Phase transitions in Ising magnetic films and superlattices

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Abstract

Within the framework of mean field theory, we examine the phase transitions in Ising magnetic films and superlattices. By transfer matrix method, we derive two general nonlinear equations for phase transition temperatures of Ising magnetic films and superlattices, respectively. The equations can be applied to the films and superlattices with arbitrary exchange interaction constants and arbitrary layer number. Numerical results for phase transition temperatures as a function of exchange interaction constants are presented.

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I. INTRODUCTION

Considerable effort has been recently devoted to the understanding of magnetic films, layered structures and superlattices[1-7]. With the development of molecular beam epitaxy, it is now possible to grow in a very controlled way magnetic films with few atomic layers or even monolayer atop nonmagnetic substrates. A superlattice in which the atoms vary from one monolayer to another can also be envisaged. Very often one finds unexpected and interesting properties in these systems. For example, experimental studies[8-10] on the magnetic properties of surfaces of Gd,Cr and Tb have shown that a magnetically ordered surface can coexist with a magnetically disordered bulk phase.

Most work has been devoted to the free surface problem in which spins on the surface interact with each other through an exchange interaction $J_s$ different from that of bulk material[11-20]. For the values of $J_s/J$ above a certain critical value $(J_s/J)_{\text{crit}}$ the system orders on the surface before it orders in the bulk. Below this critical value only two phases are expected, namely the bulk ferromagnetic and paramagnetic phases.

Magnetic excitations in superlattices were studied in numerous papers (see, e.g., Ref.21 for a brief review). Yet less attention has been paid to critical behaviour. The phase transition temperatures for a Heisenberg magnetic superlattices have been studied [22-24]. Hinchey and Mills have investigated a superlattice structure with alternating ferromagnetic and antiferromagnetic layers[25-26].

In this paper, we are concerned with phase transitions in Ising magnetic films and superlattices. we study them within the framework of mean field theory. The transfer matrix method is used to derive nonlinear equations for magnetic Ising films and superlattices. The equations are general ones for arbitrary exchange interaction constants. In section II, we outline the formalism and derive the nonlinear equation for phase transition temperatures of magnetic films. The transition temperatures as a function of surface exchange constants are studied. The nonlinear equation for
transition temperatures of superlattices are given in section III. The last section IV
is devoted to a brief discussion.

II. FORMALISM AND PHASE TRANSITIONS IN ISING MAGNETIC
FILMS

We start with a lattice of localized spins with spin equal to $1/2$. The interaction
is of the nearest-neighbor ferromagnetic Ising type. The Ising Hamiltonian of the
system is given by

$$H = -\frac{1}{2} \sum_{(i,j)} \sum_{(r,r')} J_{ij} S_{ir} S_{jr'}, \quad (1)$$

where $(i,j)$ are plane indices, $(r,r')$ are different sites of the planes, and $S_{ir}$ is spin
variable. $J_{ij}$ denote the exchange constants and are plane dependent. We will keep
only nearest-neighbour terms.

In the mean-field theory, $S_{ir}$ is replaced by its mean value $m_i$ associated with each
plane, and is determined by a set of simultaneous equations

$$m_i = \tanh[(z_0 J_{ii} m_i + z J_{i,i+1} m_{i+1} + z J_{i,i-1} m_{i-1})/K_B T], \quad (2)$$

where $z_0$, $z$ are the numbers of nearest neighbours in the plane and between the planes,
respectively, $k_B$ is the Boltzman constant and $T$ is the temperature.

Near the transition temperature, the order parameter $m_i$ are small, Eq.(2) reduces
to

$$K_B T m_i = z_0 J_{ii} m_i + z J_{i,i+1} m_{i+1} + z J_{i,i-1} m_{i-1}. \quad (3)$$

Let us rewrite the above equation in matrix form in analogy with Ref.[27]

$$\begin{pmatrix} m_{i+1} \\ m_i \end{pmatrix} = M_{i-1} \begin{pmatrix} m_i \\ m_{i-1} \end{pmatrix} \quad (4)$$

with $M_{i-1}$ as the transfer matrix defined by

$$M_{i-1} = \begin{pmatrix} (K_B T - z_0 J_{ii})/(z J_{i,i+1}) & -J_{i,i-1}/J_{i,i+1} \\ 1 & 0 \end{pmatrix}. \quad (5)$$
We consider a magnetic film which contains $N$ layers with layer indices $i = 1, 2 \ldots N$.

From Eq.(4), we get
\begin{equation}
\begin{pmatrix}
m_N \\
m_{N-1}
\end{pmatrix} = R \begin{pmatrix}
m_2 \\
m_1
\end{pmatrix},
\end{equation}
where $R = M_{N-2} \ldots M_2 M_1$ represents successive multiplication of the transfer matrices $M_i$.

For an ideal film system, there exists symmetry in the direction perpendicular to the surface, which allows us to write $m_i = m_{N+1-i}$. Then, the following nonlinear equation for the transition temperature can be obtained from equations (3) and (6) as
\begin{equation}
R_{11}[\left(\frac{K_B T - z_0 J_{11}}{z J_{1,2}}\right)^2 + (R_{12} - R_{21})\left(\frac{K_B T - z_0 J_{11}}{z J_{1,2}}\right)] - R_{22} = 0.
\end{equation}

The above equation is the general equation for the transition temperature of symmetric films. It is suitable for arbitrary exchange interaction constants $J_{ij}$. All the information about the phase transition temperatures of the system is contained in the equation.

For a uniform system with $J_{ij} = J$, Eq.(7) reduces to
\begin{equation}
R_{11}(t - z_0/z)^2 + (R_{12} - R_{21})(t - z_0/z) - R_{22} = 0,
\end{equation}
where $t = K_B T/(J z)$ is the reduced temperature and $R = D^{N-2}$. Here the matrix
\begin{equation}
D = \begin{pmatrix}
t - z_0/z & -1 \\
1 & 0
\end{pmatrix}.
\end{equation}

Note that det($D$) = 1, we can linearalize matrix $R$ as[28]
\begin{equation}
R = U_{N-2} A - U_{N-3} I,
\end{equation}
where $I$ is the unit matrix ,$U_N = (\lambda_+^N - \lambda_-^N)/(\lambda_+ - \lambda_-)$, and $\lambda_\pm = (t - z_0/z \pm \sqrt{(t - z_0/z)^2 - 4})/2$. Substituting Eq.(10) into Eq.(8), we reduce Eq.(8) to its simplest form
\begin{equation}
U_{N+1} = 0.
\end{equation}
$U_{N+1}$ can be rewritten as

$$U_{N+1} = \sin[(N + 1)\phi]/\sin \phi$$

(12)

for $(t - z_0/z)^2 \leq 4$. Here $\phi = \arccos[(t - z_0/z)/2]$. For $(t - z_0/z)^2 \geq 4$, $\phi$ becomes $i\theta$, and the trigonometric functions become hyperbolic functions of $\theta$.

Eq.(11) gives

$$t = 2 \cos[\pi/(N + 1)] + z_0/z.$$  

(13)

In the limit $N \to \infty$, the reduced bulk temperature $t_B$ is obtained as

$$t_B = 2 + z_0/z.$$  

(14)

Fig.1 shows the reduced transition temperature vs. layer number $L$. It can be seen that the film transition temperature is lower than the bulk one, i.e., the film disorders at a lower temperature than the bulk ones. Throughout this paper, we take $J$ as the unit of energy.

In the above discussions, we have assumed the surface exchange constants $J_s$ are the same as the bulk exchange constants $J$. Now we consider a $(l, n, l)$ film consisting $l$ top surface layers, $n$ bulk surface layers and $l$ bottom surface layers, and assume that the exchange constants in a surface layer is denoted by $J_s$ and that in a bulk layer or between successive layers by $J$. In this case the total transfer matrix $R$ becomes

$$R = P^{l-1}Q^nP^{l-1},$$  

(15)

where the matrix $P$ and $Q$ are

$$P = \begin{pmatrix} t - 4J_s/J & -1 \\ 1 & 0 \end{pmatrix}, \quad Q = \begin{pmatrix} t - 4 & -1 \\ 1 & 0 \end{pmatrix}.$$  

(16)

Here we have assumed that the spins lie on a simple cubic lattice, i.e., $z_0 = 4, z = 1$.

Since $\text{Det}(P) = \text{Det}(Q) = 1$, the matrix $P^{l-1}$ and $Q^n$ can be linearalized in analogous to Eq.(10). In this case, the nonlinear Eq.(7) reduces to

$$R_{11}(t - 4J_s/J)^2 + (R_{12} - R_{21})(t - 4J_s/J) - R_{22} = 0.$$  

(17)
The numerical results for transition temperatures of a magnetic \((l, n, l)\) film as a function of \(J_s/J\) are shown in Fig.2. It is can be seen that the transition temperature increase as \(J_s/J\) increases. For \(J_s/J \leq 1\), the transition temperatures in film \((10, 10, 10)\) are nearly equal to the bulk temperature \(T_B\). It is interesting that the transition temperature increases linearly with the increase of \(J_s/J\) when \(J_s/J\) is large enough. We can also see that the transition temperature increases as layer number increases.

**III. PHASE TRANSITIONS IN ISING MAGNETIC SUPERLATTICES**

The \((l, n)\) superlattice structure we study is formed from two types of atoms. In each elementary unit with layer indices \(i = 1, 2...l + n\), there are \(l\) atomic layers of type \(A\) and \(n\) atomic layers of type \(B\). The interlayer exchange constants are given by \(J_a\) and \(J_b\), whereas the exchange constants between different layers is described by \(J\). For the above model of the superlattice, the transfer matrix \(M_i\)(Eq.(5)) reduce to different types of matrix

\[
A = \begin{pmatrix} X_A & -1 \\ 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} X_B & -1 \\ 1 & 0 \end{pmatrix}, \tag{18}
\]

where \(X_A = t - 4J_A/J\) and \(X_B = t - 4J_B/J\). From Eq.(4), we can obtain the following equation as

\[
\begin{pmatrix} m_{t+n+2} \\ m_{t+n+1} \end{pmatrix} = R \begin{pmatrix} m_2 \\ m_1 \end{pmatrix}, \tag{19}
\]

where

\[
R = AB^nA^{l-1} \tag{20}
\]

is the total transfer matrix.

Due to the periodicity of the superlattice, we know \(m_{t+n+2} = m_2\) and \(m_{t+n+1} = m_1\). Then from Eq.(19), we get

\[
Det(R) - Tr(R) + 1 = 0. \tag{21}
\]
It can be easily seen that $\text{Det}(A) = \text{Det}(B) = \text{Det}(R) = 1$. Then the Eq.(21) reduces to the simplest form

$$Tr(R) = 2. \quad (22)$$

Actually, the above equation is a general equation for phase transition temperature of superlattices. It is valid for arbitrary exchange constants $J_{ij}$. The nonlinear equation for films are dependent on both diagonal and nondiagonal terms of the total transfer matrix $R$, while the nonlinear equation for superlattices are only depend on diagonal terms of $R$.

For the total transfer matrix $R = AB^nA^{l-1}$, we get

$$Tr(A^lB^n) = 2. \quad (23)$$

The matrix $A^l$ and $B^n$ can be linearized as

$$A^l = E_iA - E_{i-1}I$$
$$B^n = F_nB - F_{n-1}I, \quad (24)$$

where $E_i = (\alpha^l_+ - \alpha^l_-)/\alpha_+ - \alpha_-$, $F_n = (\beta^n_+ - \beta^n_-)/\beta_+ - \beta_-$, $\alpha_\pm = (X_A \pm \sqrt{X_A^2 - 4})/2$ and $\beta_\pm = (X_B \pm \sqrt{X_B^2 - 4})/2$. From Eq.(23), we get the equation

$$(E_iX_a - E_{i-1})(F_nX_b - F_{n-1}) - 2E_iF_n + E_{i-1}F_{n-1} = 2. \quad (25)$$

For $l = 1$, $n = 1$, the above equation reduces to

$$X_aX_b = 4, \quad (26)$$

which is identical with the result of Ref.(2) and (29). Next we numerically calculate the phase transition temperatures from Eq.(25).

In figure 3, we have shown the results for the superlattices $(3,1), (2,2), (10,5)$ and $(20,20)$. The transition temperature is plotted as a function of $J_A/J$. For $J_A/J < 1$, the transition temperature is smaller that the bulk transition temperature. For $J_A/J = 1$, the transition temperature of the superlattice is independent of $m$ and $n$, and are equal to the bulk temperature $T_B$ as expected. On the other hand,
for $J_A/J > 1$, the transition temperature is greater than the bulk temperature $T_B$.

The transition temperature increases with the layer number in one unit cell and approaches $T_B$ asymptotically as the number become large. The transition temperature increases nearly linearly with $J_A/J$ when $J_A/J$ is large enough. The layer number of superlattices $(3, 1)$ and $(2, 2)$ are same, but the transition temperatures are different. For $J_A/J < 1$, the transition temperatures of superlattice $(2, 2)$ are larger than those of superlattice $(3, 1)$. In contrary to this, the transition temperatures of superlattice $(2, 2)$ are smaller than those of superlattice $(3, 1)$ for $J_A/J > 1$.

**IV. DISCUSSIONS**

In summary, we have studied phase transitions in Ising magnetic films and superlattices with the framework of mean field theory. By transfer matrix method, we have derived two general nonlinear equations for phase transition temperatures in Ising films and superlattices, respectively. The transition temperatures as a function of exchange interaction constants are calculated. In addition, the equations can be easily solved and the parameters involved can be adjusted at will.

**Figure Captions**

Fig.1, Transition temperatures of a uniform film as a function of layer number $L$.

Fig.2, Transition temperatures of a magnetic film $(l, n, l)$ as a function of $J_s/J$.

Fig.3, Transition temperatures of a magnetic superlattice $(l, n)$ as a function of $J_A/J$. 
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Figure 1
Figure 2
Figure 3