Application of the two-site cluster approximation to the semi-infinite Ising model

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Using a recently introduced two-site cluster approximation, we investigate a semi-infinite Ising cubic lattice with three different exchange parameters (J_s couples surface spins, J_1 is the exchange interaction between spins in the surface and second layer, and J is the interaction in the bulk). Phase diagrams for surface ordering and temperature dependencies of surface and bulk magnetizations are studied for various ratios J_1/J and J_s/J. Our results show that the existence of a dip in the temperature dependence of the surface magnetization near the bulk critical temperature depends strongly on the number of the layers considered in the calculations. The magnetization as a function of the distance from the surface is obtained as well.

I. INTRODUCTION

During recent years, surface magnetism has attracted considerable interest both experimentally and theoretically. Experimentally, surface magnetism has been studied mainly using crystalline systems such as Ni, Cr, and Gd. On theoretical grounds surface magnetic order has been treated within different frameworks: the mean-field approximation,[1–3], effective-field theories,[4–9], series expansion,[10] Kikuchi-type theories,[11,12] spin-fluctuation theories,[13] the random-phase approximation,[14] renormalization-group methods,[15–20] and Monte Carlo techniques.[21–24] A number of the studies is devoted to the Mills model[1] with two exchange parameters (J_s for spins on a free surface and J for all others spins). However, in our opinion a great influence on the surface magnetic order has the exchange interaction between surface and second layer (denoted J_1). Therefore, in the present work, we study an extended and more realistic model with three exchange parameters J_s, J_1, and J (see Fig. 1). In our analysis we have used the so-called "two-site cluster approximation,"[25] which is based on the introduction of differential operators into the exact identity for a cluster of two neighboring spins. Unlike standard effective-field treatments, the present method can explicitly and systematically include correlation effect[26] and has already been applied to several situations such as site-random,[27] bond-random,[28] and random-field[29] Ising bulk problems. Moreover, the method is able to discern between lattices of the same coordination number but different structure[30] (e.g., plane triangular and simple cubic lattices). In the present paper we apply this method to the semi-infinite simple cubic ferromagnetic spin-$\frac{1}{2}$ Ising model. For simplicity we restrict ourselves to the approximation where thermal correlations are neglected.

The outline of the paper is as follows. In Sec. II we briefly review the basic points of the two-site cluster approximation when it is applied to the Ising ferromagnetic system with a free surface. In Sec. III we examine phase diagrams and show that if the exchange parameter J_1 is greater than J_1^* ($J_1^*=6.1899J$), then the surface magnetism exists always above the bulk critical temperature (T_c^b), regardless of how weak the surface exchange parameter is. In Sec. IV the temperature dependence of the surface magnetization (m_s) and some characteristic magnetization profiles as a function of distance are presented. The surface magnetization is studied near T_c^b in detail, and the influence of increasing the number of layers on the accuracy of numerical results is demonstrated. In Sec. V a brief discussion of our results is presented.

II. GENERAL FORMALISM

The Hamiltonian for a three-dimensional spin-$\frac{1}{2}$ Ising ferromagnetic system is given by

$$H=-\sum_{\langle i,j\rangle} J_{ij}\sigma_i\sigma_j \ , \tag{1}$$

where $\sigma_i=\pm 1$ is the usual Ising variable and $\langle i,j\rangle$ runs over all nearest-neighbor (NN) spins; J_{ij} is the exchange parameter, which has the value J_s if both spins lie in the free surface, the value J_1 between the surface and second layer spins, and the bulk value J otherwise (see Fig. 1).

The starting point for the statistics of our spin system is the exact equation for a pair of neighboring spins:[25]

$$\tfrac{1}{2}\langle\sigma_i+\sigma_j\rangle=\left\langle\frac{\sinh(h_i+h_j)}{\cosh(h_i+h_j)+\exp(-2t_{ij})\cosh(h_i-h_j)}\right\rangle \ , \tag{2}$$

where $t_{ij}=\beta J_{ij}$, $\beta=(k_BT)^{-1}$, and

$$h_i=\sum_k t_{ik}\sigma_k, \quad h_j=\sum_l t_{jl}\sigma_l \ ,$$

with the terms $k=j$ and $l=i$ excluded from the summations over k and l, respectively. The symbol $\langle\cdots\rangle$ indicates the usual thermal average.

It should be noted here that the exact equation (2) is a two-spin cluster analog of the Callen single-site identity,[31] which has been used as a basis for effective-field

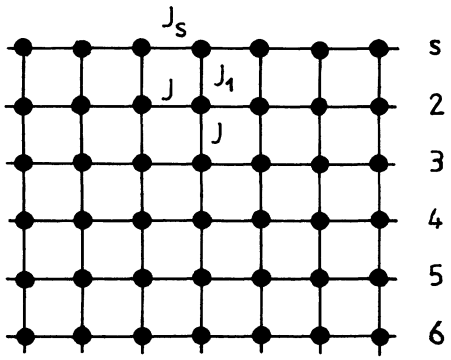

FIG. 1. Part of a two-dimensional cross section through a semi-infinite Ising system. J_s denotes the exchange parameter between surface spins, J_1 is the exchange parameter between surface and second-layer spins, and J is the exchange parameter between all other spins.

theories,[4–9] recently applied to the semi-infinite simple cubic ferromagnetic spin-$\frac{1}{2}$ Ising model. If the average of the right-hand side in (2) is taken as the arguments of hyperbolic functions, we obtain the usual Oguchi approximation.[32] For obtaining a better result, the following identity will be used:

$$\exp(\gamma D_x+\delta D_y)f(x,y)=f(x+\gamma,y+\delta)\ , \tag{3}$$

where $D_x=\partial/\partial x$ and $D_y=\partial/\partial y$ are the differential operators.

Now, by using Eq. (3) and the fact that

$$\exp(\alpha\sigma_k)=\cosh(\alpha)+\sigma_k\sinh(\alpha),\quad \sigma_k=\pm 1\ , \tag{4}$$

Eq. (2) can be rewritten as

$$\tfrac{1}{2}\langle\sigma_i+\sigma_j\rangle = \left\langle \prod_k (A_{ik}+\sigma_k B_{ik}) \prod_l (F_{jl}+\sigma_l G_{jl}) \right\rangle f(x,y)_{x=0,y=0}\ , \tag{5}$$

where

$$\begin{aligned} A_{ik}&=\cosh[t_{ik}(D_x+D_y)]\ ,\\ B_{ik}&=\sinh[t_{ik}(D_x+D_y)]\ ,\\ F_{jl}&=\cosh[t_{jl}(D_x-D_y)]\ ,\\ G_{jl}&=\sinh[t_{jl}(D_x-D_y)]\ , \end{aligned} \tag{6}$$

and

$$f(x,y)=\frac{\sinh(x)}{\cosh(x)+\exp(-2t_{ij})\cosh(y)}\ . \tag{7}$$

Let us assume the statistical independence of all multispin correlations and apply Eq. (5) to the simple cubic structure ($z=6$) with a (100) free surface. We obtain a set of mutually coupled equations, which have the general form

$$m_k=P_k(m_{k-1},m_k,m_{k+1};J_s,J_1,J,T),\quad k=1,2,3,\ldots\ , \tag{8}$$

where $m_k=\langle\sigma_k\rangle$ is the magnetization per site in the kth layer ($m_1\equiv m_s$) and P_k represent polynomial functions of m_{k-1}, m_k, and m_{k+1}. The coefficients of these polynomial functions are complicated hyperbolic functions, which depend on J_s, J_1, J, and T. As an example, we show the equation for the first layer:

$$\begin{aligned} m_s=&\,2m_s[3X_1+m_s^2(X_2+9X_5)+3m_s^4X_8]\\ &+2m_2[X_3+3m_s^2(X_4+4X_6+X_9)\\ &\quad+3m_s^4(X_7+3X_{12}+X_{11})+m_s^6X_{10}]\\ &+2m_sm_2^2[3X_{13}+m_s^2(X_{14}+X_{15})+3m_s^4X_{16}]\ , \end{aligned} \tag{9}$$

where $X_i=X_i(J_s,J_1,J,T)$ ($i=1,\ldots,46$) are the above-mentioned hyperbolic functions.[33]

Our aim in the next sections is to obtain from Eq. (8) the various phase diagrams which our model may exhibit and to study the temperature dependence of the surface magnetization. For this purpose it is necessary to solve an infinite set of equations given by (8). Obviously, this is impossible; therefore, for obtaining, for obtaining a finite set of equations, we can put $m_k=m_{k+1}$ for a certain value of k, because the difference between m_k and m_{k+1} is very small if k is sufficiently large. It is clear from the physical point of view that the assumption $m_k=m_{k+1}$ is equivalent to the assumption $m_k=m_b$ (m_b is the bulk magnetization obtained by using the same technique for the present model without a free surface). However, from the mathematical point of view, for $m_k=m_{k+1}$ and $m_k=m_b$ we obtain two different systems of equations, i.e., two different types of approximation. These two systems of equations differ only in the last equation, but their solutions can differ both quantitatively and qualitatively if we take into account only a small number of layers. On the other hand, it is clear that the difference between these solutions must decrease if k increases. Theoretically, if we take into account an infinite number of layers (i.e., $k\to\infty$), then we obtain the same solutions. For this reason we analyzed Eqs. (8) numerically under the assumptions $m_k=m_{k+1}$ and $m_k=m_b$ for $k=3$, 5, 10, 15, and 20. We found that in the case $k=3$ there is a quantitative difference of about 3%–4% between numerical solutions of Eqs. (8) for $m_3=m_4$ and $m_3=m_b$. Moreover, for $m_3=m_b$ the surface magnetization curve has near T_c^b an evident dip (in the case $m_3=m_4$, there is only a very small dip). If k increases, the quantitative difference between these solutions decreases and the above-mentioned dip disappears. For $k=20$ we obtain practically the same solutions for the cases $m_{20}=m_{21}$ and $m_{20}=m_b$. Therefore, in the next numerical calculations, we shall consider 20 layers. Let us note here that our previous considerations will be illustrated at the end of Sec. IV.

III. PHASE DIAGRAMS

In this section we are interested in studying the transition temperature of the system. The usual argument that m_k tends toward zero as the temperature approaches a critical temperature allows us to consider only linear terms in m_k. Then, from (8), we obtain

$$(6X_1-1)m_s+2X_3m_2=0\ , \tag{10}$$

$$2X_2(m_{k-1}+m_{k+1})+(6X_2-1)m_k=0\ , \tag{11}$$

$$2X_2m_{10}+(8X_2-1)m_{20}=0\ . \tag{12}$$

Equation (10)–(12) can be rewritten in matrix form (i.e., as a secular equation), and consequently the critical ferromagnetic frontiers can be derived from the condition

$$\det(M)=0\ , \tag{13}$$

where M is the determinant of the above-mentioned secular equation.

Initially, after introducing the parameters

$$\Delta_s=J_s/J-1,\quad \Delta_1=J_1/J-1\ , \tag{14}$$

we calculate, from Eq. (13), Δ_s as a function of Δ_1 at the bulk critical temperature $T_c^b=5.0392J/k_B$. We note that in the present treatment T_c^b is determined by putting $m_{k-1}=m_k=m_{k+1}$ into (11), namely, $10X_2=1$. From Fig. 2 we can see that for $\Delta_1>\Delta_1^*$ ($\Delta_1^*=5.1899$) the system would order on the surface always before it ordered in the bulk, regardless of the value Δ_s. On the other hand, if $\Delta_1<\Delta_1^*$, then we obtain two well-known cases: (i) For Δ_2 greater than a certain critical value Δ_{sc}, the system may order on the surface before it orders in the bulk. (ii) For $\Delta_s<\Delta_{sc}$ the system becomes ordered at the bulk critical temperature. For comparison with other theories, we calculate the critical value Δ_{sc} for Mills model ($\Delta_1=0$, i.e., $J_1=J$). We obtain $\Delta_{sc}=0.3157$, which is in good agreement with the results obtained by Honmura *et al.*[4] ($\Delta_{sc}=0.3068$), by Tamura *et al.*[5] ($\Delta_{sc}=0.3293$), and by Burkhardt and Eiseriegler[15] ($\Delta_{sc}=0.307$ and 0.357). We recall that the best estimate for Δ_{sc} is due to Binder and Hohenberg,[10] who used high-temperature expansions ($\Delta_{sc}=0.6$).

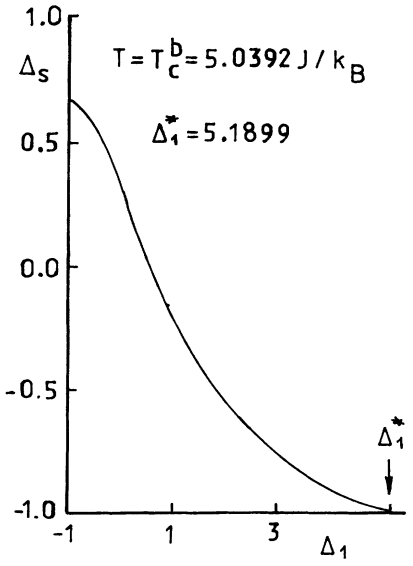

FIG. 2. Dependence of the parameter Δ_s as a function of Δ_1 for the simple cubic semi-infinite lattice at $T=T_c^b=5.0392J/k_B$.

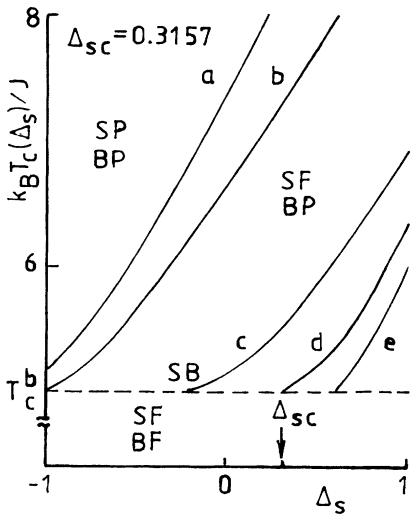

FIG. 3. Phase diagrams in (T,Δ_s) space for the simple cubic semi-infinite lattice, when the parameter Δ_1 is changed as follows: $\Delta_1=9$ (curve *a*), $\Delta_1=\Delta_1^*=5.1899$ (curve *b*), $\Delta_1=1$ (curve *c*), $\Delta_1=0$ (curve *d*), and $\Delta_1=-0.9$ (curve *e*).

In Fig. 3 we present the results for phase diagrams in (T,Δ_s) space obtained from (13) for $\Delta_1>\Delta_1^*$, $\Delta_1=\Delta_1^*$, and

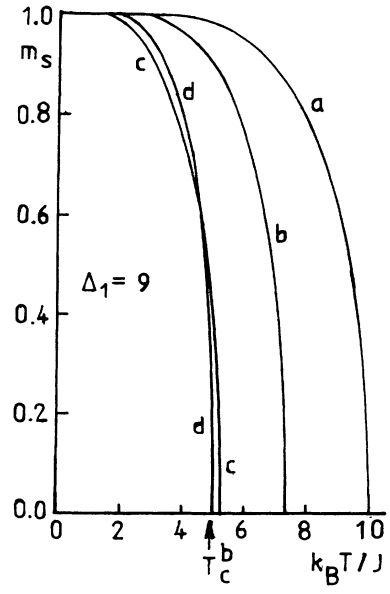

FIG. 4. Temperature dependences of the surface magnetization m_s for $\Delta_1=9$, when $\Delta_s=1$ (curve *a*), $\Delta_s=0$ (curve *b*), and $\Delta_s=-1$ (curve *c*). For comparison the bulk magnetization is plotted as well (curve *d*).

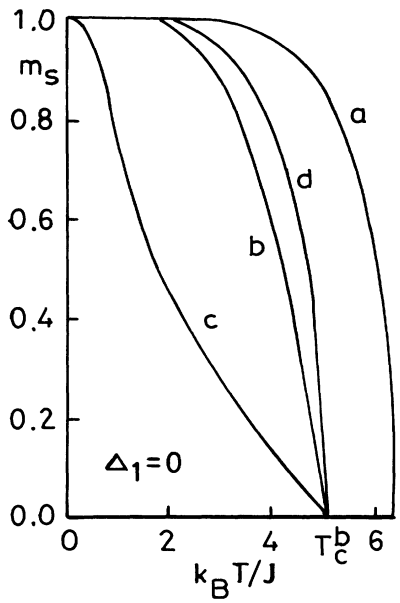

FIG. 5. Temperature dependences of the surface magnetization m_s for $\Delta_1=0$, when $\Delta_s=1$ (curve a), $\Delta_s=0$ (curve b), and $\Delta_s=-1$ (curve c). Curve d is the bulk magnetization.

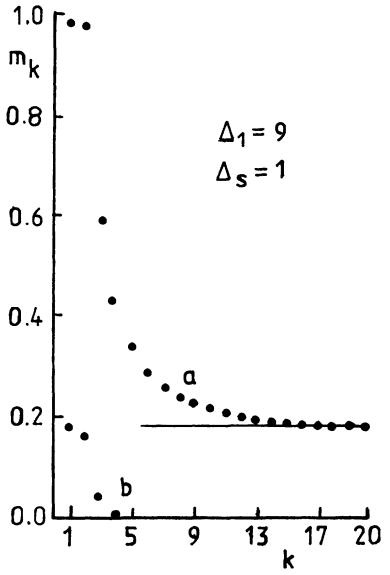

FIG. 7. Layer magnetization m_k vs the number of atomic layers, k, when $\Delta_1=9$ and $\Delta_s=1$. In the case of curve a, $T=10J/k_B$, and in the case of curve b, $T=5J/k_B$.

$\Delta_1<\Delta_1^*$. Above each curve in this figure exists a bulk-paramagnetic (BP) and a surface-paramagnetic (SP) phase. Within the region between each curve and the bulk critical temperature, coexistence of the BP and surface-ferromagnetic (SF) phases is possible. For $T<T_c^b$ we obtain SF and bulk-ferromagnetic (BF) phases. Figure 3 clearly illustrates our previous estimation of the behavior of the surface magnetization. Moreover, we can see that the coordinates $(\Delta_{sc},k_BT_c^b/J)$ denoting the multicritical point of the surface-bulk (SB) transition depend on Δ_1. Consequently, for $\Delta_1>\Delta_1^*$ this type of transition, which is usually called a "special transition," cannot exist in our system.

IV. MAGNETIZATION

It is now interesting to investigate the behavior of the magnetization curves. In the following we show numerical results for the temperature dependences of the surface

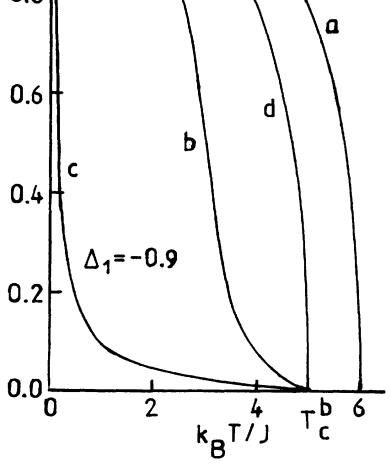

FIG. 6. Temperature dependences of the surface magnetization m_s for $\Delta_1=-0.9$, when $\Delta_s=1$ (curve a), $\Delta_s=0$ (curve b), and $\Delta_s=-1$ (curve c). Curve d is the bulk magnetization.

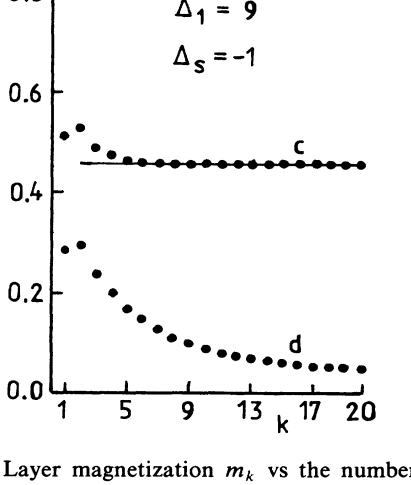

FIG. 8. Layer magnetization m_k vs the number of atomic layers, k, when $\Delta_1=9$, $\Delta_s=-1$, and the temperature is changed as follows: $T=3J/k_B$ (curve a), $T=3.5J/k_B$ (curve b), $T=4.75J/k_B$ (curve c), and $T=5.05J/k_B$ (curve d).

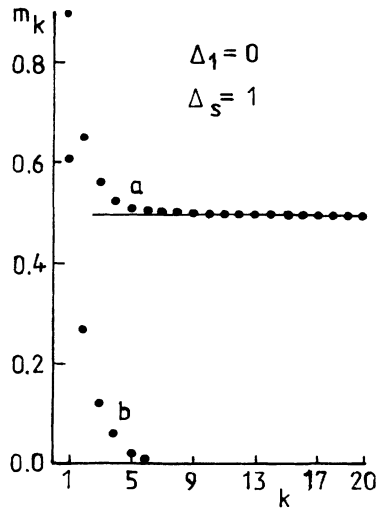

FIG. 9. Layer magnetization m_k vs the number of atomic layers, k, when $\Delta_1=0$ and $\Delta_s=1$. In the case of curve a, $T=4.7J/k_B$, and in the case of curve b, $T=5.8J/k_B$.

magnetization obtained by solving Eq. (8) under the assumption $m_{20}=m_{21}$.

In Fig. 4 are plotted the temperature dependences of the surface magnetization for $\Delta_1=9$ and $\Delta_s=1$, 0, and -1. Because in this case $\Delta_1>\Delta_1^*$, the critical temperature in the surface layer, $T_c(\Delta_s)$ is consequently greater than the bulk critical temperature for arbitrary values of Δ_s. Curve c in this figure illustrates the fact that if $\Delta_1>\Delta_1^*$ and $\Delta_s\rightarrow -1$, then for low temperatures $m_s<m_b$ and near T_c^b we find $m_s>m_b$.

Now we shall study our system for $\Delta_1<\Delta_1^*$, namely, for $\Delta_1=0$ (Mills model), $\Delta_1=-0.9$ and for the same values Δ_s as in the previous case. As can be seen from Fig. 5 for the Mills model, the present method qualitatively reproduces well-known results.[10,21,24] Namely, for $\Delta_s>\Delta_{sc}$ we obtain $m_s>m_b$ and the surface critical temperature $T_c(\Delta_s)$ is greater than T_c^b. On the other hand, for $\Delta_s<\Delta_{sc}$ we have $m_s<m_b$ and the surface magnetization disappears at T_c^b.

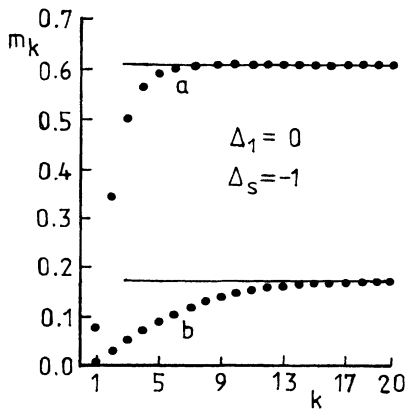

FIG. 10. Layer magnetization m_k vs the number of atomic layers, k, when $\Delta_1=0$ and $\Delta_s=-1$. In the case of curve a, $T=4.5J/k_B$, and in the case of curve b, $T=5J/k_b$.

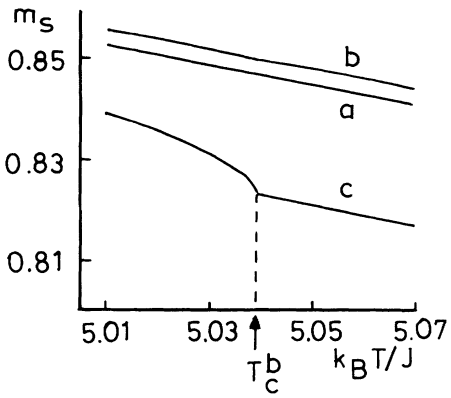

FIG. 11. Temperature dependences of the surface magnetization in different approximations. Curve a, $m_{20}=m_{21}$ or $m_{20}=m_b$; curve b, $m_3=m_4$; and curve c, $m_3=m_b$.

In Fig. 6 is illustrated that for $\Delta_1\rightarrow -1$ the surface layer behaves like a two-dimensional Ising system in which the exchange parameter is J_s.

In Figs. 7–10 the layered magnetizations are presented as functions of the layer number k (i.e., as functions of distance from the surface) for some typical values of Δ_1 and Δ_s. The most interesting results are obtained for $\Delta_1=9$ and $\Delta_s=-1$ (Fig. 8). In this case we find two different types of the magnetization profiles for $T<T_c^b$ and $T>T_c^b$. For the Mills model we obtain the layered magnetizations that exponentially decrease ($\Delta_s>\Delta_{sc}$) or increase ($\Delta_s<\Delta_{sc}$) into the bulk, as shown in Figs. 9 and 10.

Finally, we shall study the behavior of m_s for Mills model near the bulk critical temperature in detail, and we shall show the influence of increasing the number of layers k on the accuracy of results. In Fig. 11 are presented the temperature dependences of m_s obtained by the present technique for different approximations. From this figure we can see that for $m_{20}=m_{21}$ and $m_{20}=m_b$ we obtain the same results (curve a), and there is no evidence for a discontinuous slope at T_c^b. On the other hand, the difference between the results for $m_3=m_4$ (curve b) and for $m_3=m_b$ (curve c) is apparent. Moreover, in the case $m_3=m_b$ we find a clear dip near T_c^b, similarly as in Ref. 5. If we verify this fact for other values of Δ_1 and Δ_s, we obtain similar results, i.e., the existence of a dip for $m_3=m_b$ and nonexistence for $m_{20}=m_b$ or $m_{20}=m_{21}$. Let us note here that the continous dependence of the surface magnetization near T_c^b has been recently obtained by using the different methods of Refs. 24 and 34.

V. CONCLUSION

In the present treatment we have studied the semi-infinite Ising model with three different exchange parameters (J_s, J_1, and J) by using a two-site cluster approximation. Applying the formalism to the simple cubic lat-

tice has shown that the exchange parameter J_1 between the surface and second layers has a fundamental influence on surface magnetic order.

We have found that for $J_1 > 6.1899J$ the surface magnetization exists always above T_c^b, regardless of how weak J_s is. Consequently, as has been discussed in Sec. III, the special transition cannot exist for $J_1 > 6.1899J$. On the other hand, for $J_1 < 6.1899J$ we have found that for J_s greater than a certain critical value J_{sc} the system may order on the surface before it orders in the bulk, and for $J_s < J_{sc}$ the system becomes ordered at the bulk critical temperature.

The temperature dependences of the surface magnetization and magnetization profiles have been calculated as well and the most interesting results shown in Sec. IV. Moreover, at the end of Sec. IV, it has been illustrated that numerical results depend on the number of layers considered in calculations. On the basis of our analysis, we can conclude that the existence of a dip near T_c^b for surface magnetization can be only a consequence of the small number of atomic layers considered in numerical calculations.

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