Magnetic properties of mixed spin Ising system with modified surface-bulk coupling: Monte Carlo treatment

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A Monte Carlo simulation is used to study the three dimensional mixed spin-$\frac{1}{2}$ and spin-1 Ising model with intrasurface J_S and surface-bulk $J_\perp$ interactions modified with respect to the bulk exchange interaction J_B. In this investigation, the new parameter $J_\perp$ strongly affects the phase diagram obtained in the case $J_\perp = J_B$. We have found three types of phase diagrams which show some qualitatively interesting features, i.e. variety of phase transitions and multicritical points. One of the most qualitatively interesting features of the surface is the existence of two possible ferrimagnetic orderings, when the ratio $R_1 = J_\perp/J_B$ belongs to an appropriate range. A compensation point in the surface magnetization is found when the ratio of the surface and bulk exchange interactions belong to certain ranges. This phenomenon may have important applications in technology such as thermodynamic writing and erasing at the compensation point. Comparison between Monte Carlo results and those obtained by mean field theory is also made.
Keyword: xed spin; Surface magnetism; Monte Carlo simulation; Phase diagrams; Magnetizations; Compensation points.
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I. INTRODUCTION

Surface magnetism is a subject that presents great richness from the theoretical and experimental standpoints due to its important technological applications. The magnetic ordering and critical behaviour at surfaces are expected to be different from those of the bulk materials due to the different coordination number and symmetry of the atoms at the surface. Indeed, both theoretical perdictions [1, 2] and experimental observations suggest surface magnetic behavior different from the bulk [3-5]. These effects have been modeled, by the spin-$\frac{1}{2}$ semi-infinite simple cubic Ising ferromagnet with intrasurface exchange interaction J_S different from the bulk value J_B. It has been extensively studied using a variety of techniques such as mean-field theory [6, 7], and Monte Carlo techniques [9, 10].

In recent years, some interest has developed in the study of the semi-infinite simple cubic consisting of two sublattices of spin-$\frac{1}{2}$ and spin-1 Ising alloy with a free $(1, 0, 0)$ surface. It has been studied using effective-field theory with correlations [16, 17] and the real-space renormalization-group method [18]. Attention has been devoted to the case where the two exchange interactions, J_S on the surface and J_B in the bulk, are both positive (or negative). In this case, the only possible states of the surface and bulk are paramagnetic and ferromagnetic (or ferrimagnetic) ordering. Recently, attention has been devoted to the case of the Ising ferromagnet ($J_B > 0$) with a ferrimagnetic surface exchange interaction ($J_S < 0$) and a surface anisotropy perpendicular to the surface. Such systems may describe a variety of magnetic materials, such as thin films of rare-earth-transition-metal alloys which are important from the technological point of view, because of the large magnetic anisotropy perpendicular to the film plane and their magneto-optic applications. This system has been investigated [19, 20] by one of us (N.B.), using the finite cluster approximation (FCA). However, a modified surface-bulk coupling has to be considered since it describes a more realistic situation. We expect that it has important influences on the surface magnetic behaviours.

The purpose of this work is to investigate such a system on a simple cubic lattice. In particular, we examine the influence of the surface-bulk coupling ($J_\perp$) on the surface phase diagram and the magnetic properties obtained in the case $J_\perp = J_B$ [19, 20] . In our analysis we use the Monte Carlo (MC) technique [21] and compare the simulation results with those of mean field theory (MFT).

The outline of the paper is as follows: In Section 2 we briefly describe the model and review the basic points of the Monte Carlo approach and the mean field theory. In Section 3, we investigate the phase daigrams and we present our concluding remarks in Section 4.

II. MODEL AND METHODS

We consider a semi-infinite simple-cubic two sublattices spin-$\frac{1}{2}$ and spin-1 mixed Ising system, with three exchange interactions between nearest-neighbours namely: $-J_S(J_S > 0)$ if spins lie in the free surface, $J_\perp(J_\perp > 0)$ between the surface and second layer spins, and $J_B(J_B > 0)$ otherwise. The Hamiltonian of our system takes the form:

$$\mathcal{H} = J_S \sum_{<ij>} \sigma_i S_j - J_\perp \sum_{<il>} \sigma_i S_l - J_B \sum_{<kl>} \sigma_k S_l, \quad (1)$$

where S takes the values ± 1 and 0, σ can be $+\frac{1}{2}$ or $-\frac{1}{2}$. The first is carried out over nearest-neighbour sites

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located on the free surface. The second summation is carried out over nearest-neighbour sites, one located on the free surface and the other on the second layer. The third summation runs over all pairs of remaining nearest-neighbour sites.
Our three-dimensional $L\times L\times L$ simple cubic lattice contains $L\times L$ spins at the surface and $L\times L\times(L-1)$ spins in the bulk. We use the well-known Metropolis standard single-spin-flip Monte Carlo algorithm [22] with periodic boundary conditions in the two perpendicular directions of the surface and free condition in the other.
In this work, data were generated with 25000 MCS, after discarding the first 5000 steps, for linear lattice size $L=30$ spins. The magnetization M of a configuration is defined by the summation over the all spin values of the lattice sites. In order to determine the phase boundaries, we use the fluctuations of the internal energy E and the magnetization M.
On the other hand, in the framework of the well known mean-field theory, we limit our selves to give the state equations for each layer as

$$\mu_S = \frac{1}{2}tanh[\frac{1}{2}(-4K_S m_S + K_\perp m_1)], \qquad (2)$$

$$m_S = \frac{2sinh[-4K_S\mu_S + K_\perp \mu_1]}{2cosh[-4K_S\mu_S + K_\perp\mu_1]+1}, \qquad (3)$$

$$\mu_n = \frac{1}{2}tanh[\frac{K_B}{2}(4m_n + m_{(n+1)} + \epsilon_n m_{(n-1)})], \qquad (4)$$

$$m_n = \frac{2sinh[K_B(4\mu_n + \mu_{(n+1)} + \epsilon_n\mu_{(n-1)})]}{2cosh[K_B(4\mu_n + \mu_{(n+1)} + \epsilon_n\mu_{(n-1)})]+1}, \qquad (5)$$

where $K_B=\beta J_B$, $K_S=\beta J_S$,$K_\perp=\beta J_\perp$,$\beta=(k_BT)^{-1}$ and ϵ_n takes the value $K_\perp/K_B$ for $n=1$ and 1 otherwise. $\mu_S(m_S)$ and $\mu_n(m_n)$ are the $\sigma(S)$-sublattice magnetizations respectively for the surface and the n^{th} layer. The bulk magnetizations μ_B and m_B are determinated by setting in Eqs. (4) and (5) $\mu_{n-1}=\mu_n=\mu_{n+1}=\mu_B$ and $m_{n-1}=m_n=m_{n+1}=m_B$. So, μ_B and m_B are given by

$$\mu_B = \frac{1}{2}tanh[3K_Bm_B] \quad , \quad m_B = \frac{2sinh[6K_B\mu_B]}{2cosh[6K_B\mu_B]+1} \qquad (6)$$

III. PHASE DIAGRAMS AND DISCUSSIONS

We are first concerned with the evaluation of the order-disorder reduced transition temperatures K_B^C and K_S^C respectively for the bulk and surface orderings. In the framework of MC simulation, they are determined from remarkably pronounced picks in the bulk and surface magnetic susceptibilities. The MC value of K_B^C is 0.526, to be compared with the MFA result 0.408. We notice that for $J_\perp=J_B=0$, our system reduces to the two-dimensional mixed spin-1/2 and spin-1 Ising model. The MC value of the reduced critical temperature K_S^C is 1.025 which is very close to 1.026 obtained from the high-temperature series expansion [12] and a previous Monte Carlo simulation [15]. In Figs.1 obtained by MC simulation for various values of $R_1=J_\perp/J_B$, we represent the second-order phase boundary of ferrimagnetic-paramagnetic surface transition (S) obtained for $K_B\leq K_B^C$. As seen from these figures, if the ratio $R=J_S/J_B$ is greater than a critical value R_C, the surface may ferrimagnetically order at a temperature$(K_S^C)^{-1}$ higher than the bulk. K_S^C and R_C depend on the value of R_1 . In particular, for $R_1=1$ ($J_\perp=J_B$), the MC critical value of R_C is 1.939 to be compared with the mean-field result 1.474.
The remaining part of the phase diagrams ($K_B\geq K_B^C$) shows other surface transitions. Indeed, any two nearest neighbours on the surface interact via a ferrimagnetic coupling. At the ground state of the Hamiltonian (1), the surface makes a first-order transition from a ferrimagnetically ordered state for $R>R_1/4$ to a ferromagnetically ordered state for $R<R_1/4$. In fact, the analysis of this area ($K_B\geq K_B^C$) of the phase diagram leads to very interesting surface phenomena. The surface behaviours and their dependencies on the ratio R_1 are shown in the Figs.1a-c obtained by MC simulation for various values of R_1. We observe three types of phase diagram, depending on the value of R_1. For R_1 less than a critical value $R_1^c=2.802$ (Figs.1a,b), to be compared with the MFT result 4.152, five physically different phases are identified. These phases are indi-

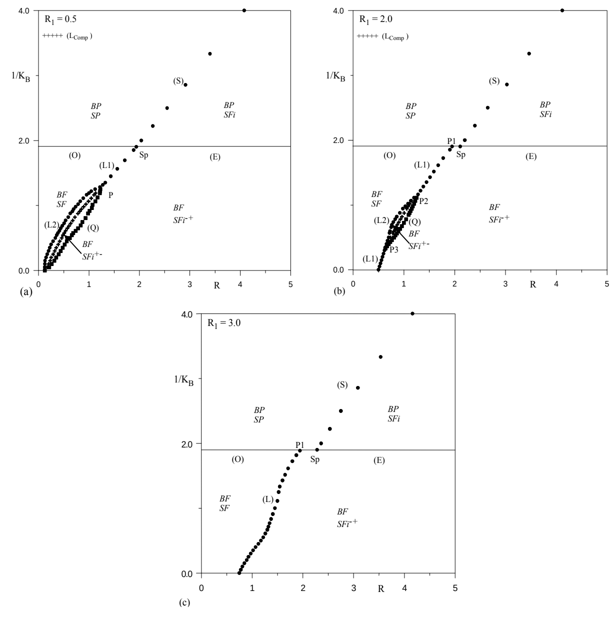

FIG. 1: The phase diagrams of MC in the $K_B^{-1}-R$ plane for various values of R_1.

cated on the phase diagrams by the following symbols : SP, BP, surface and bulk are paramagnetic; SF, BF, surface and bulk are ferromagnetic; SFi, BP, surface ferrimagnetic and bulk paramagnetic; SF_i^{-+}, BF, surface ferrimagnetic and bulk ferromagnetic with $\mu_S < 0$ and $m_S > 0$; and SF_i^{+-}, BF, surface ferrimagnetic and bulk ferromagnetic with $\mu_S > 0$ and $m_S < 0$. As is also seen from the figures, 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 [8,10,11]. They correspond to the surface (S), the extraordinary (E), the ordinary (O) and the special (SP) transitions. One of the most interesting feature of the surface is the existence of two possible ferrimagnetic ordering $(SF_i^{+-} and SF_i^{-+})$, which are separated by a first order transition line (Q) found in a previous results [19, 20] obtained for $R_1 = 1(J_\perp = J_B)$. In this case, the surface and the bulk order ferromagnetically at $(K_B^C)^{-1}$ for appropriate values of R. And at a lower temperature, the surface undergoes a second-order transition $(L1 \cup L2)$ from the ferromagnetically ordered state (SF) to the ferrimagnetically ordered state. The kind of this ferrimagnetic order depends on the ratios R and R_1. The first type of the phase diagram corresponds to $0 < R_1 < 1$, the obtained phase diagram is qualitatively similar to that found for $R_1 = 1$(see Fig.1.a), noting that the domain of $BFSF_i^{+-}$ phase becomes wider for decreasing values of the surface-bulk interaction. The second type of phase diagram is shown (Fig.1.b) for $1 < R < R_1^c$. The domain and the location of SF_i^{+-} is qualitatively and quantitatively different from case $0 < R_1 \leq 1$. In particular, the domain of SF_i^{+-} becomes more and more narrow when R_1 approaches to R_1^c. Further, this phase disappears at very low temperatures, giving rise to an other multicritical point P_3. As we can note from Fig.1.b, the transition lines (S) and (L1) does not meet at the special point (S_P) (which is the case for $R_1 = 1$). Therefore, and in contrast with $R_1 = 1$ case, the system can exhibit a transition from $BPSP$ phase to $BFSF_i^{-+}$ phase when the ratio R belongs to an appropriate range. The third type of phase diagram is obtained for $R_1 > R_1^c$. In this case, the phase $SF_i^{+-}BF$ totally disappears as indicated in Figs.1.c, for $R_1 = 3.0$. As is seen from this Figure, we have four phases instead of five. The two lines (L2) and (Q) disappear and therefore the surface undergoes a second-order transition from ferromagnetic state SF to the unique ferrimagnetic state SF_i^{-+}. Here again, the system can exhibit a transition from $BPSP$ phase to $BFSF_i^{-+}$ for appropriate range of the ratio R. We also point out that for $R < R_1/4$ (for any R_1), the bulk promotes its order to the surface in such a way that the bulk and the surface are both paramagnetic and ferromagnetic for $K_B < K_B^C$ and $K_B > K_B^C$, respectively.

It is worthy of notice here that when the system is in $BFSF_i^{+-}$ phase, it presents an important phenomenon; namely the total magnetization $M_S = (\mu_S + m_S)/2$ vanishes while the two-sublattice magnetizations are nonzero. This indicates that the system exhibits a compensation points. Their location L_{Comp} (when they exist) are plotted in Figs.1.a,b.

Finally, using Eqs.(2-6), we have investigated the phase diagram of the system described by the Hamiltonian (1) within the mean-field theory. We have found only two types of phase diagrams according to the value of the surface-bulk interaction. These phase diagrams are plotted in Fig.2.a and Fig.2.b which correspond respectively to values of R_1 less and greater than $R_1^c = 4.152$. Thus, the mean-field approximation does not expect a phase diagram like that one obtained by our MC simulation shown in Fig.1.b.

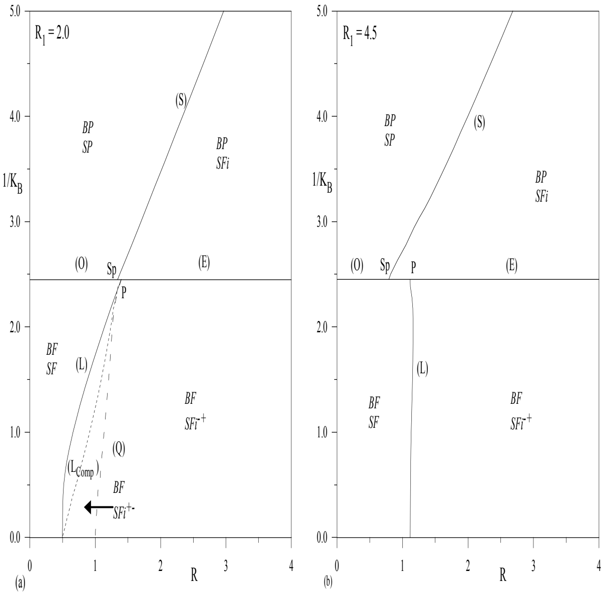

FIG. 2: The phase diagrams of MFT in the $K_B^{-1} - R$ plane for various values of R_1

IV. CONCLUSION

In this work we have studied the semi-infinite simple cubic Ising system with intrasurface and surface-bulk exchange interactions modified with respect to the bulk exchange interaction. The three types of phase diagrams, obtained by the Monte Carlo simulation show very interesting features. In particular, the system exhibits various phase transitions and multicritical points. Indeed, one of the most qualitatively interesting features of the surface is the existence of two possible ferrimagnetic orderings $SF_i^{+-}BF$ and $SF_i^{-+}BF$ when the surface-bulk and bulk interactions ratio R_1 is less than a critical value R_1^c. For $R_1 > R_1^c$, the phase $BFSF_i^{+-}$ completely disappears from the phase diagram. On the other hand, a compensation points in the surface are found when the ratios R and R_1 belong to certain ranges. This phenomenon may have important applications in technology such as thermodynamic writing and erasing at the compensation

point.
The phase diagram of the system have also been investigated using the mean-field theory. This latter predicts only two types of phase diagrams, which differs from the MC types throw the second one where the phase $BFSF_i^{+-}$ does not exist at very low temperatures.

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