Bond diluted surface phase diagrams of the transverse Ising model

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The effects of diluted surface on the phase diagram of the transverse Ising spin model is studied by the use of an effective field method within the framework of single-site cluster theory. The state equations are derived using the differential operator technique. The complete phase diagrams are investigated when the exchange interactions J_{ij}^S at the surface, is randomly distributed. J_{ij}^S is in competition with the bulk interactions. In particular, the influence of the surface transverse field and the dilution parameter on the three-dimensional transverse Ising model is examined in detail.

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I. INTRODUCTION

The problems related to the nature of phase transitions at surfaces of magnetic materials generated considerable interest both theoretically and experimentally[1,2].One of the simplest three dimensional semi-infinte models is the spin-1/2 simple cubic lattice Ising ferromagnet with a free (1,0,0) surface. It has been extensively studied using a variety of approximations and mathematical techniques . Such as mean-field theory[3,4], cluster variation method[5], effective field theory[6], finite cluster approximation[7,8], renormalization group methods[8-12], Monte Carlo techniques[13,14] and series expansions[15]. The standard example is the semi-infinite cubic ferromagnetic Ising model in which the spins on the surface interact among one another with an exchange parameter $\overline{J_S}$ different from the bulk exchange J_B. It exhibits different types of phase transitions associated with surface. If the ratio $R=J_S/J_B$ is greater than a critical value R_C, the system may order on the surface before it orders in the bulk. The system exhibits two successive transitions, namely the surface and extraordinary transitions, as the temperature is lowered. If R is less than R_C, the system becomes ordered at the bulk transition temperature. This is the ordinary phase transition. If $R=R_C$, the system orders at the bulk transition temperature but in this case the critical exponents differ from those of ordinary transition. This is the special phase transition.

The simple cubic Ising ferromagnet with a ferromagnetic exchange interaction ($J_B>0$) in the bulk and an antiferromagnetic exchange interaction ($\overline{J_S}<0$) between surface spins has been studied using mean-field approximation[15], renormalization group method[16], and Monte Calro simulation (MC)[17,18]. In this case the surface layer behaves roughly like an Ising antiferromagnet in a (temperature-dependent) field. Below the bulk critical temperature, the bulk is ordered ferromagnetically for all $\overline{J_S}$. For $\overline{J_S}$ less than some temperature dependent value of surface exchange, the surface is also in an ordered ferromagntic state, but for large negative values, the surface is antiferromagnetic instead. As the temperature increases, the bulk disorders, but for strongly negative $\overline{J_S}$ the surface remains ordered up to some higher temperature. The phase boundaries for the bulk and the surface transitions cross at a tetracritical point.

The transverse Ising model (TIM) is a system originally introduced by De Gennes[19] as a valuable model for the tunnelling of the proton in hydrogen-bonded ferroelectrics[20] type. Since then, it has been successfully applied to several physical systems, such as co-operative Jahn-Teller systems[21],ordering in rare earth compounds with a singled crystal-field ground state[22] and also to some real magnetic materials with strong uniaxial anisotropy in transverse field[23]. It has been extensively studied by the use of various techniques[24-28], including the effective field treatment[29,30] based on a generalized but approximated Callen-Suzuki relation derived by Sà Barreto, Fittipaldi and Zeks. The system shows a phase transition somewhat different from the usual Ising model case in two or more dimensions. It presents a finite-temperature phase transition which can be depressed to zero by increasing the transverse field to a certain critical value. Using the effective field theory[31], similar transition have been fund for three-dimensional semi-infinite spin-1/2 ferromagnetic Ising model in the random transverse field.

In this paper, we are interested in the study of surface phase transitions in the spin-1/2 transverse Ising ferromagnet with a diluted antiferromagnetic surface. The purpose is to describe the phase diagrams of the system, by the use of an effective field method based on differential operator technique within the framework of a single-site cluster theory. We focus our attention on the effects of the

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transverse fields and the surface random bond concentration on the phase transitions associated with the surface.

Our presentation is as follows. In section II, we review the basic points of the effective-field theory with correlations (EFT) as applied to the present model. In section III, the phase diagrams of the system as a function of the transverse field and surface random bond are examined and discussed. Finally, we comment on our results in section IV .

II. THEORETICAL FRAMEWORK

We consider a semi-infinite surface bond-diluted Ising model in transverse field which is described by the following Hamiltonian.

$$H=-\sum_{\langle ij\rangle} J_{ij}\sigma_i^z\sigma_j^z-\Omega_S\sum_{i\in S}\sigma_i^x-\Omega_B\sum_{i\notin S}\sigma_i^x \tag{1}$$

Where $\sigma_i^\alpha\,(\alpha=x,z)$ is component of spin-1/2 operator at site i. Ω_B and Ω_S represent transverse fields in the bulk and at the surface, respectively. J_{ij} is the nearest-neighbour exchange interaction between spins at sites i and j, that takes the value J_{ij}^S if both spins lie on the surface and J_B $(J_B>0)$ otherwise. J_{ij}^S obey to the following distribution.

$$Q\left(J_{ij}^S\right)=p_S\delta\left(J_{ij}^S+J_S\right)+\left(1-p_S\right)\delta\left(J_{ij}^S\right), \tag{2}$$

where $J_S>0$ and the parameter p_S measures the concentration of antiferromagntic bonds.

The theoretical framework we adopt in the study of the system described by the Hamiltonian (1), is the effective-field theory based on single-site cluster theory. In this approach, attention is focused on a cluster consisting of just a single selected spin, labelled o, and the neighbouring spins with which it directly interacts. To this end, the total Hamiltonian is split in two parts, $H=H_o+H'$, where H_o includes all those terms of H associated with the lattice site o, namely

$$H_o=-\left(\sum_j J_{oj}\sigma_j^z\right)\sigma_o^z-\Omega_\theta\sigma_o^x, \tag{3}$$

with $\theta\equiv S$ or B whether the lattice site o belongs to the surface or to the bulk, respectively. The problem consists in evaluating the longitudinal and transverse site magnetizations. The starting point of our calculation will be a generalised, but approximate, Callen-Suzuki relation[32,33].

$$\left\langle \hat{O}_o\right\rangle=\left\langle\frac{trace_o\left[\hat{O}_o\exp(-\beta H_o)\right]}{trace_o\left[\exp(-\beta H_o)\right]}\right\rangle, \tag{4}$$

derived by Sà barreto et al.[29] for the transverse Ising model. $trace_o$ means the partial trace with respect to the site o. $\langle\ldots\rangle$ indicates the canonical thermal average and $\beta=\frac{1}{k_BT}$. As pointed out by those authors, this relation is not exact since H_o and H' do not commute.

Nevertheless, they have been successfully applied to a number of interesting transverse Ising systems. We emphasize that in the limit $\Omega_\theta=0$ ($\theta\equiv S$ or B) the hamiltonian contains only σ_i^z. Then, relation (4) becomes exact identity. The application of (4) for the longitudinal and transverse site magnetizations of the n^th^ layer, leads to the following expressions.

$$\left\langle\sigma_{on}^z\right\rangle=\left\langle\frac{A}{2E_o}\tanh\left(\frac{\beta}{2}E_o\right)\right\rangle, \tag{5}$$

$$\left\langle\sigma_{on}^x\right\rangle=\left\langle\frac{\Omega_\theta}{2E_o}\tanh\left(\frac{\beta}{2}E_o\right)\right\rangle, \tag{6}$$

with

$$A=\sum_j J_{oj}\sigma_j^z, \tag{7}$$

$$E_o=\left[\left(\Omega_\theta\right)^2+A^2\right]^{1/2}. \tag{8}$$

Introducing the differential operator technique[34], (5) and (6) can be written as follows

$$\left\langle\sigma_{on}^z\right\rangle=\left\langle e^{A\nabla}\right\rangle F_\theta(x)\Big|_{x=o}, \tag{9}$$

$$\left\langle\sigma_{on}^x\right\rangle=\left\langle e^{A\nabla}\right\rangle G_\theta(x)\Big|_{x=o}, \tag{10}$$

where $\nabla=\partial/\partial x$ is a differential operator (defined as $e^{A\nabla}F(x)=F(x+A)$) and functions $F_\theta(x)$ and $G_\theta(x)$ are defined b

$$F_\theta(x)=\frac{x}{2\left[\left(\Omega_\theta\right)^2+x^2\right]^{1/2}}tanh\left(\frac{\beta}{2}\left[\left(\Omega_\theta\right)^2+x^2\right]^{1/2}\right), \tag{11}$$

$$G_\theta(x)=\frac{\Omega_\theta}{2\left[\left(\Omega_\theta\right)^2+x^2\right]^{1/2}}tanh\left(\frac{\beta}{2}\left[\left(\Omega_\theta\right)^2+x^2\right]^{1/2}\right). \tag{12}$$

By assuming the statistical independence of the lattice sites, that is $\langle\sigma_i,\sigma_j,\ldots,\sigma_l\rangle\approx\langle\sigma_i\rangle\langle\sigma_j\rangle\ldots\langle\sigma_l\rangle$ and using the spin-1/2 identity $\exp(\lambda\sigma_i)=\cosh\left(\frac{\lambda}{2}\right)+2\sigma_i\sinh\left(\frac{\lambda}{2}\right)$, (9) and (10) may be written as follows

$$\left\langle\sigma_{on}^z\right\rangle=\prod_j\left[cosh\left(\frac{J_{oj}}{2}\nabla\right)+2\left\langle\sigma_j^z\right\rangle sinh\left(\frac{J_{oj}}{2}\nabla\right)\right]\times F_\theta(x)\Big|_{x=o}, \tag{13}$$

$$\langle\sigma_{on}^{x}\rangle=\prod_{j}\left[\cosh\left(\frac{J_{oj}}{2}\nabla\right)+2\langle\sigma_{j}^{z}\rangle\sinh\left(\frac{J_{oj}}{2}\nabla\right)\right]\times G_{\theta}(x)\Big|_{x=o}. \quad (14)$$

Since the surface exchange interactions are randomly distributed, we have to perform the random average of J_{oj}^{S} according to the probability distribution function $Q(J_{ij}^{S})$ given by (2) when the lattice site o belongs to the surface $(n\equiv S)$. The surface ordering parameters μ_S^z and μ_S^x are then defined as $\mu_S^z=\overline{\langle\sigma_{oS}^{z}\rangle}$ and $\mu_S^x=\overline{\langle\sigma_{oS}^{z}\rangle}$, where the bar denotes the random bond average.

Therefore, the surface longitudinal magnetization μ_S^z per site and the magnetization μ_n^z of the n[th] layer are given by

-For the surface $(n\equiv S)$

$$\begin{cases}(\mu_S^z)_1=\left[a_S+2(\mu_S^z)_2 b_S\right]^4\times\left[a_B+2(\mu_1^z)_2 b_B\right]F_S(x)\Big|_{x=o}\\ (\mu_S^z)_2=\left[a_S+2(\mu_S^z)_1 b_S\right]^4\times\left[a_B+2(\mu_1^z)_1 b_B\right]F_S(x)\Big|_{x=o}\end{cases}, \quad (15)$$

-For the first layer

$$\begin{cases}(\mu_1^z)_1=\left[a_B+2(\mu_S^z)_2 b_B\right]\times\left[a_B+2(\mu_1^z)_2 b_B\right]^4\times\left[a_B+2(\mu_2^z)_2 b_B\right]F_B(x)\Big|_{x=o}\\ (\mu_1^z)_2=\left[a_B+2(\mu_S^z)_1 b_B\right]\times\left[a_B+2(\mu_1^z)_1 b_B\right]^4\times\left[a_B+2(\mu_2^z)_1 b_B\right]F_B(x)\Big|_{x=o}\end{cases}, \quad (16)$$

-For any layer n≥2

$$\begin{cases}(\mu_n^z)_1=\left[a_B+2(\mu_{n-1}^z)_2 b_B\right]\times\left[a_B+2(\mu_n^z)_2 b_B\right]^4\times\left[a_B+2(\mu_{n+1}^z)_2 b_B\right]F_B(x)\Big|_{x=o}\\ (\mu_n^z)_2=\left[a_B+2(\mu_{n-1}^z)_1 b_B\right]\times\left[a_B+2(\mu_n^z)_1 b_B\right]^4\times\left[a_B+2(\mu_{n+1}^z)_1 b_B\right]F_B(x)\Big|_{x=o}\end{cases}. \quad (17)$$

where

$$a_S=p_S\cosh\left(\frac{J_S}{2}\nabla\right)+(1-p_S), \quad b_S=-p_S\sinh\left(\frac{J_S}{2}\nabla\right)$$

$$a_B=\cosh\left(\frac{J_B}{2}\nabla\right), \quad b_B=\sinh\left(\frac{J_B}{2}\nabla\right)$$

$(\mu_n^z)_1$ and $(\mu_n^z)_2$ indicate the two-sublattice longitudinal magnetizations of the n[th] layer, respectively. We note that the bulk longitudinal magnetization μ_B^z is determined by setting $\mu_{n-1}^z=\mu_n^z=\mu_{n+1}^z$ in (17). Thus, μ_B^z is solution of the equation

$$\mu_B^z=\left[a_B+2\mu_B^z b_B\right]^6 F_B(x)\Big|_{x=o}. \quad (18)$$

III. PHASE DIAGRAMS AND DISCUSSIONS

In order to investigate the phase diagrams of the system described by the Hamiltonian (1), we have to solve the coupled eqs (15)-(17). However, we are unable to solve them analytically. Even if we use a numerical method, they must be terminated at a certain layer. Note that as n goes to infinity, the magnetization μ_n^z should approach the bulk value μ_B^z. For this purpose, let us assume that the magnetizations remain unaltered after the third layer i.e.

$$\mu_3^z=\mu_4^z=\ldots=\mu_B^z,$$

which may be called the four-layer approximation.

We are first concerned with evaluation of the order-disorder transition temperatures for the bulk and surface ordering based on the four-layer approximation. From (18), the bulk critical temperature $k_B T_c/J_B$ is solution of the equation

$$1=12a_B^5 b_B F_B(x)\Big|_{x=o}. \quad (19)$$

In order to obtain the surface order-disorder critical temperature, we have to linearize (15)- (17). Thus, neglecting high-order terms in magnetization near the critical temperature, and within the four-layer approximation, we obtain

$$\begin{cases}(\mu_S^z)_1=A_1(\mu_S^z)_2+A_2(\mu_1^z)_2\\ (\mu_S^z)_2=A_1(\mu_S^z)_1+A_2(\mu_1^z)_1\end{cases}, \quad (20)$$

$$\begin{cases}(\mu_1^z)_1=B_1\left((\mu_S^z)_2+4(\mu_1^z)_2+(\mu_2^z)_2\right)\\ (\mu_1^z)_2=B_1\left((\mu_S^z)_1+4(\mu_1^z)_1+(\mu_2^z)_1\right)\end{cases}, \quad (21)$$

$$\begin{cases}(\mu_2^z)_1=B_1\left((\mu_1^z)_2+4(\mu_2^z)_2+(\mu_B^z)_2\right)\\ (\mu_2^z)_2=B_1\left((\mu_1^z)_1+4(\mu_2^z)_1+(\mu_B^z)_1\right)\end{cases}. \quad (22)$$

The coefficients A_1,A_2 and B_1 are given by

$$\begin{aligned}A_1&=8a_S^3 b_S a_B F_S(x)\Big|_{x=o}\\ A_2&=2a_S^4 b_B F_B(x)\Big|_{x=o}\\ B_1&=2a_B^5 b_B F_B(x)\Big|_{x=o}\end{aligned}. \quad (23)$$

Therefore, the critical ordering frontiers (when the bulk is disordered) are analytically obtained through a determinantal equation. In Figs.1 and 2, we represent the

critical line of antiferromagnetic-paramagnetic surface transitions (S). the steps described before are not sufficient to obtain the remaining part of the phase diagram. In fact, the three dimensional ferromagnet with antiferromagnetic surface, any two nearest neighbours of the surface interact via an antiferromagntic coupling. At the ground state of the Hamiltonian (1) (with $p_s = 1, \Omega_S = \Omega_B = 0$), the surface makes a first-order transition from an antiferromagnetically order state for R > 1/4 to a ferromagnetically ordered state for R<1/4. In order to obtain to rest of phases and transitions, we must to solve numerically the couple equations (15)-(17) within the four-layer approximation scheme. The analysis of the above equations permits us to determine the whole phase diagrams of the system. Indeed, let us first examine the effect of the surface transverse field on the surface ordering in the pure three-dimensional semi-infinite transverse Ising model. The phase diagrams, in the (K_B T / J_B , J_S /J_B) plane is represented in Fig.1 for two selected values of the bulk transverse field (Ω_B = 0, Ω_B =1.5 J_B). It shows the influence of Ω_S on the surface transitions. If the ratio *R* is greater than a critical value R_c , the surface may order antiferromagnetically at a temperature higher than the bulk. We mention that surface transition temperature and R_c depend on the value of Ω_S .

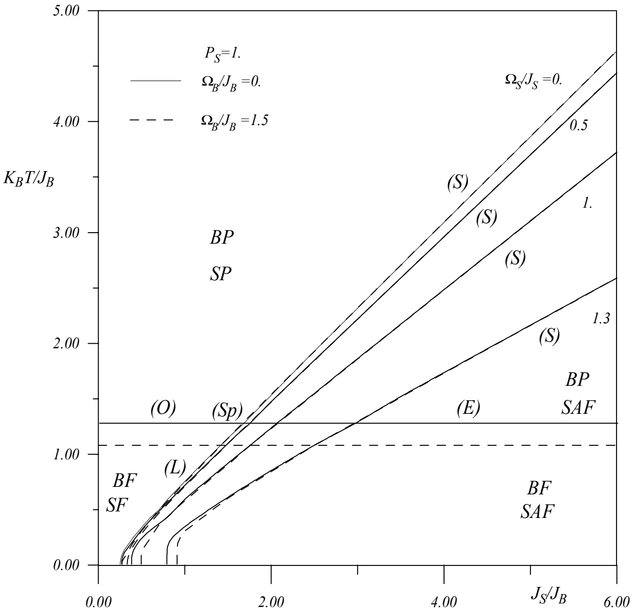

FIG.1. The phase diagram in (K_B T / J_B , J_S /J_B) plane, in the case of pure system *(p_s=1)* , with Ω_B / J_B = 0 (solid lines) and Ω_B / J_B = 1.5 (dashed lines). The number accompanying each curve denotes the value of Ω_S / J_S.

In Fig.2, we show the effects of diluted surface on the pure system behaviour *(P_S = 1)*.

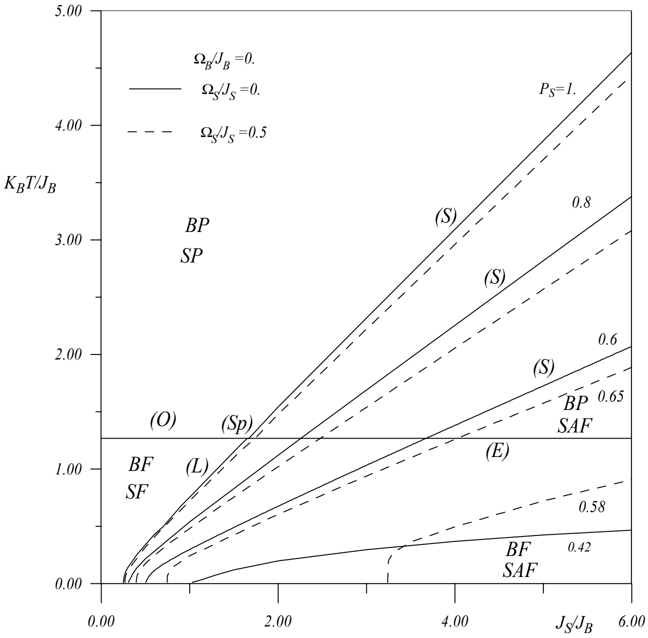

FIG.2. The phase diagram in (K_B T / J_B , J_S /J_B) plane, with Ω_S / J_S = 0, Ω_B / J_B = 0 (solid lines) and Ω_S / J_S= 0.5, Ω_B / J_B = 0 (dashed lines). The number accompanying each curve denotes the value of p_s.

Thus, some surface transition lines corresponding to various values of p_S are plotted. As clearly seen from the obtained phase diagrams, we note that for a given value of Ω_S and the ratio R = J_S / J_B (greater than 1/4), the surface critical temperature decreases with p_S , and therefore, the domain where the surface is ordered becomes less an less large when the concentration of the antiferromagnetic bonds decreases. As shown in Figs.1 and 2, four physically different phases are identified. These phases are indicated on the phase diagrams by the following symbols.

SF , BF: surface and bulk are ferromagnetic; SP,BP: surface and bulk are paramagnetic; SAF , BP: Surface antiferromagnetic and bulk paramagnetic; SAF , BF: Surface antiferromagnetic and bulk ferromagnetic. For the system under study, we extend the accepted terminology used in the classical semi-infinite Ising systems with no competing interaction[3,15,4,35]. As is seen from Figs.1 and 2, the above phases are separated by different transition lines. Among them, we find all critical lines obtained in the semi-infinite simple cubic ferromagnetic Ising model[8,14,15]. They correspond to the surface (S), the ordinary (O), the extraordinary (E), special (Sp). When the bulk is ferromagnetically ordered, the surface exhibits, at finite temperature, a second-order transition (L) from the ferromagnetic phase (SF,BF) to the antiferromagnetic

phase (BF,SAF). Moreover, we note the existence of critical value p_S^* of p_S (p_S^* =0.424) which depends on the surface transverse field strength. For $p_c < p_S \le p_S^*$ (p_c=0.393 is the percolation threshold), the (SAF,BP) phase disappear for any value of R. In Fig.3, we present the critical ratio R_c as a function of p_S when Ω_B/J_B =0 and 1.5 for different values of Ω_S/J_S.

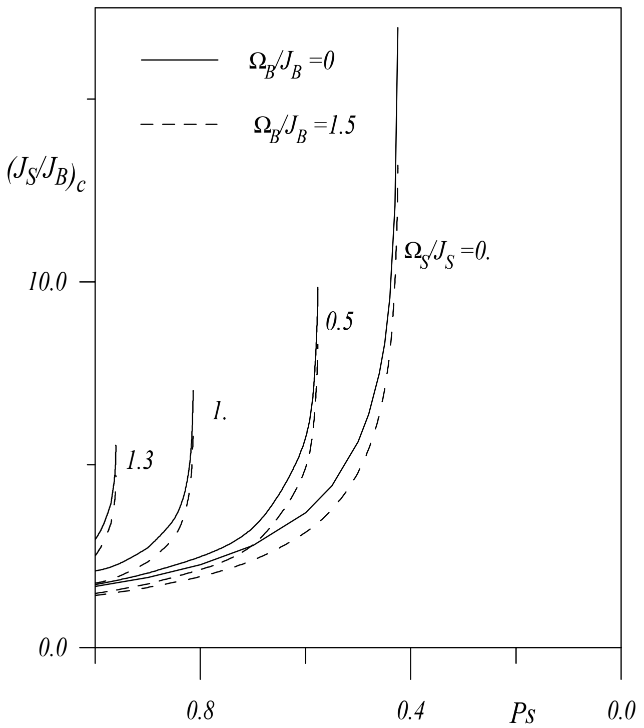

FIG.3. The dependence of the critical ratio of exchange interactions $(J_S / J_B)_C$ as a function of the surface dilution parameter p_S, with $\Omega_B / J_B = 0$ (solid lines) and $\Omega_B / J_B = 1.5$ (dashed lines). The number accompanying each curve denotes the value of Ω_S / J_S, .

We notice that for a given value of Ω_S / J_S, and p_S close to 1, the critical ratio R $_C$= $(J_S / J_B)_C$ increases weakly with decreasing p_S ; while it varies rapidly with p_S when this latter approaches to p_S^*. As seen from this figure, there is no critical exchange interaction strength ratio R_c, when $p_S \le p_S^*$. This means that there isno surface , extraordinary and special transition and therefore the phase (SAF,BP) disappears. The dependence of the critical value p_S^* with the surface transverse field is presented in Fig 4

As it can be expected, the critical value p_S^* decreases with increasing Ω_S/J_S . It is worthy of notice here that the variation of p_S^* with Ω_S/J_S is nearly independ of the bulk transverse field.

IV. CONCLUSION

In this work, we have studied the surface phase transitions in semi-infinite spin-1/2 transverse Ising model, where the antiferromagnetic exchange interactions at the surface is randomly distributed and having aconcentration p_s. The competing surface and bulk exchange interactions are denoted by J_S and J_B ,

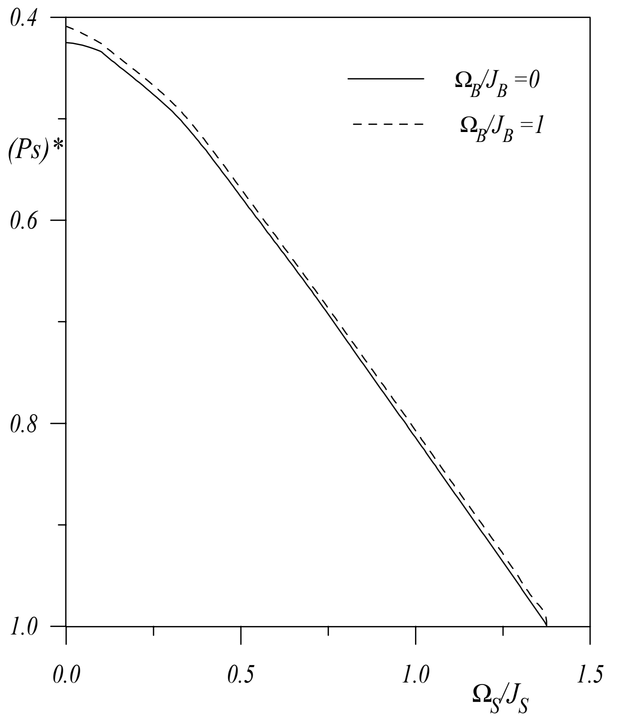

FIG.4. The variation of critical value p_S^* with the surface transverse field Ω_S / J_S, with $\Omega_B / J_B = 0$ (solid line) and Ω_B / J_B =1

respectively. To do this, we have used an effective field method within the framework of a single-site cluster theory. Let us summarize by stating the main results of this investigation. We identified four physically different phases. When the bulk is disordered (BP), if the ratio $R = (J_S/J_B)$ is greater than a critical value R_c, the surface may antiferromagntically order at a temperature higher than bulk. When the bulk is ferromagnetically ordered (BF), the surface may undergo, at finite temperature, second-order transition (L) from ferromagnetic order (SF) to the antiferromagnetic one (SAF).

Finally, the effects of the surface transverse field, and the dilution parameter on the surface ordering have been investigated and some characteristic behaviours for the surface have been found. In particular, the existence of critical value p_S^* of p_S, indicating two qualitatively

different behaviour of the surface which depend on the range of p_S. Thus for $p_S^* < p_S \leq 1$, the system exhibits five different phase transitions cited in section III. But for $p_c < p_S < p_S^*$, the phase where the surface antiferromagnetic and bulk paramagnetic disappears for any value of the ratio R; which means that the extraordinary phase transition does not exist in this range of p_S.

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