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Curie temperature for a finite alternating magnetic superlattice

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Abstract. We study a spin-one-half Ising model of an alternating magnetic superlattice. We use the mean-field approximation and express our results for the Curie temperature in terms of two types of determinants. The dependence of the Curie temperature on the film thickness is obtained. The effects of surface modification on finite superlattices are studied numerically for two types of modification to the surface exchange constants.

1. Introduction

Over the years, the magnetic properties of ordinary lattices and artificially fabricated superlattices have been widely studied. The effect of a surface on the magnetic behaviour has also been the subject of many theoretical investigations [1–7].

It is widely accepted that the magnetic properties of a surface may differ from those in the bulk of the solid. This is expected since the atoms in the surface region are in a different environment, and the interactions (exchange constants) associated with them may differ from those in the bulk. If the surface exchange constants are above some critical values, the surface will order at a temperature $T_s > T_0$ (Curie temperature for the bulk); and in the temperature region $T_0 < T < T_s$, we have surface magnetic structure, with the magnetization decaying exponentially into the bulk with a characteristic length. This surface magnetism has been confirmed by recent experimental results [8–11].

In most of the theoretical work, the lattice is considered to be compositionally uniform, consisting of only one kind of magnetic atom. The system is also assumed to be infinite, or in the surface problem, semi-infinite.

With the advent of modern vacuum science, and in particular epitaxial-growth techniques, it is nowadays possible to grow very thin magnetic films of controllable thickness or even monolayers atop non-magnetic substrates [12–18]. For example, monolayers of cobalt [12, 13] iron [14, 15] and nickel [16] have been grown on copper; an iron monolayer has been grown on gold [17] and a gadolinium monolayer has also been grown on tungsten [18]. Ferromagnetic order in some of these monolayers has also been reported. A superlattice in which the atoms vary from one monolayer to another can also be envisaged.

In a recent theoretical paper [7], the phase transitions in a finite system with one kind of bulk atom were studied using the Ising model in the mean-field approximation. The effects of surface modification are also considered.

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In the present article, we generalize the method of [7] to an alternating magnetic superlattice. We consider a spin-$\frac{1}{2}$ Ising model with alternate layers having atoms with exchange constants J_A, J_B. The mean-field approximation is employed and the results are expressed in terms of two types of determinant which can be evaluated. For a finite pure alternating superlattice, the Curie temperature can be solved analytically.

We next investigate finite superlattices with surface modifications. We have considered two cases: (i) in which only one of the surface layer exchange constants J_0 is different, and (ii) in which both the top and the bottom surface layer constants J_0, J_{00} are allowed to change. Our results for the Curie temperatures can be obtained by solving an equation involving the same two determinants. Finally, numerical results are shown for some typical values of the exchange constants.

2. Finite superlattice with no modification

We consider a lattice of localized spins with spin equal to one-half. The interaction is of the nearest-neighbour ferromagnetic Ising type and the strength of the interaction (exchange constant) is modulated to reflect a superlattice structure and possible surface modification.

$$H = -\tfrac{1}{2}\sum_{i,j}\sum_{r,r'} J_{ij}\sigma_{ir}\sigma_{jr} - h\sum_{i,r}\sigma_{ir}. \tag{1}$$

Here (i, j) are plane indices and (r, r') are different sites of the planes, σ_{ir} is the spin variable, h is the external magnetic field, and J_{ij} is plane-dependent. We will retain only nearest-neighbour terms.

In the mean-field approximation, σ_{ir} is replaced by its mean value M_i associated with each plane, and is determined by a set of simultaneous equations

$$M_i = \tanh\beta[z_0 J_{ii} M_i + z J_{i,i+1} M_{i+1} + z J_{i,i-1} M_{i-1} + h] \tag{2}$$

where z_0, z are the numbers of nearest neighbours in the plane and between the planes respectively.

Near the transition temperature, the order parameters M_i are small, and in the absence of an external field, (2) reduces to

$$\mathbf{A}M = 0 \tag{3}$$

where the matrix $\mathbf{A}$ is symmetric and tridiagonal with elements

$$A_{mn} = (k_B T - z_0 J_{mm})\delta_{m,n} - z J_{mn}(\delta_{m+1,n} + \delta_{m,n+1}). \tag{4}$$

The transition temperature is given by the determinant equation,

$$\det \mathbf{A} = 0. \tag{5}$$

Let us start with a simple alternating lattice of $2n$ layers. Layers $i = 0, 2, \ldots, 2n-2$ are made up of atoms of type A with exchange constant J_A; whereas layers $i = 1, 3, \ldots, 2n-1$ consist of atoms of type B with exchange constant J_B.

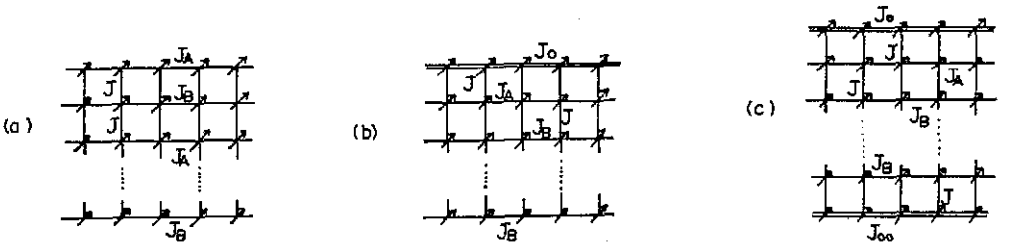

Figure 1. (*a*) Simple alternating structure. (*b*) Superlattice with modified top layer. (*c*) Superlattice with modification to top and bottom layers.

The exchange constant between successive layers is assumed to be $J_{i,i+1} = J$ (figure 1(*a*)).

We will define two basic determinants D_{2m}, C_{2m-1}

$$D_{2m} = \begin{bmatrix} x_A & -1 & & & \\ -1 & x_B & -1 & & \\ & -1 & x_A & -1 & \\ & & & \ddots & \\ & & & & x_B \end{bmatrix}_{2m\times 2m}$$

$$C_{2m-1} = \begin{bmatrix} x_B & -1 & & & \\ -1 & x_A & -1 & & \\ & -1 & x_B & -1 & \\ & & & \ddots & \\ & & & & x_B \end{bmatrix}_{(2m-1)\times(2m-1)} \tag{6}$$

where

$$x_A = (k_B T - z_0 J_A)/zJ \qquad x_B = (k_B T - z_0 J_B)/zJ. \tag{7}$$

Then for this simple alternating lattice, (5) reduces to

$$\det \mathbf{A} = (zJ)^{2n} D_{2n}(T). \tag{8}$$

The determinants C and D satisfy the recurrence relations

$$D_{2m} = x_A C_{2m-1} - D_{2m-2} \qquad C_{2m-1} = x_B D_{2m-2} - C_{2m-3}. \tag{9}$$

Eliminating Cs, we have

$$D_{2m} = \alpha D_{2m-2} - D_{2m-4} \tag{10}$$

where

$$\alpha = x_A x_B - 2 = 2\cosh\phi. \tag{11}$$

The difference equation (10) has the solution

$$D_{2m} = (1/\sinh\phi)[\sinh(m+1)\phi + \sinh(m\phi)] \tag{12}$$

and hence

$$C_{2m-1} = (2/x_A \sinh\phi)\sinh(m\phi)[\cosh\phi + 1] \qquad m \geqslant 1. \tag{13}$$

Notice that in (12) and (13), ϕ is real when $\alpha \geqslant 2$. For $\alpha \leqslant 2$, ϕ is purely imaginary and equal to $i\theta$, and the hyperbolic functions become the trigonometric functions of θ.

For the simple lattice, the Curie temperature is given by (8)

$$D_{2n}(T) = 0.$$

This has no solution for $\alpha > 2$.

For $\alpha \leqslant 2$, the solution is $\theta = 2\pi/(2n+1)$, or solving for T_c in (11), we have

$$t_c = \tfrac{1}{2}\{(j_A + j_B) + [(j_A - j_B)^2 + 16\cos^2(\pi/(2n+1))]^{1/2}\} \tag{14}$$

where we have introduced the dimensionless quantities

$$j_A = z_0 J_A / zJ \qquad j_B = z_0 J_B / zJ \qquad t_c = kT_c/zJ. \tag{15}$$

If we had started with a lattice of $(2n-1)$ layers, with B atoms at both ends, we would have obtained almost the same result as (14), but with $2n$ replaced by $(2n-1)$.

The bulk Curie temperature is obtained by taking the limit $n \to \alpha$ and is given by

$$t_0 = \tfrac{1}{2}\{j_A + j_B + [(j_A - j_B)^2 + 16]^{1/2}\} \tag{16}$$

For a finite lattice, the Curie temperature is always less than t_0. In figure 2, we have shown the dependence of t_c/t_0 on the number of layers. The parameters used are for curve (*a*) $j_A = 2$, $j_B = 1$ and for curve (*b*) $j_A = 8$, $j_B = 4$. Notice that the bulk values of 3.56 and 8.83 are reached quite rapidly. This limiting value is approached faster in the case of curve (*b*).

3. Superlattice with modified top layer

The effects of the surface on the magnetism depend on how the surface modifies the surface atoms and their interactions [1–7, 19]. In this paper, we only consider modification to the exchange constants of the Ising model. In the first model, we allow one surface (top) intralayer exchange constant J_0 to vary; in the second model, we allow changes in both the top and the bottom surface intralayer exchange constants J_0 and J_{00}. Other types of modification, such as to the intralayer exchange constants, or to more than two surface layers, can be considered. Some of these have been discussed earlier for uniform [6] and alternating [19] semi-infinite superlattices.

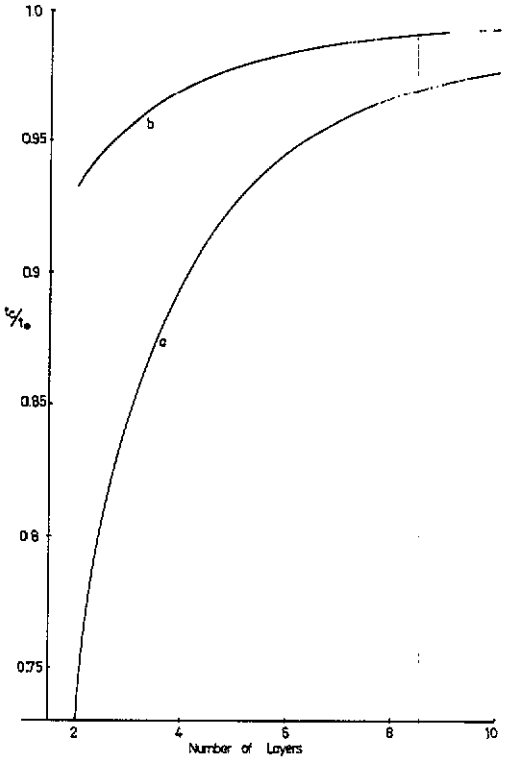

Figure 2. Dependence of Curie temperature t_c/t_0 on thickness for (*a*) $j_A = 2$, $j_B = 1$ and (*b*) $j_A = 8$, $j_B = 4$.

The first model is shown in figure 1(*b*). Here we consider a lattice of $2n + 1$ layers. Layer $i = 0$ has atoms of exchange constant J_0; layers 1, 2, ..., $2n - 1$ consist of A atoms of exchange J_A, whereas layers $i = 2, 4, \ldots, 2n$ are composed of B atoms with J_B. The interlayer exchange is J.

In this case, (5) is given by

$$\det_1(T) = \begin{bmatrix} x_0 & -1 & & & \\ -1 & x_A & -1 & & \\ & -1 & x_B & -1 & \\ & & & \ddots & \\ & & & -1 & x_B \end{bmatrix}_{(2n+1)\times(2n+1)} \tag{17}$$

and

$$x_0 = (k_B T - z_0 J_0)/zJ \qquad j_0 = z_0 J_0/zJ. \tag{18}$$

Expanding about the first row, this is

$$x_0 D_{2n}(T) - C_{2n-1}(T) = 0. \tag{19}$$

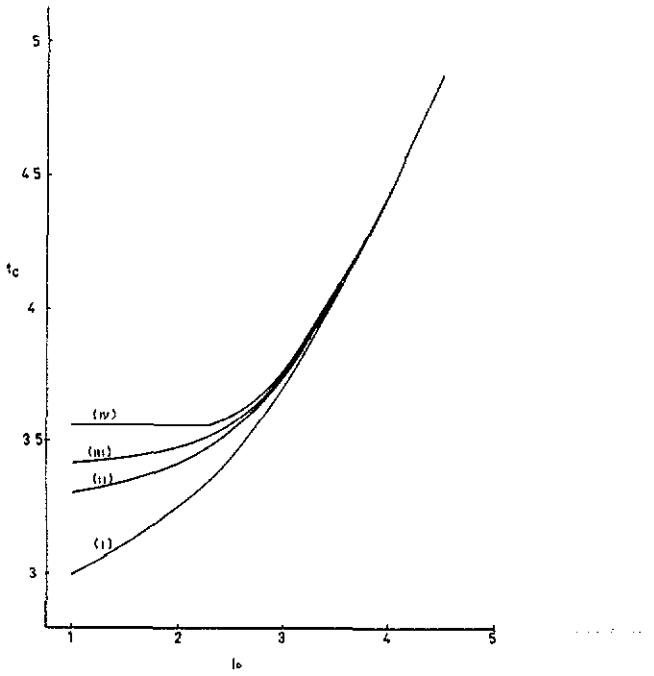

Figure 3. Dependence of t_c on j_0 for $j_A = 2$, $j_B = 1$, and for (i) three, (ii) five, (iii) seven and (iv) infinite layers.

This equation can be solved numerically for the Curie temperature $t_c = kT_c/zJ$ for any thickness n, and exchange constants j_A, j_B and j_0.

In figures 3 and 4, we have shown our results for the Curie temperature t_c as a function of j_0 for the two choices (*a*) $j_A = 2$, $j_B = 1$ and (*b*) $j_A = 8$, $j_B = 4$ respectively. In figure 3, the curves are for superlattices of three, five and seven layers as well as for a semi-infinite superlattice. In figure 4, we have shown our results for three and seven layers and the semi-infinite case. We notice that the finite case is significantly different from the semi-infinite case only for small j_0.

For a superlattice of many (infinite) layers, the system always orders at the bulk Curie temperature until a critical j_{0c} is reached. This can be evaluated [19] in terms of j_A, j_B as 2.28 and 6.41 respectively. Above j_{0c}, surface magnetism occurs, with the magnetic moment decaying into the bulk.

4. Superlattice with modification to top and bottom layers

The second model is shown in figure 1(*c*). Here we consider a lattice of $2n + 2$ layers. Layers $i = 1, 3, \ldots, 2n - 1$ consist of A atoms and layers $i = 2, \ldots, 2n$ consist of B atoms. The top layer $i = 0$ and bottom layer $i = 2n + 1$ have exchange constants j_0 and j_{00} respectively. The intralayer exchange J remains the same.

In this case, (5) becomes

$$\det \mathbf{A} = (zJ)^{2n+2} \det_2(T) = 0 \tag{20}$$

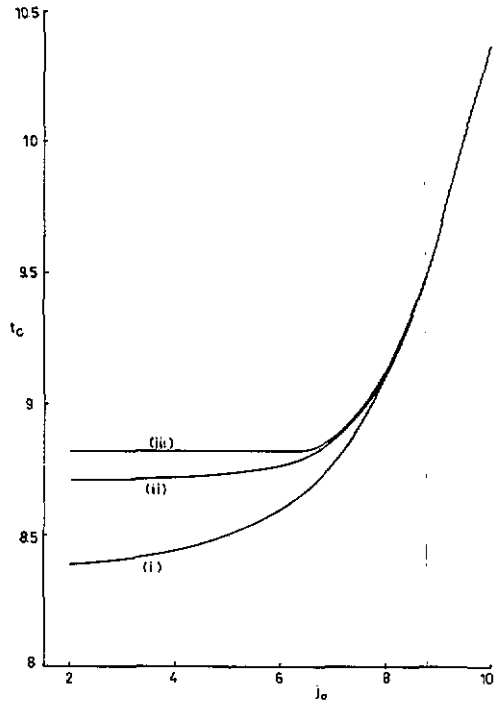

Figure 4. Dependence of t_c on j_0 for $j_A = 8$, $j_B = 4$ and for (i) three, (ii) seven and (iii) infinite layers.

where

$$\det_2(T) = \begin{bmatrix} x_0 & -1 & & & \\ -1 & x_A & -1 & & \\ & -1 & x_B & -1 & \\ & & & \ddots & \\ & & -1 & x_B & -1 \\ & & & -1 & x_{00} \end{bmatrix}_{(2n+2)\times(2n+2)} \tag{21}$$

and

$$x_{00} = (k_B T - z_0 J_{00})/zJ \qquad j_{00} = z_0 J_{00}/zJ.$$

By interchanging rows and expanding, we can write

$$\det_2(T) = x_{00}x_0 D_{2n} - (x_{00} + x_0 x_A/x_B)C_{2n-1} + D_{2n-2} = 0 \tag{22}$$

with the D and Cs from (12) and (13).

For any finite superlattice, (22) can again be solved numerically for different j_A, j_B, j_0 and j_{00}. To reduce our parameters, we have chosen $j_{00} = cj_A$, $j_0 = cj_B$, where c is the single modification parameter ($c = 1$ is our simple alternating lattice).

In figures 5 and 6, we have plotted t_c versus c for the two cases (*a*) $j_A = 2$, $j_B = 1$ and (*b*) $j_A = 8$, $j_B = 4$ respectively. The results for four and six layers, as

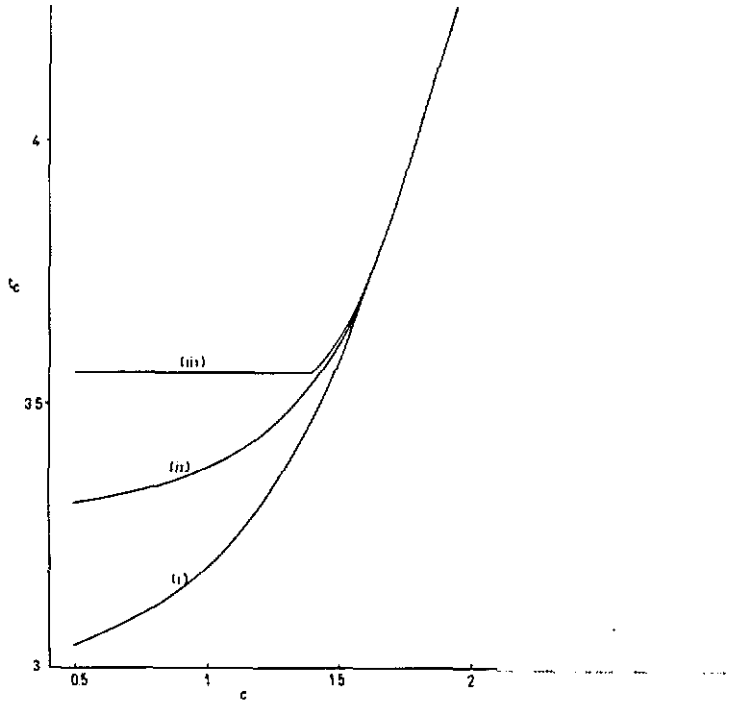

Figure 5. Variation of t_c with c for $j_A = 2$, $j_B = 1$ and for (i) four, (ii) six and (iii) infinite layers.

well as for the infinite limit, are shown. Again, the dependence of t_c on the layer thickness is significant only for small c. For larger c, the infinite limit is approached rapidly.

For the infinite case, the system again orders at the bulk t_c below a critical C_c. This critical value can be solved as in [19] by taking the limit

$$D_{2n-2}/D_{2n} \to 1 \qquad C_{2n-1}/D_{2n} = 2/x_A.$$

The values for our two cases are $C_c = 1.39$ and 1.05 respectively.

Although we have shown our numerical results for only two types of modification, the method can be used for other situations by considering different determinants, and expressing them in terms of the Cs and Ds.

At the moment, iron and cobalt may be the best candidates for alternating superlattices. Since these are itinerant magnets with nearly isotropic magnetic interaction, one may have to use an itinerant model, or at least a Heisenberg model, to describe the system properly.

In recent work on finite-size scaling [20], the transition temperature size dependence is given by $T_c(n) - T_c(\alpha) \propto n^{-\lambda}$, where λ is the shift exponent. Since we are applying the mean-field approximation, our results for large n (number of layers) are consistent with the expected mean-field exponent of $\lambda = 1/\nu$, where $\nu = \frac{1}{2}$ is the mean-field correlation length exponent. This is different from the results of more accurate calculations [20]. For example, Capehart and Fisher [21] have studied the Ising layer system with a uniform exchange by high-temperature series expansion and obtained the value $\lambda = 1.56$.

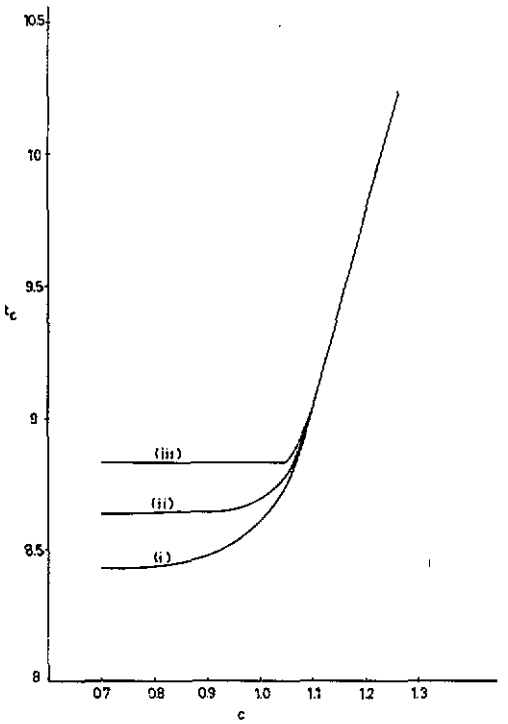

Figure 6. Variation of t_c with c for $j_A = 8$, $j_B = 4$ and for (i) four, (ii) six and (iii) infinite layers.

In conclusion, we hope our work will stimulate other theoretical studies, and our results will have relevance to some future experiments.

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