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Critical behaviour of a transverse Ising ferromagnetic thin film with spin 1

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Abstract. A correlation effective-field treatment is presented for a transverse Ising ferromagnetic thin film with $S = 1$. The critical behaviour of transverse Ising ferromagnetic thin films with $S = 1$ and, in particular, the transverse field dependences of the critical temperature and thickness dependences of the critical transverse field are investigated.

1. Introduction

There has been an increasing interest in studying the Ising model with a transverse field (TIM). It is described by the following Hamiltonian [1]:

$$\mathcal{H} = -\sum_i \Omega S_i^x - \sum_{ij} J_{ij} S_i^z S_j^z \tag{1}$$

where S_i^x and S_i^z are the components of the spin operator at site i, Ω represents a transverse field and J_{ij} is an exchange interaction between spins at sites i and j.

Along with the development of new types of magnetic material, research on the properties of magnetic thin films has received much attention [2, 3]. However, workers have only investigated a transverse Ising ferromagnetic thin film with $S = \frac{1}{2}$. They have not studied a thin film with $S = 1$ yet.

In the present work we shall investigate the critical behaviour of transverse Ising ferromagnetic thin films with $S = 1$ using the effective-field theory [4], which is based on the introduction of a differential operator. The transverse field dependences of the critical temperature and thickness dependences of the critical transverse field for the film are also investigated by us.

2. Theory

We consider a thin film consisting of L layers parallel to the surfaces, chosen as (100) layers (as shown in figure 1). This is a quasi-two-dimensional system with a finite thickness. The Hamiltonian of the system is described by equation (1).

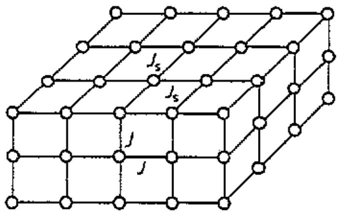

Figure 1. The ferromagnetic thin film for the simple cubic lattice. J_s denotes the exchange interaction at the surface and J is the exchange interaction in the inside.

In a series of papers where $\Omega = 0$ is used, the starting point for the statistics of the system is Callen's [5] identity. However, what we intend to discuss here is the TIM, $\mathcal{H}_i$ and $\mathcal{H}'$ which do not commute with each other. $\mathcal{H}_i$ and $\mathcal{H}'$ are two parts separating the total Hamiltonian $\mathcal{H} = \mathcal{H}_i + \mathcal{H}'$, where $\mathcal{H}_i$ includes all parts of $\mathcal{H}$ associated with the lattice site i and $\mathcal{H}'$ represents the rest of the Hamiltonian. Therefore we cannot apply Callen's identity to the present problem. According to the relation in our earlier paper [6], the expectation value of the longitudinal magnetization at i for the TIM is as follows:

$$\langle S_i^z\rangle = \left\langle \prod_j [(S_j^z)^2 \cosh(\mathrm{D}J_{ij}) + (S_j^z)\sinh(\mathrm{D}J_{ij}) + 1 - (S_j^z)^2] \right\rangle F(x)|_{x=0} \tag{2}$$

with

$$F(x) = (x/\sqrt{x^2+\Omega^2})\{2\sinh(\beta\sqrt{x^2+\Omega^2})/[1+2\cosh(\beta\sqrt{x^2+\Omega^2})]\} \tag{3}$$

where $\mathrm{D} = \partial/\partial x$ is a differential operator. Different from the TIM with $S = \frac{1}{2}$, there exists a new kind of order parameter $(S_j^z)^2$ in the TIM with $S = 1$. Its expectation value is as follows:

$$\langle (S_i^z)^2\rangle = \left\langle \prod_j [(S_j^z)^2 \cosh(\mathrm{D}J_{ij}) + (S_j^z)\sinh(\mathrm{D}J_{ij}) + 1 - (S_j^z)^2] \right\rangle U(x)|_{x=0} \tag{4}$$

with

$$\begin{aligned} U(x) &= (1/\beta)H(x) + W(x) \\ H(x) &= \{1/\sqrt{\Omega^2+x^2} - x^2/(\Omega^2+x^2)^{3/2}\} \\ &\quad \times \{2\sinh(\beta\sqrt{\Omega^2+x^2})/[1+2\cosh(\beta\sqrt{\Omega^2+x^2})]\} \\ W(x) &= [x^2/(\Omega^2+x^2)]\{2\cosh(\beta\sqrt{\Omega^2+x^2})/[1+2\cosh(\beta\sqrt{\Omega^2+x^2})]\}. \end{aligned} \tag{5}$$

For simplicity, we shall assume that exchange interactions exist only between nearest neighbours, with $J_{ij} = J > 0$. With the above approximation, the atomic magnetizations for the various layers are easily obtained:

$$\begin{aligned} m_1^z = \langle S_1^z\rangle &= [y_1\cosh(\mathrm{D}J) + m_1^z\sinh(\mathrm{D}J) + 1 - y_1]^4 \\ &\quad \times [y_2\cosh(\mathrm{D}J) + m_2^z\sinh(\mathrm{D}J) + 1 - y_2]F(x)|_{x=0} \end{aligned} \tag{6}$$

$\vdots$

$$\begin{aligned} m_n^z = \langle S_n^z\rangle &= [y_n\cosh(\mathrm{D}J) + m_n^z\sinh(\mathrm{D}J) + 1 - y_n]^4 \\ &\quad \times [y_{n-1}\cosh(\mathrm{D}J) + m_{n-1}^z\sinh(\mathrm{D}J) + 1 - y_{n-1}] \\ &\quad \times [y_{n+1}\cosh(\mathrm{D}J) + m_{n+1}^z\sinh(\mathrm{D}J) + 1 - y_{n+1}]F(x)|_{x=0} \end{aligned} \tag{7}$$

$\vdots$

$$m_L^z = \langle S_L^z \rangle = [y_L \cosh(DJ) + m_L^z \sinh(DJ) + 1 - y_L]^4$$
$$\times [y_{L-1} \cosh(DJ) + m_{L-1}^z \sinh(DJ) + 1 - y_{L-1}] F(x)|_{x=0} \tag{8}$$

where

$$y_m \equiv \langle (S_n^z)^2 \rangle.$$

Near the critical points where the atomic magnetization in each layer is very small, we can linearize equations (6)–(8). At the same time, as a result of the symmetry of the system, it is understood that $y_L = y_1$, $y_{L-1} = y_2$ and $y_n = y$ when $3 \leqslant n \leqslant L-2$. Consequently, we obtain a set of simultaneous equations

$$\begin{pmatrix} \frac{1-E_1}{E_2}, -1 & & & & \\ -1, \frac{1-E_3}{E_4}, -1 & & & & \\ & \cdots & & & \\ & & -1, \frac{1-E_3}{E_4}, -1 & & \\ & & \cdots & & \\ & & & -1, \frac{1-E_3}{E_4}, -1 & \\ & & & & -1, \frac{1-E_1}{E_2} \end{pmatrix} \begin{pmatrix} m_1 \\ m_2 \\ \vdots \\ m_n \\ \vdots \\ m_{L-1} \\ m_L \end{pmatrix} = 0. \tag{9}$$

Here the coefficients E_1 to E_4 in the simultaneous equations can be written out explicitly after linearizing equations (6)–(8):

$$E_1 = 4[y_1 \cosh(DJ) + 1 - y_1]^3 [y_2 \cosh(DJ) + 1 - y_2] \sinh(DJ)\, F(x)|_{x=0} \tag{10}$$

$$E_2 = [y_1 \cosh(DJ) + 1 - y_1]^4 \sinh(DJ)\, F(x)|_{x=0} \tag{11}$$

$$E_4 = [y \cosh(DJ) + 1 - y]^5 \sinh(DJ)\, F(x)|_{x=0} \tag{12}$$

$$E_3 = 4E_4$$

and y_1, y_2 and y in these equations can be also evaluated from (4) after the approximation concerning nearest neighbours has been performed:

$$y_1 = [y_1 \cosh(DJ) + 1 - y_1]^4 [y_2 \cosh(DJ) + 1 - y_2] U(x)|_{x=0} \tag{13}$$

$$y_2 = [y_2 \cosh(DJ) + 1 - y_2]^4 [y_1 \cosh(DJ) + 1 - y_1]$$
$$\times [y \cosh(DJ) + 1 - y] U(x)|_{x=0} \tag{14}$$

$$y = [y \cosh(DJ) + 1 - y]^6 U(x)|_{x=0}. \tag{15}$$

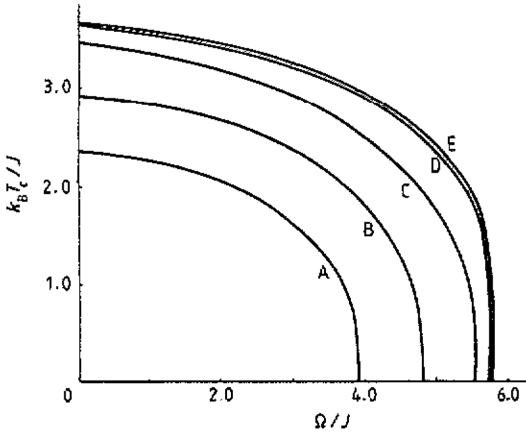

Figure 2. The phase diagrams in (T_c, Ω) for some selected values of L: curve A, $L = 1$; curve B, $L = 2$; curve C, $L = 5$; curve D, $L = 10$; curve E, $L = 80$.

The phase transition temperature T_c can be derived from the condition det $A = 0$, where det A is the secular determinant of (9). This condition can be transformed to

$$\begin{vmatrix} x-a, -1 & & & & \\ -1, x, -1 & & & & \\ & \cdots & & & \\ & & -1, x, -1 & & \\ & & & -1, x-a \end{vmatrix} = 0 \tag{16}$$

where

$$x = (1 - E_3)/E_4 = (1/E_4 - 4) \tag{17}$$

$$x - a = (1 - E_1)/E_2. \tag{18}$$

On inserting $x = 2\cos k$ and applying the addition theorem for determinants, one can reduce the secular determinant (16) to Wolstenholme determinants [7] and can obtain [8]

$$\tan(kL) = (r_0 \sin k)/(\cos k - t) \tag{19}$$

$$r_0 = (a^2 - 1)/(a^2 + 1) \tag{20}$$

$$t = 2a/(a^2 + 1). \tag{21}$$

From the many formal solutions of equation (19), we choose the one corresponding to the highest possible transition temperature as the critical temperature $T_c(\Omega/J)$ of the film under a given transverse field. It can correspond to a value of k which is the smallest of the set yielding the solutions.

3. Numerical results and discussion

By solving equation (19), the critical frontier characterizing the ferromagnetic phase stability limit as a function of transverse field Ω and thickness L can be obtained. Therefore, the phase diagrams can be plotted as well (figure 2). As shown in figure 2,

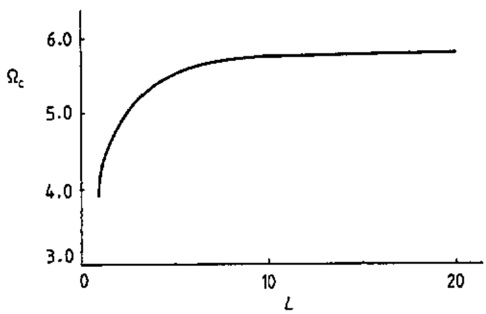

Figure 3. Thickness dependences of the critical transverse field.

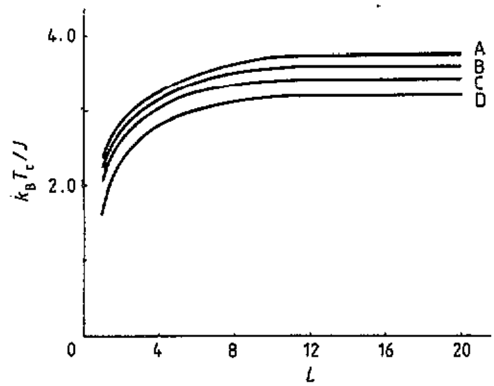

Figure 4. The thickness dependences of the values of critical temperature for some selected values of transverse field: curve A, $\Omega/J = 0$; curve B, $\Omega/J = 1.0$; curve C, $\Omega/J = 2.0$; curve D, $\Omega/J = 3.0$.

when the transverse field Ω in the film increases from zero and the number of atomic layers is given, the phase transition temperature T_c decreases from its value in the Ising model and reaches zero at a critical value of the transverse field Ω_c. The role of the transverse field in a transverse ferromagnetic thin film is essentially to inhibit the ordering of the S^z component. On the other hand, it can be seen from figure 2 that the critical values of the transverse field Ω_c increase together with the increase in the thickness L. In order to reveal this behaviour more clearly, we plotted figure 3.

From figure 3, we shall discover that at first the critical values Ω_c scale rapidly but, when the number of the atomic layers $L > 10$, the values of Ω_c approach the bulk values. In fact, in the case $L = 1$, which is a pure two-dimensional case, we obtain the critical value of the transverse field $\Omega_c/J = 3.902$. This result is the same as that in [6] previously reported by us. All values of the critical transverse field should interpolate between the two values $\Omega_c/J(L = 1) = 3.902$ and $\Omega_c/J(L = \infty) = 5.8099$.

Figure 4 displays the thickness dependences of the values of critical temperature for some selected values of transverse field. As shown in figure 4, all values of critical temperature $k_B T_c/J$ when $\Omega = 0$ should interpolate between the two values $k_B T_c/J(L = 1) = 2.3644$ and $k_B T_c/J(L = \infty) = 3.7107$. This can be seen more clearly from figure 1.

Up to now, we have applied the correlation effective-field theory and TIM to study the critical behaviour of a ferromagneic thin film. It is seen that there is a direct relation between the thickness of a film and its critical behaviour; in particular, when the number of atomic layers is small, the effect of thickness is very sharp.

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