Magnetization Profiles of Ferromagnetic Ising Films in a Transverse Field

WANG Xiao-Guang (王晓光), PAN Shao-Hua (潘少华), YANG Guo-Zhen (杨国桢)
Laboratory of Optical Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080

(Received 7 June 1999)

Within the framework of the mean field theory, we study the magnetization profiles of ferromagnetic Ising films in a transverse field. By the transfer matrix method, we first derive a general nonlinear equation for phase transition temperatures and then calculate the magnetization profiles of the system. The method proposed here can be applied to ferromagnetic films with arbitrary surface layer number, bulk layer number, exchange interaction constants and transverse fields.

PACS: 75.10.−b, 75.50.Rr, 75.70.Ak

The development of the molecular epitaxy technique and its application to the growth of thin films has stimulated renewed interest in the thin film magnetism. Very often one finds unexpected and interesting properties. For instance, the experimental studies\(^1\)\(^-\)\(^3\) 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.

From the theoretical point of view, two models widely used to study the magnetic properties of thin films are the Ising model and Ising model in a transverse field. The effects produced by surfaces can be simulated by assuming that the surface exchange interaction \(J_s\) is different from the bulk interaction \(J\). The surface magnetism of the system is very interesting.\(^4\)\(^-\)\(^14\) For values of \(J_s/J\) above a critical value \((J_s/J)_c\), the system orders on the surface before it orders in the bulk and a surface ferromagnetic phase is possible. Below this critical value only two phases are expected, namely the bulk ferromagnetic and paramagnetic phases.

In this paper, we are concerned with the magnetization profiles of ferromagnetic Ising films in a transverse field. The transverse field may be either an applied magnetic field or at the surface it may represent a surface field due to the presence of a substrate or adjacent magnetic layers of different materials. Within the framework of the mean field theory, we first obtain a general nonlinear equation for phase transition temperatures and then determine the magnetization profiles by transfer matrix method. The transfer matrix method proposed here is very effective to calculating the phase transition temperatures and magnetization profiles of ferromagnetic films.

We start with the Ising model in a transverse field\(^14\)\(^-\)\(^16\)

\[
H = -\frac{1}{2} \sum_{(i,j)} \sum_{(r,r')} J_{ij} S^x_i S^x_j + \sum_{ir} \Omega_i S^z_i,
\]  

where \(S^x_i, S^z_i\) are the \(x\) and \(z\) components of a spin-1/2 operator, \((i,j)\) are the plane indices and \((r,r')\) represent different sites of the planes, and \(J_{ij}\) denote the exchange interaction. We consider the interaction between neighboring sites and assume that the transverse field \(\Omega_i\) is dependent only on layer index.

The spin average \(\langle S^z_i \rangle\) obtained from the mean field theory\(^15\)\(^,\)\(^16\) is as follows:

\[
\langle S^z_i \rangle = \frac{H_i}{2|H_i|} \tanh \left( \frac{|H_i|}{2k_B T} \right),
\]

where \(H_i(\Omega_i, 0, \sum_j J_{ij} \langle S^z_j \rangle)\) is the mean field acting on the \(i\)-th spin, \(k_B\) is the Boltzmann constant and \(T\) is the temperature.

At a temperature close and just below the Curie temperature, \(\langle S^z_i \rangle\) and \(\langle S^z_i \rangle\) are small, \(|H_i| \approx \Omega_i\), Eq. (2) can be approximated as

\[
\langle S^z_i \rangle = \frac{1}{2} \frac{\Omega_i}{2k_B T} \tanh \left( \frac{\Omega_i}{2k_B T} \right),
\]

\[
\langle S^z_i \rangle = \frac{1}{2} \frac{\Omega_i}{2k_B T} \left[ z_0 J_{ii} \langle S^z_i \rangle + z_0 J_{ii} \langle S^z_{i+1} \rangle + \frac{z_0 J_{ii} \langle S^z_{i-1} \rangle}{2k_B T} \right].
\]

Here \(z_0\) and \(z\) are the numbers of nearest neighbors on a certain plane and that between a pair of successive planes, respectively. By defining

\[
K_i = \frac{z_0 J_{ii}}{z J}, \quad K_i, i=\pm 1 = \frac{J_{i,i+1}}{J},
\]

\[
m_i = \langle S^z_i \rangle, \quad \tau_i = \frac{2 \Omega_i}{z J} \frac{1}{\coth \left( \frac{\Omega_i}{2k_B T} \right)},
\]

Eq. (4) can be rewritten as

\[
(\tau_i - K_i) m_i - K_{i,i+1} m_{i+1} - K_{i,i-1} m_{i-1} = 0,
\]

where \(J\) is the interlayer exchange constant in the bulk.

Let us rewrite the above equation in matrix form in analogy with Ref. 17:

\[
\left( \begin{array}{c} m_{i+1} \\ m_i \\ m_{i-1} \end{array} \right) = M_i \left( \begin{array}{c} m_{i+1} \\ m_i \\ m_{i-1} \end{array} \right),
\]

with \(M_i\) as the transfer matrix defined by

\[
M_i = \left( \begin{array}{ccc} (\tau_i - K_{i})/K_{i,i+1} & -K_{i,i-1}/K_{i,i+1} & 1 \\ 0 & 0 & 0 \end{array} \right)
\]
We assume that the ferromagnetic film contains $N+1$ layers with layer indices $i = 0, 1, 2, \cdots, N$. From Eq. (7), we get
\begin{equation}
\begin{pmatrix} m_N \\ m_{N-1} \end{pmatrix} = R \begin{pmatrix} m_1 \\ m_0 \end{pmatrix},
\end{equation}
where $R = M_{N-1} \cdots M_2 M_1$ represents the successive multiplication of the transfer matrices.

For an ideal film system, there exists symmetry in the direction perpendicular to the surface, which allows us to write $m_i = m_{N-i}$. Then, the following nonlinear equation for phase transition temperatures can be derived from Eqs. (6) and (9) as
\begin{equation}
R_{11} \left( \tau_0 - \frac{K_0}{K_{0,1}} \right)^2 + (R_{12} - R_{21}) \left( \tau_0 - \frac{K_0}{K_{0,1}} \right) - R_{22} = 0.
\end{equation}

The above equation is the general equation for Curie temperature for arbitrary exchange constants $J_{ij}$ and transverse fields $\Omega_i$.

As an example, we consider a $(l, n, l)$ film consisting of $l$ top surface layers, $n$ bulk layers and $l$ bottom surface layers. We assume that the spins lie on a simple cubic lattice and that the transverse fields $\Omega_i = \Omega$. The coupling strength in a surface layer is denoted by $J_s$ and in that a bulk layers or successive layers is denoted by $J$. Then the transfer matrix (8) reduces to two different types of matrices:
\begin{equation}
P = \begin{pmatrix} X & 1 \\ 0 & 0 \end{pmatrix}, \quad Q = \begin{pmatrix} Y & 1 \\ 0 & 0 \end{pmatrix},
\end{equation}
and the total transfer matrix $R = P^{l-1} Q^n P^{l-1}$. Here $X = \tau - 4J_s/J$ and $Y = \tau - 4$. Equation (10) for phase transition temperatures thus reduces to
\begin{equation}
R_{11}X^2 + (R_{12} - R_{21})X - R_{22} = 0.
\end{equation}

From the above equation, the phase transition temperatures can be calculated, then the magnetization profiles can be determined from Eq. (7) if we know the magnetizations $m_1$ and $m_0$. We use $m_0$ to scale the magnetization $m_i$, i.e., take $m_0$ as the unit of the magnetization, $m_1$ is obtained from the equation $m_1 = (\tau - 4J_s/J)m_0$. Figure 1 shows the reduced magnetization $m_i/m_0$ for a $(10, 5, 10)$ film with $n = 5, 10, 15$. All these figures are symmetric because of the symmetry of the system. For $n = 5$, we observe the positive maximum magnetization in the bulk layer $i = 12$ and the negative maximum magnetization in the bulk layers $i = 11$ and 13. The absolute value of the magnetization in the bulk layer $i = 12$ is comparable to those in the bulk layers $i = 11$ and 13. For $n = 10$ and 15, there are maximal at surface layer $i = 4$. As $i$ increases from 0, the magnetization first increases, then decreases, the minimum of the magnetization is not at the outermost surface layer. The magnetizations in the surface layers are like the characteristics of the ferromagnetic coupling and those in the bulk layers are like the characteristics of the antiferromagnetic coupling. The perfect symmetry of the figures also indicates the efficiency of the transfer matrix method.

In conclusion, we propose a general method to calculate the phase transition temperatures and magnetization profiles of a ferromagnetic Ising film in a transverse field. As an example, we study the magnetization profiles of a $(l, n, l)$ film. The method proposed here can be applied to ferromagnetic films with arbitrary surface layer number, bulk layer number, exchange interaction constants and transverse fields and is expected to be able to study layered ferromagnetic structures and superlattices.

REFERENCES