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Surface Phase Diagram and Tricritical Point of a Semi-Infinite Ising Model with a Spin-One Free Surface

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Abstract Within the framework of an effective field theory with correlations, we have investigated the effects of surface single ion anisotropy on the surface phase transition of a semi-infinite Ising model with a spin-one free surface. Behavior characteristic of surface magnetism is found, and comparison is made with standard molecular field results.

1. INTRODUCTION

The magnetic behavior of semi-infinite solids has been extensively investigated for many years. In particular surface effects on phase transitions have received much attention and have been studied by using a variety of approximations and mathematical techniques, such as mean-field approximation[1], various effective-field theories[2,3], series expansions[4], Monte Carlo techniques[5], and renormalization-group methods[6]. For details, the reader is referred to recent reviews: that of Binder[7] for a general introduction and that of Diehl[8] for reciprocal space renormalization group treatments. The standard example is the semi-infinite simple cubic ferromagnetic Ising model with $S = 1/2$ (S is the spin magnitude), in which the spins on the surface interact with an exchange parameter J_s different from the bulk exchange J. It exhibits different types of phase transitions associated with the surface; if the ratio $\Delta = (J_s/J)-1$ is greater than a critical value Δ_c, the system may order on the surface before it orders in the bulk. The system exhibits two successive transitions, namely the surface and bulk phase transitions, as the temperature is lowered. If $\Delta < \Delta_c$, the system becomes

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ordered at the bulk transition temperature.

In Ising models, on the other hand, there exist many systems exhibiting the tricritical point at which the phase transition changes from second order to first order. Their critical behavior has been the subject of numerous studies. In this way some works[9-11] have studied semi-infinite systems which undergo first-order and tricritical phase transitions.

The purpose of this work is to study a semi-infinite ferromagnetic simple cubic Ising system with a spin-one free surface ($S = 1$), different from $S = 1/2$ of the bulk spins. The spin-one atoms have a single-ion crystal-field interaction. In particular, it is known that the two-dimensional spin-one Ising model with a crystal-field interaction exhibits a tricritical behavior. Therefore, the main aim is to investigate the effects of surface single-ion anisotropy on the surface transition temperature, and under what conditions the system can exhibit tricritical behavior on the surface.

The outline of this paper is as follows. In section 2, we briefly review the basic points of the effective-field theory with correlations (EFT), when applied to the present model. In section 3, expressions for evaluating the transition temperature of surface ordering, surface tricritical point and phase diagram are derived within the framework of the EFT. In section 4, analogous expressions are obtained for the standard molecular field theory (MFT). In section 5, the numerical results are studied within the two frameworks of EFT and MFT.

2. FORMULATION

We consider a semi-infinite simple cubic $S = 1/2$ system with a spin-one free surface which is described by the mixed Ising Hamiltonian, as follows

$$H = -\sum_{<i,j>} J_{ij}\, S_i^z S_j^z - \sum_{<m,n>} J_{mn}\, \mu_m^z \mu_n^z - \sum_{<i,m>} J_{im}\, S_i^z \mu_m^z + D_s \sum_i (S_i^z)^2 \qquad (1)$$

where the spin variable S_i^z takes the values ±1 and 0, μ_m^z can be ±1, and the summations are carried out only over nearest-neighbor pairsof spins. J_{ij} is the exchange interaction between spins one at sites i and j on the surface, which is assumed to be J_s. J_{im} is the exchange pararneter between spins one at the surface and its nearest-neighbor spin-1/2 in the first layer denoted by J_1, and J_{mn} = J is the bulk ferromagnetic interaction, between spins 1/2 otherwise. D_s is the single-ion crystal field interaction parameter. Fig.1 shows a two-dimensional cross section of this system.

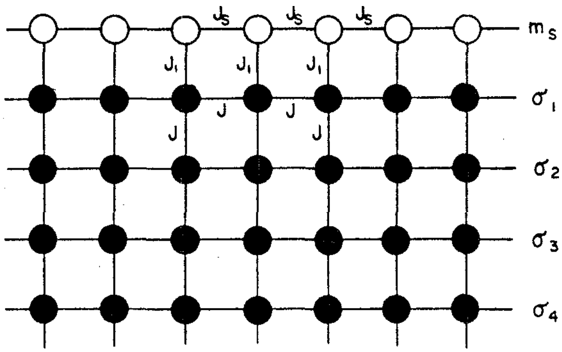

Fig.1 - Part of two-dimensional cross section through a semi-infinite Ising lattice. Black points denote lattice points which are occupied by spins μ_m=±1. On the (1,0,0) surface lattice points are occupied by S_i = ±1 and 0.

The problem is now the evaluation of the mean values $\langle S_i^z\rangle$ and $\langle\mu_m^z\rangle$. As discussed by Kaneyoshi[13], the formal identities for the spin correlation functions for the Ising models can be used. The starting point for the evaluation of the mean values of $\langle S_i^z\rangle$ and $\langle\mu_m^z\rangle$ are the spin correlation exact identities,

$$m_i = \langle S_i^z\rangle = \left\langle \frac{2\sinh(\beta \sum_i J_{ij} S_j^z)}{2\cosh(\beta \sum_j J_{ij} S_j^z) + \exp(D_i\beta)} \right\rangle \qquad (2)$$

$$\sigma_m = \langle\mu_m^z\rangle = \langle\tanh(\beta \sum_n J_{mn}\ \mu_n^z)\rangle \tag{3}$$

where $\beta = 1/k_BT$. As discussed in a series of works, for example ref. 14, by introdycing the differential operator $D = \partial/\partial x$ into eqs. (2) and (3), one may rewrite them in the following forms

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

$$\sigma_m = \langle\prod_n \left[\cosh(\beta J_{mn}D) + \mu_n\ \sinh(\beta J_{mn}D)\right]\rangle\ \tanh x\big|_{x=0} \tag{5}$$

where

$$F_i(x) = \frac{2\ \sinh(\beta x)}{2\ \cosh(\beta x) + \exp(\beta D)} \tag{6}$$

The eqs. (4) and (5) constitute a set of exact relations according to which we can study the present system. However, if we try to treat exactly all the spin-spin correlations for that set of equations, the problem quickly becomes intractable. A first obuious attempt todeal with it is to ignore correlations; the decoupling approxirnations

$$\begin{aligned} &\langle S_i^z\ (S_j^z)^2\ \ldots\ S_n^z\rangle \simeq \langle S_i^z\rangle\ \langle (S_j^z)^2\rangle\ \ldots\ \langle S_n^z\rangle \\ &\langle\mu_m^z\ \mu_n^z\ \ldots\ \mu_\ell^z\rangle \simeq \langle\mu_m^z\rangle\ \langle\mu_n^z\rangle\ \ldots\ \langle\mu_\ell^z\rangle \end{aligned} \tag{7}$$

with $i\neq j\neq\ldots\neq k$ and $m\neq n\neq\ldots\neq\ell$ have been introduced within the effective-field theory with correlations (EFT). In fact, the approximation corresponds essentially to the Zernike approximation[12] in the bulk problem and has been successfully applied to a great number of magnetic systems including the surface problems (refs. 15, 16 and references therein).

Taking account of the decoupling approxirnations (7), eqs. (4) and (5) can be written in a compact form

$$m_i = \left[qc_i + ms_i + 1 - q\right]^z\ F_i(x)\big|_{x=0} \tag{8}$$

$$\sigma_m = \left[c_i + \sigma_n\ s_i\right]\ \ \tanh(\beta x)\big|_{x=0} \tag{9}$$

where $c_i = \cosh(J_i D)$, $s_i = \sinh(J_i D)$ $(i = s,1)$, and z is the number of nearest-neighbors. In order to obtain m, it is necessary to calculate the parameter q. In the sameway as for the evaluation of m, we can easily obtain

$$q = [qc_i + ms_i + 1 - q]^z \; G_i(x)|_{x=0} \tag{10}$$

with

$$G_i(x) = \frac{2\cosh(\beta x)}{2\cosh(\beta x) + \exp(\beta D_i)} \tag{11}$$

Now, let us apply eqs. (8), (9) and (10) to our layered simple cubic mixed system with a (1,0,0) surface. For the surface magnetization, eqs. (8) and (10) yield

$$m_s = [q_s\, c_s + m_s\, s_s + 1 - q_s]^4 [c_1 + \sigma_1\, s_1] \; F_s(x)\Big|_{x=0} \tag{12}$$

$$q_s = [q_s\, c_s + m_s\, s_s + 1 - q_s]^4 [c_1 + \sigma_1\, s_1] \; G_s(x)\Big|_{x=0} \tag{13}$$

The first layer magnetization is given by

$$\sigma_1 = [c + \sigma_1\, s]^4 [q_s\, c_1 + m_s\, s_1 + 1 - q_s] [c + \sigma_2\, s] \; f(x)\Big|_{x=0} \tag{14}$$

where

$$c = \cosh(JD), \quad s = \sinh(JD)$$

and

$$f(x) = \tanh(\beta x) \;, \tag{15}$$

and for the n-th layer $(n \geqslant 2)$ we have

$$\sigma_n = [c + \sigma_n\, s]^4 [c + \sigma_{n-1}\, s] [c + \sigma_{n+1}\, s] f(x)\Big|_{x=0} \tag{16}$$

where σ_{n-1} and σ_{n+1} are the magnetizations in the $(n-1)$th and $(n+1)$th layers, respectively.

In this section we have discussed the effective-field theory with correlations (EFT) in the semi-infinite ferromagnetic Ising model with a spin-one free surface. We are now in a position to examine the transition temperature and the tricritical behavior on the surface. In the following sections, within this framework, we shall study the corresponding physical properties.

3. SURFACE TRANSITION TEMPERATURE AND TRICRITICAL POINT

We are now concerned with the calculation of the critical temperature and the tricritical point for surface ordering (and the respective phase diagrams). Expanding the right-hand sides of eqs. (12), (13), (14) and (16), we obtains

$$m_s = 4A_1\, m_s + A_2\, \sigma_1 + 4A_3\, m_s^3 + 6A_4\, m_s^2\, \sigma_1 + \dots \tag{17}$$

$$q_s = B_1 + 6B_2\, m_s^2 + 4B_3\, m_s\, \sigma_1 + \dots \tag{18}$$

$$\sigma_1 = 4C_1\, \sigma_1 + C_2\, m_s + C_1\, \sigma_2 + \dots \tag{19}$$

and

$$\sigma_n = K(\sigma_{n-1} + 4\sigma_n + \sigma_{n+1}) + \dots\, , \quad n \geq 2 \tag{20}$$

where the coefficients A_j, B_j, C_j and K are given in the Appendix, and are easily calculated by the use of the mathematical relation

$$e^{\alpha D} f(x) = f(x+\alpha) \quad .$$

A. Transition Temperature

The bulk transition temperature T_c^b can be determined by putting $\sigma_n = \sigma_{n-1} = \sigma_{n+1} = \sigma$ into eq. (20), which yields

$$\tanh\left(\frac{6J}{k_B T_c^b}\right) + 4\tanh\left(\frac{4J}{k_B T_c^b}\right) + 5\tanh\left(\frac{2J}{k_B T_c^b}\right) = \frac{16}{3} \tag{21}$$

which has been obtained by Zernike[12] by the use of another method. The bulk transition temperature is given by

$$\frac{k_B T_c^b}{J} = 5.073 \quad .$$

This is an improvement on the standard HFT, which provides $k_B T_c^b / J = 6.0$.

In order to evaluate the transition temperature for surface ordering, let us assume that

$$\sigma_n = a\,\sigma_{n-1} \quad \text{for} \quad n \geq 2 \quad .$$

Upon using eq. (20), the parameter a is given by:

$$a = \frac{(1-4k) - [(6k-1)(2k-1)]^{1/2}}{2k} \tag{22}$$

Eqs. (17) to (20) then yield the following secular equation

$$\tilde{M}\begin{pmatrix} m_s \\ \sigma_1 \end{pmatrix} = \begin{pmatrix} 4A_1 - 1 & A_2 \\ C_2 & C_1(4+a) - 1 \end{pmatrix} \begin{pmatrix} m_s \\ \sigma_1 \end{pmatrix} = 0 \tag{23}$$

Thus, the critical ferromagnetic frontiers can be derived from the condition det $\tilde{M} = 0$, namely

$$(4A_1 - 1)[C_1(4+a) - 1] = A_2\, C_2 \tag{24}$$

where the parameter q_s in the coefficients A_1, A_2, C_1, C_2 and K is determined from

$$\begin{aligned} q_s &= B_1 \\ &= c_1 [q_s\, c_s + 1 - q_s]^4\, G_s(x)\big|_{x=0} \end{aligned} \tag{25}$$

From the formal solutions of eq. (24) we choose those corresponding to the highest posçible transition temperature T_c^s, which is the temperature for surface ordering.

B. Tricritical Point

In order to examine the tricritical behavior of the surface, as discussed by Kaneyoshi[14], it is necessary to retain terms up to third order in m_s in eq. (17). For this purpose, let us substitute

$$q_s = q_s^0 + q_s^1\, m_s^2 \tag{26}$$

into expression (18), which yields

$$q_s^0 = c_1 [q_s^0 c_s + 1 - q_s^0]^4 G_s(x)\Big|_{x=0} \tag{27}$$

and

$$q_s^1 = \frac{4\lambda E_2 + 6E_3}{1 - 4E_1} \tag{28}$$

where

$$\begin{aligned} E_1 &= (c_s-1)c_1 [q_s^0 c_s + 1 - q_s^0]^3 G_s(x)\Big|_{x=0} \\ E_2 &= s_s s_1 [q_s^0 c_s + 1 - q_s^0]^3 G_s(x)\Big|_{x=0} \\ E_3 &= s_s^2 c_1 [q_s^0 c_s + 1 - q_s^0]^2 G_s(x)\Big|_{x=0} \end{aligned} \tag{29}$$

with the assurnption that

$$\sigma_1 = \lambda m_s .$$

The parameter λ is found from eq. (19) using

$$\sigma_2 = a\,\sigma_1$$

Then, we obtain

$$\lambda = \frac{D_2}{1-4D_1-aD_3} \tag{30}$$

where

$$\begin{aligned} D_1 &= sc^4 [q_s^0 c_1 + 1 - q_s^0] f(x)\Big|_{x=0} \\ D_2 &= s_1 c^5 f(x)\Big|_{x=0} \\ D_3 &= sc^4 [q_s^0 c_1 + 1 - q_s^0] f(x)\Big|_{x=0} \end{aligned} \tag{31}$$

Thus, we obtain in general an equation for m_s of the form

$$ms = \tilde{a}\, m_s + \bar{b}\, m_s^3 + \dots \tag{32}$$

with

$$\bar{a} = 4I_1 + \lambda \dot{I}_2 \qquad (33)$$

$$\bar{b} = 2(6I_3\, q_s^1 + 2\lambda\, I_4\, q_s^1 + 3\lambda\, I_5 + 2I_6) \qquad (34)$$

where the coefficients I_i (i = 1 to 6) are given in the appendix.

The second order surface phase transition is then determined by $\bar{a} = 1$, or

$$4I_1 + \lambda I_2 = 1 \qquad (35)$$

which is equivalente to eq. (24). In the vicinity of the second-order surface phase transition line, the magnetization is given by

$$m_s = \frac{1-\bar{a}}{\bar{b}} \qquad (36)$$

The r.h.s. must be positive. If this is not the case, the transition is first order, and hence the point at which $\bar{a}$ = 1 and $\bar{b}$ = 0 is the surface tricritical point, if it exists above the bulk transition temperature $_c$.

We are now in a position to examine the effects of single-ion anisotropies on the second-order phase transition and tricritical point of the surface by the use of eqs. *(24)* and (34). Before discussing the results, it is worth investigating these quantities within the framework of the standard molecular field theory (MFT). In the next section, this approach is followed.

4. MEAN FIELD THEORY

In the MFT the surface magnetization m_s is given by

$$m_s = F_s(\phi_s) \qquad (37)$$

with

$$\phi_s = 4\, J_s\, m_s + J_1\, \sigma_1 \qquad (38)$$

The first and n-th layer magnetizations are

$$\sigma_1 = f(\phi_1) \qquad (39)$$

$$\sigma_n = f(\phi_n) \qquad (40)$$

with

$$\phi_1 = 4J\ \sigma_1 + J_1\ m_s + J\ \sigma_2 \tag{41}$$

$$\phi_n = J(\sigma_{n-1} + 4\sigma_n + \sigma_{n+1}) \tag{42}$$

The functions $F(x)$ and $f(x)$ are given by eqs. (6) and (15).

A. Transition Temperature

The transition temperature for surface ordering can be obtained by linearizing eqs. (37), (39) and (40), as discussed in section 3. We have, for m_s and σ_1,

$$m_s = 4J_s\ F_s\ m_s + J_1\ F_s\ \sigma_1 \tag{43}$$

$$\sigma_1 = 4J\ \beta\ \sigma_1 + J_1\ \beta\ m_s + \beta\ a\ \sigma_1 \tag{44}$$

where

$$F_s = D\ F_s(x)\Big|_{x=0} = \beta\ g_s \tag{45}$$

$$\beta = D\ f(x)\Big|_{x=0} \tag{46}$$

$$g_s = 2/(2+\exp(\beta D_s)) \tag{47}$$

where

$$\sigma_n = a\ \sigma_{n-1}\quad ,\quad (n \geq 2)$$

was used. The parameter a is determined frorn

$$\sigma_n = \beta J(\sigma_{n-1} + 4\sigma_n + \sigma_{n+i}) \tag{48}$$

as

$$a = \frac{(1-4\beta J) - \sqrt{(1-4\beta J)^2 - 4(\beta J)^2}}{2\beta J} \tag{49}$$

Upon using eqs. (43) and (44), the critical ferromagnetic fronties of the MFT can be derived from:

$$(4J_s\ F_s - 1)(4J\beta + J\beta a - 1) = J_1^2\ F_s \beta \tag{50}$$

8. Tricritical Point

In order to determine the surface tricritical point for the MFT, let us expand eq. (37) to third order in ϕ_s, since ϕ_s is proportional to m_s. We then obtain

$$m_s = [\phi_i^s D + \frac{D^3}{3!}(\phi_i^s)^3] F_s(x)|_{x=0} \quad (51)$$

$$= g_s(\beta\phi_s) + \frac{(\beta\phi_s)^3}{3} g_s(1-3g_s) \quad (52)$$

Thus, the point at which eq. (50) and $1 = 3g_s$ are simultaneously satisfied is the tricritical point of the MFT.

5. NUMERICAL RESULTS

In this section, we examine numerically the effects of the surface anisotropy parameter D_s on the transition temperature, tricritical point and phase diagram for surface ordering by solving equations discussed in section 3 and 4.

In fig.2, by solving eqs. (24) and (50) for the system, the phase diagrams are obtained within the two frameworks of EFT and MFT by changing the value of D_s. In the figure, solid lines are the results of the EFT and dashed lines are for the MFT. We denote the paramagnetic, bulk ferromagnetic, and surface-ferromagnetic phases by P, BF, and SF, respectively. When $D_s = -\infty$, the surface behaves like a bulk two-dimensional Ising model (or Mill's model[1]) for J_s larger than $J_s^{MFT} = 1.25$ (within the framework of the MFT). On the other hand, the EFT result gives the critical value of J_s as $J_{sc} = 1.30$ J, which value is also, within the numerical error, equivalent to that obtained by Kaneyoshi et al[2] ($J_{sc} = 1.3068$).

For $D_s=0.0$, the critical value of J_s is determined as $J_{sc}=2.0\,J$ for both MFT and EFT. For $D_s=1.0$ J, on the other hand, the critical values of J_s are given by $J_{sc}=2.24$ J for the MFT and $J_{sc}=2.11J$ for the EFT, respectively. Thus, for a positive value of D_s less than a critical value at which the surface phase transition changes from second order to first order, the MFT overestimates the critical value of J_s in com-

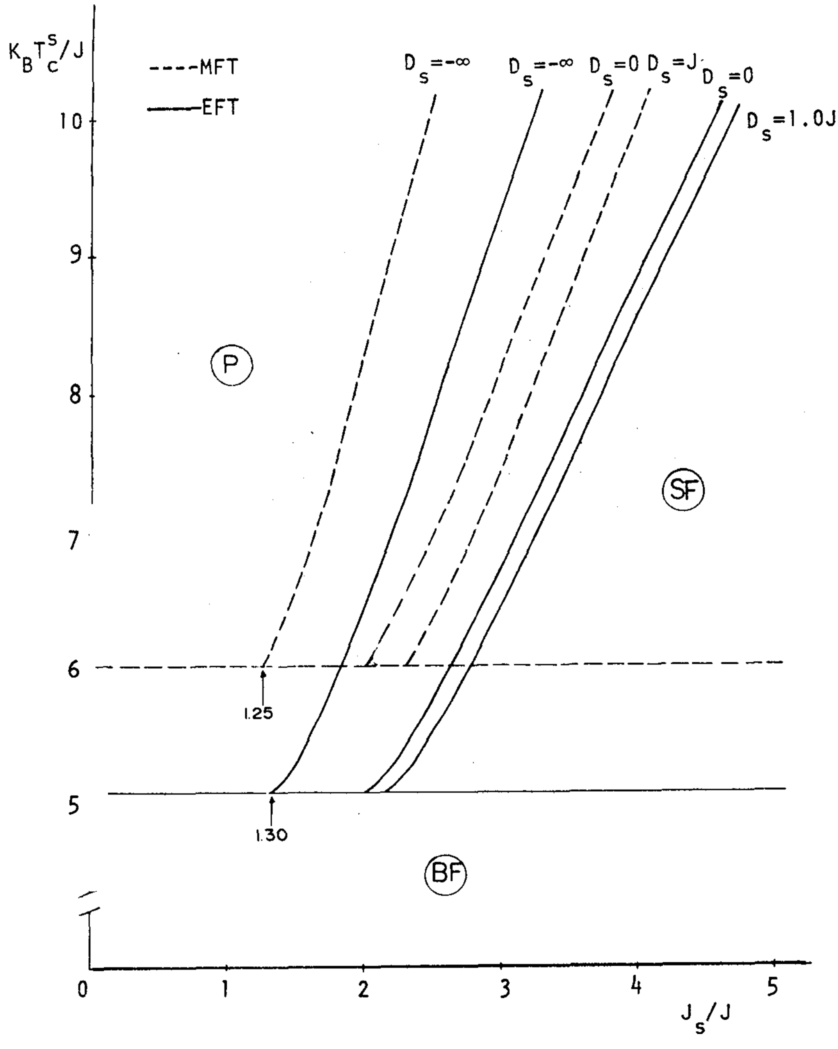

Fig.2 - Phase diagram in the (T,J_S) space for the simple cubic Ising lattice with $J_1=J$. The dashed lines are the results of the MFT. The solid lines are the results of the EFT. The curves (a) are obtained for $D_S=-\infty$. The curves (b) are for $D_S=0$. The curves (c) are for $D_S=1.0J$. The paramagnetic, bulk-ferromagnetic and surface-ferromagnetic phases are indicated by P, BF, and SF, respectively.

parison with that given by EFT, although for $D_s=-\infty$ the MFT underestimates the critical value of J_s, as compared with that given by EFT.

In fig.3, by solving eq.(24) and $\bar{b}=0$ simultaneously for the EFT (or (50) and $3g_s=1$ for the MFT), transition temperatures T_c^s for surface ordering of the system with $J_1=J$ are plotted as a function of the surface single-ion anisotropy parameter D_s. The curves (a), (b), (c) and (d) are the MFT results, when J_s is selected respectively as $J_s=3.5\ J$, $J_s=4.25\ J$, $J_s=5.0\ J$, and $J_s=5.5\ J$. For the values of J_s smaller than $J_s=4.25\ J$, the point satisfying the relations (24) and $3g_s=1$ simultaneously does not appear above the bulk transition temperature T_c^b. When $J_s=4.25\ J$, as shown in the curve (b), the MFT gives the tricritical point at T_c^s, which is denoted as the white circle in the curve. The curves (a'), (c') and (d') are the results of the EFT, when the values of J_s are selected in the same values as for curves (a), (c) and (d) of the MFT. The dashed lines in fig.3 are simply extrapolations of the solution $1-\bar{a}=0$ and do not have any physical meaning, since within our theory we are discussing the second-order phase transition line and the tricritical point. The first order phase transition line is impossible to obtain within our formulation.

6. CONCLUSIONS

We have discussed the effects of surface single-ion anisotropy on the transition temperature for surface ordering, the surface tricritical point, and the phase diagram within the two frameworks of MFT and EFT. Our discussion has revealed behavior characteristic in the Ising model. As shown in fig.2, for a positive value of D_s the MFT overestimates the critical value of J_s for surface ordering in comparison with that given by EFT, although for $D_s=-\infty$ (or Mill's model) the MFT underestimates the critical value J_{sc}, as compared with that given by EFT. In fact, a number of sophisticated theoretical works on Mill's model have revealed that the critical value $J_{sc}^{MFT}=1.25\ J$ is an underestimation for the value of J_{sc}. To our knowledge, the effect of a positive D_s on J_{sc} has not been investigated previously.

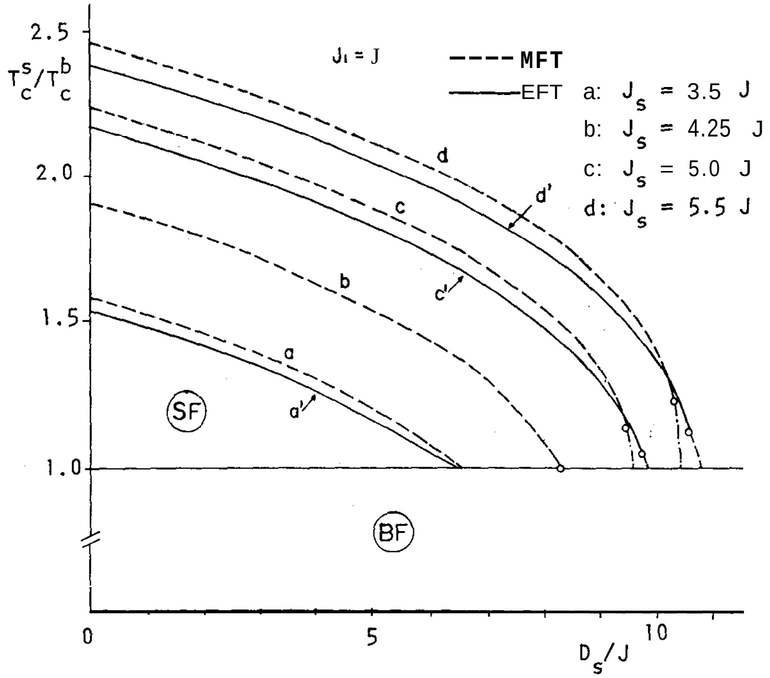

Fig.3 - Surface transition temperatures of the system with $J_1=J$, plotted as a function of surface single-ion anisotropy parameter D_S for selected values of J_S; (a), (b), (c) and (d) are obtained from the MFT for J_S=3.5 J, J_S=4.25 J, J_S=5.0 J, and J_S=5.5 J, respectively. (a'), (c') and (d') are the results of the EFT for the same values of J_S as the corresponding (a), (c) and (d). White circles denote surface tricritical points.

APPENDIX

$$A_1 = s_s \, c_1 \, [q_s \, c_s + 1 - q_s]^3 \, F_s(x)|_{x=0}$$

$$A_2 = s_1 \, [q_s \, c_s + 1 - q_s]^4 \, F_s(x)|_{x=0}$$

$$A_3 = s_s^3 \, c_1 \, [q_s \, c_s + 1 - q_s] \, F_s(x)|_{x=0}$$

$$A_4 = s_s^2 \, s_1 \, [q_s \, c_s + 1 - q_s]^2 \, F_s(x)|_{x=0}$$

$$B_1 = c_1 \left[q_s c_s + 1 - q_s\right]^4 G_s(x)\big|_{x=0}$$

$$B_2 = s_s^2 c_1 \left[q_s c_s + 1 - q_s\right]^2 G_s(x)\big|_{x=0}$$

$$B_3 = s_s s_1 \left[q_s c_s + 1 - q_s\right]^3 G_s(x)\big|_{x=0}$$

$$C_1 = s c^4 \left[q_s c_1 + 1 - q_s\right] f_s(x)\big|_{x=0}$$

$$C_2 = s_1 c^5 f(x)\big|_{x=0}$$

$$K = s c^5 f(x)\big|_{x=0}$$

$$I_1 = s_s c_1 \left[q_s^0 c_s + 1 - q_s^0\right]^3 F_s(x)\big|_{x=0}$$

$$I_2 = s_1 \left[q_s^0 c_s + 1 - q_s^0\right]^4 F_s(x)\big|_{x=0}$$

$$I_3 = s_s c_1 (c_s-1) \left[q_s^0 c_s + 1 - q_s^0\right]^2 F_s(x)\big|_{x=0}$$

$$I_4 = s_1 (c_s-1) \left[q_s^0 c_s + 1 - q_s^0\right]^3 F_s(x)\big|_{x=0}$$

$$I_5 = s_s^2 s_1 \left[q_s^0 c_s + 1 - q_s^0\right]^2 F_s(x)\big|_{x=0}$$

$$I_6 = s_s^3 c_1 \left[q_s^0 c_s + 1 - q_s^0\right] F_s(x)\big|_{x=0}$$

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Resumo

Dentro de um modelo de teoria de campo efetivo com correlações, investigamos os efeitos de uma anisotropia uniaxial de superfície na transição de fase de superficie de um meio semi-infinito (Ising) com uma superfície livre de spins-1. Algumas características de magnetismo de superficie são encontradas e os resultados são comparados com aqueles fornecidos pela teoria de campo médio.