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Phase transitions in a magnetic superlattice: effective-field-theory approach

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Abstract. The critical behaviour of a magnetic superlattice is examined within the framework of the effective-field theory with correlations. For a spin- $\frac{1}{2}$ Ising model of a superlattice with arbitrary number of magnetic layers in a unit cell we obtain the general formalism of transition temperature T_c derivation. For the case of an alternating superlattice, the transition temperatures T_c are calculated as a function of the film thickness and of the inter- and intralayer exchange constants. The effects of surface modification on finite superlattices are also studied numerically.

1. Introduction

In the past few years, there has been growing interest in the magnetic properties of both naturally and artificially layered structures, especially in the nature of spin waves, giant magnetoresistance and critical phenomena (for a review, see [1]). With the advance of modern vacuum science, in particular the epitaxial growth technique, it is now possible to grow very thin films of predetermined thickness, even of a few monolayers. Superlattice structures composed of two different ferromagnetic layers (Fe/Co, Fe/Cr, Fe/Ni, Co/Cr, Dy/Gd, etc) have already been artificially fabricated. The critical properties of such systems have been studied, either experimentally [2–5] or theoretically [6–12]. Camley and Tilley [8] have calculated the critical temperature in the same superlattice using the Ginzburg–Landau formalism. Hinchey and Mills [6] have used a localized spin model in the investigation of a superlattice composed of alternating ferromagnetic and antiferromagnetic layers. Recently Sy and Ow [10] studied the phase transitions in an alternating magnetic superlattice using the Ising model in the mean-field approximation.

We study in this article the critical properties of a magnetic superlattice using the differential operator technique within the effective-field theory with correlations. This technique, first proposed by Honmura and Kaneyoshi [13], has been widely developed and applied to various magnetic systems [14], including thin films and superlattices [15–18], and it is believed to give more exact results compared to the standard mean-field approximation. So, recently, using this method Hai *et al* studied the critical temperature of a magnetic slab as a function of slab thickness and surface exchange coupling [16], and the critical behaviour of an infinite superlattice consisting of two different ferromagnets [17].

In section 2 we present the model of the superlattice and derive the equation that determines the transition temperature. In section 3 we apply the obtained formalism to calculate the transition temperatures of an alternating superlattice with two layers in the unit cell. We consider first an infinite superlattice, then a finite one and last a finite superlattice with modified surface. Finally, the discussion and brief conclusion are given in section 4.

2. Model and formalism

We consider a model of an infinite superlattice with the unit cell consisting of an arbitrary number N of magnetic layers. Each magnetic layer j ($j = 1, \dots, N$) contains n_j atomic layers. The same model of a magnetic superlattice was considered recently [12, 19] for study of the bulk and surface spin-wave spectrum. The unit cell of the superlattice under consideration is shown in figure 1.

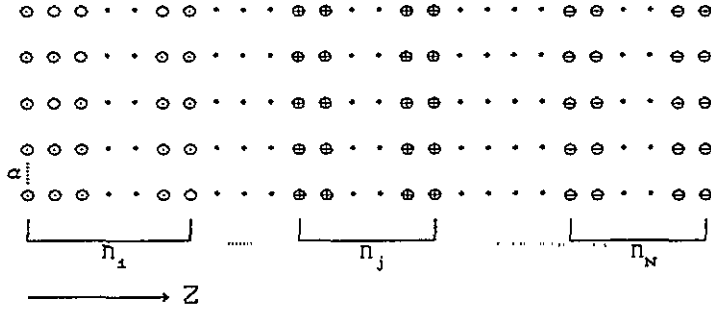


Figure 1. The unit cell of the superlattice consisting of N different ferromagnetic materials. The same lattice parameter a is assumed for all the materials and $l = La$ is the superlattice parameter. The layers are infinite in the directions perpendicular to the axis z .

The spin- $\frac{1}{2}$ Ising Hamiltonian of the system is given by

$$H = \sum_{n,n'} \sum_{r,r'} J_{nn'} S_{nr} S_{n'r'} \tag{1}$$

where $S_{nr} = \pm 1$ is the usual Ising variable, (n, n') are plane indices and (r, r') are different sites of the plane. We will retain only nearest-neighbour (NN) terms. In (1), $J_{nn'}$ is only plane dependent, and in NN terms is given as

$$J_{nn} = J^{(j)} \quad kL + \sum_{\sigma=1}^{j-1} n_{\sigma} + 1 \leq n \leq kL + \sum_{\sigma=1}^j n_{\sigma}$$

$$J_{n,n+1} = \begin{cases} J^{(j)} & kL + \sum_{\sigma=1}^{j-1} n_{\sigma} + 1 \leq n \leq kL + \sum_{\sigma=1}^j n_{\sigma} - 1 \\ J^{(j,j+1)} & n = kL + \sum_{\sigma=1}^j n_{\sigma} \end{cases}$$

for $j = 1, \dots, N$. Here L is the number of atomic layers in the unit cell and is defined as $L = \sum_{j=1}^N n_j$, k is the index of the unit cell ($k = 0, \pm 1, \pm 2, \dots$ for an infinite system) and $j + 1 \rightarrow 1$ for $j = N$.

To evaluate the mean spin $\langle S_{nr} \rangle$ we use the exact Callen identity [20]:

$$\langle S_{nr} \rangle = \left\langle \tanh \left(\sum_{n'} \sum_{r'} K_{nn'} S_{n'r'} \right) \right\rangle \tag{2}$$

where $K_{ij} = J_{ij}/k_B T$, and $\langle \dots \rangle$ indicates the usual canonical ensemble average for a given configuration of $\{J_{ij}\}$. For derivation of the right-hand side of expression (2) we use the

differential operator technique [13]. Now we introduce the differential operator $D \equiv \partial/\partial x$ and recall that the displacement operator $\exp(\alpha D)$ satisfies the relation

$$\exp(\alpha D)f(x) = f(x + \alpha). \quad (3)$$

Then equation (2) can be rewritten with the help of equation (3) as

$$\begin{aligned} \langle S_{nr} \rangle &= \left\langle \exp \left(\sum_{n'} \sum_{r'} K_{nn'} S_{n'r'} D \right) \right\rangle \tanh(x) \Big|_{x=0} \\ &= \left\langle \prod_{n'} \prod_{r'} [\cosh(K_{nn'} D) + S_{n'r'} \sinh(K_{nn'} D)] \right\rangle \tanh(x) \Big|_{x=0}. \end{aligned} \quad (4)$$

On the right-hand side of equation (4) we have obtained the multi-spin correlation function, which must be decoupled. We follow the Kaneyoshi decoupling approximation [21]

$$\langle x_1 x_2 \dots x_n \rangle = \langle x_1 \rangle \langle x_2 \rangle \dots \langle x_n \rangle.$$

Then, as $\langle S_{nr} \rangle$ is independent of r , we introduce the mean atomic magnetization of the n th layer $m_n = \langle S_{nr} \rangle$. Hence equation (4) in NN approximation and in terms of m_n reduces to

$$\begin{aligned} m_n &= [\cosh(K_{nn} D) + m_n \sinh(K_{nn} D)]^{z_0} [\cosh(K_{n,n-1} D) + m_{n-1} \sinh(K_{n,n-1} D)]^z \\ &\quad \times [\cosh(K_{n,n+1} D) + m_{n+1} \sinh(K_{n,n+1} D)]^z \tanh(x) \Big|_{x=0} \end{aligned} \quad (5)$$

where $n = 1, \dots, L$, and z_0 and z are the numbers of nearest neighbours in the plane and between adjacent planes, respectively ($z_0 = 4$, $z = 1$ in the case of a simple cubic lattice; $z_0 = 6$, $z = 1$ for a hexagonal lattice; $z_0 = 3$, $z = 1$ for a honeycomb lattice; etc). Since the periodic condition of the superlattice is satisfied, we have $m_0 = m_L$ and $m_{L+1} = m_1$. So we have a set of L coupled equations for m_1, m_2, \dots, m_L . The magnetization in the n th layer, m_n , depends on the magnetizations in adjacent $(n+1)$ th and $(n-1)$ th layers and via these on exchange couplings in these layers. We can see that, in general, owing to interface effects, the magnetizations in n_j atomic layers of magnetic layer j are not the same.

As the temperature becomes higher than the critical temperature T_c , the whole system becomes demagnetized and the mean atomic magnetization in every layer approaches zero. Using this condition we can determine T_c . Hence, all terms of order higher than linear in equation (5) can be neglected. This leads to a set of L linear simultaneous equations:

$$m_n = z_0 A_{nn} m_n + z A_{n,n-1} m_{n-1} + z A_{n,n+1} m_{n+1} \quad (6)$$

where $n = 1, \dots, L$, and coefficients $\{A\}$ are given by

$$A_{nn} = \cosh^{z_0-1}(K_{nn} D) \sinh(K_{nn} D) \cosh^z(K_{n,n-1} D) \cosh^z(K_{n,n+1} D) \tanh(x) \Big|_{x=0} \quad (7a)$$

$$A_{n,n-1} = \cosh^{z-1}(K_{n,n-1} D) \sinh(K_{n,n-1} D) \cosh^{z_0}(K_{nn} D) \cosh^z(K_{n,n+1} D) \tanh(x) \Big|_{x=0} \quad (7b)$$

$$A_{n,n+1} = \cosh^{z-1}(K_{n,n+1} D) \sinh(K_{n,n+1} D) \cosh^{z_0}(K_{nn} D) \cosh^z(K_{n,n-1} D) \tanh(x) \Big|_{x=0} \quad (7c)$$

The set of linear equations (6) can be rewritten in matrix form:

$$\mathbf{B}m = 0 \quad (8)$$

where

$$B_{ij} = (1 - z_0 A_{ij})\delta_{ij} - z A_{ii}(\delta_{i,j-1} + \delta_{i,j+1}). \quad (9)$$

The secular equation of the set of coupled equations (6) is

$$\begin{vmatrix} 1 - z_0 A_{11} & -z A_{12} & \cdots & -z A_{1L} \\ -z A_{21} & 1 - z_0 A_{22} & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & 1 - z_0 A_{L-1,L-1} & -z A_{L-1,L} \\ -z A_{L1} & \cdots & -z A_{L,L-1} & 1 - z A_{LL} \end{vmatrix} = 0. \quad (10)$$

From the numerical calculation of equation (10) we can determine the critical temperature T_c for a given configuration of exchange constants $\{J_{ij}\}$ and superlattice structure (z_0, z) . Thus the formalism we have obtained is general and applicable for an arbitrary superlattice.

3. Superlattice with two layers in the unit cell

3.1. Infinite lattice

Now let us apply the obtained formalism to a superlattice where the adjacent layers consist of atoms of two different magnetic materials A and B and alternate as ...ABABA... The exchange coupling constant between the NN spins in A (B) is denoted by J_a (J_b), while J_{ab} stands for the exchange coupling between the NN spins across the interface. Let us assume that the superlattice is infinite and has a simple cubic structure ($z_0 = 4$, $z = 1$). Since the unit cell includes only two layers, we have two different mean magnetizations, m_a for layers A and m_b for layers B. Evidently, for arbitrary n , the relation $m_{n-1} = m_{n+1}$ is satisfied. Hence the set of equations (6) has the form

$$m_a = 4A_{aa}m_a + 2A_{ab}m_b \quad (11a)$$

$$m_b = 4A_{bb}m_b + 2A_{ba}m_a \quad (11b)$$

where the coefficients $\{A\}$ may be obtained with the help of equations (7):

$$A_{aa}(K_a, K_{ab}) = [\tanh(4K_a + 2K_{ab}) + \tanh(4K_a - 2K_{ab}) + 2 \tanh(2K_a + 2K_{ab}) + 2 \tanh(2K_a - 2K_{ab}) + 2 \tanh(4K_a) + 4 \tanh(2K_a)]/32 \quad (12a)$$

$$A_{ab}(K_a, K_{ab}) = [\tanh(4K_a + 2K_{ab}) - \tanh(4K_a - 2K_{ab}) + 4 \tanh(2K_a + 2K_{ab}) - 4 \tanh(2K_a - 2K_{ab}) + 6 \tanh(2K_{ab})]/32 \quad (12b)$$

$$A_{bb}(K_b, K_{ab}) = A_{aa}(K_a \rightarrow K_b, K_{ab}) \quad (12c)$$

$$A_{ba}(K_b, K_{ab}) = A_{ab}(K_a \rightarrow K_b, K_{ab}). \quad (12d)$$

The set of equations (11) reduces to the secular equation

$$\begin{vmatrix} 1 - 4A_{aa} & -2A_{ab} \\ -2A_{ba} & 1 - 4A_{bb} \end{vmatrix} = 0. \quad (13)$$

From the numerical calculation of secular equation (13) we can determine the critical temperature of the infinite alternating superlattice as a function of J_a , J_b and J_{ab} . Let us assume that $J_a \geq J_b$ and hence $T_c^{(a)} \geq T_c^{(b)}$, where $T_c^{(a)} = 5.073J_a/k_B$ is the bulk critical temperature of a uniform lattice of material A and $T_c^{(b)} = (J_b/J_a)T_c^{(a)}$. Then we take J_a as the unit of energy. In figure 2 we show the dependence of the critical temperature T_c on interlayer exchange constant J_{ab} for various values of J_b . It is easy to see that this dependence is approximately linear in agreement with results of other methods [9-11]. It is interesting to note that, for every choice of J_a and J_b , there exists some critical value of interface exchange constant $J_{ab}^{(c)}$ such that, when $J_{ab} > J_{ab}^{(c)}$ and consequently $T_c > T_c^{(a)}$, $T_c^{(b)}$, the system may order in the interface layers before the intralayer ordering, i.e. the interface magnetism dominates. For $J_{ab} < J_{ab}^{(c)}$, $T_c < T_c^{(a)}$, $T_c^{(b)}$, we have the contrary situation. Initially it has a place intralayer ordering, i.e. the intralayer magnetism dominates and the system behaves like metamagnets. For the plots in figure 2 we obtained the following critical values of $J_{ab}^{(c)}$: for (a) $J_b = 0.25J_a$ and $J_{ab}^{(c)} = 1.33J_a$; for (b) $J_b = 0.5J_a$ and $J_{ab}^{(c)} = 1.22J_a$; for (c) $J_b = 0.75J_a$ and $J_{ab}^{(c)} = 1.11J_a$; for (d) $J_b = J_a$ and $J_{ab}^{(c)} = J_a$. Recently Hai *et al* [17] considered a similar model of an infinite superlattice consisting of two different ferromagnetic materials A and B, where each magnetic sublayer contained several monolayers, and calculated the critical temperature as a function of sublayer thicknesses. It was found also that there exists for each set of values of J_a , J_b and number of layers some critical interface coupling $J_{ab}^{(c)}$ that satisfies the same conditions as $J_{ab}^{(c)}$ introduced in the present work.

3.2. Finite lattice

Now we consider an alternating superlattice of finite thickness. In the case of the infinite superlattice we restricted our discussion to one unit cell because of the periodic condition. Now, taking 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.

Let us assume that the lattice has $2l$ layers. Layers $n = 0, 2, \dots, 2l - 2$ are made up of atoms of type A with J_a , whereas layers $n = 1, 3, \dots, 2l - 1$ are made up of atoms of type B with J_b . The exchange constant between all successive layers is given by J_{ab} . Such a type of superlattice was considered recently [10] in the mean-field approximation.

Therefore matrix equation (8) can be performed now as a set of $2l$ linear equations, and m has $2l$ components, i.e. l mean magnetizations m_a and l mean magnetizations m_b . Matrix \mathbf{B} will have the form

$$\mathbf{B}_{(ab)} = \begin{bmatrix} 1 - z_0 A_{aa} & -z A_{ab} & & & \\ -z A_{ba} & 1 - z_0 A_{bb} & -z A_{ba} & & \\ & \dots & \dots & \dots & \\ & & \dots & \dots & \dots \\ & & & -z A_{ba} & 1 - z_0 A_{bb} \end{bmatrix} \quad (14)$$

and the critical temperature T_c is given as before by the determinant equation:

$$\det \mathbf{B}_{(ab)} = 0. \quad (15)$$

We can represent $\det \mathbf{B}_{(ab)}$ as

$$\det \mathbf{B}_{(ab)} = (z A_{ab})^l (z A_{ba})^l C_{2l}(T) \quad (16)$$

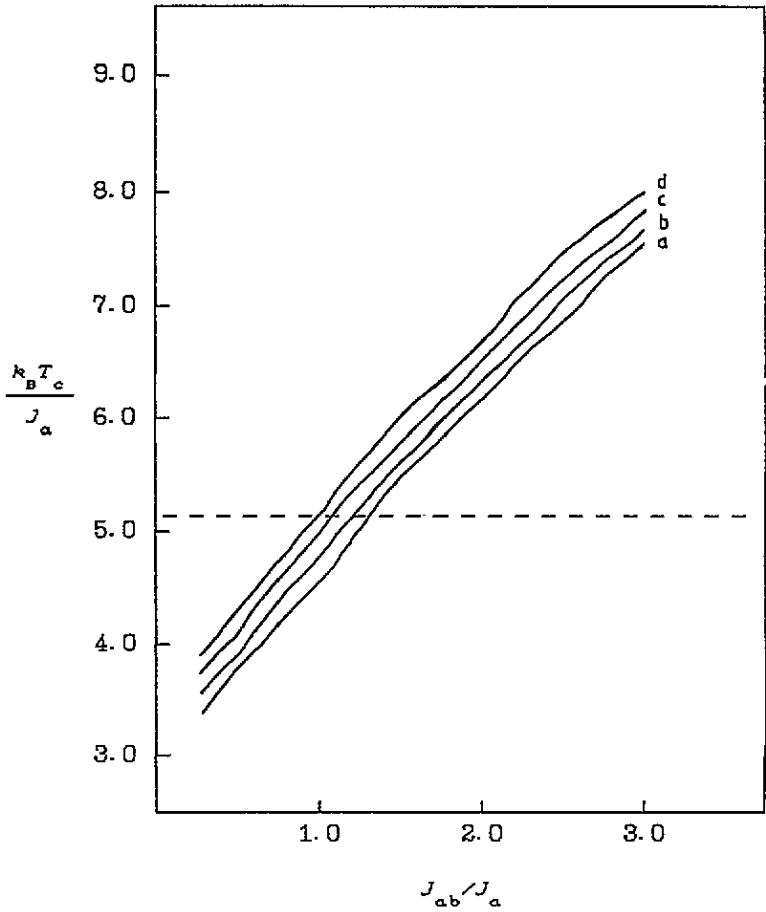


Figure 2. Dependence of critical temperature T_c on interface coupling J_{ab} for (a) $J_b = 0.25J_a$, (b) $J_b = 0.5J_a$, (c) $J_b = 0.75J_a$ and (d) $J_b = J_a$. The broken line shows the critical temperature of a uniform lattice, $k_B T_c = 5.073$, i.e. when $J_b = J_a$ and $J_{ab} = J_a$.

where

$$C_{2l} = \begin{bmatrix} x_a & -1 & & & \\ -1 & x_b & -1 & & \\ & -1 & x_a & -1 & \\ & & \dots & \dots & \\ & & & -1 & x_b \end{bmatrix}_{(2l) \times (2l)} \tag{17}$$

and

$$x_a = (1 - z_0 A_{aa}) / (z A_{ab}) \quad x_b = (1 - z_0 A_{bb}) / (z A_{ba}) \tag{18}$$

where $\{A\}$ are given in (12).

Now let us evaluate C_{2l} . The determinant of such a symmetric tridiagonal matrix satisfies the recurrence relation

$$C_{2l} = (x_a x_b - 2) C_{2l-2} - C_{2l-4} \tag{19}$$

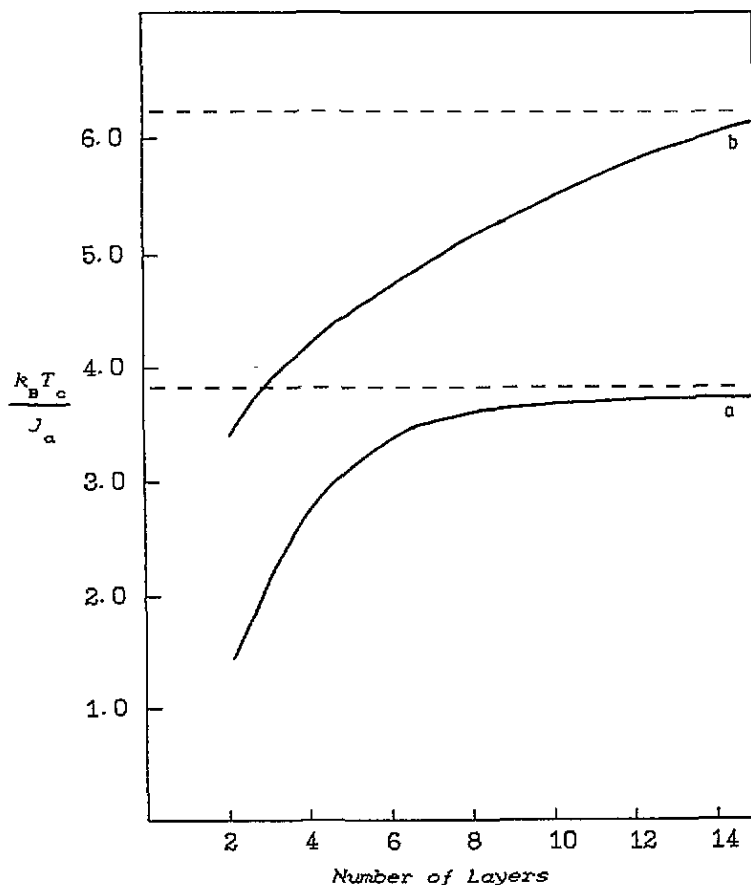


Figure 3. Dependence of critical temperature T_c on thickness for (a) $J_b = 0.5J_a$, $J_{ab} = 2J_a$, and (b) $J_b = 0.5J_a$, $J_{ab} = 0.5J_a$.

and where x_0 and x_{00} differ from x_a and x_b by putting J_0 instead of J_a and J_{00} instead of J_b , respectively, in expressions (12).

Expanding the determinant $C_{2l}^{(S)}$ about the first and last rows we can write

$$C_{2l}^{(S)} = [x_0 x_{00} - (x_0/x_a + x_{00}/x_b)]C_{2l-2} + [1 - (x_0/x_a + x_{00}/x_b)]C_{2l-4} \quad (26)$$

where C_{2l} is given in (20).

From the condition of critical temperature derivation

$$C_{2l}^{(S)}(T) = 0 \quad (27)$$

we can numerically calculate T_c for various values of J_a , J_b , J_{ab} , J_0 and J_{00} and the number of layers $2l$. For simplicity we have chosen

$$J_0 = cJ_a \quad J_{00} = cJ_b \quad (28)$$

where c is the single modification parameter ($c = 1$ is our simple alternating superlattice).

In figures 4 and 5 we have plotted critical temperature T_c versus c for two cases: $J_b = 0.5J_a$, $J_{ab} = 0.5J_a$, and $J_b = 0.5J_a$, $J_{ab} = 2J_a$, respectively. The results are shown for simple cubic structure and for various numbers of layers. Notice that the dependence of T_c on the layer thickness is significant only for small c .

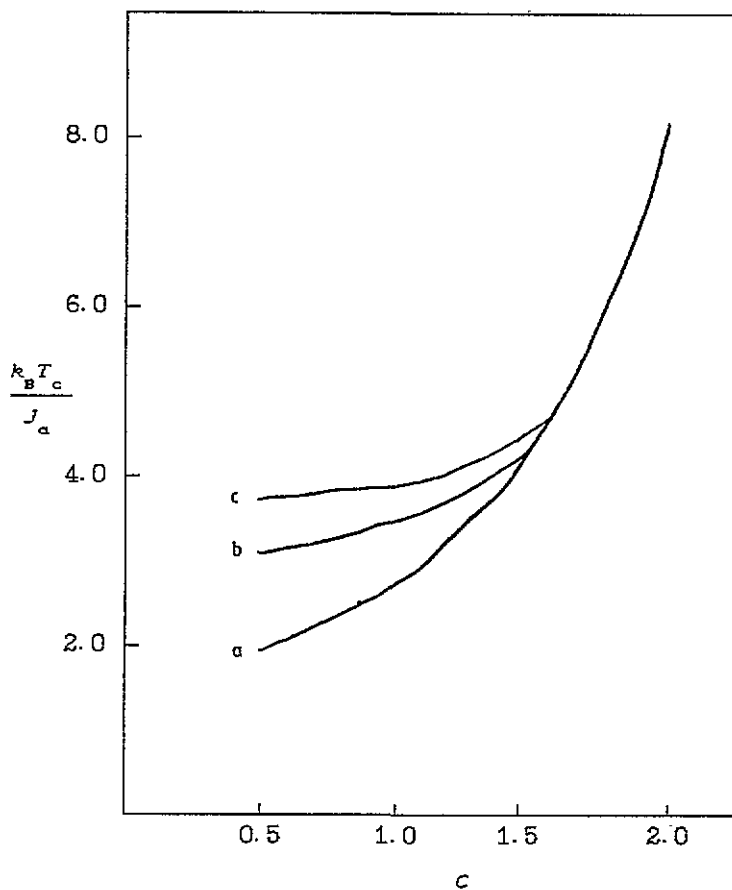


Figure 4. Dependence of critical temperature T_c on c for $J_b = 0.5J_a$, $J_{ab} = 0.5J_a$ and for (a) six, (b) ten and (c) an infinite number of layers.

4. Conclusion

We have examined a spin- $\frac{1}{2}$ Ising model of a magnetic superlattice. The formalism of transition temperature derivation obtained above is universal and can be used for study of a 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 several monolayers in a magnetic layer, a superlattice with impurity layers, a superlattice in transverse applied field, and so on. The more complex the model, the more complicated are the computer calculations required.

Although we have considered a superlattice with only ferromagnetic exchange (all $J > 0$), the formulation is also applicable for antiferromagnetic coupling (some or all $J < 0$). It is easy to see, for example, that, if exchange interactions between the successive layers are antiferromagnetic (i.e. we have to replace K_{ab} by $-K_{ab}$ in expressions (15)), the values of T_c are not changed, which is consistent with the discussion in [9].

In this paper we also introduce some critical value of interlayer exchange constant $J_{ab}^{(c)}$ so that for $J_{ab} > J_{ab}^{(c)}$ ($J_{ab} < J_{ab}^{(c)}$) the interlayer (intralayer) ordering dominates.

Although superlattices of alternating magnetic monolayers have not been studied

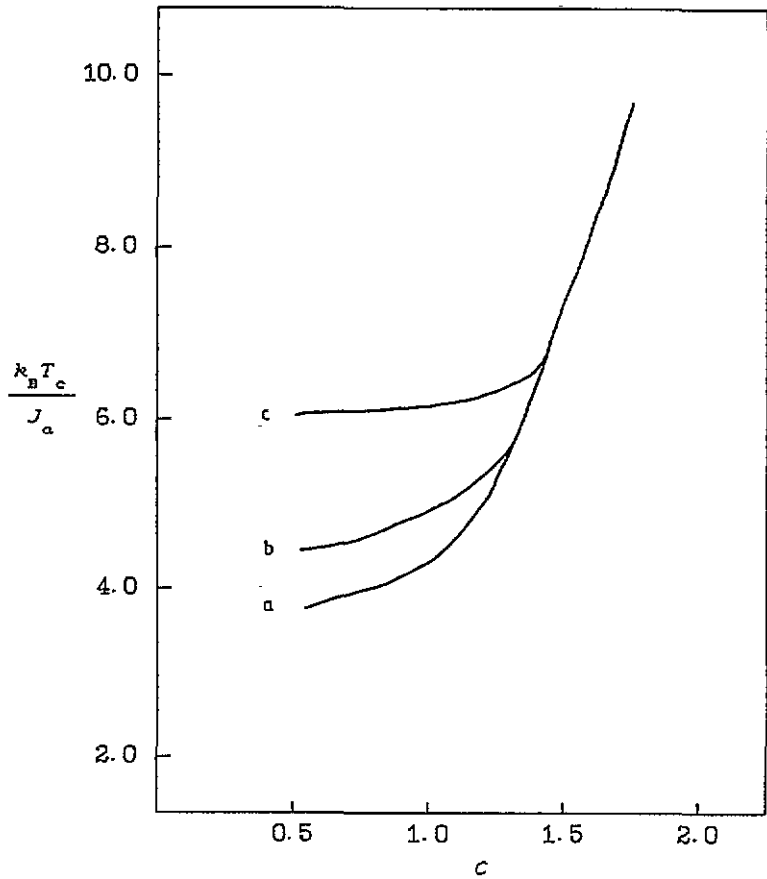


Figure 5. Dependence of critical temperature T_c on c for $J_b = 0.5J_a$, $J_{ab} = 2J_a$ and for (a) six, (b) ten and (c) an infinite number of layers.

experimentally yet, it is expected that such systems can be fabricated in the near future, and a possible candidate is a structure with alternating Fe and Co monolayers. Investigation of the transition temperatures on magnetic superlattices in which the atoms vary from one monolayer to another will be most useful and enlightening.

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References

- [1] Camley R E and Stamps R L 1993 *J. Phys.: Condens. Matter* 5 3727
- [2] Thompson M and Erskine J L 1985 *Phys. Rev. B* 31 6832
- [3] Onellion M F, Fu C L, Thompson M A, Erskine J L and Freeman A J 1986 *Phys. Rev. B* 33 7322

- [4] Farle M and Baberschke K 1987 *Phys. Rev. Lett.* **58** 511
- [5] Durr W, Taborelli M, Paul O, German R, Gudat W, Pescia D and Landolt M 1989 *Phys. Rev. Lett.* **62** 206
- [6] Hinchey L L and Mills D L 1986 *Phys. Rev. B* **33** 3329; 1986 *Phys. Rev. B* **34** 1689
- [7] Fishman F, Schwable F and Schwenk D 1987 *Phys. Lett.* **121A** 192
- [8] Camley R E and Tilley D R 1988 *Phys. Rev. B* **37** 3413
- [9] Tilley D R 1988 *Solid State Commun.* **65** 657
- [10] Sy H K and Ow M H 1992 *J. Phys.: Condens. Matter* **4** 5891
- [11] Sy H K 1992 *Phys. Rev. B* **45** 4454
- [12] Barnas J 1988 *J. Phys. C: Solid State Phys.* **21** 1021
- [13] Honmura R and Kaneyoshi T 1979 *J. Phys. C: Solid State Phys.* **12** 3979
- [14] Balcerzak T 1991 *J. Magn. Magn. Mater.* **97** 152
- [15] Kaneyoshi T and Beyer H 1980 *J. Phys. Soc. Japan* **49** 1306
- [16] Hai T and Li Z Y 1989 *Phys. Status Solidi b* **156** 641
- [17] Hai T, Li Z Y, Lin D L and George T F 1991 *J. Magn. Magn. Mater.* **97** 227
- [18] Jascur M and Kaneyoshi T 1993 *J. Phys.: Condens. Matter* **5** 6313
- [19] Seidov Yu M and Shaulov G R 1992 *Preprint IF-464*, Institute of Physics, Baku
Shaulov G R 1989 *MS Thesis* Baku State University (unpublished)
- [20] Callen H B 1963 *Phys. Lett.* **4** 161
- [21] Kaneyoshi T 1986 *Phys. Rev. B* **33** 526, 7688
- [22] Kaneyoshi T 1991 *J. Phys.: Condens. Matter* **3** 4497