if $F/J=F_0/J=1.78$, $F/J>F_0/J$, and $F/J<F_0/J$ for a given $J_s/J=2.0$, respectively, as n is increased. The cases that the critical concentration of magnetic atoms cannot change with n and can increase with the increase in n are first found in the diluted Ising film. c_c always decreases with the increase in n when J_s/J is smaller (for example, $J_s/J=1.0$).

In conclusion, we have found some interesting properties in the system. They are (i) the critical temperature can decrease from its maximum with increase in the surface coupling constant when the system is in a smaller transverse field; (ii) the critical concentration as a function of the film thickness has different behaviors in the different transverse fields when the surface coupling constant is larger (such as $J_s/J=2.0$ or $J_s/J=1.5$), i.e., as the increase in the thickness of the film the critical concentration increases, decreases, and remains unchanged in a higher transverse field, in a lower one, and for a certain transverse field, respectively.

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