Phase diagrams of site diluted ferromagnetic semi infinite system

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The spin correlations functions of face-centered cubic semi-infinite system are investigated by using the high temperature series expansions extrapolated with the Padé approximant method for Heisenberg, XY and Ising models. The magnetic phase diagrams $\tau_c(\nu)$ versus the dilution x are obtained. The value obtained of the percolation threshold is $x_p \approx 0.2$. The x_p is defined as the concentration at which $\tau_c = 0$.

Keywords: Correlation functions; Semi-infinite film; Magnetic phase diagrams; Percolation threshold.

I. INTRODUCTION

Laosiritaworn and al [1] have used Monte-Carlo simulations and mean filed analysis to study the magnetic behavior of Ising thin film with cubic lattice structures as a function of temperature and thickness, especially in the critical region. It is finding that the magnetic behavior changes from the two-dimensional to three dimensional characters with increasing film thickness. Amazonas and al [2] have studied the influence of the lattice structure on the Curie temperature of a thin quantum spin $1/2$ Heisenberg film by using the varaitional principles of the mean field approximation and Oubelkacem and al [3] have investigated the tricritical behavior of the classical three dimensional Heisenberg model of spin ½ in a random field. In this work, we have applied the high temperature series expansions (HTSE) extrapolated with the Padé (PA) approximant method to the correlation functions of the semi infinite system. The three first correlation functions between spins at surface and between spin at the surface and in the nearest neighbor layer have been obtained. The magnetic phase diagrams, i.e. the reduced critical temperature $\tau_c(\nu)$ versus the dilution x, for the three models: Ising, XY and Heisenberg. The threshold percolations of the surface and the neighbored layers are deduced.

II. METHOD AND FORMALISM:

The theoretical method used in this study has been developed in previous papers [4, 5]. Here we only give a brief description of the essentials of the method. We consider a semi-infinite system with face-centered cubic lattice symmetry. The exchange coupling between spins at sites i and j takes the value J_s if both spins are nearest neighbors within the surface, $J_\perp$ if it is between a spin on the surface and its nearest - neighbor in the next layer, and the value J_b for nearest-neighbor interactions within the bulk. Starting with zero-field Heisenberg Hamiltonian:

$$H = -2\sum_{ij} J_{ij}\vec{S}_i.\vec{S}_j \qquad (1)$$

where the summation runs over all pairs of nearest-neighbor pair interactions. The strength of J_{ij} is assumed to be positive (ferromagnetic interactions). $\vec{S}_i$ is the operator of spin at site i of length $\bar{S}$, where $\bar{S}^2 = S(S+1)$. The correlation functions between spins at sites i and j, in powers of β [6]:

$$\gamma_{ij} = \langle \vec{S}_i\vec{S}_j \rangle = \sum_{l=0}^{\infty} \frac{(-1)^l}{l!}\alpha_l \beta^l \qquad (2)$$

where $\beta = \dfrac{1}{k_B T}$ and k_B being the Boltzmann constant.

In our case, we have to deal with nearest-neighbor coupling J_{ij}. The coefficient α_l may be expressed for each topological graph as [6]:

$$\alpha_l = \bar{S}^2(-2\bar{S}^2)^l (J_{ik_1}^{m_1} J_{k_2k_3}^{m_2} ... J_{k_wj}^{m_\nu})[\alpha_l] \qquad (3)$$

with the condition $\sum_{r=1}^{\nu} m_r = l$ for $m_r = 0,1,....,l$. The ‘‘weight’’ $[\alpha_l]$ of each graph is tabulated and given in Ref. [6] and $k_1, k_2, ..., k_w$ represent the sites surrounding the sites i and j. Here HTSE method is developed for the magnetic correlation function γ_{ij} with arbitrary exchange

interaction couplings J_S, J_b and $J_\perp$, up to order 6 in β. For the semi-infinite system with centered face cubic structure, we obtain the following function:

$$\gamma_{ij} = \sum_{n=1}^{6}\left(\sum_{p=0}^{n}\sum_{q=0}^{n} a(p,q,n) R_1^p R_2^q\right)\tau^{-n} \qquad (4)$$

Where $R_1 = \frac{J_\perp}{J_b}$, $R_2 = \frac{J_s}{J_b}$,

$\tau_c(\nu) = \frac{k_B T_c}{2S(S+1)J_b}$ and the condition $p+q \le n$.

The non zero coefficients $a(p,q,n)$ are computed till order $n = 6$, for the case of two sites situated at the surface $(L=0)$ and two sites situated in the nearest neighbor layer $(L=1)$ and are available on request. The coefficients of Ising and XY models are deducted by a transformation of the coefficients of Heisenberg model given in [7]. The values of $[\alpha_l]$ (Eq. (3)) depend only on the dimension ν of the spin (i.e.: $\nu = 1$ for Ising type, $\nu = 2$ for XY type and $\nu = 3$ for Heisenberg type). We use the well-known *Padé* approximants method [8] to estimate the critical reduced temperature $\tau_c(\nu)$. In this method, the reduced critical temperature $\tau_c(\nu)$ is determinate by locating the singularity in the *Padé* approximants to the HTSE of the correlation functions. In order to study the effect of dilution of magnetic ions by non magnetic ones, we introduce a ratio of dilution x in the system. To introduce the dilution x in the correlation function expressions, we adopt a distribution function of bonds J_i^{np} ($i = s$, $\perp$ or b denotes the interactions in the surface, between the surface and the nearest-neighbor layer and in the bulk). The interaction is between the nearest-neighbor site n and p. The probability distribution is:

$$P(J_i^{np}) = x\delta(\sigma_n - 1)[x\delta(J^{np} - J_i) + (1-x)\delta(J^{np})] \qquad (5)$$

n is considered as the central magnetic site. If $\sigma_n = 1$ there is an interaction of type J_i whenever the p site is occupied by a magnetic ion. If $\sigma_n = 0$ the central site is unoccupied, thus there is not contribution. The obtained results in the case of a face centered cubic structure are:

$$J_s(x) = (x^5 - 3x^4 + 3x^3)J_s .$$

$$J_b(x) = (210x^{13} - 1386x^{12} + 3850x^{11} - 5775x^{10} + 4950x^9 - 2310x^8 + 462x^7)J_b$$

$$J_\perp(x) = (x^5 - 3x^4 + 3x^3)J_\perp \qquad (6)$$

III. DISCUSSIONS AND CONCLUSION:

We have studied the variation of the reduced critical temperature $\tau(\nu) = \frac{k_B T(\nu)}{2S(S+1)J_b}$ with the ratio of exchange interactions R_1 and R_2 for a semi-infinite system with face centered cubic structure the three models: Ising (I), XY and Heisenberg (H). $\tau_c(\nu)$ is determinate from the divergence of the correlation functions. *Figure 1* shows the variations of $\tau_c(\nu)$ with R_2 in the surface $(L=0)$ and in the neighbored layer $(L=1)$ for $R_1 = 1$. We see that for a given model the curves intersect at the abscises $R_2^c(I) = 0.817$, $R_2^c(XY) = 0.819$, $R_2^c(H) = 0.823$ and ordinate point : $\tau_c(I) = 4.790$, $\tau_c(XY) = 2.386$ and $\tau_c(H) = 1.594$. At R_2^C, $\tau_c(\nu)$ is independent of the localisation of the spins and becomes similar to three-dimensional infinite system. R_2^c is the special point corresponding to the separation between the ordinary and the extraordinary transitions.

We have also studied the magnetic phase diagrams, i.e. $\tau_c(\nu)$ versus the dilution x. The obtained results are given in *figures.2* and *3*. We note that $\tau_c(\nu)$ decreases with x and vanishes at the percolation point x_p. The obtained values of x_p in the surface for $R_1 = 1$, is 0.27 and in the neighbored layer of the surface is 0.22.

From these results one can see that the reduced critical temperature, for the three models, of the surface is greater than that of the neighbored layer.

Our results obtained by HTSE, in the case of Ising model, are situated between previous studies based effective field theory [10] and Monte Carlo simulation [1] (see table 1)

$\frac{K_B T_c}{J_b}$ present work	$\frac{K_B T_c}{J_b}$
7.18	9.86 [1] 5.73 [10]

Table1: Values of $\frac{K_B T_c}{J_b}$ by different models.

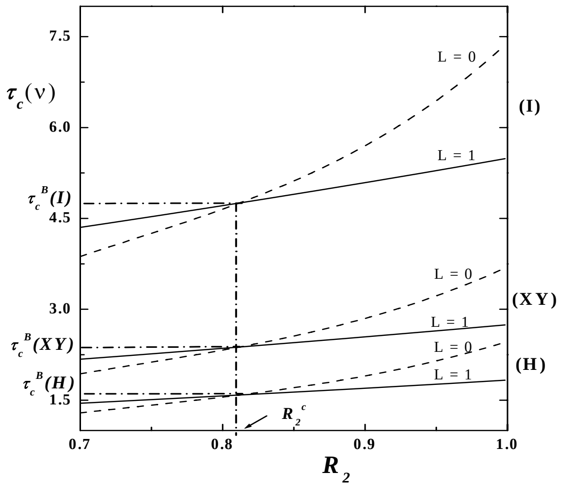

FIG. 1 : The reduced critical temperature $\tau_c(\nu)$ as a function of the ratio R_2 (for the case of $R_1 = 1$) for Ising, XY and Heisenberg models. L=0 corresponds to surface, L=1 corresponds to the neighbored layer.

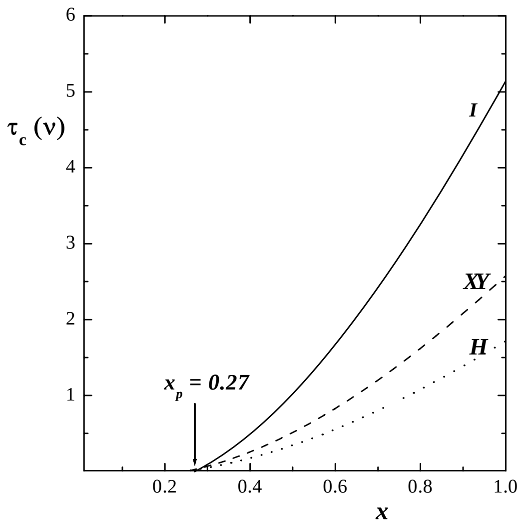

FIG. 2: Phase diagram, $\tau_c(\nu)$ versus dilution x, for the three models: Ising (I), XY and Heisenberg (H), for $R_1 = 1$ and $R_2 = 0.85 \approx R_2^c$ of the surface.

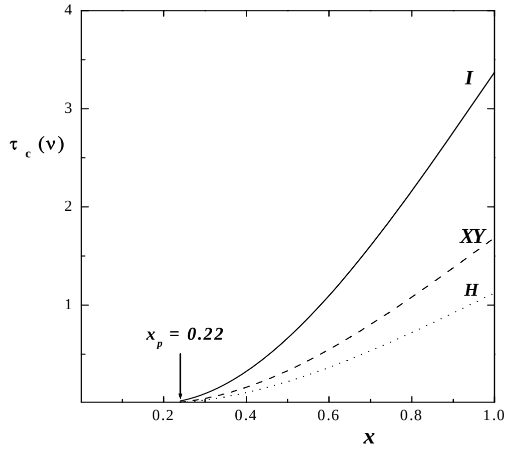

FIG. 3: Phase diagram $\tau_c(\nu)$ versus dilution x for the three models: Ising (I), XY and Heisenberg (H), for $R_1 = 1$ and $R_2 = 0.6$ of the surface.

Acknowledgements
This study is a part of the PROTARS III D12/10.

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