Eur. Phys. J. B **23**, 235–241 (2001)

THE EUROPEAN PHYSICAL JOURNAL B
EDP Sciences

Phase transitions of a spin-one alternating magnetic superlattice

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Received 2 March 2001

Abstract. We examine the critical behavior of a magnetic superlattice which made up of two magnetic materials, A and B. Using the effective field theory with a probability distribution technique that accounts for the single-site spin correlation, we derive the analytical equation for the Curie temperature of the superlattice which alternates as $ABAB\ldots AB$. The dependence of the Curie temperature on the interface coupling strength J_{ab} and the layer number of the finite superlattice was calculated. The effects of the surface modification are also studied.

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

1 Introduction

Magnetic superlattices artificially fabricated that consists of two or more ferromagnets materials have been studied in great detail because their physics properties differ dramatically from simple solids formed from the same materials. The development of film deposition technique 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 behaviour depending on the materials, the thickness and the number of slabs and of the applied field [1–5]. A number of theoretical works have been devoted to the magnetic and phase transition properties of superlattices formed from alternating layers of different materials [6–14].

In this article, we study the critical properties of alternating magnetic superlattices using the 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 derived the equation that determine the transition temperature. Numerical results are discussed in Section 3. A brief conclusion is given in Section 4.

2 Formalism

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

$$H = -\sum_{n,n'}\sum_{r,r'} J_{nn'}\sigma^z_{nr}\sigma^z_{n'r'}, \tag{1}$$

where σ^z_{nr} denotes the z component of a quantum spin $\boldsymbol{\sigma}_{nr}$ 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 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 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

$$H_{nr} = -\left(\sum_{n',\ r'} J_{nn'}\sigma^z_{n'r'}\right)\sigma^z_{nr}. \tag{2}$$

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

$$\langle\langle(\sigma^z_{nr})^p\rangle_c\rangle = \left\langle \frac{\mathrm{Tr}_{nr}\left[(\sigma^z_{nr})^p \exp\left(-\beta H_{nr}\right)\right]}{\mathrm{Tr}_{nr}\left[\exp\left(-\beta H_{nr}\right)\right]}\right\rangle \tag{3}$$

where $\langle(\sigma^z_{nr})^p\rangle_c$ denotes the mean value of $(\sigma^z_{nr})^p$ for a given configuration c of all other spins, $\langle ... \rangle$ denotes the average over all spin configurations σ_{nr}, Tr_{nr} means the trace performed over $(\sigma^z_{nr})^p$ only, $\beta = 1/k_{\mathrm{B}}T$ with k_{B} the Boltzmann constant and T the absolute temperature. For a fixed configuration of neighbouring spins of the site (n, r) the longitudinal and the transverse magnetizations

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

and quadrupolar moments of any spin at site (n,r) are given by,

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

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

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 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 [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

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

$$\left\langle\left\langle(\sigma_{nr}^z)^2\right\rangle_c\right\rangle = \int \mathrm{d}\omega f_{2z}(\omega,B)\frac{1}{2\pi}\int \mathrm{d}t\exp(\mathrm{i}\omega t) \times \prod_{n'r'}\langle\exp(-\mathrm{i}tJ_{n,n'}\sigma_{n'r'}^z)\rangle \cdot \quad (10)$$

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

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

Then, as $\langle\langle\sigma_{nr}^z\rangle_c\rangle$ and $\left\langle\left\langle(\sigma_{nr}^z)^2\right\rangle_c\right\rangle$ are independent of r, we introduce the longitudinal magnetization and the longitudinal quadrupolar moment of the nth 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 equations (4, 9, 12) yields the following set of equations for the layer longitudinal magnetizations

see equation (13) above,

where

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

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 $q_{0z} = q_{Lz}$, 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

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

In this work we are interested with 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 equations (13) that give the expressions of

$$M_{n,n-1} = 2^{-N-2N_0} \sum_{\mu=0}^{N} \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu_1} \sum_{j=0}^{N_0-(\mu_1+\nu_1)} (-1)^i \, 2^{\mu+\mu_1+\mu_2} \delta_{1,i+j}$$
$$\times C_\mu^N C_\nu^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} C_i^{\nu_1} C_j^{N_0-(\mu_1+\nu_1)} (1-t_n)^\mu$$
$$\times (1-t_{n-1})^{\mu_1} (1-t_{n+1})^{\mu_2} \, t_n^{N-\mu} t_{n-1}^{(N_0-\mu_1)-(i+j)} t_{n+1}^{N_0-\mu_2} f_{1z}(y_n) \quad (21)$$

$$M_{n,n} = 2^{-N-2N_0} \sum_{\mu=0}^{N} \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu} \sum_{j=0}^{N_-(\mu+\nu)} (-1)^i \, 2^{\mu+\mu_1+\mu_2} \delta_{1,i+j}$$
$$\times C_\mu^N C_\nu^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} C_i^{\nu} C_j^{N-(\mu+\nu)} (1-t_n)^\mu$$
$$\times (1-t_{n-1})^{\mu_1} (1-t_{n+1})^{\mu_2} \, t_n^{N-\mu-(i+j)} t_{n-1}^{(N_0-\mu_1)} t_{n+1}^{N_0-\mu_2} f_{1z}(y_n) - 1 \quad (22)$$

$$M_{n,n+1} = 2^{-N-2N_0} \sum_{\mu=0}^{N} \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} \sum_{i=0}^{\nu_2} \sum_{j=0}^{N_0-(\mu_2+\nu 2)} (-1)^i \, 2^{\mu+\mu_1+\mu_2} \delta_{1,i+j}$$
$$\times C_\mu^N C_\nu^{N-\mu} C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} C_i^{\nu_1} C_j^{N_0-(\mu_2+\nu 2)} (1-t_n)^\mu$$
$$\times (1-t_{n-1})^{\mu_1} (1-t_{n+1})^{\mu_2} \, t_n^{N-\mu} t_{n-1}^{(N_0-\mu_1)} t_{n+1}^{N_0-\mu_2-(i+j)} f_{1z}(y_n) \quad (23)$$

m_{nz} can be neglected. This leads to the set of simultaneous equations

$$m_{nz} = A_{n,n-1} m_{n-1,z} + A_{n,n} m_{nz} + A_{n,n+1} m_{n+1,z} \quad (16)$$

or

$$A\mathbf{m}_z = \mathbf{m}_z \quad (17)$$

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

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

The system of equations (17) is of the form

$$M\mathbf{m_z} = \mathbf{0} \quad (19)$$

where

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

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

see equations (21–23) above,

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

see equation (24) below,

All the information about the Curie temperature of the system is contained in equation (19). Up to know 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 for L different values of the Curie temperature T_c. We denote by J_{aa} and J_{bb} the coupling strength between nearest-neighbouring spins in A and B respectively, while J_{ab} stands for the exchange coupling between the nearest-neighbour spins for all successive layers. 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 begin with the evaluation of the Curie temperature with an example: the Curie temperature of the spin-1 Ising model for the simplest possible "bulk case" of a material A (*i.e.* $N = 4$, $N_0 = 1$, $J_{i,j} = J_{aa}$).

$$t_n = 2^{-N-2N_0} \sum_{\mu=0}^{N} \sum_{\nu=0}^{N-\mu} \sum_{\mu_1=0}^{N_0} \sum_{\nu_1=0}^{N_0-\mu_1} \sum_{\mu_2=0}^{N_0} \sum_{\nu_2=0}^{N_0-\mu_2} 2^{\mu+\mu_1+\mu_2} C_\mu^N C_\nu^{N-\mu}$$
$$\times C_{\mu_1}^{N_0} C_{\nu_1}^{N_0-\mu_1} C_{\mu_2}^{N_0} C_{\nu_2}^{N_0-\mu_2} (1-2t_n)^\mu \, t_n^{N-\mu} (1-t_{n-1})^{\mu_1} \, t_{n-1}^{(N_0-\mu_1)}$$
$$\times (1-2t_{n+1})^{\mu_2} \, t_{n+1}^{N_0-\mu_2} f_{2z}(y_n). \quad (24)$$

Then we can reduce det$M$ to the following form

$$\det M = \begin{vmatrix} a & b & & & & & & & b \\ b & a & b & & & & & & \\ & b & a & b & & & & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & b & a & b & & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & & & b & a & b & \\ & & & & & & b & a & b \\ b & & & & & & & b & a \end{vmatrix}_{(L,L)} \quad (26)$$

whose value is

$$\det M_{\mathrm{bulk}} = \prod_{k=1}^{L} \left[a + 2b \cos\left(\frac{2\pi (k-1)}{L} \right) \right] \quad (27)$$

where the elements in the above determinant are given by

$$a = M_{n,n} \left(J_{n,n} = J_{n,n-1} = J_{n,n+1} = J_{aa} \right) \quad (28)$$

$$b = \frac{1}{4} (a+1) \quad (29)$$

and L in the "bulk" case is an arbitrary number. Now we obtain the Curie temperature from the condition given by

$$\det M_{\mathrm{bulk}} = 0. \quad (30)$$

We apply the obtained formalism to an alternating magnetic superlattice consisting of atoms of type A and B which alternate as $...ABABAB...AB...$ The periodic conditions suggests that we only have to consider one unit cell which interacts with its nearest neighbours *via* the interlayer coupling. Let us consider a simple alternating lattice of $2L$ layers $n = 1, 3, 5...2L-1$ consist of atoms of type A, whereas layers $n = 2, 4, ...2L$ consist of atoms of type B. In this case we can represent $\det M_{ab}$ as

$$\det M_{ab} = \begin{vmatrix} a_1 & b_1 & & & & & & b_1 \\ b_2 & a_2 & b_2 & & & & & \\ & b_1 & a_1 & b_1 & & & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & & b_2 & a_2 & b_2 & \\ & & & & & b_1 & a_1 & b_1 \\ b_2 & & & & & & b_2 & a_2 \end{vmatrix}_{(2L,2L)} \quad (31)$$

whose value is

$$\det M_{ab} = (a_1 a_2)^L \times \prod_{k=1}^{L} \left(1 - \frac{2 b_1 b_2}{a_1 a_2} \left[1 + \cos\left(\frac{2\pi (k-1)}{L} \right) \right] \right), \quad (32)$$

where the elements in the determinant are given by

$$\begin{cases} a_1 = M_{n,n} \left(J_{n,n} = J_{aa}, J_{n,n-1} = J_{n,n+1} = J_{ab} \right) \\ b_1 = M_{n,n-1} \left(J_{n,n} = J_{aa}, J_{n,n-1} = J_{n,n+1} = J_{ab} \right) \\ \quad = M_{n,n+1} \left(J_{n,n} = J_{aa}, J_{n,n-1} = J_{n,n+1} = J_{ab} \right) \end{cases}$$
$$\text{for} \quad n = 1, 3, ... \, 2L-1 \quad (33)$$

$$\begin{cases} a_2 = M_{n,n} \left(J_{n,n} = J_{bb}, J_{n,n-1} = J_{n,n+1} = J_{ab} \right) \\ b_2 = M_{n,n-1} \left(J_{n,n} = J_{bb}, J_{n,n-1} = J_{n,n+1} = J_{ab} \right) \\ \quad = M_{n,n+1} \left(J_{n,n} = J_{bb}, J_{n,n-1} = J_{n,n+1} = J_{ab} \right) \end{cases}$$
$$\text{for} \quad n = 2, 4, ... \, 2L \quad (34)$$

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

$$\det M_{ab} = 0. \quad (35)$$

3 Results and discussion

For the pure Ising model, we obtain the critical value of the temperature $T_{\mathrm{c}}/J_{aa} = 3.519$ from equation (30) which is intermediate between the low-temperature series expansion result, $T_{\mathrm{c}}^{\mathrm{SE}}/J_{aa} = 3.194$ [17], and the mean-field theory result, $T_{\mathrm{c}}^{\mathrm{MFT}}/J_{aa} = 4$ [18] and is the same result reported by Fittipaldi *et al.* [19] for the bulk media.

In the case of a finite superlattice we restricted our discussion to take into account the effects of finite thickness of the superlattice, we have to consider all unit cells because the periodicity is broken on the surface layers. In this case, for the alternating superlattice described before, $\det M$ reduces to

$$\det M = \begin{vmatrix} a_1 & b_1 & & & & & 0 \\ b_2 & a_2 & b_2 & & & & \\ & b_1 & a_1 & b_1 & & & \\ & & & & & & \\ & & & & b_2 & a_2 & b_2 \\ & & & & & b_1 & a_1 & b_1 \\ 0 & & & & & b_2 & a_2 \end{vmatrix}_{2L} \quad (36)$$

or

$$\det M_{2L} = c \det C_{2L} \quad (37)$$

with

$$\det C_{2L} = \begin{vmatrix} x_a & -1 & & & & & 0 \\ -1 & x_a & -1 & & & & \\ & -1 & x_a & -1 & & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & -1 & x_a & -1 & \\ & & & & -1 & x_a & -1 \\ 0 & & & & & -1 & x_a \end{vmatrix}_{2L} \quad (38)$$

and the coefficients x_a, x_b and c given by

$$x_a = -a_1/b_1 \quad (39)$$

$$x_b = -a_2/b_2 \quad (40)$$

$$c = a_1^L b_2^L. \quad (41)$$

Equation (36) satisfies the recurrence relation

$$\det C_{2L} = (x_a x_b - 2) \det C_{2L-2} - \det C_{2L-4}. \quad (42)$$

This difference equation has the solution [20]

$$\det C_{2L} = \frac{1}{\sinh(\varphi)} \left(\sinh\left[(L+1)\varphi\right] + \sinh(L\varphi)\right), \quad (43)$$

where

$$x_a x_b - 2 = 2\cosh(\varphi). \quad (44)$$

If $x_a x_b < 2$ then $\varphi = \mathrm{i}\theta$ and the hyperbolic functions become trigonometric functions of θ. The Curie temperature is given by

$$\det C_{2L} = 0. \quad (45)$$

This equation has no solution for $x_a x_b > 2$. For $x_a x_b \leq 2$, the solution is

$$\theta = \frac{2\pi}{2L+1} \quad (46)$$

and we have

$$x_a x_b - 2 = 2\cos\left(\frac{2\pi}{2L+1}\right). \quad (47)$$

From this equation, we can obtain the Curie temperature of the finite alternating superlattice $k_{\mathrm{B}}T_{\mathrm{c}}/J_{aa}$ for a given values of the coupling exchanges J_{bb} and J_{ab} and a fixed number of layers. For the case of $J_{ab} = 0$, the superlattice reduces to two layers, so there exists separated phase transitions in two layers. But we are interested in the case of $J_{ab} \neq 0$. Without loss of generality, we assume the Curie temperature of layer B is higher than that of layer A, that is, $J_{bb} > J_{aa}$. By numerical treatment, we can obtain the dependence of the Curie temperature on the interface coupling J_{ab}, shown in Figure 1. Generally, the Curie temperature of both infinite and finite superlattice increases with increase in J_{ab}. L fixed, the Curie temperature of the superlattice increases with increase in J_{bb} (see Fig. 1). While fixing J_{bb}, the Curie temperature increases with L and approaches the bulk one for large values of L.

The effects of surface magnetism have been the subject of many investigations in recent years (for a review see [22]). We consider a finite lattice when the magnetic properties of the surface differ from those in the bulk. This is expected since the atoms at the surface are in a different environment, and the interaction (exchange constant) associated with them may differ from those in the bulk. We consider the simplest model of surface modification.

Let us assume that only for the first surface (top and bottom) layers the exchange constant differs from that in the bulk, *i.e.* for $n = 1$ we have $J_0 \neq J_{aa}$ and for $n = 2L$ we have $J_{00} \neq J_{bb}$; layers $n = 2, 4, ..., 2L-2$ are composed of atoms B with J_{bb} and layers $n = 3, 5, ...2L-1$ are composed of atoms A with J_{aa}. The exchange interaction between all successive layers is given by J_{ab}. In this case $\det C$ has the form

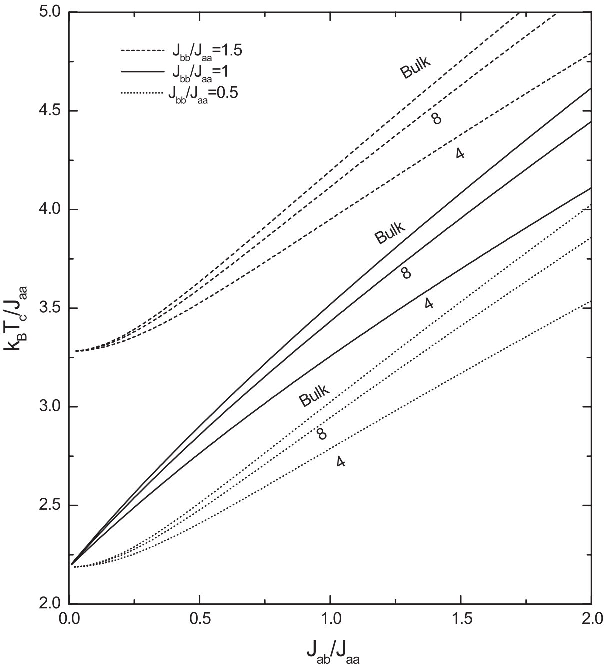

Fig. 1. The Curie temperature $k_{\mathrm{B}}T_{\mathrm{c}}/J_{aa}$ *versus* J_{ab}/J_{aa} for three values of J_{bb}/J_{aa}= 1.5, 1 and 0.5 corresponding respectively to the dashed, solid and dotted curves. The number accompanying each curve denotes the number of layers in the finite superlattice case. The line labeled by "bulk" corresponds to the infinite superlattice.

$$\det C_2^s = \begin{vmatrix} x_0 & -1 & & & & & & 0 \\ -1 & x_b & -1 & & & & & \\ & -1 & x_a & -1 & & & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & & -1 & x_b & -1 & \\ & & & & & -1 & x_a & -1 \\ 0 & & & & & & -1 & x_{00} \end{vmatrix}_{2L} \quad (48)$$

where x_0 and x_{00} are obtained from x_a and x_b by putting J_0 instead of J_{aa} and J_{00} instead of J_{bb}, respectively, in expressions (39) and (40),

$$x_0 = x_a \left(J_{aa} \to J_0\right) \quad (49)$$

$$x_{00} = x_b \left(J_{bb} \to J_{00}\right), \quad (50)$$

By expanding equation (48) about the first and last rows, we get

$$\det C_{2L}^s = \left[x_0 x_{00} - \left(\frac{x_0}{x_a} + \frac{x_{00}}{x_b}\right)\right] \det C_{2L-2} + \left[1 - \left(\frac{x_0}{x_a} + \frac{x_{00}}{x_b}\right)\right] \det C_{2L-4}, \quad (51)$$

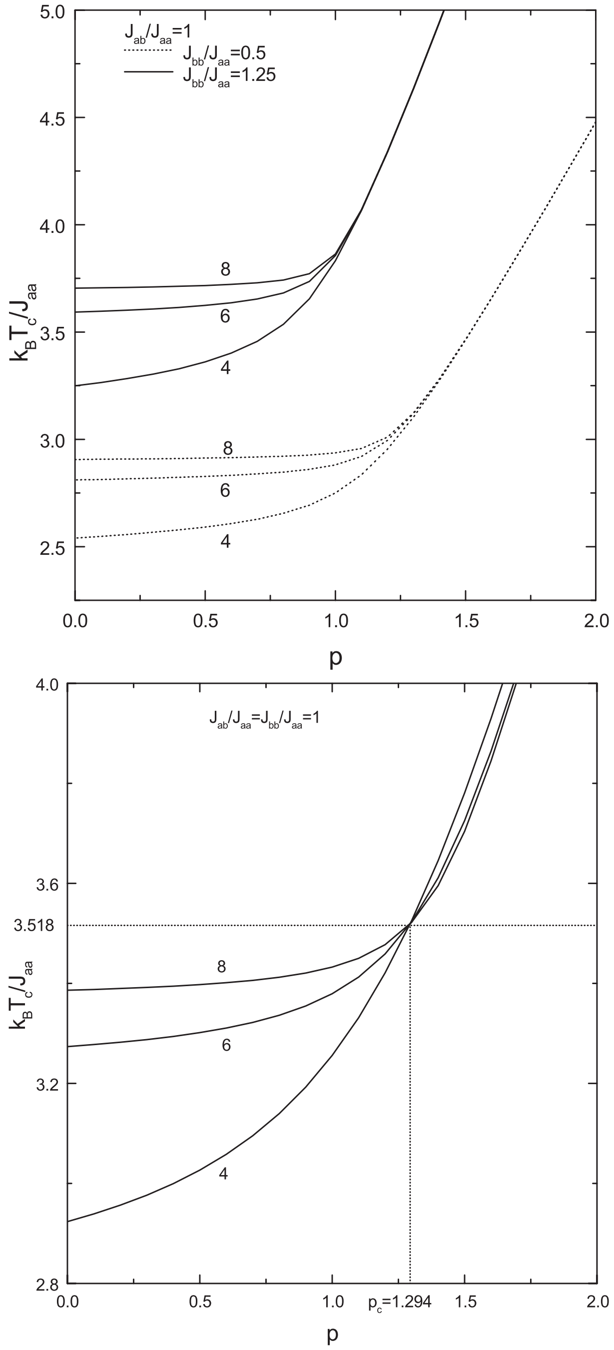

Fig. 2. The Curie temperature $k_{\rm B}T_{\rm c}(L)/J_{aa}$ as a function of the parameter p for different thickness L indicated by numbers 4, 6 and 8 and for (a) $J_{ab}/J_{aa} = 1$ and two values of $J_{bb}/J_{aa} = 0.5$ (dotted lines) and 1.25 (solid lines) (b) $J_{ab}/J_{aa} = J_{bb}/J_{aa} = 1$. The dotted horizontal line corresponds to the bulk Curie temperature.

where $\det C_{2L}$ is given by equation (43). The Curie temperature is given by

$$\det C^s_{2L} = 0. \tag{52}$$

For any finite superlattice, equation (52) can be solved numerically for different $R_1 = J_{bb}/J_{aa}$, $R_2 = J_{ab}/J_{aa}$, $R_0 = J_0/J_{aa}$ and $R_{00} = J_{00}/J_{bb}$ and the number of the

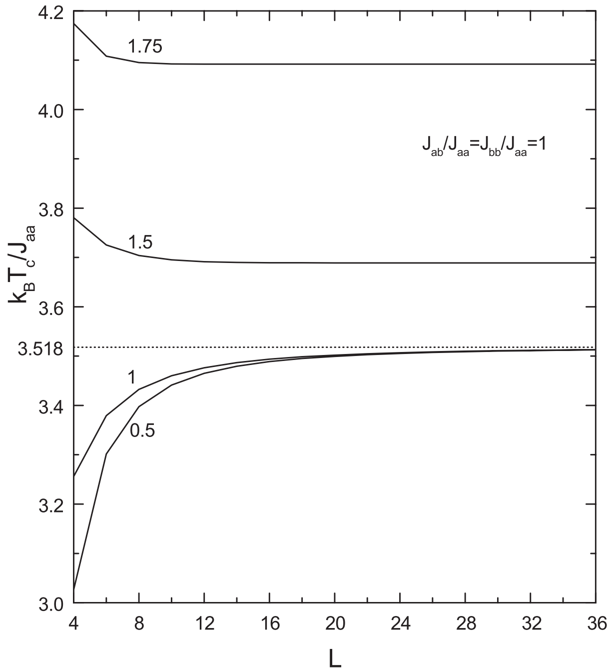

Fig. 3. Dependence of the Curie temperature on film thickness L in the case when $J_{ab}/J_{aa} = J_{bb}/J_{aa} = 1$. The number accompanying each curve denotes the value of the parameter p. The dotted horizontal line corresponds to the bulk Curie temperature at which $p = p_{\rm c} = 1.294$.

layers L. For simplicity we choose $R_0 = p$ and $R_{00} = pR_1$ where p is the single modification parameter ($p = 1$ is our simple alternating superlattice). In Figures 2a, b, we have plotted the Curie temperature *versus* p for $L = 4$, 6 and 8 and for three values of R_1 and R_2 fixed. Notice that the dependence of the Curie temperature on the thickness is significant only for small values of p. For large p the Curie temperature is quasi linear and increases with the increase of J_{bb}/J_{aa} (see Fig. 2a).

In Figure 2b, we show the phase diagram $(p, k_{\rm B}T/J_{aa})$ plane for the case when $J_{ab}/J_{aa} = J_{bb}/J_{aa} = 1$ in which the finite superlattice is reduced to a simple film and for several film thickness that are indicated by the numbers. The dotted line labeled by "bulk" corresponds to the bulk Curie temperature. Critical value $p_{\rm c} = 1.294$ can also be compared with the result of Monte Carlo simulation which is 1.452 [21] (parameter $p_{\rm c}$ at which $k_{\rm B}T_{\rm c}/J_{aa}$ being greater than $k_{\rm B}T_{\rm c}^B/J_{aa}$ is independent of the film thickness and is equal to one coordinate of the multicritical point of the surface bulk transition in the semi-infinite case), see [22].

We can clearly see this behaviour in Figure 3, where the film Curie temperatures $k_{\rm B}T_{\rm c}(L)/J_{aa}$ are presented for films with various thickness L. The curves refer to two different parameter modification surface p labeled by number. The characteristic property of the curves refer to $p > p_{\rm c}$, as indicated in figure obtained for $J_{ab}/J_{aa} = J_{bb}/J_{aa} = 1$ is a decrease of the film Curie temperature $k_{\rm B}T_{\rm c}(L)/J_{aa}$ when the film thickness increases. We see that for an enhanced value of p, the film Curie temperature

$k_B T_c(L)/J_{aa}$ exceeds $k_B T_c^B/J_{aa}$ despite the reduced number of nearest neighbours. In this case, $k_B T_c(L)/J_{aa}$ exhibits a maximum for small film thickness L. The same qualitative results have been obtained by Monte Carlo simulation [21].

On the other hand, for the curves referring to $p < p_c$, we note just the opposite tendency. For $p = p_c$, the film Curie temperature $k_B T_c/J_{aa}$ is equal to the bulk one regardless of the film thickness (dotted horizontal line).

4 Conclusion

In conclusion, the properties of the phase transition, a ferromagnetic alternating superlattice described the spin-one Ising model in effective field theory, have been discussed in this paper. The dependence of the Curie temperature on the strength of the coupling at the interface of the simplest case when the superlattice is infinite and the layer-number of a finite superlattice has been obtained. We studied also the effects of the surface.

The author, A. Saber would like to thank "ICTP Programme for Training and Research in Italian Laboratories, Trieste, Italy" for the financial support.

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