

## Phase diagrams of the site-diluted spin- $\frac{1}{2}$ Ising superlattice

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Using the effective-field theory with a probability distribution technique that accounts for the single-site spin correlations, the critical behavior of a diluted spin- $\frac{1}{2}$  Ising superlattice consisting of two different ferromagnet materials is examined. The critical temperature of the system is studied as a function of the thickness of the constituents in a unit cell, the concentration of magnetic atoms, and the exchange interactions in each material. It is shown that the properties of the diluted system are different from those of the corresponding pure system. [S0163-1829(99)02529-1]

### I. INTRODUCTION

Magnetic layered structures and superlattices have attracted significant attention recently because of a wide array of fascinating properties. The study of a magnetic superlattice that consists of two or more ferromagnets with different bulk properties has been motivated by the idea that the properties of the superlattice can be significantly different from those of their constituents. A detailed review of the properties of magnetic multilayers and superlattices has appeared.<sup>1</sup>

With the advance of modern vacuum science, in particular the epitaxial growth technique, it is possible to grow very thin magnetic films, of predetermined thickness, even of a few monolayers. Superlattice structures composed of two different ferromagnetic layers have already been artificially fabricated. Ferromagnetic ordering in some of these monolayers has been reported and the critical properties of such systems have been studied, either experimentally<sup>2-5</sup> or theoretically.<sup>6-15</sup>

For a periodic multilayer system formed from two different ferromagnetic materials, Fishman *et al.*<sup>8</sup> have discussed its statics and dynamics within the framework of the Ginzburg-Landau formulation. They have computed the transition temperature and spin-wave spectra. The Landau formalism of Camley and Tilley<sup>9</sup> has been applied to calculate the critical temperature in this system.<sup>10</sup> For more complicated superlattices with an arbitrary number of different layers in an elementary unit, Barnas<sup>11</sup> has derived some general dispersion equations for the bulk and surface magnetic polaritons. These equations are then applied to magnetostatic modes and retarded wave propagation in the Voigt geometry.<sup>12</sup>

On one hand, from both the experimental and theoretical points of view, the spin- $\frac{1}{2}$  Ising magnetic superlattice is very important. Aguilera-Granja and Morán-López<sup>16</sup> studied some experimental results by modeling the ferromagnetic thin film within the framework of the spin- $\frac{1}{2}$  Ising Hamiltonian. As a

result, analytical expression of the thickness dependence of the critical temperature was obtained and the model was applied to estimate the magnetic interaction in Fe and Gd ultrathin films. The experimental results in the case of Fe films on Au substrates<sup>5</sup> were very well reproduced. Hai *et al.*,<sup>18</sup> using the effective-field theory, studied the critical properties in a superlattice consisting of two ferromagnetic materials with different bulk transition temperatures. The critical temperatures were obtained as functions of the thickness of the superlattice with various couplings strengths between nearest-neighbor spins in the same material and across the interface. Sy and Ow<sup>13</sup> and Sy,<sup>14</sup> using the mean-field approximation, and Saber *et al.*,<sup>15</sup> using the effective-field theory,<sup>17</sup> investigated alternating magnetic superlattices. The critical temperatures were calculated as a function of the thickness of the superlattice for various couplings strengths.

On the other hand, there is a class of magnetic substances that are well approximated by simple or site-diluted Ising systems.<sup>19-22</sup> Notable examples are Cs<sub>3</sub>Cl<sub>5</sub>, DyPO<sub>4</sub>, Fe<sub>p</sub>Mg<sub>1-p</sub>Cl<sub>2</sub>, Fe<sub>p</sub>Co<sub>1-p</sub>Cl<sub>2</sub>, and Cd<sub>1-p</sub>Mn<sub>p</sub>Te. Each of them may be a promising candidate for being prepared in the form of a superlattice and the critical temperature measurements. From the experimental point of view it is possible to synthesize the multilayered systems in which each layer thickness is regulated on the atomic scale.<sup>23</sup> Therefore it is possible to design the structure of the sample so as to fit it to the study of a specific fundamental physics problem. Examples of such experimental studies dealing with the interface and dealing with the surface magnetic order problem when the bulk of the sample is paramagnetic were reported by Shinjo *et al.*<sup>23</sup> and Rau *et al.*,<sup>24</sup> respectively. For the site-diluted systems, the magnetic atoms on some lattice sites 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. Kaney-

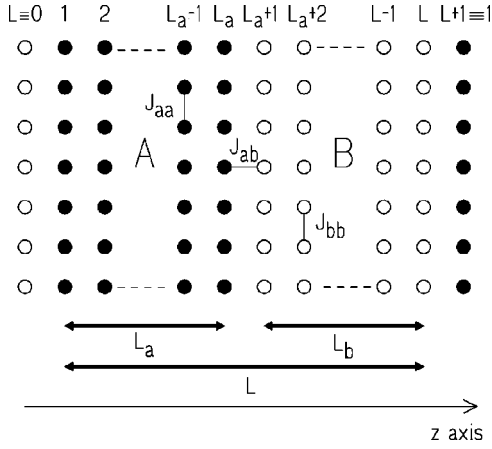


FIG. 1. Two-dimensional cross section of a unit cell of the superlattice composed of two ferromagnetic materials *A* and *B*, where  $L=L_a+L_b$  is the thickness of the cell.

oshi *et al.*<sup>25</sup> investigated a semi-infinite system with surface dilution by means of the effective-field theory with correlations. Qiang Hong<sup>26,27</sup> and Benyoussef *et al.*<sup>28</sup> studied the diluted semi-infinite system using the mean-field theory and renormalization-group method, respectively. Ferchmin and Maciejewski<sup>29</sup> have studied 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 this paper, we study a diluted spin- $\frac{1}{2}$  Ising superlattice consisting of two ferromagnetic materials with different bulk properties as our model system. For simplicity, we restrict our attention to the case of simple cubic structures but other structures can be treated without any difficulty. In particular, we consider the two constituents *A* and *B* with different bulk transition temperatures, i.e.,  $T_c^A \neq T_c^B$ . The interface is, in general, different in nature from both bulks, even if the bulk critical temperatures are the same. We use the effective-field theory with a probability distribution technique<sup>17</sup> in the present work, as it is believed to be far superior to the standard mean-field approximation since it does not predict a zero critical concentration for diluted magnets. For the sake of simplicity, we assume that the concentration of magnetic atoms of the superlattice is homogeneous. In Sec. II we outline the formalism and derive the equation that determines the transition temperature. Numerical results are discussed in Sec. III where the existence of the interface magnetic phase transition is discovered and the critical value of the interface coupling relative the bulk coupling is determined. A brief conclusion is given in Sec. IV.

## II. MODEL AND FORMULATION

We consider a superlattice consisting of two different ferromagnetic materials *A* and *B* stacked alternately: material *A* with  $L_a$  layers and material *B* with  $L_b$  layers. The coupling strength between nearest-neighboring spins in *A* (*B*) is denoted by  $J_{aa}$  ( $J_{bb}$ ), while  $J_{ab}$  stands for the exchange coupling between the nearest-neighbor spins across the interface. The periodic condition suggests that we only have to consider one unit cell of the thickness  $L=L_a+L_b$ , which interacts with its nearest neighbors via the interface coupling. The situation is depicted in Fig. 1. The Hamiltonian of the system

is given by

$$H = - \sum_{(i,j)} J_{ij} c_i c_j \sigma_{iz} \sigma_{jz}, \quad (1)$$

where the first sum runs over all nearest-neighbor pairs and the second sum is taken over all the spins,  $\sigma_{iz}$  denotes the  $z$  component of a quantum spin  $\vec{\sigma}_i$  of magnitude  $\sigma = \frac{1}{2}$  at site  $i$ ,  $J_{ij}$  stands for one of the three coupling constants depending on where the spin pair is located, and  $c_i$  is the occupation number on the lattice site  $i$ ,  $c_i = 1$  if the lattice site is occupied by a magnetic atom and zero otherwise.

The method we use is the effective-field theory, fully described by Saber,<sup>17</sup> that employed the probability distribution technique to account for the single-site spin correlations. Following that procedure, we find in the current situation that for a fixed configuration of neighboring spins the thermal average  $\langle \sigma_{iz} \rangle$  is given by

$$\langle \sigma_{iz} \rangle = c_i f_z \left( \sum_{j=1}^Z J_{ij} c_j \sigma_{jz} \right), \quad (2)$$

where

$$f_z \left( \sum_{j=1}^Z J_{ij} c_j \sigma_{jz} \right) = \frac{1}{2} \tanh \left( \frac{1}{2} \beta \sum_{j=1}^Z J_{ij} c_j \sigma_{jz} \right) \quad (3)$$

and  $\beta = 1/k_B T$ . The sum in Eqs. (2) and (3) is over the nearest neighbors of the site  $i$ ,  $Z$  being the nearest-neighbor coordination number of the lattice. In a mean-field approximation one would simply replace these spin operators by their thermal values  $m_z$  and these occupation numbers by the concentration  $c$  of magnetic atoms. However, it is at this point that a substantial improvement to the theory is made by noting that the spin operators and their occupation numbers have a finite set of base states, so that the average over the function  $f_z$  can be expressed as an average over a finite polynomial of spin operators and their occupation numbers belonging to the neighboring spins. This procedure can be effected by the combinatorial method and correctly accounts for the single-site kinematic relations. Up to this point the theory is exact, but the right-hand side of Eq. (2) will contain multiple correlation functions. Usually, at this stage a Zernike-type decoupling of the multiple correlation functions is made that neglects the correlation between quantities pertaining to different sites.

The above thermal average was for a fixed spatial configuration. In the next step, we have to carry out the spatial configurational averaging, to be denoted by  $\langle \dots \rangle_r$ . To make progress, the simplest approximation of neglecting the correlations between different sites will be made. This is achieved by introducing the probability distribution of the spin variable  $\sigma_{iz}$  with its occupation number  $c_i$ ,  $P(c_i, \sigma_{iz})$ , which is given by<sup>17</sup>

$$\begin{aligned} P(c_i, \sigma_{iz}) = & \frac{1}{2} (1-c) \delta(c_i) [ \delta(\sigma_{iz} + \frac{1}{2}) + \delta(\sigma_{iz} - \frac{1}{2}) ] \\ & + \frac{1}{2} \delta(c_i - 1) [ (c - 2m_z) \delta(\sigma_{iz} + \frac{1}{2}) \\ & + (c + 2m_z) \delta(\sigma_{iz} - \frac{1}{2}) ], \end{aligned} \quad (4)$$

with

$$c = \langle \langle c_i \rangle \rangle_r \quad (5)$$

and

$$m_z = \langle \langle c_i \sigma_{iz} \rangle \rangle_r = \langle \langle \sigma_{iz} \rangle \rangle_r. \quad (6)$$

### III. RESULTS

Allowing for the site magnetizations to take different values in each atomic layer parallel to the surface of the superlattice, and labeling them in accordance with the layer number in which they are situated, the application of Eqs. (2) and (4) leads to the following equation for the  $n$ th layer magnetization:

$$\begin{aligned} m_{nz} = & 2^{-N-2N_0} c \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} 2^{\mu+\mu_1+\mu_2} (1-c)^{\mu+\mu_1+\mu_2} \\ & \times C_{\mu}^N C_{\nu}^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} (c-2m_{nz})^{\nu} (c+2m_{nz})^{N-(\mu+\nu)} \\ & \times (c-2m_{n-1,z})^{\nu_1} (c+2m_{n-1,z})^{N_0-(\mu_1+\nu_1)} (c-2m_{n+1,z})^{\nu_2} (c+2m_{n+1,z})^{N_0-(\mu_2+\nu_2)} \\ & \times f_z \left( \frac{1}{2} \{ J_{nn} [N - (\mu + 2\nu)] + J_{n,n-1} [N_0 - (\mu_1 + 2\nu_1)] + J_{n,n+1} [N_0 - (\mu_2 + 2\nu_2)] \} \right), \end{aligned} \quad (7)$$

where  $n = 1, 2, 3, \dots, L, N$ , and  $N_0$  are the numbers of nearest neighbors in the plane and between adjacent planes, respectively ( $Z = N + 2N_0$ ).  $C_k^l$  are the binomial coefficients  $C_k^l = l! / k!(l-k)!$ .

The periodic condition of the superlattice has to be satisfied, namely,  $m_{0z} = m_{Lz}$  and  $m_{1z} = m_{L+1,z}$ .

We have thus obtained the self-consistent equation Eq. (7) for the magnetization  $m_{nz}$ , that can be solved directly by numerical iteration. No further algebraic manipulation is necessary. This is the advantage of introducing the probability distribution technique. The same equations hold for an arbitrary superlattice structure with a coordination number,  $Z$ , and therefore results for different structures can be obtained without carrying out the detailed algebra encountered when employing other techniques. For the case of a simple cubic lattice, which we will consider here, one has  $N=4$  and  $N_0=1$ . As we are interested with the calculation of the ordering near the transition critical temperature, the usual ar-

gument that  $m_{nz}$  tends to zero as the temperature approaches its critical value, allows us to consider only terms linear in  $m_{nz}$  because higher-order terms tend to zero faster than  $m_{nz}$  on approaching a critical temperature. Consequently, all terms of the order higher than linear terms in Eq. (7) can be neglected. This leads to the set of simultaneous equations

$$m_{nz} = A_{n,n-1} m_{n-1,z} + A_{n,n} m_{nz} + A_{n,n+1} m_{n+1,z}, \quad (8)$$

which can be written as

$$M m_z = 0, \quad (9)$$

where  $M$  is a matrix acting on the vector  $m_z$  containing the magnetizations  $m_{nz}$ . The elements of the matrix  $M$  are given by

$$M_{ij} = (A_{ii} - 1) \delta_{i,j} + A_{i,j} (\delta_{i,j-1} + \delta_{i,j+1}). \quad (10)$$

The only nonzero elements of the matrix  $M$  are given by

$$\begin{aligned} M_{n,n-1} = & 2^{-N-2N_0} c \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu} \sum_{j=0}^{N_0-(\mu_1+\nu_1)} (-1)^i 2^{\mu+\mu_1+\mu_2+i+j} \\ & \times \delta_{1,i+j} (1-c)^{\mu+\mu_1+\mu_2} c^{N+2N_0-(\mu+\mu_1+\mu_2+i+j)} C_{\mu}^N C_{\nu}^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} C_i^{\nu} C_j^{N_0-(\mu_1+\nu_1)} \\ & \times f_z \left( \frac{1}{2} \{ J_{nn} [N - (\mu + 2\nu)] + J_{n,n-1} [N_0 - (\mu_1 + 2\nu_1)] + J_{n,n+1} [N_0 - (\mu_2 + 2\nu_2)] \} \right), \end{aligned} \quad (11)$$

$$\begin{aligned} M_{n,n} = & 2^{-N-2N_0} c \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu} \sum_{j=0}^{N-(\mu+\nu)} (-1)^i 2^{\mu+\mu_1+\mu_2+i+j} \\ & \times \delta_{1,i+j} (1-c)^{\mu+\mu_1+\mu_2} c^{N+2N_0-(\mu+\mu_1+\mu_2+i+j)} C_{\mu}^N C_{\nu}^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} C_i^{\nu} C_j^{N-(\mu+\nu)} \\ & \times f_z \left( \frac{1}{2} \{ J_{nn} [N - (\mu + 2\nu)] + J_{n,n-1} [N_0 - (\mu_1 + 2\nu_1)] + J_{n,n+1} [N_0 - (\mu_2 + 2\nu_2)] \} \right) - 1, \end{aligned} \quad (12)$$

$$\begin{aligned}
 M_{n,n+1} &= 2^{-N-2N_0} c \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu_2} \sum_{j=0}^{N_0-(\mu_2+\nu_2)} (-1)^i 2^{\mu+\mu_1+\mu_2+i+j} \\
 &\quad \times \delta_{1,i+j} (1-c)^{\mu+\mu_1+\mu_2} c^{N+2N_0-(\mu+\mu_1+\mu_2+i+j)} C_{\mu}^N C_{\nu}^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} C_i^{\nu_2} C_j^{N_0-(\mu_2+\nu_2)} \\
 &\quad \times f_z \left( \frac{1}{2} \{ J_{nn} [N - (\mu + 2\nu)] + J_{n,n-1} [N_0 - (\mu_1 + 2\nu_1)] + J_{n,n+1} [N_0 - (\mu_2 + 2\nu_2)] \} \right), \quad (13)
 \end{aligned}$$

with the periodic-boundary conditions  $M_{1,0} = M_{1,L}$  and  $M_{L,L+1} = M_{L,1}$ .

All the information about the critical temperature of the system is contained in Eq. (9). Up to now, we did not assign precise values to the coupling constants, concentration of magnetic atoms and the thickness of the superlattice: the terms in matrix (9) are general ones.

In a general case, for arbitrary values of these parameters, the evaluation of the critical temperature relies on numerical solution of the system of linear equations (9). These equations are fulfilled if and only if

$$\det M = 0. \quad (14)$$

This condition can be satisfied for  $L$  different values of the critical temperature  $T_c$  from which we choose the highest possible one.<sup>29</sup>

This value of the critical temperature corresponds to a solution where  $m_{1z}, m_{2z}, \dots, m_{Lz}$  are all positive, which is compatible with a ferromagnetic ordering. The other solutions correspond, in principle, to other types of ordering that usually do not occur here.

In this paper, we take  $J_{aa}$  as the unit of energy, the length is measured in units of the lattice constant and we introduce the reduced exchange couplings  $R_1 = J_{bb}/J_{aa}$  and  $R_2 = J_{ab}/J_{aa}$ .

Let us begin with the evaluation of the critical temperature with an example: the critical temperature of the site-diluted spin- $\frac{1}{2}$  Ising model for the simplest possible ‘‘bulk case’’ of a material  $A$  (i.e.,  $N=4$ ,  $N_0=1$ ,  $J_{i,j} = J_{aa}$ ). Then we can reduce  $\det M$  to the following form:

$$\det M = \begin{vmatrix} a & b & & & & & & & & b \\ b & a & b & & & & & & & \\ & b & a & b & & & & & & \\ & & & & \dots & \dots & & & & \\ & & & & & & b & a & b & \\ & & & & & & & & \dots & \dots \\ & & & & & & & & & b & a & b \\ & & & & & & & & & b & a & b \\ & & & & & & & & & b & a & \\ b & & & & & & & & & & & b \end{vmatrix}_{(L,L)}, \quad (15)$$

whose value is

$$\det M_{bulk} = \prod_{k=1}^L \left[ a + 2b \cos\left(\frac{2\pi(k-1)}{L}\right) \right], \quad (16)$$

where the elements in the above determinant are given by

$$a = M_{n,n} (J_{n,n} = J_{n,n-1} = J_{n,n+1} = J_{aa}), \quad (17)$$

$$b = \frac{1}{4}(a+1), \quad (18)$$

and  $L$  in the ‘‘bulk’’ case is an arbitrary number. Now, we obtain the critical temperature from the condition  $\det M = 0$ .

In Fig. 2, we show the behavior of the bulk critical temperature  $T_c^A/J_{aa}$  of the bulk material  $A$  as a function of the concentration  $c$  of magnetic atoms. With the decrease of  $c$

the phase region in which the ferromagnetic ordering is realizable gradually becomes small and vanishes at the bulk critical concentration  $c_B = 0.2928$  at which the bulk critical temperature  $T_c^A/J_{aa}$  reduces to zero. The series methods<sup>30</sup> and the Monte Carlo simulations<sup>30</sup> give, respectively,  $c_B = 0.307$  and  $c_B = 0.325$ . In particular, for the pure system with  $c=1$  (or the regular simple cubic lattice) the  $T_c^A/J_{aa}$  value at  $c=1$  is given by  $T_c^A/J_{aa} = 1.2683$ , which is to be compared with the mean-field approximation result  $T_c^A/J_{aa} = 1.5$  and the series methods result<sup>30</sup>  $T_c^A/J_{aa} = 1.1277$ .

Now let us turn to the study of the critical temperatures for the diluted ferromagnet spin- $1/2$  superlattice. We remember that the exchange couplings between the nearest-neighbor spins in the slabs  $A$  and  $B$  and across the interface are different. These differences influence the form of  $\det M$ , which can be written as

$$\det M = \alpha \left| \begin{array}{cccccccccccc} a_1 & 1 & & & & & & & & & & & & & & b_1 \\ 1 & c_1 & 1 & & & & & & & & & & & & & \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \\ & & & & 1 & c_1 & 1 & & & & & & & & & \\ & & & & & & 1 & a_1 & b_1 & & & & & & & \\ & & & & & & & b_2 & a_2 & 1 & & & & & & \\ & & & & & & & & & 1 & c_2 & 1 & & & & \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \\ & & & & & & & & & & 1 & c_2 & 1 & & & \\ b_2 & & & & & & & & & & & 1 & a_2 & & & \end{array} \right|_{(L,L)}, \quad (19)$$

where the coefficients  $\alpha$ ,  $a_1$ ,  $a_2$ ,  $b_1$ ,  $b_2$ ,  $c_1$ , and  $c_2$  are given by

$$\alpha = \left(\frac{1}{M_{1,1}/4}\right)^2 \left(\frac{1}{M_{2,1}}\right)^{2(L_a-2)} \times \left(\frac{1}{M_{L_a+1,L_a+1}/4}\right)^2 \left(\frac{1}{M_{L_a+2,L_a+1}}\right)^{2(L_b-2)}, \quad (20)$$

$$\begin{aligned} a_1 &= M_{1,1}/M_{1,2}, & a_2 &= M_{L_a+1,L_a+1}/M_{L_a+1,L_a+2}, \\ b_1 &= M_{1,0}/M_{1,2}, & b_2 &= M_{L_a+L_b,1}/M_{L_a+1,L_a+2}, \\ c_1 &= M_{2,2}/M_{2,1}, & c_2 &= M_{L_a+2,L_a+2}/M_{L_a+2,L_a+1}. \end{aligned} \quad (21)$$

In order to calculate the critical temperatures of the superlattice, we have to solve Eq. (14) numerically in which we substitute  $\det M$  by its expression given by Eq. (19).

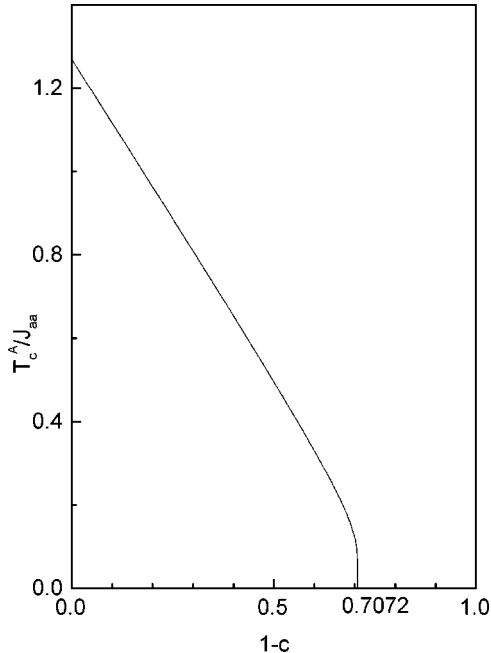


FIG. 2. Dependence of the critical temperature  $T_c^A/J_{aa}$  of an infinite bulk simple cubic lattice of material A on the concentration  $c$  of magnetic atoms.

We note that for the case of  $J_{ab}=0$  ( $R_2=0$ ), the superlattice reduces to two sets of simple films, so there exists separated phase transitions in two slabs. But here, we are interested in the case of  $J_{ab} \neq 0$  ( $R_2 \neq 0$ ). Therefore, without loss of generality, we assume the critical temperature of slab A higher than that of slab B, that is  $J_{aa} \geq J_{bb}$  ( $R_1 = J_{bb}/J_{aa} \leq 1$ ), and hence  $T_c^A/J_{aa} \geq T_c^B/J_{aa}$ , where  $T_c^A/J_{aa}$  is the bulk critical temperature of a uniform lattice of material A and  $T_c^B/J_{aa} = R_1 T_c^A/J_{aa}$ .

We have calculated many dependencies of the critical temperature of the superlattice on the reduced interface coupling, superlattice thickness, and concentration of magnetic atoms but here we will present only some particular interesting results.

We first show the critical temperature of the superlattice  $T_c/J_{aa}$  as a function of the unit cell width  $L=L_a+L_b$  in Fig. 3 when  $R_1=0.9$ ,  $R_2=0.5$ , and various values of the concentration  $c$  of magnetic atoms. Three cases of different  $L_b$  are

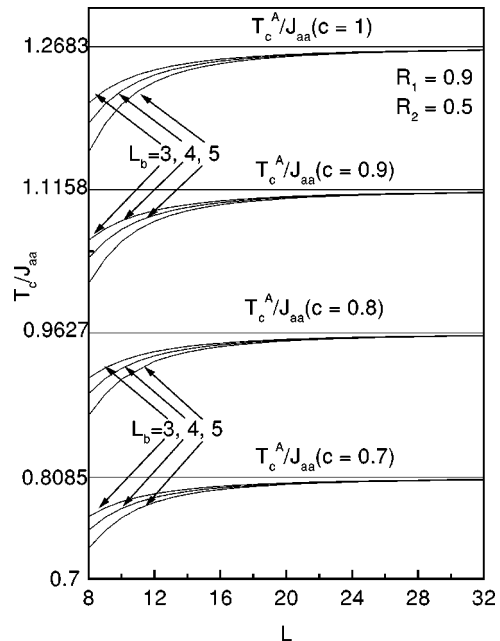


FIG. 3. Dependence of the critical temperature  $T_c/J_{aa}$  of the superlattice on the thickness  $L$  for  $R_1=0.9$ ,  $R_2=0.5$ , various values of  $c$ , and various values of  $L_b$ .

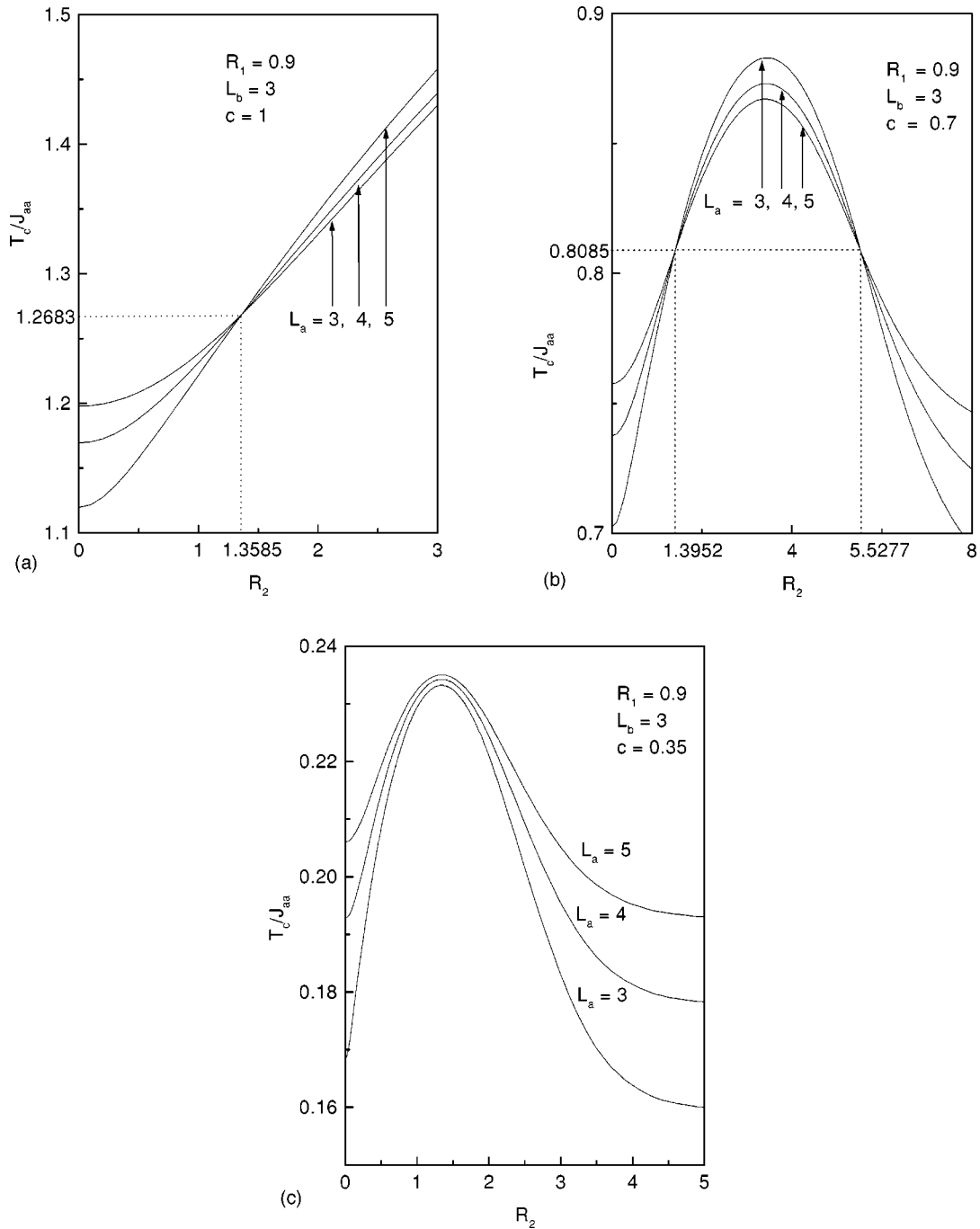


FIG. 4. The critical temperature  $T_c/J_{aa}$  of the superlattice versus the reduced interface exchange interaction  $R_2=J_{ab}/J_{aa}$  for  $L_b=3$ ,  $R_1=J_{bb}/J_{aa}=0.9$ , and several values of  $c$ . The number accompanying each curve denotes the value of  $L_a$ . (a)  $c=1$ ; (b)  $c=0.7$ ; (c)  $c=0.35$ .

plotted  $L_b=3, 4$ , and  $5$ . We first note that for a given value of  $c(L_b)$ ,  $T_c/J_{aa}$  decreases with increasing (decreasing)  $L_b$  ( $c$ ). For a given  $L_b$ , it is observed that  $T_c/J_{aa}$  increases steadily as  $L$  increases indefinitely. For each value of  $c$ , all the curves approach the limiting value that is the bulk critical temperature of material A,  $T_c^A/J_{aa}$ , which depends on  $c$ . This is, of course, easily understood.

To study the effects of the reduced interface exchange coupling  $R_2=J_{ab}/J_{aa}$  and the concentration of magnetic atoms  $c$  on the critical temperature  $T_c/J_{aa}$  of the superlattice,

$T_c/J_{aa}$  is calculated as a function of  $R_2$  for fixed  $R_1=0.9$  and  $L_b=3$ , but various values of  $L_a$  and various values of the concentration  $c$ .

Figure 4(a) corresponds to the pure case  $c=1$  and it shows that for  $R_2>1$  the dependence of  $T_c/J_{aa}$  on  $R_2$  is approximately linear in agreement with the results of other methods.<sup>10,13,14</sup> It is easy to see from this figure that there exists a critical value of the reduced interface exchange  $R_2^c$  such that, when  $R_2>R_2^c$  and consequently  $T_c/J_{aa}>T_c^A/J_{aa}$ ,  $T_c^B/J_{aa}$ , the system may order in the interface



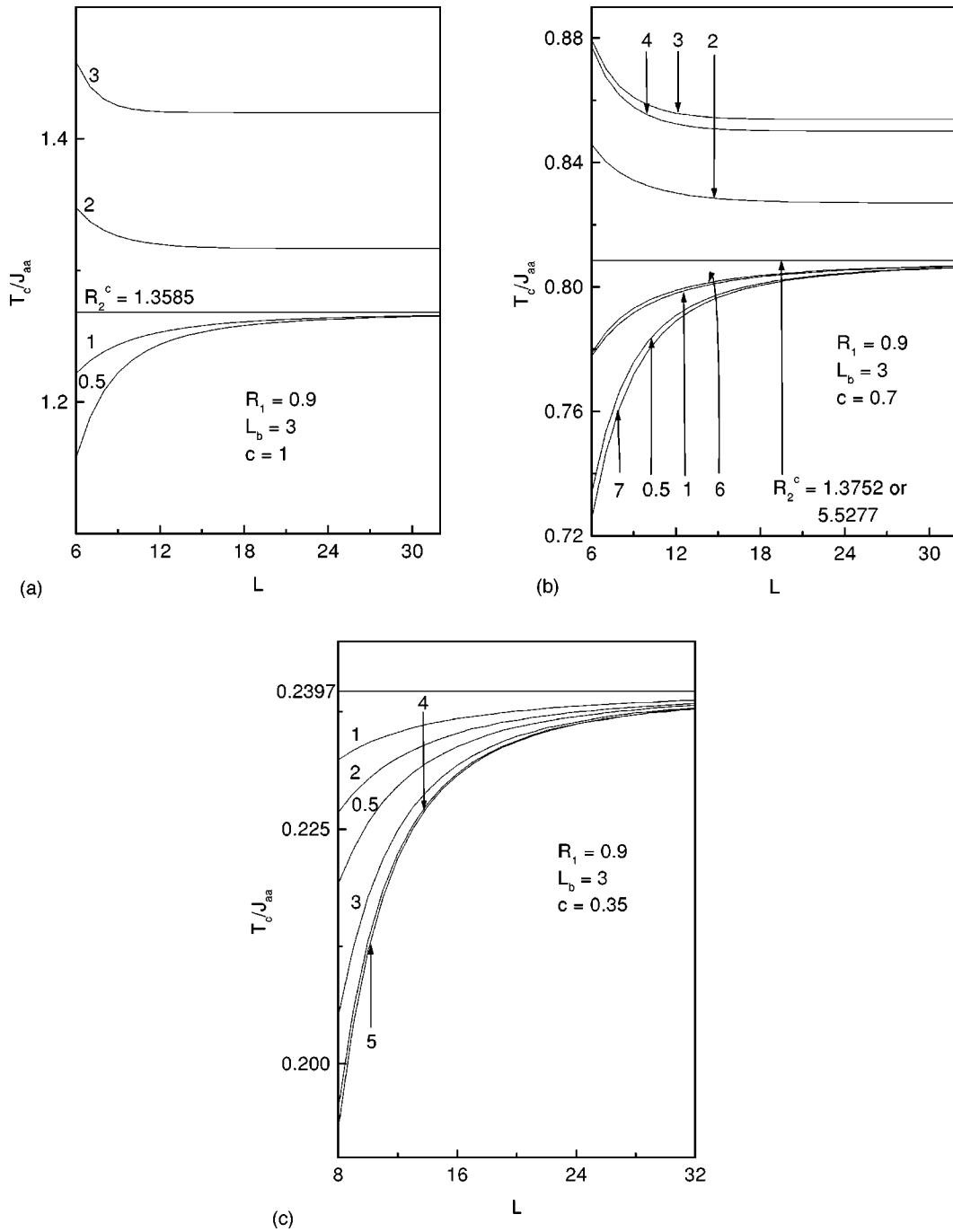


FIG. 5. The critical temperature  $T_c/J_{aa}$  of the superlattice versus the thickness for  $L_b=3$ ,  $R_1=J_{bb}/J_{aa}=0.9$ , and several values of  $c$ . The number accompanying each curve denotes the value of reduced exchange coupling  $R_2=J_{ab}/J_{aa}$ . (a)  $c=1$ ; (b)  $c=0.7$ ; (c)  $c=0.35$ .

layers before the intralayer ordering, i.e., the interface magnetism dominates. For  $R_2 < R_2^c$ ,  $T_c/J_{aa} < T_c^A/J_{aa}$ ,  $T_c^B/J_{aa}$ , we have the contrary situation. Initially it has a plane intralayer ordering, i.e., the intralayer magnetism dominates and the system behaves like metamagnets.

Figure 4(b) shows the dependence of  $T_c/J_{aa}$  on  $R_2$  for the same values of the parameters as Fig. 4(a), except here the concentration of magnetic atoms is  $c=0.7$ . This figure exhibits some new interesting results for the diluted case. First, as is seen from this figure, the critical temperature curves show the reentrant phenomena that may be attributed to the competition between the effects due to the exchange couplings and the dilution. Second, the dependence of  $T_c/J_{aa}$  on

$R_2$  is not linear and it is interesting to note that there exist two critical values of the reduced interface exchange  $R_2^c$ ,  $R_2^c=1.3952$  and  $R_2^c=5.5277$ , such that when  $R_2 < 1.3952$  or  $R_2 > 5.5277$ , and consequently,  $T_c/J_{aa} < T_c^A/J_{aa}$ ,  $T_c^B/J_{aa}$ , the system may order in the intralayers before the interface ordering; and when  $1.3952 < R_2 < 5.5277$ , and consequently,  $T_c/J_{aa} > T_c^A/J_{aa}$ ,  $T_c^B/J_{aa}$ , the system may order in the interface layers before the intralayer ordering, i.e., the interface magnetism dominates.

Figure 4(c) shows the dependence of  $T_c/J_{aa}$  on  $R_2$  for the same values of the parameters as Fig. 4(a) except here the concentration of magnetic atoms is  $c=0.35$ . This figure exhibits also some interesting results for the diluted case (the

reentrant phenomena in the critical temperature curves). Here, the dependence of  $T_c/J_{aa}$  on  $R_2$  is not linear and the critical temperature of the superlattice  $T_c/J_{aa}$  increases with the increase of  $L_a$  for  $L_b$  fixed. We note that the interface magnetism disappears in this case.

In Figs. 5(a)–5(c) we show the critical temperature of the superlattice as a function of the unit cell thickness  $L$  for fixed  $L_b=3$ ,  $R_1=0.9$ , various values of  $R_2$ , and various values of  $c$ .

Figure 5(a) corresponds to the pure case  $c=1$ . The horizontal line corresponds to the case of  $R_2=R_2^c=1.3585$ , such that  $T_c/J_{aa}=T_c^A/J_{aa}=1.2683$  and remains constant for any  $L_a$ . We see that  $T_c/J_{aa}$  increases with the increase of  $R_2$ . For  $R_2>R_2^c$  the critical temperature of the superlattice is higher than the bulk critical temperature  $T_c^A/J_{aa}$  and  $T_c/J_{aa}$  decreases with the increase of  $L$  to reach an asymptotic value. For  $R_2<R_2^c$  the critical temperature of the superlattice is smaller than the bulk critical temperatures  $T_c^A/J_{aa}$  and  $T_c/J_{aa}$  increases with the increase of  $L$  to reach  $T_c^A/J_{aa}$  for large values of  $L$ . This suggests that there exists an interface magnetism in the system, i.e., for  $R_2>R_2^c$  the system may order in the interface layers before it orders in the other layers.

Figure 5(b) corresponds to the diluted case with  $c=0.7$ . The horizontal line corresponds to two critical values of  $R_2=R_2^c=1.3752$  or  $5.5277$  such that  $T_c/J_{aa}=T_c^A/J_{aa}=0.8085$  and remains constant for any  $L_a$ . Contrary to the pure case, we see that  $T_c/J_{aa}$  does not increase with the increase of  $R_2$ . For  $1.3752<R_2<5.5277$  the critical temperature of the superlattice is higher than the bulk critical temperature  $T_c^A/J_{aa}$  and  $T_c/J_{aa}$  decreases with the increase of  $L$  to reach an asymptotic value. For  $R_2<1.3752$  or  $R_2>5.5277$  the critical temperature of the superlattice is smaller than the bulk critical temperatures  $T_c^A/J_{aa}$  and  $T_c/J_{aa}$  increases with the increase of  $L$  to reach  $T_c^A/J_{aa}$  for large values of  $L$ . Here the interface magnetism in the system exists only in the region  $1.3752<R_2<5.5277$ .

Figure 5(c) corresponds to the diluted case with  $c=0.35$ . Contrary to the pure case, we see that  $T_c/J_{aa}$  does not increase with the increase of  $R_2$ . For any value of  $R_2$ , the critical temperature of the superlattice is always smaller than the bulk critical temperature  $T_c^A/J_{aa}$  and  $T_c/J_{aa}$  increases with the increase of  $L$  to reach an asymptotic value. In this case there is no interface magnetism.

#### IV. CONCLUSION

In conclusion, we have studied the phase transitions in a diluted spin- $\frac{1}{2}$  Ising model of magnetic superlattice using the

effective-field theory with a probability distribution technique that accounts for the self-spin-correlation function. For the pure case, a critical value  $R_2^c$  of the reduced interlayer exchange interaction  $R_2$  has been found such that for  $R_2>R_2^c$  ( $R_2<R_2^c$ ) the interlayer (intralayer) ordering dominates. For ( $R_2<R_2^c$ ) we found that the critical temperature of the superlattice  $T_c/J_{aa}$  is always less than the bulk critical temperature  $T_c^A/J_{aa}$  and reaches the last one when the thickness  $L$  becomes large, but for ( $R_2>R_2^c$ ),  $T_c/J_{aa}$  is always greater than  $T_c^A/J_{aa}$ .

The study of the effect of the dilution of magnetic atoms on the critical temperatures of the system is very significant as it has been seen in these two investigated cases  $c=0.7$  and  $c=0.35$ . For  $c=0.7$  the behavior of the system is different from the pure case. In particular, two critical values of the reduced exchange coupling have been found and the interface magnetism does not dominate even if the interface exchange interaction  $R_2$  is strong enough. For  $c=0.35$  the interface magnetism is absent even if the critical concentration  $c$  of magnetic atoms is larger than the bulk critical concentration  $c_B=0.2928$ .

As discussed in Sec. III, a number of interesting phenomena such that the reentrant phenomena have been found in the critical temperature curves that are due to the competition between the exchange couplings and the dilution. We hope that the results obtained in this work may be helpful from both a theoretical and experimental aspect.

The formalism of transition temperature derivation obtained above is general and can be used for the study of superlattices of various thicknesses and structures. Although we have discussed only ferromagnetic exchanges (all  $J>0$ ), the formulation is applicable to antiferromagnetic couplings as well. Hence, some or all of the  $J$ 's can be negative. A simple observation can be made: If the exchange interactions between the successive layers are antiferromagnetic [i.e., we have to replace  $J_{ab}$  by  $-J_{ab}$  ( $R_2$  by  $-R_2$ ) in the equations], the values of the critical temperature are not changed, which is consistent with the discussion of Tilley.<sup>10</sup>

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