

Phase Transitions in a Two Component Spin-One Ising Ferromagnetic Superlattice

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Using effective field theory with a probability distribution technique, the magnetic properties in an infinite superlattice consisting of two different ferromagnets are studied in a spin-one Ising model. The dependence of the Curie temperature is calculated as a function of the thickness of the two slabs in one period and as a function of the intra- and interlayer exchange interactions. A critical value of the exchange reduced interaction, above which the interface magnetism appears, is found.

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I. Introduction

The magnetic properties of artificially fabricated superlattices that consist of two or more ferromagnetic materials have been widely studied over the years, because their physical properties differ dramatically from simple solids formed from the same materials. The development of film deposition techniques has aroused great interest in the synthesis and study of superlattices in other materials. In layered ferromagnetic materials, it has been found experimentally that one can obtain a rich variety of magnetic behaviours depending on the materials, the thickness and the number of slabs and the applied field [1-5]. A number of theoretical works have been devoted to the magnetic and phase transition properties of superlattices formed from layers of different materials [6-14].

In the present paper, we will study the critical properties of infinite superlattices made up of elementary units of two kinds of atoms. In each elementary unit, there are L_a atomic layers of magnetic ions of type A and L_b atomic layers of magnetic ions of type B . We use effective field theory with the probability distribution technique in its simplest form [15, 16]. This technique is believed to give more exact results than those of the standard mean-field approximation. In section 2 we outline the formalism and derive the equation that determines the transition temperature. Numerical results are discussed in section 3. A brief conclusion is given in section 4.

II. Formalism

Consider an infinite superlattice consisting of two different ferromagnetic materials A and B . For simplicity, we restrict our attention to the case of the simple Ising-type structure. The

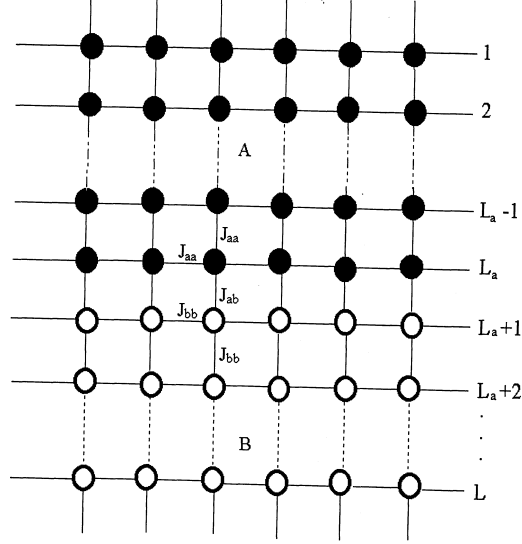


FIG. 1. Sketch of a unit cell of the superlattice.

periodic condition suggests that we only have to consider one unit cell. The situation is shown in Fig. 1. The exchange coupling between the nearest-neighbor spins in $A(B)$ is denoted by $J_{aa}(J_{bb})$; we take J_{aa} as the unit of energy. Here, we consider the interface to be composed of two layers (L_a and $L_a + 1$). J_{ab} stands for the exchange coupling between the nearest-neighbor spins across the interface. The number of atomic layers in material $A(B)$ is $L_a(L_b)$ and the thickness of the unit cell is $L = L_a + L_b$. The spin-one Ising Hamiltonian of the system is given by

$$H = - \sum_{n,n'} \sum_{r,r'} J_{nn'} \sigma_{nr}^z \sigma_{n'r'}^z, \quad (1)$$

where σ_{nr}^z denotes the z component of a quantum spin σ_{nr} of magnitude $\sigma_{nr} = 1$ at site (n, r) , (n, n') are plane indices, (r, r') are different sites of the planes, and $J_{nn'}$, is the strength of the ferromagnetic exchange interaction which is only plane dependent. The statistical properties of the system are studied using an effective field theory that employs the probability distribution technique, which is based on a single-site cluster comprising just a single selected spin, labeled (n, r) , and the neighbouring spins with which it directly interacts. To this end, the Hamiltonian is split into two parts, $H = H_{nr} + H'$, where H_{nr} is that part of the Hamiltonian containing the spin (n, r) , namely

$$H_{nr} = - \left(\sum_{n',r'} J_{nn'} \sigma_{n'r'}^z \right) \sigma_{nr}^z, \quad (2)$$

The starting point of effective field theory is a set of formal identities of the type

$$\langle \langle (\sigma_{nr}^z)^p \rangle_c \rangle = \left\langle \frac{\text{Tr}_{nr} [(\sigma_{nr}^z)^p \exp(-\beta H_{nr})]}{\text{Tr}_{nr} [\exp(-\beta H_{nr})]} \right\rangle, \quad (3)$$

where $\langle (\sigma_{nr}^z)^p \rangle_c$ denotes the mean value of $(\sigma_{nr}^z)^p$ for a given configuration c of all other spins, $\langle \dots \rangle$ denotes the average over all spin configurations $\sigma_{n'r'}^z$, $T r_{nr}$ means the trace performed over $(\sigma_{nr}^z)^p$ only, $\beta = 1/k_B T$ with k_B the Boltzmann constant and T is the absolute temperature. For a fixed configuration of neighbouring spins of the site (n, r) . the longitudinal and the transverse magnetizations and quadrupolar moments of any spin at site (n, r) are given by

$$m_{nrz} = \langle \langle \sigma_{nr}^z \rangle_c \rangle = \langle f_{1z}(A) \rangle, \quad (4)$$

$$q_{nrz} = \langle \langle (\sigma_{nr}^z)^2 \rangle_c \rangle = \langle f_{2z}(A) \rangle, \quad (5)$$

where

$$f_{1z}(A) = \frac{2 \sinh(\beta A)}{1 + 2 \cosh(\beta A)}, \quad (6)$$

$$f_{2z}(A) = \frac{2 \cosh(\beta A)}{1 + 2 \cosh(\beta A)}, \quad (7)$$

with

$$A = \sum_{n'} \sum_{r'} J_{nn'} \sigma_{n'r'}^z, \quad (8)$$

where the first and second sums run over all possible configurations of atoms neighboring or lying on the (n, r) site, respectively. Each of these configurations can be characterized by the number of magnetic atoms in the planes $n - 1$, n , $n + 1$. To perform thermal averaging on the right-hand side of equations (4) and (5) one now follows the general approach described in [15, 16]. Thus with the use of the integral representation method of Dirac δ -distribution, equations (4) and (5) can be written in the form,

$$\langle \langle \sigma_{nr}^z \rangle_c \rangle = \int d\omega f_{1z}(\omega, B) \frac{1}{2\pi} \int dt \exp(i\omega t) \prod_{n'r'} \langle \exp(-it J_{n,n'} \sigma_{n'r'}^z) \rangle, \quad (9)$$

$$\langle \langle (\sigma_{nr}^z)^2 \rangle_c \rangle = \int d\omega f_{2z}(\omega, B) \frac{1}{2\pi} \int dt \exp(i\omega t) \prod_{n'r'} \langle \exp(-it J_{n,n'} \sigma_{n'r'}^z) \rangle. \quad (10)$$

In the derivation of the equations (9) and (10), the commonly used approximation has been made according to which the multi-spin correlation functions are decoupled into products of the spin averages (the simplest approximation of neglecting the correlations between different sites has been made). That is

$$\langle \sigma_j^z (\sigma_k^z)^2 \dots \sigma_l^z \rangle \approx \langle \sigma_j^z \rangle \langle (\sigma_k^z)^2 \rangle \dots \langle \sigma_l^z \rangle, \quad \text{for } j \neq k \dots \neq l. \quad (11)$$

Then, as $\langle \langle \sigma_{nr}^z \rangle_c \rangle$ and $\langle \langle (\sigma_{nr}^z)^2 \rangle_c \rangle$ are independent of r , we introduce the longitudinal magnetization and the longitudinal quadrupolar moment of the n -th layer, on the basis of equations (4) and (5), with the use of the probability distribution of the spin variables [15, 16],

$$P(\sigma_{nr}^z) = \frac{1}{2} [(q_{nz} - m_{nz}) \delta(\sigma_{nr}^z + 1) + 2(1 - q_{nz}) \delta(\sigma_{nr}^z) + (q_{nz} + m_{nz}) \delta(\sigma_{nr}^z - 1)]. \quad (12)$$

Allowing for the site magnetizations and quadrupolar moments to take different values in each atomic layer parallel to the surfaces of the superlattice, and labeling them in accordance with the layer number in which they are situated, the application of Eqs. (4), (9) and (12) yields the following set of equations for the layer longitudinal magnetizations:

$$\begin{aligned}
m_{nz} = & 2^{-N-2N_0} \sum_{\mu=0}^n \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} 2^{\mu+\mu_1+\mu_2} C_{\mu}^N C_{\nu}^{N-\mu} \\
& C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} (1 - 2q_{nz})^{\mu} (q_{nz} - m_{nz})^{\nu} (q_{nz} + m_{nz})^{N-\mu-\nu} \\
& (1 - 2q_{n-1,z})^{\mu_1} (q_{n-1,z} - m_{n-1,z})^{\nu_1} (q_{n-1,z} + m_{n-1,z})^{N_0-\mu_1-\nu_1} \\
& (1 - 2q_{n+1,z})^{\mu_2} (q_{n+1,z} - m_{n+1,z})^{\nu_2} (q_{n+1,z} + m_{n+1,z})^{N_0-\mu_2-\nu_2} f_{1z}(y_n),
\end{aligned} \tag{13}$$

where

$$y_n = [J_{n,n}(N - \mu - 2\nu) + J_{n,n-1}(N_0 - \mu_1 - 2\nu_1) + J_{n,n+1}(N_0 - \mu_2 - 2\nu_2)]. \tag{14}$$

N and N_0 are the numbers of nearest neighbours in the plane and between adjacent planes, respectively ($N = 4$ and $N_0 = 1$ in the case of a simple cubic lattice which is considered here), and C_k^l are the binomial coefficients, $C_k^l = \frac{l!}{k!(l-k)!}$. The periodic condition of the superlattice has to be satisfied, namely $m_{0z} = m_{Lz}$, $m_{L+1,z} = m_{1z}$ and $q_{0z} = q_{L+1,z}$, and $q_{L+1,z} = q_{1z}$. The equations of the longitudinal the quadrupolar moments are obtained by substituting the function f_{1z} by f_{2z} in the expression of the layer longitudinal magnetizations. This yields

$$q_{nz} = m_{nz}[f_{1z}(y_n) \rightarrow f_{2z}(y_n)]. \tag{15}$$

In this work we are interested in the calculation of the ordering near the transition Curie temperature. The usual argument, 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 Curie temperature. Consequently, all terms of the order higher than linear terms in Eqs. (13) that give the expressions of m_{nz} can be neglected. This leads to the set of simultaneous equations

$$m_{nz} = A_{n,n-1}m_{n-1,z} + A_{n,n}m_{nz} + A_{n,n+1}m_{n+1,z}, \tag{16}$$

or

$$A\mathbf{m}_z = \mathbf{m}_z, \tag{17}$$

where \mathbf{m}_z is a vector of components $(m_{1z}, m_{2z}, \dots, m_{nz}, \dots, m_{Lz})$ and the matrix A is symmetric and tridiagonal with elements

$$A_{i,j} = A_{i,i}\delta_{i,j} + A_{i,j}(\delta_{i,j-1} + \delta_{i,j+1}). \tag{18}$$

The system of Eqs. (17) is of the form

$$M\mathbf{m}_z = \mathbf{0}, \tag{19}$$

where

$$M_{i,j} = (A_{i,j} - 1)\delta_{i,j} + A_{i,j}(\delta_{i,j-1} + \delta_{i,j+1}). \quad (20)$$

The only non-zero elements of the matrix M are given by

$$M_{n,n-1} = 2^{-N-2N_0} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu_1} \sum_{j=0}^{N_0-(\mu_1+\nu_1)} (-1)^i 2^{\mu+\mu_1+\mu_2} \delta_{1,i+j} \quad (21)$$

$$C_{\mu}^N C_{\nu}^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} C_i^{\nu_1} C_j^{N_0-(\mu_1+\nu_1)} (1-t_n)^{\nu}$$

$$(1-t_{n-1})^{\mu_1} (1-t_{n+1})^{\mu_2} t_n^{N-\mu} t_{n-1}^{(N_0-\mu_1)-(i+j)} t_{n+1}^{N_0-\mu_2} f_{1z}(y_n),$$

$$M_{n,n} = 2^{-N-2N_0} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu} \sum_{j=0}^{N-(\mu+\nu)} (-1)^i 2^{\mu+\mu_1+\mu_2} \delta_{1,i+j} \quad (22)$$

$$C_{\mu}^N C_{\nu}^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} C_i^{\nu} C_j^{N-(\mu+\nu)} (1-t_n)^{\mu}$$

$$(1-t_{n-1})^{\mu_1} (1-t_{n+1})^{\mu_2} t_n^{N-\mu-(i+j)} t_{n-1}^{(N_0-\mu_1)} t_{n+1}^{N_0-\mu_2} f_{1z}(y_n) - 1,$$

$$M_{n,n+1} = 2^{-N-2N_0} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu_2} \sum_{j=0}^{N_0-(\mu_2+\nu_2)} (-1)^i 2^{\mu+\mu_1+\mu_2} \delta_{1,i+j} \quad (23)$$

$$C_{\mu}^N C_{\nu}^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} C_i^{\nu_1} C_j^{N_0-(\mu_2+\nu_2)} (1-t_n)^{\mu}$$

$$(1-t_{n-1})^{\mu_1} (1-t_{n+1})^{\mu_2} t_n^{N-\mu} t_{n-1}^{(N_0-\mu_1)} t_{n+1}^{N_0-\mu_2-(i+j)} f_{1z}(y_n),$$

where the t_n are the values of the q_{nz} when $m_{nz} = 0$ at the critical point, which are given by

$$t_n = 2^{-N-2N_0} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} 2^{\mu+\mu_1+\mu_2} C_{\mu}^N C_{\nu}^{N-\mu} \quad (24)$$

$$C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} (1-2t_n)^{\mu} t_n^{N-\mu} (1-2t_{n-1})^{\mu_1} t_{n-1}^{(N_0-\mu_1)}$$

$$(1-2t_{n+1})^{\mu_2} t_{n+1}^{N_0-\mu_2} f_{2z}(y_n).$$

All the information about the Curie temperature of the system is contained in Eq. (19). Up to now we did not define the values of the exchange interactions; the terms in matrix (19) are general ones. In a general case, for arbitrary coupling constants and superlattice thickness the evaluation of the Curie temperature relies on the numerical solution of the system of linear equations (19). These equations are fulfilled if and only if

$$\det M = 0. \quad (25)$$

This condition can be satisfied or L different values of the Curie temperature T_c . In this paper, we take J_{aa} as the unit of the energy, the length is measured in units of the lattice constant. Let us

where the elements in the determinant are given by

$$c = \left(\frac{1}{M_{1,1}} \right)^2 \left(\frac{1}{M_{2,1}} \right)^{L_a-2} \left(\frac{1}{M_{L_a+1,L_a+1}} \right)^2 \left(\frac{1}{M_{L_a+2,L_a+1}} \right)^{L_b-2}, \quad (32)$$

$$\begin{aligned} a_1 &= M_{1,1}/M_{1,2}, & a_2 &= M_{L_a+1,L_a+1}/M_{L_a+1,L_a+2}, \\ b_1 &= M_{1,1}/M_{1,L}, & b_2 &= M_{L_a+L_b-1,L_a+1}/M_{L_a+1,L_a+2}, \\ c_1 &= M_{2,2}/M_{2,1}, & c_2 &= M_{L_a+2,L_a+2}/M_{L_a+2,L_a+1}, \end{aligned} \quad (33)$$

By solving Eq. (31) numerically, we can obtain the critical properties of the superlattice.

III. Results an discussion

For the pure Ising model, we obtain the critical value of the temperature $k_B T_c^B / J_{aa} = 3.518$ from Eq. (30), which is intermediate between the low-temperature series expansion result, $T_c^{SE} / J_{aa} = 3.194$ [17], and the mean-field theory result, $k_B T_c^{MFT} / J_{aa} = 4$ [18], and is the same result reported by Fittipaldi *et al.* [19] for the bulk media.

From Eq. (31), we can obtain the Curie temperature of the infinite superlattice $k_B T_c / J_{aa}$ for given values of the coupling exchanges J_{bb} and J_{ab} and a fixed number of layers of the two components. For the case of $J_{ab} = 0$, the superlattice reduces to two slabs, so there exists separated phase transitions in the two slabs. But we are interested in the case $J_{ab} \neq 0$. We study the dependence of the phase transition temperature on the interface coupling J_{ab} . We fix the layer-number of slab A ($L_a = 2$) and let the layer-number L_b of slab B change. Such results are shown in Fig. 2. Generally, the Curie temperature of the infinite superlattice increases with an increase in J_{ab} . With L_a fixed, the Curie temperature of the superlattice increases with an increase in L_b for fixed values of $J_{bb}/J_{aa} = 0.75$, for large J_{ab}/J_{aa} ; while it is almost independent of L_b when J_{ab}/J_{aa} is sufficiently small. Fixing L_b , the Curie temperature increases with J_{ab}/J_{aa} .

We can clearly see this behavior in Fig. 3, where the Curie temperatures $k_B T_c(L_b) / J_{aa}$ are presented for superlattices with various layer-number L_b of the slab B . The characteristic properties of the curves, as indicated in the figure, obtained for the fixed values, $J_{bb}/J_{aa} = 0.75$, $L_a = 2$ and two different values, $J_{ab}/J_{aa} = 1$ and 2 , is a decrease of the superlattice Curie temperature $k_B T_c(L_b) / J_{aa}$ when the layer-number of slab B increases and an increase with J_{ab}/J_{aa} for fixed L_b .

In Fig. 4, we plot the Curie temperature of the infinite superlattice against J_{ab}/J_{aa} for fixed values of J_{bb}/J_{aa} , L_b , while the layer-number of slab A changes. It is easy to see from this figure that there exists a critical value of the reduced interface coupling strength $(J_{ab}/J_{aa})_{crit} = 1.586$ which is independant of the thickness L_b of slab B . As the layer-number L_a of slab A increases, the Curie temperature of the superlattice decreases for $(J_{ab}/J_{aa})_{crit} < J_{ab}/J_{aa}$ and is approximately linear, in good agreement with the result of the spin-1/2 case [13], but increases for $(J_{ab}/J_{aa})_{crit} > J_{ab}/J_{aa}$. At this critical point, the Curie temperature does not depend on the layer-number L_a of slab A an is equal to its bulk Curie temperature.

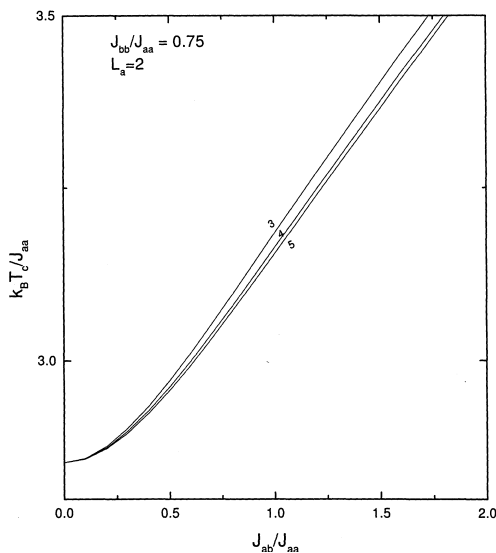


FIG. 2. The Curie temperature $k_B T_c / J_{aa}$ versus J_{ab} / J_{aa} for fixed values of $L_a = 2$ and $J_{bb} / J_{aa} = 0.75$. The number accompanying each curve denotes the value of L_b .

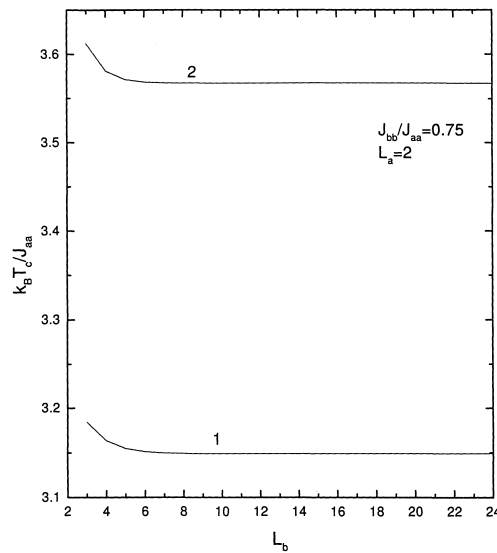


FIG. 3. The dependence of the Curie temperature $k_B T_c(L_b) / J_{aa}$ on the layer-number L_b of the slab B for fixed values of $L_a = 2$ and $J_{bb} / J_{aa} = 0.75$. The number accompanying each curve denotes the value of J_{ab} / J_{aa} .

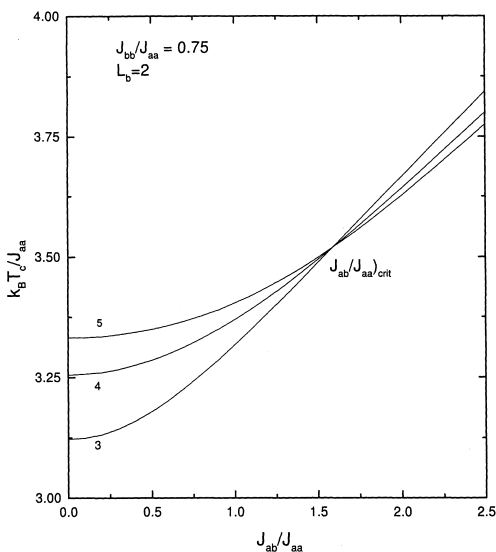


FIG. 4. The Curie temperature $k_B T_c / J_{aa}$ versus J_{ab} / J_{aa} for fixed values of $L_b = 2$ and $J_{bb} / J_{aa} = 0.75$. The number accompanying each curve denotes the value of L_a .

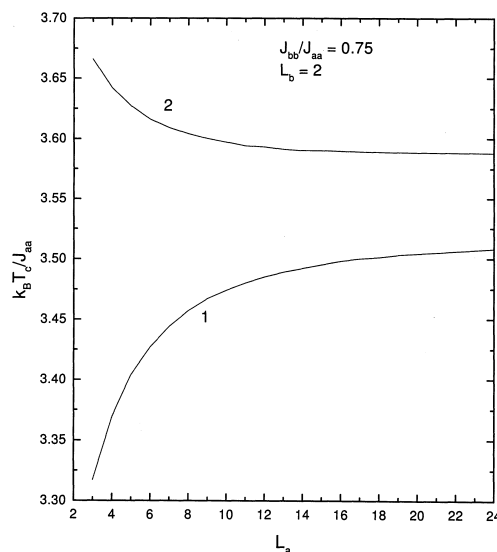


FIG. 5. The dependence of the Curie temperature $k_B T_c(L_a) / J_{aa}$ on the layer-number L_a of the slab A for fixed values of $L_b = 2$ and $J_{bb} / J_{aa} = 0.75$. The number accompanying each curve denotes the value of J_{ab} / J_{aa} .

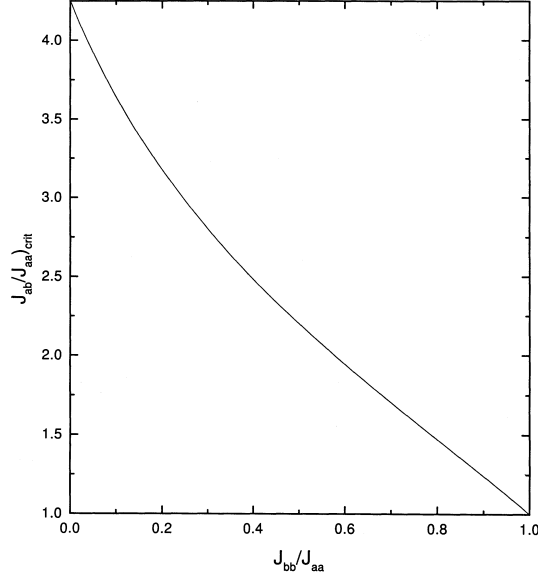


FIG. 6. The reduced critical interface exchange interaction $(J_{ab}/J_{aa})_{crit}$ on the reduced exchange interaction J_{bb}/J_{aa} .

Fig. 5 corresponds to $J_{bb}/J_{aa} = 0.75$ and $L_b = 2$. The horizontal line corresponds to the case of $(J_{ab}/J_{aa})_{crit} = 1.586$, such that $k_B T_c^B/J_{aa} = k_B T_c/J_{aa} = 3.518$ and remains constant for any L_a . We see that $k_B T_c(L_a)/J_{aa}$ increases with increase of J_{ab}/J_{aa} . For $(J_{ab}/J_{aa})_{crit} < J_{ab}/J_{aa} = 2$, the Curie temperature of the superlattice is higher than the bulk Curie temperature of slab A, $k_B T_c^B/J_{aa}$, and $k_B T_c(L_a)/J_{aa}$ decreases with an increase of L_a to reach an asymptotic value. For $(J_{ab}/J_{aa})_{crit} > J_{ab}/J_{aa} = 1$, the Curie temperature of the superlattice is smaller than the bulk Curie temperature $k_B T_c^B/J_{aa}$ and $k_B T_c(L_a)/J_{aa}$ increases with an increase of L_a to reach asymptotically $k_B T_c^B/J_{aa}$ for large values of L_a .

Fig. 6 shows the dependence of $(J_{ab}/J_{aa})_{crit}$ on J_{bb}/J_{aa} for fixed values of L_b ; the critical coupling exchange J_{ab}/J_{aa} is independent of the layer-number L_a of slab A [see Fig. 4]. We note that when J_{bb}/J_{aa} decreases, the value of $(J_{ab}/J_{aa})_{crit}$ increases, and when $J_{bb}/J_{aa} = 1$, $(J_{ab}/J_{aa})_{crit} = 1$ as expected.

In Figs. 7a(b), we show the Curie temperature $k_B T_c/J_{aa}$ against J_{bb}/J_{aa} , for fixed $L_a(L_b) = 2$ and different values of $L_b(L_a) = 3, 4, \text{ and } 5$ and for $J_{ab} = (J_{aa} + J_{bb})/2$. For $J_{bb}/J_{aa} > 1$, the Curie temperature decreases (increases) with the increase of $L_b(L_a)$ and is always larger than the bulk Curie temperature of the slab A $k_B T_c^B/J_{aa} = 3.518$. For $J_{bb}/J_{aa} < 1$, we have just the opposite situation. Notice that, for small values of J_{bb}/J_{aa} , the Curie temperature is insensitive to L_a [see Fig. 7b]. or $J_{bb}/J_{aa} = 1$, the Curie temperature is independent of $L_b(L_a)$, the layer-number of the slab B(A) of the two component superlattice, and is equal to $k_B T_c^B/J_{aa}$, as expected.

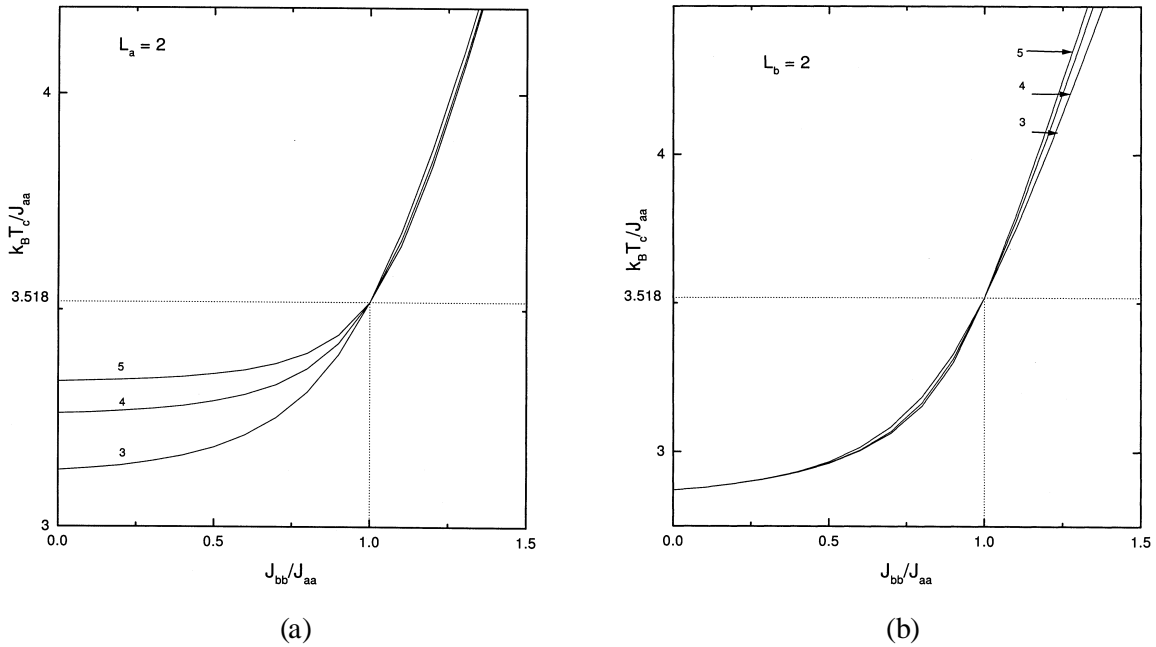


FIG. 7. a(b). The dependence of the Curie temperature on J_{bb}/J_{aa} for $L_a(L_b) = 2$, $J_{ab} = (J_{aa} + J_{bb})/2$ with different values of $L_b(L_a) = 3, 4$ and 5 denoted by the numbers.

IV. Conclusion

In conclusion, the properties of the phase transition of a ferromagnetic infinite superlattices describing the spin-one Ising model in effective field theory, have been discussed in this paper. The dependence of the Curie temperature on the inter- and intralayer strength coupling of the simplest case when the superlattice is infinite has been obtained.

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