

The transverse ferromagnet spin-1 Ising model of alternating magnetic superlattice

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Abstract. Within the framework of the effective field theory with a probability distribution technique that accounts for the single-site spin correlations, we examine the critical behavior of the transverse ferromagnetic spin-1 Ising model of an alternating magnetic superlattice. The critical temperature of the alternating magnetic superlattice has been studied as a function of the interlayer and intralayer exchange interactions and the strength of the transverse field and the thickness of the finite superlattice.

PACS. 77.80.Bh Phase transitions and Curie point – 75.70.Cn Interfacial magnetic properties (multilayers, magnetic quantum wells, superlattices, magnetic heterostructures)

1 Introduction

During the last few years much effort has been directed towards the study of the critical phenomena in various magnetic layered structures and superlattices [1–7]. The basic theoretical problem is the examination of the magnetic excitation and the phase transitions in these systems. Magnetic excitations in superlattices were considered in numerous papers (see *e.g.* [8] for a brief review). Yet, less attention has been paid to the critical behavior and in particular to the critical temperatures in superlattices. Ma and Tasi [9] have studied the variation with modulation wavelength of the Curie temperature for a Heisenberg magnetic superlattice. Their results agree qualitatively with experiments on Cu/Ni films [10]. Superlattice structures composed of alternating ferromagnetic and antiferromagnetic layers have been investigated by Hinckey and Mills [11,12], using a localized spin model. A sequence of spin transitions is found to be different for superlattices with antiferromagnetic component consisting of an even or odd number of spin layers. In two earlier papers [5,6] one of the present authors has studied the effects of a uniform transverse and surface magnetism on the critical behavior of an alternating ferromagnetic spin-1/2 Ising superlattice, we study in this paper the effect of a uniform transverse field on the critical temperature of a spin-1 Ising superlattice consisting of two ferromagnetic materials with different bulk properties, with a simple cubic

structure. 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 in its simplest form [13–15]. This technique is believed to give more exact results than those of the standard mean-field approximation and it has been applied successfully to the study of various physical problems, in particular to the transverse spin-1/2 Ising multilayers [16]. In Section 2 we outline the formalism and derived the equation that determines the transition temperature. Both analytical and numerical results are discussed in Section 3 for the case of an infinite superlattice where the interface magnetic phase transition is studied and the critical value of the reduced interlayer exchange interaction is determined. The case of a finite superlattice is discussed in Section 4. The last section is devoted to a short conclusion.

2 Model and formulation

We consider an infinite simple cubic superlattice with a unit cell consisting of arbitrary number L of magnetic layers. The transverse spin-1 Ising Hamiltonian of the system is given by

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

where σ_{nr}^z and σ_{nr}^x denote respectively the z and x components of a quantum spin σ_{nr} of magnitude $\sigma_{nr} = 1$ at site (n, r) , (n, n') , are plane indices and (r, r') are different sites of the planes, and $J_{nn'}$ is the strength of the

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ferromagnetic exchange interaction which is only plane dependent, and Ω_n is the strength of the transverse field.

The statistical properties of the system are studied using an effective field theory that employs the probability distribution technique, which 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

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

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

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

where $\alpha = z, x$, $p = 1, 2$, $\langle \langle (\sigma_{nr}^\alpha)^p \rangle_c \rangle$ denotes the mean value of $(\sigma_{nr}^\alpha)^p$ for a given configuration c of all other spins, $\langle \dots \rangle$ denotes the average over all spin configurations $\sigma_{n', r'}$, Tr_{nr} means the trace performed over $(\sigma_{nr}^\alpha)^p$ only, $\beta = 1/k_B T$ with k_B the Boltzmann constant (we take $k_B = 1$ for simplicity) and T 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

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

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

where

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

$$f_{2z}(A, B) = \frac{1}{[A^2 + B^2]} \times \frac{B^2 + (2A^2 + B^2) \cosh(\beta [A^2 + B^2]^{1/2})}{1 + 2 \cosh(\beta [A^2 + B^2]^{1/2})} \quad (7)$$

and

$$f_{1x}(A, B) = f_{1z}(B, A) \quad (8)$$

$$f_{2x}(A, B) = f_{2z}(B, A) \quad (9)$$

with

$$A = \sum_{n'} \sum_{r'} J_{nn'} \sigma_{n', r'}^z, \quad (10)$$

$$B = \Omega_n \quad (11)$$

where the first and second sums run over all possible configurations of atoms environing or lying on the (n, r) site, respectively. Each of these configurations can be characterized by numbers 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 [13–15]. Thus with the use of the integral representation method of Dirac δ -distribution, equations (4) and (5) can be written in the form

$$\langle \langle \sigma_{nr}^\alpha \rangle_c \rangle = \int d\omega f_{1\alpha}(\omega, B) \frac{1}{2\pi} \times \int dt \exp(i\omega t) \prod_{n', r'} \langle \exp(-it J_{n, n'} \sigma_{n', r'}^z) \rangle \quad (12)$$

$$\langle \langle (\sigma_{nr}^\alpha)^2 \rangle_c \rangle = \int d\omega f_{2\alpha}(\omega, B) \frac{1}{2\pi} \times \int dt \exp(i\omega t) \prod_{n', r'} \langle \exp(-it J_{n, n'} \sigma_{n', r'}^z) \rangle. \quad (13)$$

In the derivation of the equations (12) and (13), 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

$$\langle \sigma_j^z (\sigma_k^z)^2 \dots \sigma_l^z \rangle \approx \langle \sigma_j^z \rangle \langle (\sigma_k^z)^2 \rangle \dots \langle \sigma_l^z \rangle \quad \text{for } j \neq k \dots \neq l. \quad (14)$$

Then, as $\langle \langle \sigma_{nr}^\alpha \rangle_c \rangle$ and $\langle \langle (\sigma_{nr}^\alpha)^2 \rangle_c \rangle$ 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 [13–15]

$$P(\sigma_{nr}^z) = \frac{1}{2} [(q_{nz} - m_{nz}) \delta(\sigma_{nr}^z + 1) + 2(1 - q_{nz}) \delta(\sigma_{nr}^z) + (q_{nz} + m_{nz}) \delta(\sigma_{nr}^z - 1)]. \quad (15)$$

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 equations (4, 12, 15) yields

$$\begin{aligned}
m_{n\alpha} &= 2^{-N-2N_0} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} 2^{\mu+\mu_1+\mu_2} C_\mu^N C_\nu^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} \\
&\times (1-2q_{nz})^\mu (q_{nz}-m_{nz})^\nu (q_{nz}+m_{nz})^{N-\mu-\nu} (1-2q_{n-1,z})^{\mu_1} (q_{n-1,z}-m_{n-1,z})^{\nu_1} (q_{n-1,z}+m_{n-1,z})^{N_0-\mu_1-\nu_1} \\
&\times (1-2q_{n+1,z})^{\mu_2} (q_{n+1,z}-m_{n+1,z})^{\nu_2} (q_{n+1,z}+m_{n+1,z})^{N_0-\mu_2-\nu_2} f_{1\alpha}(y_n, \Omega_n), \tag{16}
\end{aligned}$$

$$\begin{aligned}
M_{n,n-1} &= 2^{-N-2N_0} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu_1} \sum_{j=0}^{N_0-(\mu_1+\nu_1)} (-1)^i 2^{\mu+\mu_1+\mu_2} \delta_{1,i+j} C_\mu^N C_\nu^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} \\
&\times C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} C_i^{\nu_1} C_j^{N_0-(\mu_1+\nu_1)} (1-r_n)^\mu (1-r_{n-1})^{\mu_1} (1-r_{n+1})^{\mu_2} r_n^{N-\mu} r_{n-1}^{(N_0-\mu_1)-(i+j)} r_{n+1}^{N_0-\mu_2} f_{1z}(y_n, \Omega_n) \tag{24}
\end{aligned}$$

$$\begin{aligned}
M_{n,n} &= 2^{-N-2N_0} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu} \sum_{j=0}^{N-(\mu+\nu)} (-1)^i 2^{\mu+\mu_1+\mu_2} \delta_{1,i+j} C_\mu^N C_\nu^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} \\
&\times C_{\nu_2}^{N_0-\mu_2} C_i^\nu C_j^{N-(\mu+\nu)} (1-r_n)^\mu (1-r_{n-1})^{\mu_1} (1-r_{n+1})^{\mu_2} r_n^{N-\mu-(i+j)} r_{n-1}^{(N_0-\mu_1)} r_{n+1}^{N_0-\mu_2} f_{1z}(y_n, \Omega_n) - 1 \tag{25}
\end{aligned}$$

$$\begin{aligned}
M_{n,n+1} &= 2^{-N-2N_0} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu_2} \sum_{j=0}^{N_0-(\mu_2+\nu_2)} (-1)^i 2^{\mu+\mu_1+\mu_2} \delta_{1,i+j} C_\mu^N C_\nu^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} \\
&\times C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} C_i^{\nu_2} C_j^{N_0-(\mu_2+\nu_2)} (1-r_n)^\mu (1-r_{n-1})^{\mu_1} (1-r_{n+1})^{\mu_2} r_n^{N-\mu} r_{n-1}^{(N_0-\mu_1)} r_{n+1}^{N_0-\mu_2-(i+j)} f_{1z}(y_n, \Omega_n), \tag{26}
\end{aligned}$$

the following set of equations for the layer longitudinal magnetizations

see equation (16) above

where

$$\begin{aligned}
y_n &= [J_{n,n}(N-\mu-2\nu) + J_{n,n-1}(N_0-\mu_1-2\nu_1) \\
&+ J_{n,n+1}(N_0-\mu_2-2\nu_2)] \tag{17}
\end{aligned}$$

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 $m_{0\alpha} = m_{L\alpha}$, $m_{L+1,\alpha} = m_{1\alpha}$, $q_{0\alpha} = q_{L\alpha}$, and $q_{L+1,\alpha} = q_{1\alpha}$.

The equations of the longitudinal and transverse quadrupolar moments are obtained by substituting the function $f_{1\alpha}$ by $f_{2\alpha}$ in the expressions of the layer longitudinal and transverse magnetizations respectively. This yields

$$q_{n\alpha} = m_{n\alpha} [f_{1\alpha}(y_n, \Omega_n) \rightarrow f_{2\alpha}(y_n, \Omega_n)]. \tag{18}$$

In this work we are interested with the calculation of the ordering near the transition critical 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 critical temperature. Consequently, all terms of the order higher than linear terms in equation (16) that give the expressions of m_{nz} can be neglected.

This leads to the set of simultaneous equations

$$m_{nz} = A_{n,n-1}m_{n-1,z} + A_{n,n}m_{nz} + A_{n,n+1}m_{n+1,z} \tag{19}$$

or

$$A\mathbf{m}_z = \mathbf{m}_z \tag{20}$$

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

$$A_{i,j} = A_{i,i}\delta_{i,j} + A_{i,j}(\delta_{i,j-1} + \delta_{i,j+1}). \tag{21}$$

The system of equations (20) is of the form

$$M\mathbf{m}_z = 0 \tag{22}$$

where

$$M_{i,j} = (A_{i,j} - 1)\delta_{i,j} + A_{i,j}(\delta_{i,j-1} + \delta_{i,j+1}). \tag{23}$$

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

see equations (24–26) above,

where the r_n are the values of the q_{nz} when $m_{nz} = 0$ at

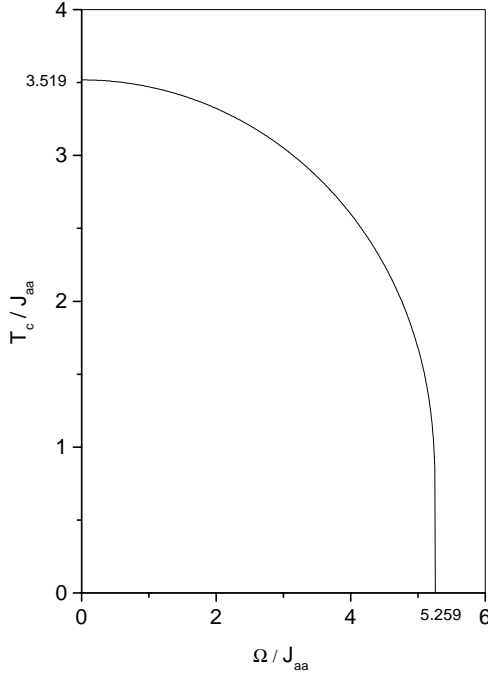


Fig. 1. The variation of the bulk critical temperature T_c/J_{aa} versus the strength of the transverse field Ω/J_{aa} for the transverse spin-1 Ising model on a simple cubic lattice.

whose value is

$$\det M_{ab} = (a_1 a_2)^L \prod_{k=1}^L \left\{ 1 - \frac{2b_1 b_2}{a_1 a_2} \times \left[1 + \cos \left(\frac{2\pi(k-1)}{L} \right) \right] \right\}, \quad (35)$$

where the elements in the determinant are given by

$$\begin{cases} a_1 = M_{n,n} (J_{n,n} = J_{aa}, J_{n,n-1} = J_{n,n+1} = J_{ab}, \Omega) \\ b_1 = M_{n,n-1} (J_{n,n} = J_{aa}, J_{n,n-1} = J_{n,n+1} = J_{ab}, \Omega) \\ \quad = M_{n,n+1} (J_{n,n} = J_{aa}, J_{n,n-1} = J_{n,n+1} = J_{ab}, \Omega) \\ \quad \quad n = 1, 3, \dots, 2L-1 \end{cases} \quad (36)$$

$$\begin{cases} a_2 = M_{n,n} (J_{n,n} = J_{bb}, J_{n,n-1} = J_{n,n+1} = J_{ab}, \Omega) \\ b_2 = M_{n,n-1} (J_{n,n} = J_{bb}, J_{n,n-1} = J_{n,n+1} = J_{ab}, \Omega) \\ \quad = M_{n,n+1} (J_{n,n} = J_{bb}, J_{n,n-1} = J_{n,n+1} = J_{ab}, \Omega) \\ \quad \quad n = 2, 4, \dots, 2L \end{cases} \quad (37)$$

L in the case of an infinite alternating superlattice is an arbitrary number. Now we obtain the critical temperature of the system from the condition given by

$$\det M_{ab} = 0. \quad (38)$$

From the numerical treatment of equation (38), we can determine the critical temperature of the infinite alternating superlattice as a function of the reduced exchange interactions R_1 and R_2 . We assume that $R_1 \leq 1$ and denote

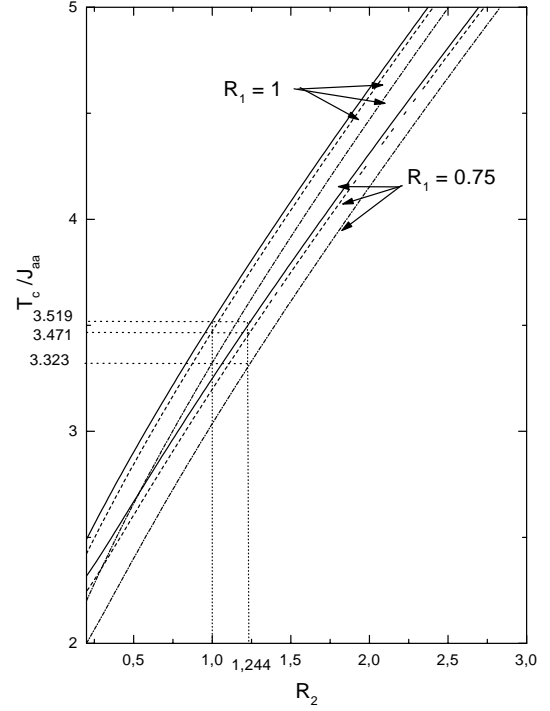


Fig. 2. Dependence of the bulk critical temperature T_c/J_{aa} on the reduced interface exchange interaction R_2 , for different values of the reduced exchange interaction R_1 and different values of the strength of the transverse field. The dotted horizontal lines show the bulk critical temperatures of a uniform cubic lattice *i.e.* when $R_1 = R_2 = 1$. $T_c/J_{aa} = 3.519, 3.471, 3.323$, and for $\Omega/J_{aa} = 0, 1$ and 2 respectively.

by $T_c^a/J_{aa} = 3.519$ and by $T_c^b/J_{aa} = (T_c^a/J_{aa}) R_1$ the bulk critical temperature of a uniform lattice of material A and of material B. In Figure 2 we show the dependence of the critical temperature T_c/J_{aa} on the reduced interlayer exchange coupling R_2 for various values of R_1 and Ω/J_{aa} . This dependence is approximately linear, in agreement with the spin-1/2 case [20] and in disagreement with the results of [5]. It is interesting to note that for every choice of R_1 and Ω/J_{aa} , there exists a critical value R_2^c of the interface exchange coupling such that when $R_2 > R_2^c$ we have $T_c/J_{aa} > T_c^a/J_{aa}$; T_c^b/J_{aa} the system may order in the interface layers before the intralayer ordering, *i.e.* the interlayer magnetism dominates. For $R_2 < R_2^c$, $T_c/J_{aa} < T_c^a/J_{aa}$; we have the contrary situation. Initially it has a place intralayer magnetism dominates and the system behaves like metamagnets. From Figure 2, we obtained the critical values of R_2^c for different values of R_1 and Ω/J_{aa} , and are collected together in Table 1. We see that for each value of R_1 , R_2^c is independent of Ω/J_{aa} .

4 Finite superlattice

In the case of the finite superlattice we restricted our discussion to take into account the effects of finite thickness of our superlattice, we have to consider all unit cells, because the periodicity is broken on the surface layers.

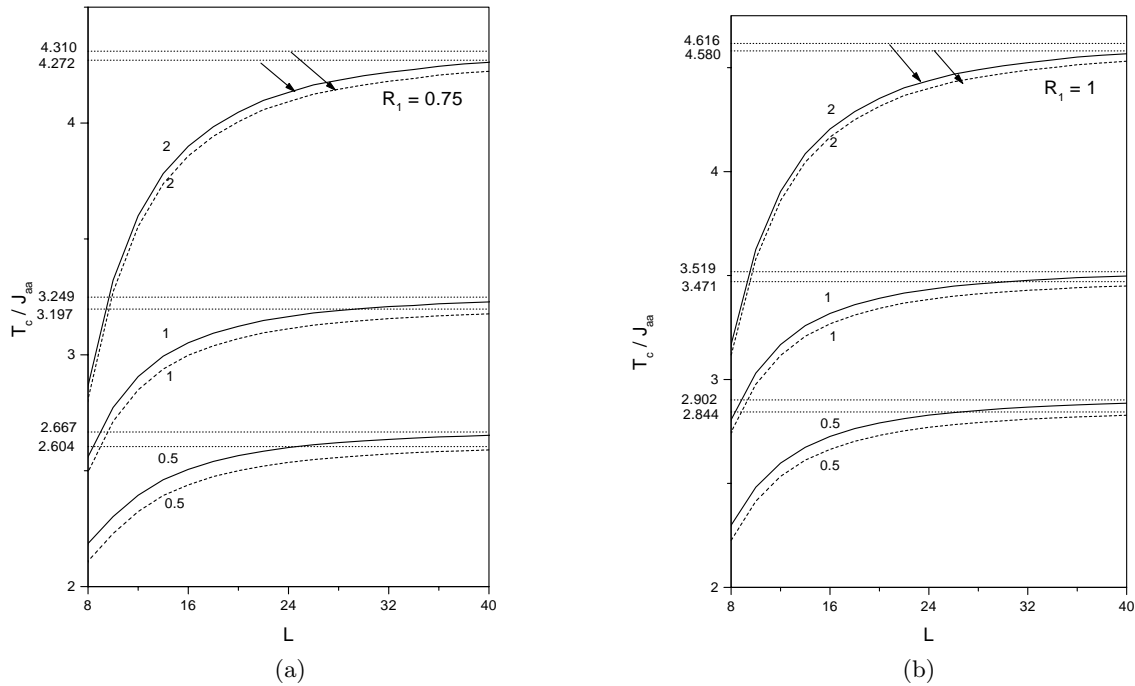


Fig. 3. The dependence of the critical temperature T_c/J_{aa} of the finite superlattice on the thickness for various values of R_1 and R_2 . (a) $R_1 = 0.75$, (b) $R_1 = 1$. The number accompanying each curve denote the values of R_2 . The dotted lines shows the critical temperature of the infinite superlattice (bulk critical temperature). The solid and dashed curves correspond respectively to $\Omega/J_{aa} = 0$, and 1.

Table 1. Critical values of R_2^c

R_1	Ω/J_{aa}	R_2^c
0.75	0	1.244
"	1	1.244
"	2	1.244
1	0	1
"	1	1
"	2	1

The dependence of the critical temperature T_c/J_{aa} on the superlattice thickness (the thickness is measured in units of the lattice constant in our calculations) is shown in Figures 3a,b for various values of R_1 and R_2 and Ω/J_{aa} , the critical temperature of the finite superlattice increases with the increase of R_2 (R_1). The critical temperature of the finite superlattice is always less than that of the corresponding infinite superlattice and reaches the last one for large values of L . As expected, the critical temperature of the finite superlattice decreases with the increase of the strength of the transverse field Ω/J_{aa} , for fixed values of R_1 and R_2 .

5 Conclusion

In conclusion, we have examined a spin-1 Ising model of an alternating magnetic superlattice. The formalism of transition temperature derivation obtained above is universal and can be used for study of superlattice of various thicknesses and structures. The authors are presently working on extension and application of this formalism to more complicated models: a superlattice with an arbitrary number of layers, a superlattice with dilution, a superlattice with high spin, and so on.

Although we have discussed our results using only ferromagnetic exchanges (all J 's > 0), the formalism is applicable to antiferromagnetic coupling (some or all J 's < 0).

In this paper we also introduce some critical value of interlayer exchange constant R_2^c so that for $R_2 > R_2^c$ ($R_2 < R_2^c$) the interlayer (intralayer) ordering dominates. We found that the critical temperature of the finite superlattice is always less than the critical temperature of the bulk system (infinite superlattice) and reaches the last one when the thickness L becomes large. The critical temperature decreases with the increase of the strength of the transverse field.

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