Magnetic properties of a transverse Ising film with s=1/2

1992 J. Phys.: Condens. Matter 4 3651

(http://iopscience.iop.org/0953-8984/4/13/024)

J. Phys.: Condens. Matter 4 (1992) 3651–3658. Printed in the UK

Magnetic properties of a transverse Ising film with $s = 1/2$

Xuan-Zhang Wang, Xiu-Ye Jiao and Jing-Ju Wang
Department of Physics, Harbin Normal University, Harbin 150080, People's Republic of China

Received 29 October 1991

Abstract. A transverse Ising film, for $s = 1/2$, with a body-centred cubic structure and two (001) surfaces is studied by means of the effective-field theory with correlations. The layer magnetizations and average magnetization of the film as functions of temperature and transverse field are calculated numerically and some interesting results are obtained.

1. Introduction

Using the technique of molecular-beam expitaxy, high-quality thin films can be fabricated. Of these, magnetic films are very important from both the theoretical standpoint and the experimental standpoint [1, 2] and can be studied as models of the magnetic size effect [3] and quasi-two-dimensional system. The magnetic and phase transition properties of semi-infinite Ising systems have been investigated for many years. The surface magnetism of these systems is very interesting [4–9]. When the surface exchange parameter J_s is larger than a critical value J_{sc}, the system becomes ordered on the surface before it is ordered in the bulk, and the critical temperature of the surface is higher than that of the bulk. For a film composed of a few atomic layers, one cannot differentiate between the critical temperatures of the surface and the internal layers, and the film possesses a unified critical temperature [10–12]. For a film in which there are a great number of atomic layers parallel to the surfaces, in the central region of the film the magnetism is similar to that of the bulk, and in this case the film may be considered as a semi-infinite system. Recently the critical properties of ordinary and transverse Ising films were calculated and discussed [10–12], but the magnetization properties of a transverse Ising film were not investigated. In addition, in previous work on Ising films and semi-infinite Ising systems, the lattice structures used are almost simple cubic. In this paper, we use the effective-field theory with correlations [4, 13] to investigate the temperature and transverse field dependences of the magnetizations, including the average and sublattice (layer) magnetizations, of a transverse Ising film with $s = \frac{1}{2}$ and a body-centred cubic (BCC) lattice.

2. Theory

We consider a transverse Ising film, for $s = \frac{1}{2}$, with BCC lattice structure and (001) surfaces as shown in figure 1. The Hamiltonian of the film can be written as

$$H = -\tfrac{1}{2}\sum_{ij} J_{ij} S_i^z S_j^z - \Omega_{\mathrm{I}} \sum_{i\in I} S_i^x - \Omega_{\mathrm{S}} \sum_{i\in S} S_i^x \tag{1}$$

where S^x and S^z are components of spin-$\frac{1}{2}$ operators, and Ω_I and Ω_S represent transverse fields in the internal and surface layers, respectively; the symbols $\sum_{i\in I}$ and $\sum_{i\in S}$ express the sums over the internal and surface lattice points; J_{ij} is an exchange interaction between spins at nearest-neighbour sites i and j, and J_{ij} is J_S between spins on the surface layer and its nearest-neighbour layer, otherwise J. There is no interaction between spins on the same layer parallel to the surfaces.

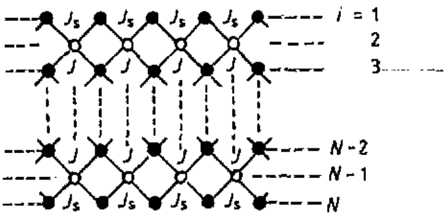

Figure 1. Section of the film with the BCC lattice: O, ●, different lattice points in the BCC lattice; i is the layer index; J_S and J are interaction parameters.

According to the effective-field theory with correlations, the layer magnetizations of the film are given by

$$\sigma_1 = 2\langle S_1^z\rangle = [\cosh(J_{12}\mathrm{D}) + \sigma_2 \sinh(J_{12}\mathrm{D})]^4 f_S(x)|_{x=0}$$

$$\vdots$$

$$\sigma_i = 2\langle S_i^z\rangle = [\cosh(J_{ii-1}\mathrm{D}) + \sigma_{i-1}\sinh(J_{ii-1}\mathrm{D})]^4 \times [\cosh(J_{ii+1}\mathrm{D}) + \sigma_{i+1}\sinh(J_{ii+1}\mathrm{D})] f_I(x)|_{x=0} \quad (2)$$

$$\vdots$$

$$\sigma_N = 2\langle S_N^z\rangle = [\cosh(J_{NN-1}\mathrm{D}) + \sigma_{N-1}\sinh(J_{NN-1}\mathrm{D})]^4 f_S(x)|_{x=0}$$

where we use N to represent the number of atomic layers parallel to the surfaces; $\langle S_1^z\rangle, \langle S_2^z\rangle, \ldots, \langle S_i^z\rangle, \ldots, \langle S_N^z\rangle$ are the layer magnetizations; $\mathrm{D} = \partial/\partial x$ is a differential operator and $\exp(\alpha\mathrm{D})f(x) = f(x+\alpha)$; $f(x)$ is defined by

$$f_i(x) = [x/(4\Omega_i^2 + x^2)^{1/2}] \tanh[\beta/4(4\Omega_i^2 + x^2)^{1/2}]. \quad (3)$$

In (3), $\beta = 1/k_B T$, where k_B is the Boltzmann constant and T denotes the absolute temperature.

Let us assume that the two surfaces are identical; therefore $J_{12} = J_{NN-1} = J_S$ and

$$\sigma_1 = \sigma_N, \sigma_2 = \sigma_{N-1}, \sigma_3 = \sigma_{N-2}, \cdots. \quad (4)$$

In order to calculate equations (2) numerically, it is necessary that equations (2) be expanded; thus we obtain

$$\sigma_1 = A_1\sigma_2 + A_2\sigma_2^2 + A_3\sigma_2^3 + A_4\sigma_2^4$$

$$\sigma_2 = B_1\sigma_3 + B_2\sigma_3^2 + B_3\sigma_3^3 + B_4\sigma_3^4 + \sigma_1 C_0 + C_1\sigma_1\sigma_3 + C_2\sigma_1\sigma_3^2 + C_3\sigma_1\sigma_3^3$$

$$+ C_4\sigma_1\sigma_3^4 + D_0\sigma_1^2 + D_1\sigma_1^2\sigma_3 + D_2\sigma_1^2\sigma_3^2 + D_3\sigma_1^2\sigma_3^3 + D_4\sigma_1^2\sigma_3^4 \quad (5)$$
$$+ E_0\sigma_1^3 + E_1\sigma_1^3\sigma_3^1 + E_2\sigma_1^3\sigma_3^2 + E_3\sigma_1^3\sigma_3^3 + E_4\sigma_1^3\sigma_3^4 + F_0\sigma_1^4$$
$$+ F_1\sigma_1^4\sigma_3 + F_2\sigma_1^4\sigma_3^2 + F_3\sigma_1^4\sigma_3^3 + F_4\sigma_1^4\sigma_3^4$$

$$\vdots$$

$$\begin{aligned}\sigma_i = {} & 4G_1(\sigma_{i-1} + \sigma_{i+1}) + 2G_2(3\sigma_{i-1}^2 + 8\sigma_{i-1}\sigma_{i+1} + 3\sigma_{i+1}^2) \\ & + 4G_3(\sigma_{i-1}^3 + 6\sigma_{i-1}^2\sigma_{i+1} + 6\sigma_{i-1}\sigma_{i+1}^2 + \sigma_{i+1}^3) \\ & + G_4(\sigma_{i-1}^4 + 16\sigma_{i-1}^3\sigma_{i+1} + 36\sigma_{i-1}^2\sigma_{i+1}^3 + 16\sigma_{i-1}\sigma_{i+1}^3 + \sigma_{i+1}^4) \\ & + 4G_5(\sigma_{i-1}^4\sigma_{i+1} + 6\sigma_{i-1}^3\sigma_{i+1}^2 + 6\sigma_{i-1}^2\sigma_{i+1}^3 + \sigma_{i-1}\sigma_{i+1}^4) \\ & + 2G_6(3\sigma_{i-1}^2\sigma_{i+1}^4 + 8\sigma_{i-1}^3\sigma_{i+1}^3 + 3\sigma_{i-1}^4\sigma_{i+1}^2 \\ & + 4G_7(\sigma_{i-1}^4\sigma_{i+1}^3 + \sigma_{i-1}^3\sigma_{i+1}^4 + G_8\sigma_{i-1}^4\sigma_{i+1}^4\end{aligned}$$

where A_λ and B_λ ($\lambda = 1$, 2, 3 and 4), and C_λ, D_λ, E_λ and F_λ($\lambda = 0$, 1, 2, 3 and 4), respectively, are given by

$$\begin{aligned} A_\lambda &= C_4^\lambda \cosh^{4-\lambda}(J_S D)\sinh^\lambda(J_S D) f_S(x)|_{x=0} \\ B_\lambda &= C_4^\lambda \cosh^4(J_S D)\cosh^{4-\lambda}(JD)\sinh^\lambda(JD) f_I(x)|_{x=0} \\ C_\lambda &= 4C_4^\lambda \cosh^3(J_S D)\cosh^{4-\lambda}(JD)\sinh(J_S D)\sinh^\lambda(JD) f_I(x)|_{x=0} \\ D_\lambda &= C_4^\lambda \cosh^2(J_S D)\sinh^2(J_S D)\cosh^{4-\lambda}(JD)\sinh^\lambda(JD) f_I(x)|_{x=0} \\ E_\lambda &= 4C_4^\lambda \cosh(J_S D)\sinh^3(J_S D)\cosh^{4-\lambda}(JD)\sinh^\lambda(JD) f_I(x)|_{x=0} \\ F_\lambda &= C_4^\lambda \sinh^4(J_S D)\cosh^{4-\lambda}(JD)\sinh^\lambda(JD) f_I(x)|_{x=0} \end{aligned} \quad (6)$$

with

$$C_4^\lambda = 4!/(4-\lambda)!\lambda! \quad (7)$$

and $G_\lambda(\lambda = 1\text{–}8)$ is written as

$$G_\lambda = \cosh^{8-\lambda}(JD)\sinh^\lambda(JD) f_I(x)|_{x=0}. \quad (8)$$

In the numerical calculation, we should note the symmetry of the film and thus the amount of the calculation can be decreased greatly.

For a given transverse field, as $T \to T_c$ (T_c is the critical temperature), the layer magnetization $\sigma_i/2(i = 1, 2, 3, \ldots, N)$ approaches zero. Considering σ_i as a small value, we expand equations (5) and neglect the non-linear terms; then the critical temperature of the system is determined by

$$\begin{vmatrix} 1 & A_1 & 0 & 0 & & & & \\ C_0 & 1 & B_1 & 0 & & & & \\ 0 & 4G_1 & 1 & 4G_1 & & & & \\ 0 & 0 & 4G_1 & 1 & & & & \\ & & & \ddots & \ddots & \ddots & & \\ & & & & 1 & 4G_1 & 0 & 0 \\ & & & & 4G_1 & 1 & 4G_1 & 0 \\ & & & & 0 & B_1 & 1 & C_0 \\ & & & & 0 & 0 & A_1 & 1 \end{vmatrix} = 0 \quad (9)$$

where T_c obeys equation (9) through A_1, C_0, B_1 and G_1.

3. Numerical results

Solving equations (5) numerically, we can obtain the layer magnetizations and average magnetization of the film as functions of temperature or transverse field, and solving equation (9) we can determine the critical temperature in a given transverse field. Because the magnetization behaviours of a transverse Ising film have not been studied in the past as far as we know, and in addition the transverse field dependence of the magnetization of transverse Ising systems was considered only rarely, we give mainly the temperature and transverse field dependences of the magnetizations, and use $\Omega_S = \Omega_I = \Omega$ for simplicity. Because of the symmetry of the film, we give only $N/2$ layer magnetizations as functions of temperature and transverse field in the corresponding figures.

3.1. Temperature dependences of the magnetizations

After selecting a value of the transverse field, one can obtain the layer magnetizations from equations (5) as functions of temperature, and then the average magnetization of the film is determined by

$$\overline{m} = \frac{1}{2N}\sum_{i=1}^{N}\sigma_i. \tag{10}$$

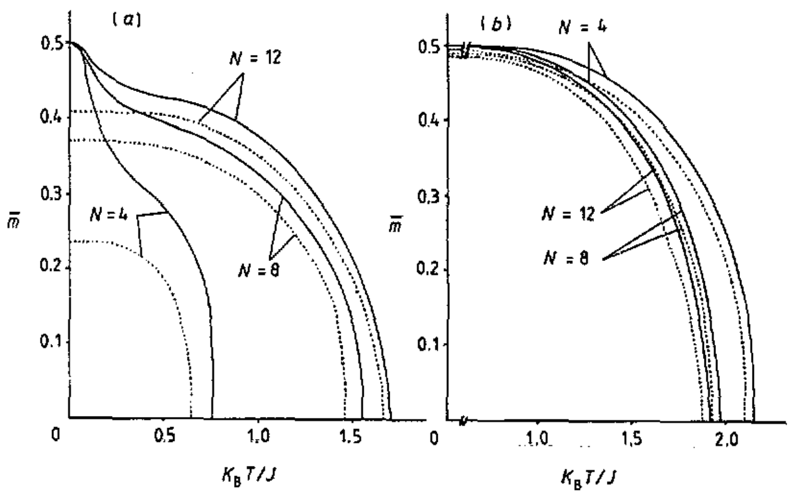

Figure 2. Average magnetization as a function of the temperature for (*a*) $J_S/J = 0.1$ and (*b*) $J_S/J = 2.0$: broken curves, transverse field $\Omega/J = 0.0$; full curves, transverse field $\Omega/J = 1.0$. N represents the number of the layers in the film.

First we consider the average magnetization $\overline{m}$; it is shown in figure 2 for $N =$ 4, 8 and 12, for two transverse fields $\Omega = 0.0$ and 1.0. Figure 2(*a*) shows how the magnetization changes with temperature for $J_S/J = 0.1$. The broken curves correspond to $\Omega/J = 1.0$ and the full curves to $\Omega/J = 0.0$. For $\Omega/J = 0.0$ and $T/J = 0.0$, the magnetizations of the film with $N =$ 4, 8 and 12 are $\frac{1}{2}$ (saturation magnetization m_0) but, for $\Omega/J = 1.0$ and $T/J = 0.0$, the magnetization decreases and, the thinner the film, the smaller the magnetization. For $N = 4$, $\overline{m} < \frac{1}{2}m_0$. Comparing the broken curves with the full curves, one can note that the transverse field changes greatly the shapes of the magnetization curves and decreases the critical temperatures. The critical temperatures for $\Omega/J = 0.0$ and $N = 4$, 8 and 12 are 0.785, 1.558 and 1.705, respectively, and those for $\Omega/J = 1.0$ and $N = 4$, 8 and 12 are 0.637, 1.497 and 1.667, respectively. Figure 2(*b*) corresponds to $J_S/J = 2.0$ and the other parameters are as in figure 2(*a*). Comparing the broken curves with the full curves in this figure, one can see that the transverse field ($\Omega/J = 1.0$) decreases the magnetizations slightly, for $T/J = 0.0$, from their saturation values $m_0 = \frac{1}{2}$, and also the critical temperatures; the shapes of two curves for $\Omega/J = 1.0$ and 0.0, for a given N, are similar. The critical temperatures for $\Omega/J = 0.0$, and $N = 4$, 8 and 12 are 2.146, 1.970 and 1.930, respectively, and those for $\Omega/J = 1.0$ and $N = 4$, 8 and 12 are 2.101, 1.920 and 1.881, respectively. As opposed to figure 2(*a*), figure 2(*b*) shows that, the thinner the film, the larger the magnetization, when the other parameters are unchanged.

The temperature dependence of the magnetization of every layer in the film, for $N = 12$ and different transverse fields $\Omega/J = 0.0$ and 1.0, is shown in figure 3. Figures 3(*a*)–3(*d*) correspond to $\Omega/J = 0.0$ and $J_S/J = 2.0$, $\Omega/J = 0.0$ and $J_S/J = 0.1$, $\Omega/J = 1.0$ and $J_S/J = 2.0$, and $\Omega/J = 1.0$ and $J_S/J = 0.1$, respectively. From figures 3(*a*) and 3(*b*), we see that the next outermost layer has a more special magnetization, and its magnetization is the largest for a finite temperature and $J_S/J = 2.0$. Comparing figure 3(*a*) with figure 3(*c*), we see that the transverse field ($\Omega/J = 1.0$) influences slightly the layer magnetizations. From figures 3(*b*) and 3(*d*) with $J_S/J = 0.1$, one sees that the magnetizations of the outermost three layers are clearly different from those of the other layers and vary greatly from each other. In figure 3(*b*), as the temperature is increased, the magnetization of the surface layer decreases rapidly and that of the next outermost layer, for $T_c/2 < T < T_c$, shows an approximately linear decrease. In figure 3(*d*), the transverse field ($\Omega/J = 1.0$) influences greatly the magnetizations of the outermost two layers, and in particular the surface layer; its magnetization is only small even for $T/J = 0.0$. In figure 3, the common characteristics are that the magnetization of the next outermost layer is always larger than that of the surface layer at a finite temperature and for any transverse field; the magnetizations of the internal layers, except those of the outermost three layers, have similar functions of temperature.

3.2. *Transverse field dependence of layer magnetizations*

Solving equations (5) numerically, we can also obtain the layer magnetizations as functions of the transverse field; magnetization–transverse field relations of this kind were rarely considered in the past. In this paper, we assume the film to be composed of 12 atomic layers parallel to the surfaces as an example to understand the transverse field dependences of layer magnetizations.

For $T = 0.0$, figures 4(*a*) and 4(*b*) show the transverse field dependences of the layer magnetizations for $J_S/J = 2.0$ and $J_S/J = 0.1$, respectively. The critical transverse field (Ω_c/J) is 3.62 for $J_S/J = 2.0$, and 3.21 for $J_S/J = 0.1$.

Figure 4(*a*) shows that the magnetization of the next outermost layer is obviously different from those of the other layers, while the magnetization of the surface layer is similar to that of the third layer. For $J_S/J = 0.1$, figure 4(*b*) shows that, as the transverse field is increased, the magnetization of the surface layer decreases rapidly

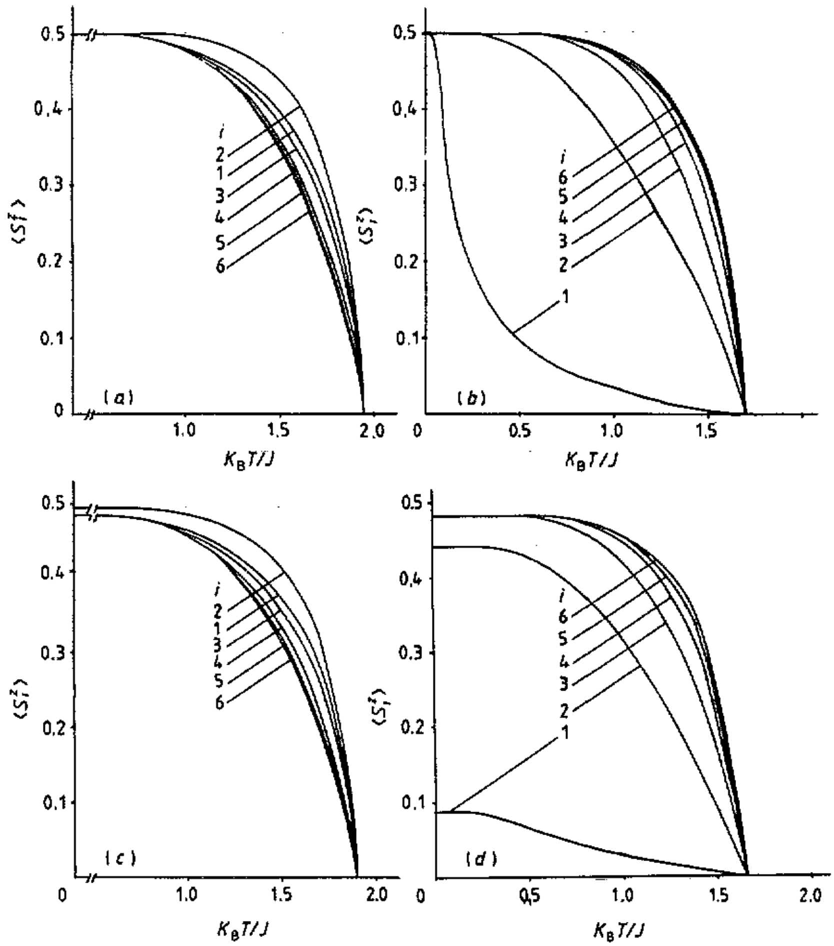

Figure 3. Layer magnetizations, for $N = 12$, as functions of the temperature: (*a*) $\Omega/J = 0.0$, $J_S/J = 2.0$; (*b*) $\Omega/J = 0.0$, $J_S/J = 0.1$; (*c*) $\Omega/J = 1.0$, $J_S/J = 2.0$; (*d*) $\Omega/J = 1.0$, $J_S/J = 0.1$. $\langle S_i^z \rangle$ represents the magnetization of the ith layer, and i is the layer index. Because of the symmetry of the film, $i = 1, 2, 3, 4, 5$ and 6.

and that of the next outermost layer decreases almost linearly over a larger temperature region. For a temperature given by $k_B T/J = 1.0$, the layer magnetizations as functions of transverse field are displayed in figures 4(*c*) and 4(*d*). $J_S/J = 2.0$ in figure 4(*c*) and $J_S/J = 0.1$ in figure 4(*d*). Comparing figure 4(*c*) with figure 4(*d*), we see that increasing temperature more obviously decreases the layer magnetizations of the film with the smaller value of J_S/J, and in particular the magnetizations of the outermost two layers. At the temperature given in figures 4(*c*) and 4(*d*), the critical transverse field $\Omega_c/J = 3.47$ for $J_S/J = 2.0$, and $\Omega_c/J = 2.96$ for $J_S/J = 0.1$.

Comparing figure 4 with figure 3, we find that the magnetization–transverse field curves and the corresponding magnetization–temperature curves have some similar features.

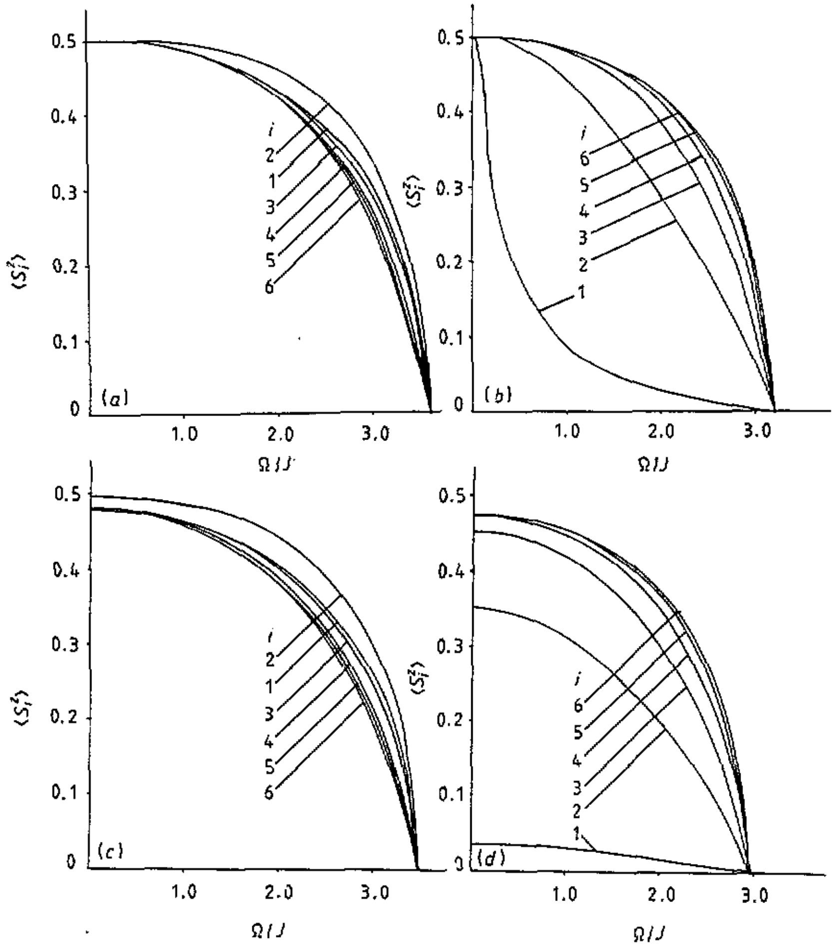

Figure 4. Layer magnetizations, for $N = 12$, as functions of the transverse field. (*a*) $k_BT/J = 0.0$, $J_S/J = 2.0$; (*b*) $k_BT/J = 0.0$, $J_S/J = 0.1$; (*c*) $k_BT/J = 1.0$, $J_S/J = 2.0$; (*d*) $k_BT/J = 1.0$, $J_S/J = 0.1$. i is the layer index.

4. Summary

In summary, using the effective-field theory with correlations, we have studied the magnetizations of the transverse Ising film with BCC structure and $s = \frac{1}{2}$. For a few sets of the selected parameters we have calculated numerically the average and layer magnetizations as functions of the temperature and transverse field and found that the magnetization of the next outermost layer is always larger than that of the surface layer for $T \neq 0$ and the magnetization–transverse field curves and the corresponding magnetization–temperature curves have some very similar features.

Acknowledgment

The authors acknowledge the financial support received from the Natural Science Foundation of Heilongjiang Province.

References

[1] Ferchimin A R 1982 *IEEE Trans. Magn.* MAG-18 714
[2] Mielnicki J, Balcerzak T and Wiatrowski G 1987 *J. Magn. Magn. Mater.* **65** 27
[3] Barber M N 1983 *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and J L Lebowits (New York: Academic)
[4] Sarmento E F and Kaneyoshi T 1988 *J. Phys. C: Solid State Phys.* **21** 3993
[5] Qing Jiang and Li Zhen-Ya 1991 *Phys. Rev.* B **43** 6198
[6] Mills D L 1971 *Phys. Rev.* B **3** 3887
[7] Binder K and Hohenberg P C 1974 *Phys. Rev.* B **9** 2194
[8] Binder K and Landau D P 1984 *Phys. Rev. Lett.* **52** 318
[9] Kaneyoshi T 1991 *Phys. Rev.* B **43** 6109
[10] Qiang Hong 1990 *Phys. Rev.* B **41** 9621
[11] Wu Z M, Yang C Z and Li Z Y 1988 *Solid State Commun.* **68** 205
[12] Wang Xuan-Zhang 1992 *Physica* submitted
[13] Monmura R and Kaneyoshi T 1979 *J. Phys. C: Solid State Phys.* **12** 3979