Magnetic properties of a transverse spin-$\frac{1}{2}$ Ising film

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Within the framework of the effective-field theory, we examine the phase transitions of a transverse spin-$\frac{1}{2}$ Ising film. The critical temperatures of the film as a function of the interactions, transverse fields, and film thickness are studied. It is found that for the ratio of the surface interactions to the bulk ones $R = J_s/J$ less than a critical value R_c, the critical temperature T_c/J of the film is smaller than the bulk critical temperature T_c^B/J and as the film thickness L is increased further, T_c/J increases and approaches asymptotically T_c^B/J for large values of L. However, for $R > R_c$, T_c/J is larger both than the bulk T_c^B/J and the surface T_c^S/J critical temperatures of the corresponding semi-infinite system and as the film thickness L is increased further, T_c/J decreases and approaches asymptotically, for large values of L, the surface magnetic transition T_c^S/J observed in the corresponding semi-infinite system. We calculate also some magnetic properties of the film such as the layer magnetizations, their averages and their profiles and the longitudinal susceptibility of the film. The film longitudinal susceptibility still diverges at the film critical temperature as does the bulk longitudinal susceptibility, but its magnitude is reduced. Also there is a rounded peak at the bulk critical temperature when $R > R_c$. The bulk related character of the susceptibility is more pronounced and the surface related character is less pronounced when the film thickness is large. [S0163-1829(99)03706-6]

I. INTRODUCTION

Over the past few years much effort has been directed towards the study of critical phenomena in various magnetic layered structures, ultrathin films, and superlattices.[1–4] The basic theoretical problem is the examination of the magnetic excitation and the phase transitions in these systems. Of these, magnetic films are very important from both the theoretical[5] standpoint and the experimental[6] standpoint and can be studied as models of the magnetic size effect and quasi-two-dimensional systems.[7] Although much is known about phase transitions in two- and three-dimensional systems, many aspects remain to be understood in systems with surfaces, thin films, etc. Very often one finds unexpected and interesting properties in these systems. For example, experimental studies[8–11] on the magnetic properties of surfaces of Gd, Cr, and Tb have shown that a surface ordered magnetically can coexist with a magnetically disordered bulk phase.

The most studied systems are those with magnetic phase transitions and much effort has been devoted to their understanding. From the theoretical point of view, one of the models more widely used to study the magnetic properties of surfaces is the semi-infinite Ising model. Within that model one can take into account in a straightforward manner the presence of the surface. The environmental effects produced by the surface can be simulated by assuming a location dependent interaction $J_{i,j}$; i and j denote the position of the magnetic atoms in the lattice. The simplest case corresponds to a situation in which only the surface interaction J_s is assumed to be different from the bulk interaction J. In that context, the surface magnetism of these systems is very interesting.[12–21] It exhibits different types of phase transitions associated with the surface; if the ratio $R = J_s/J$ is greater than a critical value $R_c = (J_s/J)_{crit}$, the system may order on the surface before it orders in the bulk. The system exhibits two successive transitions, namely the surface and the bulk phase transitions, as the temperature is lowered. If the ratio is less than R_c, the system becomes ordered at the bulk transition temperature.

Magnetic excitations in superlattices were considered in numerous papers (see, e.g., Ref. 22 for a brief review). Yet less attention has been paid to critical behavior, and in particular to critical temperatures in superlattices. Ma and Tsai[23] have studied the variation with modulation wavelength of the Curie temperature for a Heisenberg magnetic superlattice. Their results agree qualitatively with experiments on the Cu/Ni film.[24] Superlattice structures composed of alternating ferromagnetic and antiferromagnetic layers have been investigated by Hinchey and Mills,[25,26] using a localized spin model. A sequence of spin reorientation transitions are found to be different for superlattices with the antiferromagnetic component consisting of an even or odd number of spin layers.

For a periodic multilayer system formed of two different ferromagnetic materials, Fishman, Schwable, and Schwenk[27] have discussed its statics and dynamics within the framework of Ginzburg-Landau formalism. They have computed the transition temperature and spin-wave spectra. On the other hand, the Landau formalism of Camley and Tilley[28] has been applied to calculate the critical temperature in the same system.[29] Compared to Ref. 27, the formalism of Ref. 28 appears to be more general because it allows for a wider range of boundary conditions and includes the sign of interaction across the interface.

For more complicated superlattices with arbitrary number of different layers in an elementary unit, Bernás[30] has derived some general dispersion equations for the bulk and surface magnetic polaritons. These equations are then applied to magnetostatic modes and to retarded wave propagation in the Voigt geometry.[31]

Using the development of modern vacuum science and in particular the epitaxial growth technique, it is now possible to study experimentally the magnetic properties of low dimensional systems; and by depositing magnetic atoms on the top of nonmagnetic substrates, the thickness dependence of the critical temperature of ultrathin films of Gd on W(110) (Ref. 32) and of Fe on Au(100),[33] has been measured.

In addition, the effects of size and surface on the ferroelectric phase transition have been under investigation for a long time. Jaccord, Känzig, and Peter[34] and Anliker *et al.*[35] found that KDP fine particles embedded in an insulating medium show no ferroelectric phase transition if their size is less than 150 nm, while Anliker, Brugger, and Känzig[35] demonstrated that the critical temperatures of $BaTiO_3$ fine particles and $PbTiO_3$ fine particles demonstrated that the critical temperature decreases with decrease in grain size.

In this paper, we are concerned with the magnetic properties and phase transitions in ferroelectric films. As was first pointed out by De Gennes,[36] these may be described within a pseudospin model by the Ising model in a transverse field since the phase transition to ferroelectricity associated with preferential occupation by the protons of one or the other of the two equivalent wells in the hydrogen bounds. We will study the magnetic properties of a transverse spin-$\frac{1}{2}$ Ising film within the framework of the effective-field theory.[37,38] This technique is believed to give more exact results than those of the standard mean-field approximation. In Sec. II we outline the formalism and derive the equations that determine the layer magnetizations, the average magnetizations, and the critical temperatures of the film as functions of temperature, interactions, transverse fields, and film thickness. The phase diagrams of the film as functions of temperature, interactions, transverse fields, and film thickness are discussed in Sec. III. The layer longitudinal and transverse magnetizations, their averages, and their profiles are studied in Sec. IV. In Sec. V we study the magnetic longitudinal susceptibility of the film. The last Sec. VI is devoted to a brief conclusion.

II. FORMALISM

We consider a transverse spin-$\frac{1}{2}$ Ising film of L layers on a simple cubic lattice with free surfaces parallel to the (001) plane, submitted to a transverse field. The Hamiltonian of the system is given by

$$H=-\sum_{(ij)} J_{ij}\sigma_{iz}\sigma_{jz}-\sum_{i} \Omega_i\sigma_{ix}, \tag{1}$$

where σ_{iz} and σ_{ix} denote the z and x components of a quantum spin $\vec{\sigma}_i$ of magnitude $\sigma=\frac{1}{2}$ at site i, J_{ij} is the strength of the interaction between the spins at nearest-neighbor sites i and j, and Ω_i represents the transverse field. We assume $J_{ij}=J_s$ if both spins belong to surface layers and $J_{ij}=J$ otherwise.

The statistical properties of the system are studied using an effective-field theory whose starting point is a generalized, but approximate, Callen[39] relation derived by Sá Barreto, Fittipaldi, and Zeks[40] for the transverse Ising model. The longitudinal and transverse magnetizations of the spin at any site i are approximately given by (for details see Sá Barreto and Fittipaldi[41])

$$\begin{aligned} m_{iz}=\langle\sigma_{iz}\rangle&=\frac{1}{2}\left\langle \frac{\sum_j J_{ij}\sigma_{jz}}{\left(\left(\sum_j J_{ij}\sigma_{jz}\right)^2+\Omega_i^2\right)^{1/2}} \right. \\ &\quad\left.\times\tanh\left[\frac{1}{2}\beta\left(\left(\sum_j J_{ij}\sigma_{jz}\right)^2+\Omega_i^2\right)^{1/2}\right]\right\rangle \\ &=\left\langle f_z\left(\sum_j J_{ij}\sigma_{jz},\Omega_i\right)\right\rangle, \end{aligned} \tag{2}$$

$$\begin{aligned} m_{ix}=\langle\sigma_{ix}\rangle&=\frac{1}{2}\left\langle \frac{\Omega_i}{\left(\left(\sum_j J_{ij}\sigma_{jz}\right)^2+\Omega_i^2\right)^{1/2}} \right. \\ &\quad\left.\times\tanh\left[\frac{1}{2}\beta\left(\left(\sum_j J_{ij}\sigma_{jz}\right)^2+\Omega_i^2\right)^{1/2}\right]\right\rangle \\ &=\left\langle f_x\left(\sum_j J_{ij}\sigma_{jz},\Omega_i\right)\right\rangle=\left\langle f_z\left(\Omega_i,\sum_j J_{ij}\sigma_{jz}\right)\right\rangle, \end{aligned} \tag{3}$$

where m_{iz} and m_{ix} are, respectively, the longitudinal and the transverse magnetizations at site i, $\beta=1/k_BT$ (we take $k_B=1$ for sake of simplicity), $\langle\ \dots\ \rangle$ indicates the usual canonical ensemble thermal average for a given configuration, and the sum runs over all nearest neighbors of site i. We assume that the transverse field Ω_i depends only on the layer index, which we shall denote by n. Because of the translation symmetry parallel to the (001) plane, also the magnetizations only depend on n. To perform thermal averaging on the right-hand side of Eqs. (2) and (3), one now follows the general approach described in Refs. 34 and 35. Thus, with the use of the integral representation method of the Dirac's delta distribution, Eqs. (2) and (3) can be written in the form

$$\begin{aligned} m_{n\alpha}&=\int d\omega f_\alpha(y,\Omega_n)\frac{1}{2\pi} \\ &\quad\times\int dt\ \exp(i\omega t)\prod_j\ \langle\exp(-itJ_{ij}\sigma_{jz})\rangle, \end{aligned} \tag{4}$$

where $\alpha=z,x$ and

$$f_z(y,\Omega_n)=\frac{1}{2}\frac{y}{(y^2+\Omega_n^2)^{1/2}}\tanh\left[\frac{1}{2}\beta(y^2+\Omega_n^2)^{1/2}\right], \tag{5}$$

$$f_x(y,\Omega_n)=\frac{1}{2}\,\frac{\Omega_n}{(y^2+\Omega_n^2)^{1/2}}\tanh\left[\frac{1}{2}\beta(y^2+\Omega_n^2)^{1/2}\right]$$
$$=f_z(\Omega_n,y). \qquad (6)$$

In the derivation of Eq. (4), the commonly used approximation has been made according to which the multispin correlation functions are separated into products of the spin averages. On the basis of Eq. (4) and with the use of the probability distribution of the spin variables (for details see Saber[37] and Tucker, Saber, and Peliti[38])

$$P(\sigma_{nz})=\frac{1}{2}\left[(1-2m_{nz})\,\delta\left(\sigma_{nz}+\frac{1}{2}\right)+(1+2m_{nz})\,\delta\left(\sigma_{nz}-\frac{1}{2}\right)\right] \qquad (7)$$

we get the following set of equations for the layer magnetizations

$$m_{1\alpha}=2^{-N-N_0}\sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\left[C_\mu^N C_{\mu_1}^{N_0}(1-2m_{1z})^{\mu}\times(1+2m_{1z})^{N-\mu}(1-2m_{2z})^{\mu_1}\times(1+2m_{2z})^{N_0-\mu_1}f_\alpha(y_1,\Omega)\right] \qquad (8)$$

$$\vdots$$

$$m_{n\alpha}=2^{-N-2N_0}\sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\sum_{\mu_2=0}^{N_0}\left[C_\mu^N C_{\mu_1}^{N_0}C_{\mu_2}^{N_0}(1-2m_{nz})^{\mu}\times(1+2m_{nz})^{N-\mu}(1-2m_{n-1,z})^{\mu_1}\times(1+2m_{n-1,z})^{N_0-\mu_1}(1-2m_{n+1,z})^{\mu_2}\times(1+2m_{n+1,z})^{N_0-\mu_2}f_\alpha(y_n,\Omega)\right] \qquad (9)$$

$$\vdots$$

$$m_{L\alpha}=2^{-N-N_0}\sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\left[C_\mu^N C_{\mu_1}^{N_0}(1-2m_{Lz})^{\mu}\times(1+2m_{Lz})^{N-\mu}(1-2m_{L-1,z})^{\mu_1}\times(1+2m_{L-1,z})^{N_0-\mu_1}f_\alpha(y_L,\Omega)\right], \qquad (10)$$

where $y_1=y_L=(J/2)[R(N-2\mu)+(N_0-2\mu_1)]$ and $y_n=(J/2)[(N-2\mu)+(N_0-2\mu_1)+(N_0-2\mu_2)]$ for $2\leqslant n<L$.

In these equations, we have introduced the notation $R=J_s/J$, and C_k^l are the binomial coefficients. N and N_0 denote, respectively, the coordination numbers on the parallel planes and interplanes. For the case of a simple cubic lattice which is considered here, one has $N=4$ and $N_0=1$. We have thus obtained the self-consistent Eqs. (8)–(10) for the layer longitudinal and transverse magnetizations $m_{n\alpha}$, that can be solved directly by numerical iteration. For sake of simplicity, we study only the case of a uniform transverse field Ω acting on the system. As we are interested with the calculation of the longitudinal ordering near the transition critical temperature, the usual argument that the layer longitudinal magnetization m_{nz} tends to zero as the temperature approaches its critical value, allows us to consider only terms linear in m_{nz} because higher-order terms tend to zero faster than m_{nz} on approaching a critical temperature. Consequently, all terms of the order higher than linear terms in Eqs. (8)–(10) can be neglected. This leads to the set of simultaneous equations

$$m_{nz}=A_{n,n-1}m_{n-1,z}+A_{n,n}m_{nz}+A_{n,n+1}m_{n+1,z} \qquad (11)$$

or

$$Am_{nz}=m_{nz}, \qquad (12)$$

where the matrix A is symmetric and tridiagonal with elements

$$A_{i,j}=A_{i,i}\delta_{i,j}+A_{i,j}(\delta_{i,j-1}+\delta_{i,j+1}). \qquad (13)$$

The only nonzero elements of the matrix A are given by

$$A_{11}=A_{LL}=\frac{1}{2}\left[f_z\left(\frac{J}{2}(4R+1),\Omega\right)+f_z\left(\frac{J}{2}(4R-1),\Omega\right)+2f_z\left(\frac{J}{2}(2R+1),\Omega\right)+f_z\left(\frac{J}{2}(2R-1),\Omega\right)\right]\equiv A_1, \qquad (14)$$

$$A_{12}=A_{L,L-1}=\frac{1}{8}\left[f_z\left(\frac{J}{2}(4R+1),\Omega\right)-f_z\left(\frac{J}{2}(4R-1),\Omega\right)+4f_z\left(\frac{J}{2}(2R+1),\Omega\right)-4f_z\left(\frac{J}{2}(2R-1),\Omega\right)+6f_z\left(\frac{J}{2},\Omega\right)\right]\equiv A_2, \qquad (15)$$

$$\frac{A_{n,n}}{4}=A_{n,n-1}=A_{n,n+1}=\frac{1}{16}[f_z(3J,\Omega)+4f_z(2J,\Omega)+5f_z(J,\Omega)]\equiv A_3 \qquad (16)$$

for $n=2,3,\ldots,L-1$.

The system of Eq. (12) is of the form

$$Mm_{nz}=0, \qquad (17)$$

where

$$M_{i,j}=(1-A_{i,i})\delta_{i,j}-A_{i,j}(\delta_{i,j-1}+\delta_{i,j+1}). \qquad (18)$$

All the information about the critical temperature of the system is contained in Eq. (17). Up to now we did not assign precise values of the coupling constants and the transverse fields the terms in matrix (17) are general ones.

In a general case, for arbitrary coupling constants and transverse fields and film thickness the evaluation of the critical temperature relies on numerical solution of the system of linear Eq. (17). This equation can be satisfied by nonzero magnetization vectors m_{nz} only if

$$\det M=0, \qquad (19)$$

where

$$\det M = c\begin{vmatrix} a & -1 & & & & & & & & & \\ -1 & b & -1 & & & & & & & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & & -1 & b & -1 & & & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & & & & & & -1 & b & -1 \\ & & & & & & & & & -1 & a \end{vmatrix}_L . \tag{20}$$

The parameters a, b, and c that appear in Eq. (20) take into account the boundary conditions and reflect the different abilities of the surfaces and the bulk of the film to get ordered. They are given by

$$a = \frac{1-A_1}{A_2}, \tag{21}$$

$$b = \frac{1-A_{n,n}}{A_3} \quad \text{for} \quad n = 2,3, \ldots, L-1, \tag{22}$$

$$c = \left(\frac{1}{A_2}\right)^2 \left(\frac{1}{A_3}\right)^{2(L-2)}. \tag{23}$$

In general, Eq. (19) can be satisfied for L different values of the critical temperature T_c/J from which we choose the one corresponding to the highest possible transition temperature.[42,43] This value of T_c/J corresponds to a solution having $m_{1z}, m_{2z}, \ldots, m_{Lz}$ positive, which is compatible with a ferromagnetic longitudinal ordering. The other formal solutions correspond in principle to other types of ordering that usually do not occur here (Ferchmin and Maciejewski[42]).

The reduction and rearrangement of the determinant of Eq. (20) leads to the result[44–46]

$$\det M = c[(ab-1)^2 D_{L-4}(b) - 2a(ab-1)D_{L-5}(b) + a^2 D_{L-6}(b)], \tag{24}$$

where $D_L(x)$ is the determinant

$$D_L(x) = \begin{vmatrix} x & -1 & & & & & & & & & \\ -1 & x & -1 & & & & & & & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & & -1 & x & -1 & & & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & & & & & & -1 & x & -1 \\ & & & & & & & & & -1 & x \end{vmatrix}_L \tag{25}$$

whose value is given by

$$D_L(x) = \frac{1}{(x^2-4)^{1/2}}\left\{\left[\frac{x+(x^2-4)^{1/2}}{2}\right]^{L+1} - \left[\frac{x-(x^2-4)^{1/2}}{2}\right]^{L+1}\right\} \quad \text{for} \quad x^2 > 4 \tag{26}$$

and

$$D_L(x) = \frac{\sin[(L+1)k]}{\sin(k)} \quad \text{with} \quad k = \cos^{-1}\left(\frac{x}{2}\right), \quad \text{for} \quad x^2 \leqslant 4. \tag{27}$$

Throughout this paper, we take J as the unit of energy, and the length is measured in the unit of lattice constant in our numerical calculations.

III. PHASE DIAGRAMS

From Eqs. (19) and (24), we can obtain the phase diagrams of the film. The results show that there can be two phases, a film ferromagnetic phase (F) which means that the longitudinal magnetization $[\overline{m}_{nz} = (1/L)\sum_{n=1}^{L} m_{nz}]$ in the film is different from zero, and a film paramagnetic phase (P) which corresponds to $\overline{m}_{nz} = 0$. In addition, if the number of layers in the film L is very large ($L \to \infty$), the film can be considered practically as a semi-infinite Ising system. As it is well known, if the ratio of the surface interactions to the bulk ones $R=J_s/J$ is greater than a critical value $R_c=(J_s/J)_{crit}$, there are two kinds of transitions on the semi-infinite Ising system, the surface transition and the bulk transition, and the critical temperatures related to them are called the surface critical temperature T_c^S/J and the bulk critical temperature T_c^B/J, respectively.

To obtain the bulk and surface critical temperatures of the semi-infinite Ising system, we follow the approach due to Binder and Hohenberg.[15] Equation (21) yields

$$m_{1z}=A_1 m_{1z}+A_2 m_{2z}, \tag{28}$$

$$m_{2z}=A_3 m_{1z}+4A_3 m_{2z}+A_3 m_{3z} \tag{29}$$

$$\vdots$$

$$m_{nz}=A_3 m_{n-1,z}+4A_3 m_{nz}+A_3 m_{n+1,z} \quad \text{for} \quad n \geqslant 3. \tag{30}$$

According to Binder and Hohenberg,[15] let us assume that $m_{n+1,z}=\gamma m_{nz}$ for $n \geqslant 3$, e.g., the layer longitudinal magnetization m_{nz} of each layer with n larger than 2 decreases exponentially into the bulk. Equations (28) and (29) then yield the following secular equation

$$M_S\begin{pmatrix} m_{1z} \\ m_{2z} \end{pmatrix}=\begin{pmatrix} A_1 & A_2 \\ A_3 & (4+\gamma)A_3 \end{pmatrix}\begin{pmatrix} m_{1z} \\ m_{2z} \end{pmatrix}, \tag{31}$$

where the parameter γ is given by, using Eq. (30),

$$\gamma=\frac{1}{2A_3}[(1-4A_3)-[(1-4A_3)^2-4A_3^2]^{1/2}]. \tag{32}$$

Thus, the surface critical temperature T_c^S/J can be derived from the condition $\det M_S=0$, namely

$$(A_1-1)[(4+\gamma)A_3-1]-A_2A_3=0. \tag{33}$$

We are now in a position to examine the physical properties for the surface and the bulk of the semi-infinite Ising system numerically. Here it is worth noting that in our treatment the bulk transition temperature T_c^B/J can be determined by putting $m_{nz}=m_{n-1,z}=m_{n+1,z}=m_z$ into Eq. (30), i.e.,

$$1=6A_3, \quad \text{for} \quad n \geqslant 3. \tag{34}$$

This yields

$$f_z(3J,\Omega)+4f_z(2J,\Omega)+5f_z(J,\Omega)=\frac{8}{3}. \tag{35}$$

At $T_c^B/J=0$, Eq. (35) yields $\Omega_c^B=2.3529J$ which is to be compared with $\Omega_c^B=2.58J$ obtained by series expansion methods (Elliot and Wood[47]). The mean-field approximation leads to $\Omega_c^B=3J$. On the other hand, for the special case of the pure Ising model $(\Omega=0)$, Eq. (35) reduces to

$$\tanh(3\beta J)+4\tanh(2\beta J)+5\tanh(\beta J)=\frac{16}{3} \tag{36}$$

which is the Zernike[48] equation for the simple cubic lattice. The transition temperature is then determined as $T_c^B/J=1.2683$.

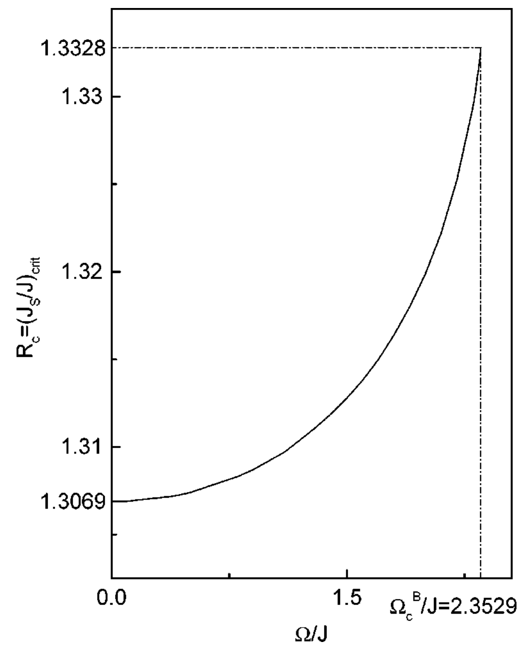

FIG. 1. The variation of $R_c=(J_s/J)_{crit}$ as a function of the transverse field Ω/J.

A useful expression for determining the critical value $R_c=(J_s/J)_{crit}$ is therefore given by the simultaneous solution of Eqs. (33) and (34). The variation of R_c as a function of the strength of the transverse field Ω/J is shown in Fig. 1. It shows that R_c increases with the increase of Ω/J. When $\Omega/J=0$, $R_c=1.3069$ which is the same value reported by Wiatrowski, Mielnicki, and Balcerzak[49] and by Sarmento and Tucker[50] and when $\Omega/J=\Omega_c^B/J=2.3529$, R_c is maximal and its value is $R_c^{\max}=1.3328$.

Now we calculate the $(T_c/J, R=J_s/J)$ phase diagrams for different numbers of layers when the strength of the transverse field is $\Omega/J=1$. The results are shown in Fig. 2. We see that our phase diagrams are different from the corresponding phase diagrams for the semi-infinite ferromagnets. The main difference is that in the film instead of the possibility of the existence of the two critical temperatures T_c^B/J and T_c^S/J we get only one well defined critical temperature T_c/J which depends on the film thickness. According to these results a new definition of the R_c parameter should be given. In semi-infinite systems R_c was defined as the value of R above which the two critical temperatures T_c^B/J and T_c^S/J exist. However, according to Fig. 2 the parameter R_c can be defined as that particular R value at which the film critical temperature T_c/J does not depend on film thickness (the crossover point in Fig. 2). The numerical values of R_c and related T_c/J parameters are exactly the same as those found for the semi-infinite system. Furthermore, according to the definition of R_c, it can be expected that the crossover point in Fig. 2 should define also the critical temperature of the three-dimensional infinite bulk system, where the surface and the R parameter are of no importance. This is really the case, which can be seen also from Fig. 2, where the bulk T_c^B/J and the surface T_c^S/J critical temperatures of the corresponding semi-infinite system are represented, respectively, by the dashed and dotted lines. Figure 2 shows also that for $R<R_c$, the critical temperature T_c/J of the film is smaller

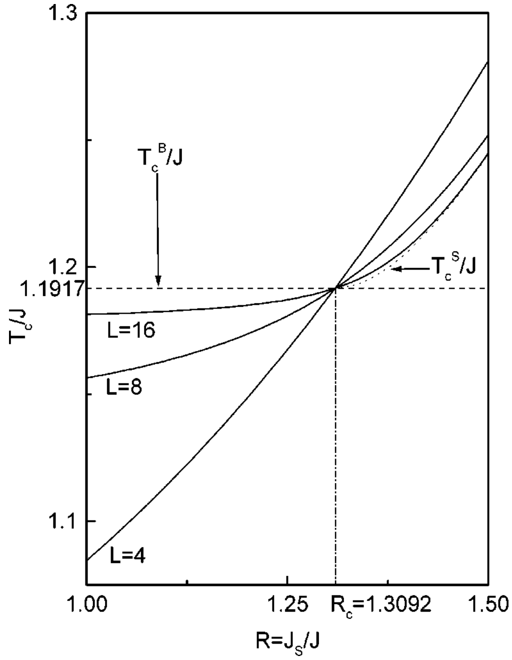

FIG. 2. The phase diagram in the $(T_c/J, R=J_s/J)$ plane for $\Omega/J=1$. The dashed and dotted lines are, respectively, the bulk T_c^B/J and the surface T_c^S/J critical temperatures of the corresponding semi-infinite system.

than the bulk critical temperature T_c^B/J. It increases with the film thickness L, and approaches T_c^B/J asymptotically as the number of layers becomes large. When $R=R_c$, the critical temperature T_c/J of the film is independent of L, and equal to T_c^B/J. On the other hand, for $R>R_c$, the critical temperature T_c/J, of the film is greater both than the bulk T_c^B/J and the surface T_c^S/J critical temperatures of the corresponding semi-infinite Ising system and larger the L is, the lower T_c/J is. The film critical temperature T_c/J approaches asymptotically the surface critical temperature T_c^S/J of the corresponding semi-infinite system as the number of layers becomes large.

In Figs. 3(a) and 3(b), we present the critical temperatures of the film and the semi-infinite system as a function of the strength of the transverse field Ω/J for different thicknesses L and for two values of R, i.e., $R=1<R_c^{\min}$ [Fig. 3(a)] and $R=1.5>R_c^{\max}$ [Fig. 3(b)]. The presence of a transverse field, of course, causes a reduction in the critical temperatures of the film and the semi-infinite system. We find that the $(T_c/J, \Omega/J)$ curve and the Ω/J axis intersect at some critical point, and the value of Ω/J corresponding to this point is called the critical transverse field Ω_c/J. When $\Omega/J>\Omega_c/J$ at any temperature, there cannot be a ferromagnetic phase. Figure 3(a) shows that the critical temperature T_c/J of the film is always less than the bulk critical temperature T_c^B/J and it increases with the increase of the film thickness L to approach asymptotically T_c^B/J for large values of L. Figure 3(b) shows that, T_c/J is greater than both T_c^B/J and T_c^S/J and it decreases with the increase of L to approach asymptotically T_c^S/J for large values of L.

We present in Fig. 4 the thickness dependence of the critical temperatures of the film and the semi-infinite system for different values of R and for $\Omega/J=1$. For $\Omega/J=1$, the critical value of the parameter R is $R_c=1.3092$. This figure shows that for any value of R below $R_c=1.3092$, the film critical temperature T_c/J is smaller than T_c^B/J and it increases with the increase of the film thickness L to approach T_c^B/J. When $R=R_c=1.3092$, T_c/J is independent of L and T_c/J is equal to T_c^B/J. For $R>R_c$, we see that T_c/J is greater than both T_c^B/J and T_c^S/J and it decreases with the increase of the film thickness L to approach asymptotically the surface critical temperature T_c^S/J of the corresponding semi-infinite system when the number of layers becomes large.

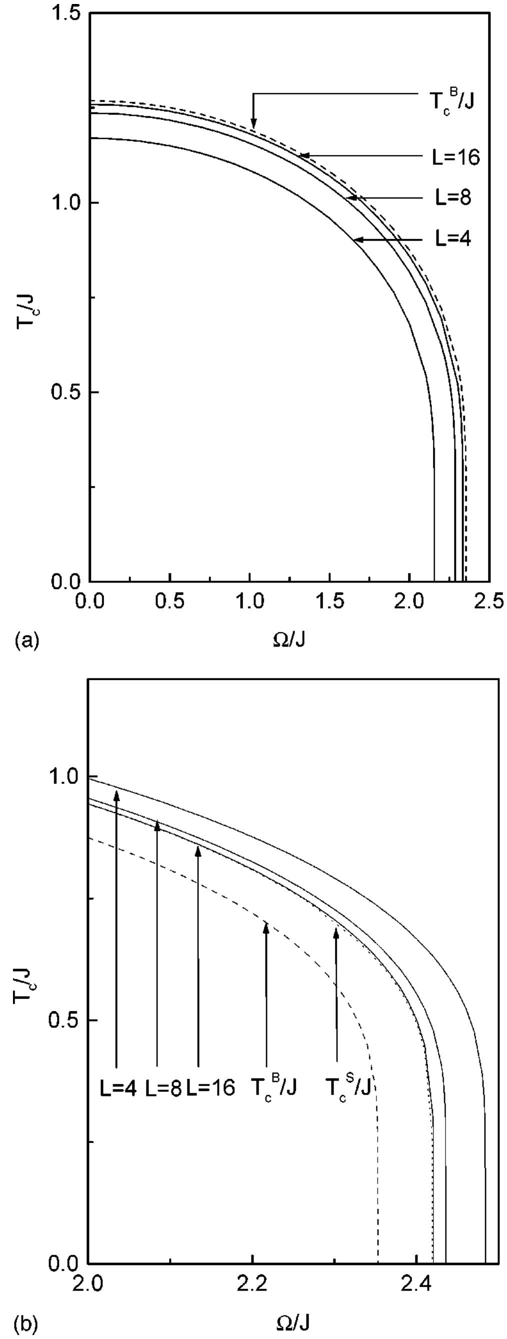

FIG. 3. The phase diagram in the $(T_c/J, \Omega/J)$ plane for (a) $R=1$ and (b) $R=1.5$. The dashed and dotted lines are, respectively, the bulk T_c^B/J and the surface T_c^S/J critical temperatures of the corresponding semi-infinite system.

Figure 5 shows the variation of the critical transverse field

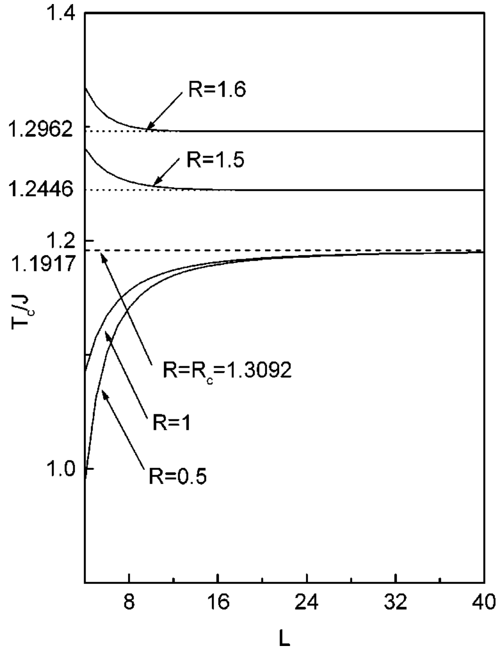

FIG. 4. Thickness dependence of the critical temperature of the film for several values of R and for $\Omega/J=1$. The dashed and dotted lines are, respectively, the bulk T_c^B/J and the surface T_c^S/J critical temperatures of the corresponding semi-infinite system.

Ω_c/J as a function of the thickness of the film L for several values of the parameter R. The dashed and dotted lines correspond, respectively, to the bulk Ω_c^B/J and the surface Ω_c^S/J critical transverse fields for the semi-infinite Ising system. For $R<R_c$, the film critical transverse field Ω_c/J is smaller than Ω_c^B/J and as the film thickness L is increased, Ω_c/J

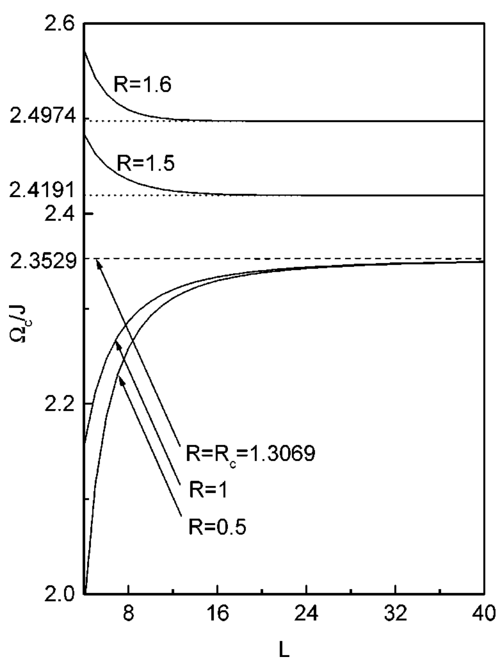

FIG. 5. The variation of the critical transverse field Ω_c/J of the film at which the critical temperature of the film T_c/J becomes zero as function of the number of layers L for several values of R. The dashed and dotted lines are, respectively, the bulk and the surface critical transverse fields of the semi-infinite Ising system.

increases and approaches asymptotically Ω_c^B/J for large values of L. However, for $R>R_c$, Ω_c/J is larger than both the bulk Ω_c^B/J and the surface Ω_c^S/J critical transverse fields and as the film thickness L is increased further, Ω_c/J decreases and approaches asymptotically Ω_c^S/J for large values of L.

IV. MAGNETIZATIONS

After selecting some values of R, Ω/J, and L one can obtain the layer longitudinal and transverse magnetizations from Eqs. (8)–(10) and then their averages (the film longitudinal and transverse magnetizations), which are determined by

$$\overline{m}_\alpha=\frac{1}{L}\sum_{n=1}^{L} m_{n\alpha}. \tag{37}$$

We have calculated many curves of the temperature dependences of the layer magnetizations for different values of the parameter $R=(J_s/J)$ and different transverse fields, but we only present several typical cases here. Because of the symmetry of the system under consideration we limit the interpretation to the first half layers of the film.

First we consider in Figs. 6(a) and 6(b) the temperature dependences of the first layers ($n=1,2,3$), the middle layer ($n=20$), and the film longitudinal magnetizations for a fixed film thickness $L=40$, fixed value of the transverse field $\Omega/J=2$, and two values of the parameter $R=J_s/J$, i.e., $R=1<R_c$ [Fig. 6(a)] and $R=1.5>R_c$ [Fig. 6(b)]. From these figures one can see that the layer and the film longitudinal magnetizations start from their saturation values at $T/J=0$ which depend on the layer and they decrease with the increase of the temperature to vanish at the film critical temperature. Figure 6(a) [6(b)] which corresponds to $R=1<R_c$ ($R=1.5>R_c$) shows that the layer longitudinal magnetization of the surface layer $n=1$ is smaller (larger) than that of its adjacent layer $n=2$, which is smaller (larger) than that of the third layer, which is smaller (larger) than that of the middle layer $n=20$.

Figures 7(a) and 7(b) show the longitudinal magnetization profiles for a film with $L=200$ layers. They are drawn for a fixed value of the transverse field $\Omega/J=2$ and for two values of the parameter R, i.e., $R=1<R_c$ [Fig. 7(a)], and $R=1.5>R_c$ [Fig. 7(b)]. The number accompanying each curve denotes the value of the temperature. All these figures are symmetric because of the symmetry of the system. For $R=1<R_c$, we observe that the longitudinal magnetization has its smallest value at the surfaces and it increases with the number of layers to reach its maximal value in the bulk ($n=100$), and for $R=1.5>R_c$, we have the opposite situation.

V. SUSCEPTIBILITIES

The magnetic properties are important in practice and in particular the longitudinal susceptibilities are interesting physical quantities which describe the characteristics of the change of the magnetizations with the fields and can show the phase transition's properties, particularly its critical temperature.[51] The phase transition is usually predicted by the abnormal behavior of the longitudinal susceptibility at the critical temperature. In order to obtain the longitudinal

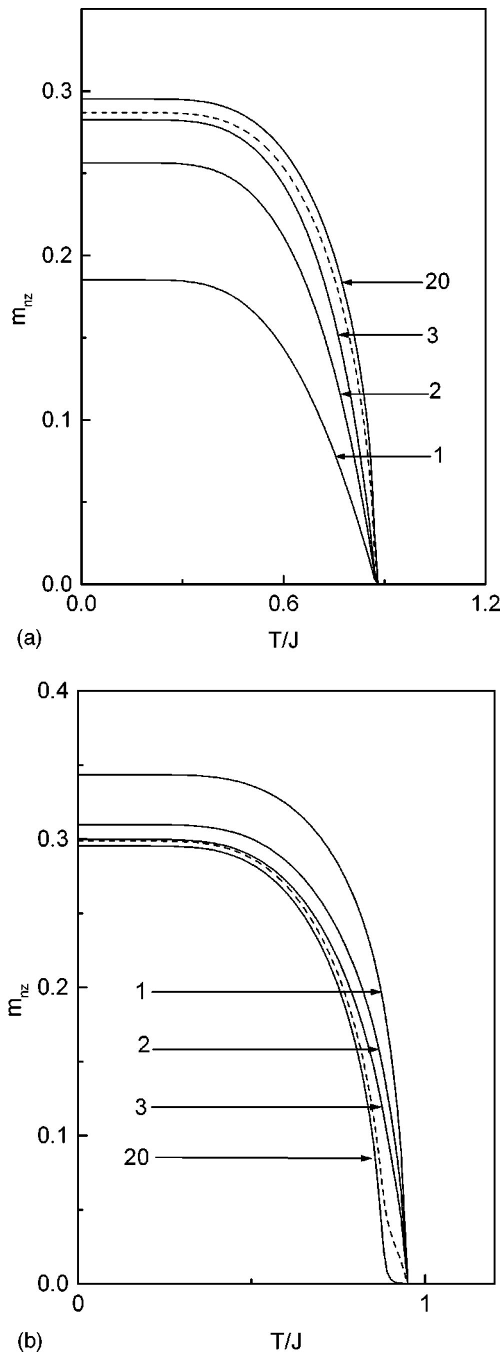

FIG. 6. Layer longitudinal magnetizations and their averages for a film with $L=40$ layers as function of the critical temperature for two values of R and fixed transverse field $\Omega/J=2$. The dashed lines correspond to the longitudinal magnetizations of the film. (a) $R=1$; (b) $R=1.5$. The number accompanying each curve denotes the layer index n.

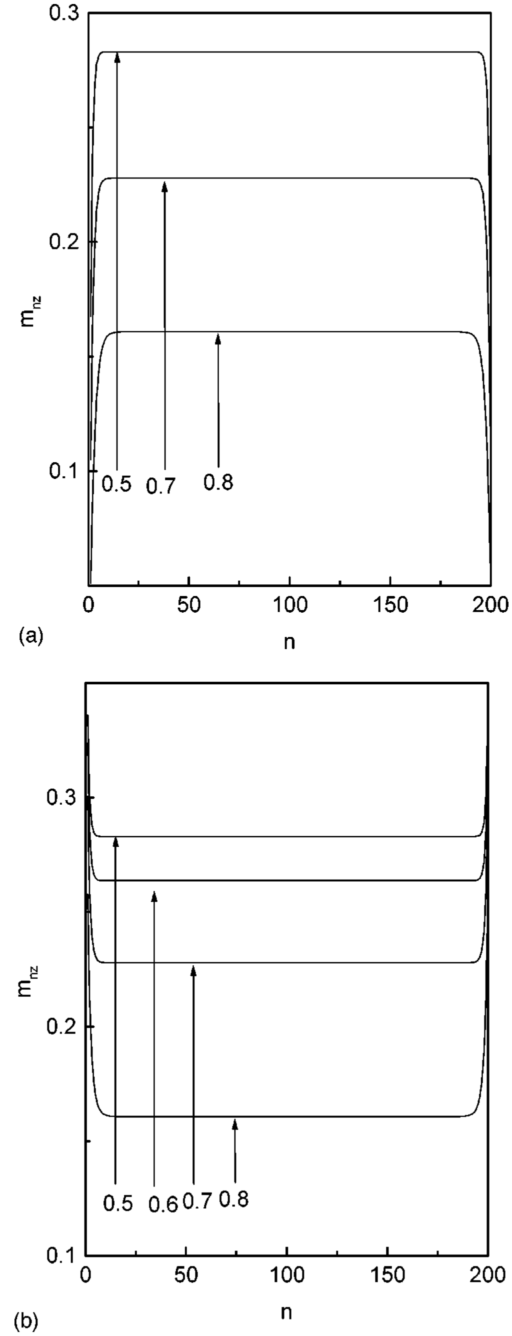

FIG. 7. Longitudinal magnetization profiles for a film with $L=200$ layers for two values of R and fixed transverse field $\Omega/J=2$. (a) $R=1$; (b) $R=1.5$. The number accompanying each curve denotes the value of the temperature.

susceptibility, we apply a uniform longitudinal magnetic field h across the film, which adds to the Hamiltonian Eq. (1) a term

$$H_1=-h\sum_{i=1}^{L}\sigma_{iz} \tag{38}$$

describing the interaction of the longitudinal magnetization with the magnetic field h. In order to calculate the magnetic longitudinal susceptibility, we apply the formalism of Sec. II. Equations (8)–(10) continue to apply but the parameter y now is replaced by $y+h$.

The longitudinal susceptibility of the nth layer is given by

$$\chi_{nz}=\left.\frac{\partial m_{nz}}{\partial h}\right|_{h=0}. \tag{39}$$

The details of the calculus of the layer longitudinal susceptibilities are given in the Appendix.

To evaluate the longitudinal susceptibility of the film, we follow the formalism of Wang, Smith, and Tilley.[52] As each

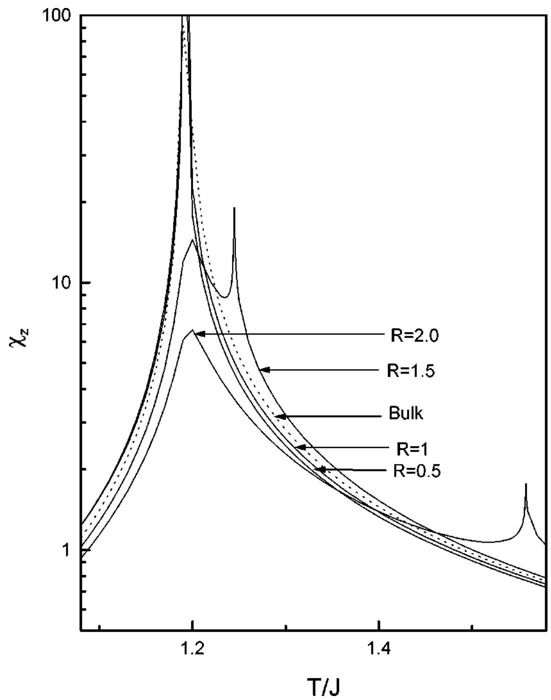

FIG. 8. The film longitudinal susceptibilities versus the temperature for a film of $L=40$ layers, when $\Omega/J=1$. The dashed line corresponds to the bulk longitudinal susceptibility.

layer can be treated as a capacitor, the capacitance of the film is the sum of the capacitance of each of the layers connected in series. The total reciprocal permittivity is the sum of the reciprocal permittivities at each of the layers. Thus the total susceptibility (the film longitudinal susceptibility) χ_z is determined from

$$(1+\chi_z)^{-1}=\frac{1}{L}\sum_{n=1}^{L}(1+\chi_{nz})^{-1}, \tag{40}$$

where L is the total number of layers.

The temperature dependences of the longitudinal susceptibilities are shown in Fig. 8 for different values of the parameter R, for a film of $L=40$ layers, and for $\Omega/J=1$. The number accompanying each curve denotes the value of R and the dashed lines correspond to the bulk susceptibility. It is easy to see from Eq. (A7) (see the Appendix) and Eq. (40) that the magnetic longitudinal susceptibility reaches infinity at the critical temperature.

When R is weaker than the critical value R_c, the curve is similar to that for the bulk, except that its peak position shifts to low temperature and its magnitude is reduced. The weaker R, the more the peak position is shifted and the smaller its magnitude. When R exceeds the critical value R_c, the peak shifts to higher temperature. The greater the deviation from its critical value, the more serious the shift and reduction in magnitude. There are other features: humps in the $R=1.5$, and $R=2$ curves around the bulk critical temperature. In fact, these are the corresponding rounded bulk peaks. The results agree qualitatively with those of Wang Smith, and Tilley.[52]

VI. CONCLUSION

In summary, we have studied the critical behavior and some magnetic properties of the transverse spin-$\frac{1}{2}$ Ising film where the interactions between spins at the surfaces are different from the interactions between spins in the bulk within the effective-field theory with a probability distribution technique. The effects of the ratio of the surface interactions to the bulk ones, transverse field, and film thickness on the phase diagrams are investigated. The film has one critical temperature which is lower than the bulk critical temperature for $R\leqslant R_c$ and larger both than the bulk T_c^B/J and the surface T_c^S/J critical temperatures of the corresponding semi-infinite Ising system for $R>R_c$. The layer magnetizations and their profiles were presented and they illustrate the existence of one defined critical temperature of the film. The longitudinal susceptibility of the film diverges at the film critical temperature as does the bulk longitudinal susceptibility, but its magnitude is reduced. Also there is a rounded peak at the bulk critical temperature for $R>R_c$. The bulk related character of the longitudinal susceptibility is more pronounced and the surface related character is less pronounced when the film thickness is large.

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APPENDIX: CALCULUS OF THE LAYER LONGITUDINAL SUSCEPTIBILITIES

By taking into account the applied longitudinal magnetic field h, the layer longitudinal magnetizations take the form

$$\begin{aligned}m_{1z}=2^{-N-N_0}&\sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\\&\times[C_\mu^N C_{\mu_1}^{N_0}(1-2m_{1z})^{\mu}(1+2m_{1z})^{N-\mu}\\&\times(1-2m_{2z})^{\mu_1}(1+2m_{2z})^{N_0-\mu_1}\\&\times f_z(y_1+h,\Omega)],\end{aligned} \tag{A1}$$

$$\vdots$$

$$\begin{aligned}m_{nz}=2^{-N-2N_0}&\sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\sum_{\mu_2=0}^{N_0}\\&\times[C_\mu^N C_{\mu_1}^{N_0}C_{\mu_2}^{N_0}(1-2m_{nz})^{\mu}(1+2m_{nz})^{N-\mu}\\&\times(1-2m_{n-1,z})^{\mu_1}(1+2m_{n-1,z})^{N_0-\mu_1}\\&\times(1-2m_{n+1,z})^{\mu_2}(1+2m_{n+1,z})^{N_0-\mu_2}f_z(y_n+h,\Omega)],\end{aligned} \tag{A2}$$

where

$$m_{Lz}=2^{-N-N_0}\sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\times[C_\mu^N C_{\mu_1}^{N_0}(1-2m_{Lz})^{\mu}(1+2m_{Lz})^{N-\mu}\times(1-2m_{L-1,z})^{\mu_1}(1+2m_{L-1,z})^{N_0-\mu_1}f_z\times(y_L+h,\Omega)], \quad \text{(A3)}$$

where $y_1=y_L=(J/2)[R(N-2\mu)+(N_0-2\mu_1)]$ and $y_n=(J/2)[(N+2N_0)-2(\mu+\mu_1+\mu_2)]$ for $2\leqslant n\leqslant L-1$.

By differentiating the equations of the layer longitudinal magnetizations [Eqs. (A1)–(A3)] with respect to h and taking the limit when h goes to zero, we get the following set of equations:

$$\left.\frac{\partial m_{1z}}{\partial h}\right|_{h=0}=A_{1,1}^z\left.\frac{\partial m_{1z}}{\partial h}\right|_{h=0}+A_{1,2}^z\left.\frac{\partial m_{2z}}{\partial h}\right|_{h=0}+B_1^z \quad \text{(A4)}$$

$$\vdots$$

$$\left.\frac{\partial m_{nz}}{\partial h}\right|_{h=0}=A_{n,n-1}^z\left.\frac{\partial m_{n-1,z}}{\partial h}\right|_{h=0}+A_{n,n}^z\left.\frac{\partial m_{nz}}{\partial h}\right|_{h=0}+A_{n;n+1}^z\left.\frac{\partial m_{n+1,z}}{\partial h}\right|_{h=0}+B_n^z \quad \text{(A5)}$$

$$\vdots$$

$$\left.\frac{\partial m_{Lz}}{\partial h}\right|_{h=0}=A_{L,L-1}^z\left.\frac{\partial m_{L-1,z}}{\partial h}\right|_{h=0}+A_{L,L}^z\left.\frac{\partial m_{Lz}}{\partial h}\right|_{h=0}+B_L^z. \quad \text{(A6)}$$

The set of equations (A4)–(A6) yields

$$C_{n,n-1}^z\chi_{n-1,z}+C_{n,n}^z\chi_{nz}+C_{n,n+1}^z\chi_{n+1,z}-1=0 \quad \text{(A7)}$$

with $1\leqslant n\leqslant L$ and $C_{1,0}^z=C_{L,L+1}^z=0$, $C_{n,n-1}^z=-(A_{n,n-1}^z/B_n^z)$, $C_{n,n}^z=(1-A_{n,n}^z/B_n^z)$, $C_{n,n+1}^z=-(A_{n,n+1}^z/B_n^z)$. Equation (A7) is a set of L linear equations from which the layer longitudinal susceptibilities are obtained.

The expressions of the coefficients appearing in the equations of the appendix are given by

$$A_{1,1}^z=2^{-N-N_0}\sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\sum_{i=0}^{\mu}\sum_{j=0}^{N-\mu}\times[(-1)^i(i+j)2^{i+j}C_\mu^N C_{\mu_1}^{N_0}C_i^{\mu}C_j^{N_0-\mu}m_{1z}^{i+j-1}\times(1-2m_{2z})^{\mu_1}(1+2m_{2z})^{N_0-\mu_1}f_z(y_1,\Omega)], \quad \text{(A8)}$$

$$A_{1,2}^z=2^{-N-N_0}\sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\sum_{i=0}^{\mu_1}\sum_{j=0}^{N_0-\mu_1}\times[(-1)^i(i+j)2^{i+j}C_\mu^N C_{\mu_1}^{N_0}C_i^{\mu_1}C_j^{N_0-\mu_1}m_{2z}^{i+j-1}\times(1-2m_{1z})^{\mu}(1+2m_{1z})^{N-\mu}f_z(y_1,\Omega)] \quad \text{(A9)}$$

$$\vdots$$

$$A_{n,n-1}^z=2^{-N-2N_0}\sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\sum_{\mu_2=0}^{N_0}\sum_{i=0}^{\mu_1}\sum_{j=0}^{N_0-\mu_1}\times[(-1)^i(i+j)2^{i+j}C_\mu^N C_{\mu_1}^{N_0}C_i^{\mu_1}C_j^{N_0-\mu_1}m_{n-1,z}^{i+j-1}\times(1-2m_{nz})^{\mu}(1+2m_{nz})^{N-\mu}(1-2m_{n+1,z})^{\mu_2}\times(1+2m_{n+1,z})^{N_0-\mu_2}f_z(y_n,\Omega)], \quad \text{(A10)}$$

$$A_{n,n}^z=2^{-N-2N_0}\sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\sum_{\mu_2=0}^{N_0}\sum_{i=0}^{\mu}\sum_{j=0}^{N-\mu}\times[(-1)^i(i+j)2^{i+j}C_\mu^N C_{\mu_1}^{N_0}C_i^{\mu}C_j^{N-\mu}m_{nz}^{i+j-1}\times(1-2m_{n-1,z})^{\mu_1}(1+2m_{n-1,z})^{N_0-\mu_1}\times(1-2m_{n+1,z})^{\mu_2}(1+2m_{n+1,z})^{N_0-\mu_2}f_z(y_n,\Omega)], \quad \text{(A11)}$$

$$A_{n,n+1}^z=2^{-N-2N_0}\sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\sum_{\mu_2=0}^{N_0}\sum_{i=0}^{\mu_2}\sum_{j=0}^{N_0-\mu_2}\times[(-1)^i(i+j)2^{i+j}C_\mu^N C_{\mu_1}^{N_0}C_i^{\mu_2}C_j^{N_0-\mu_2}m_{n+1,z}^{i+j-1}\times(1-2m_{nz})^{\mu}(1+2m_{nz})^{N-\mu}(1-2m_{n-1,z})^{\mu_1}\times(1+2m_{n-1,z})^{N_0-\mu_1}f_z(y_n,\Omega)] \quad \text{(A12)}$$

$$\vdots$$

$$A_{L,L-1}^z=2^{-N-N_0}\sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\sum_{i=0}^{\mu_1}\sum_{j=0}^{N_0-\mu_1}\times[(-1)^i(i+j)2^{i+j}C_\mu^N C_{\mu_1}^{N_0}C_i^{\mu_1}C_j^{N_0-\mu_1}m_{L-1,z}^{i+j-1}\times(1-2m_{Lz})^{\mu}(1+2m_{Lz})^{N-\mu}f_z(y_L,\Omega)], \quad \text{(A13)}$$

$$A_{L,L}^z=2^{-N-N_0}\sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\sum_{i=0}^{\mu}\sum_{j=0}^{N-\mu}\times[(-1)^i(i+j)2^{i+j}C_\mu^N C_{\mu_1}^{N_0}C_i^{\mu}C_j^{N-\mu}m_{Lz}^{i+j-1}\times(1-2m_{L-1,z})^{\mu_1}(1+2m_{L-1,z})^{N_0-\mu_1}f_z(y_L,\Omega)], \quad \text{(A14)}$$

$$B_1^z=2^{-N-N_0}\sum_{\mu=0}^{N}\sum_{\mu_1=0}^{N_0}\times[C_\mu^N C_{\mu_1}^{N_0}(1-2m_{1z})^{\mu}(1+2m_{1z})^{N-\mu}\times(1-2m_{2z})^{\mu_1}(1+2m_{2z})^{N_0-\mu_1}g_z(y_1,\Omega)] \quad \text{(A15)}$$

$$\vdots$$

$$B_n^z = 2^{-N-2N_0} \sum_{\mu=0}^{N} \sum_{\mu_1=0}^{N_0} \sum_{\mu_2=0}^{N_0} [C_\mu^N C_{\mu_1}^{N_0} C_{\mu_2}^{N_0} (1-2m_{nz})^{\mu} (1+2m_{nz})^{N-\mu} (1-2m_{n-1,z})^{\mu_1} (1+2m_{n-1,z})^{N_0-\mu_1} \times (1-2m_{n+1,z})^{\mu_2} (1+2m_{n+1,z})^{N_0-\mu_2} g_z(y_n,\Omega)] \tag{A16}$$

$$\vdots$$

$$B_L^z = 2^{-N-N_0} \sum_{\mu=0}^{N} \sum_{\mu_1=0}^{N_0} [C_\mu^N C_{\mu_1}^{N_0} (1-2m_{Lz})^{\mu} (1+2m_{Lz})^{N-\mu} (1-2m_{L-1,z})^{\mu_1} (1+2m_{L-1,z})^{N_0-\mu_1} g_z(y_L,\Omega)], \tag{A17}$$

where the function $g_z(y,\Omega)$ is given by

$$g_z(y,\Omega) = \left.\frac{\partial f_z(y,\Omega)}{\partial h}\right|_{h\to 0} = \frac{1}{2}\left\{ \frac{\Omega^2}{(y^2+\Omega^2)^{3/2}} \tanh\left(\frac{1}{2}\beta(y^2+\Omega^2)^{1/2}\right) + \frac{\beta}{2}\,\frac{y^2}{(y^2+\Omega^2)}\left[1-\tanh^2\left(\frac{1}{2}\beta(y^2+\Omega^2)^{1/2}\right)\right]\right\}. \tag{A18}$$

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