Phase diagrams of site diluted semi infinite ferromagnetic film

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The magnetic susceptibility of a semi-infinite ferromagnetic films with a simple cubic lattice and the face centered cubic lattice is investigated by the method of exact high-temperature series expansions (HTSE) extrapolated with the Padé approximants method for Heisenberg, XY and Ising models. The magnetic phase diagrams in ($\tau_c(\nu), x$) plane are obtained. The value of the percolation threshold x_p is obtained. The x_p is defined at which $\tau_c = 0$.

Keywords: magnetic susceptibility; semi-infinite film; magnetic phase diagrams; percolation threshold.

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I. Introduction

Recently, the study of magnetic multilayer has attracted considerable attention and has been stimulated by recent technological progresses. In particular, modern high-vacuum techniques, such as the epitaxial growth ones, allow us to fabricate very thin magnetic films of controllable thickness [1] The increasing technological importance of manometer scaled magnets results from the general trend of miniaturization in technical applications. These interesting magnetic properties of magnets on a nanometer scale provide both interesting opportunities for technology and questions for basic research. On the other hand, from both the experimental and theoretical points of view, one particularly important phenomenon is the dependence of the transition temperature with respect to several parameters, such as the film thickness (L), the geometrical structure or the composition of the film and magnetic excitation. Amazonas and al [2] have studied the influence of the lattice structure on the Curie temperature of a thin quantum spin ½ Heisenberg film by using the varaitional principles of the mean field approximation and Oubelkacem and al [3] have investigated the tricritical behaviour of the classical three dimensional Heisenberg model of spin ½ in a random field. The surface magnetic behaviour of a semi infinite Ising model with a spin one free surface is studied by [4]. The Laosiritaworn and al [5] have used Monte-Carlo simulations and mean filed analysis to observe the magnetic behaviour of Ising thin film with a cubic lattice structures as a function of temperature and thickness, especially in the critical region. It is finding that the magnetic behaviour changes from the two-dimensional to three dimensional characters with increasing film thickness. The Benayad and al [6] have used the Monte Carlo treatment to study the magnetic properties of mixed spin Ising system with modified surface-bulk coupling. In this work, we have applied the HTSE and the Padé approximant [7] to the magnetic susceptibility in the surface and layer nearest neighbour to the surface (bulk) to determinate the reduced critical temperature versus the R_2 ($R_2 = \frac{J_s}{J_b}, J_b$ is the exchange interactions in the bulk and J_s in the surface) and the magnetic phase diagrams in ($\tau_c(\nu), x$) plane for two structure and for the three models: Ising, XY and Heisenberg. The threshold percolations in the surface and in the bulk are deduced.

II. Theoretical method

The theoretical method used in this study has been developed in previous papers [8,9]; here we only give a brief description of the essentials of the method. We consider a semi-infinites ferromagnets Heisenberg, Ising and XY films with a simple cubic lattice and face centred cubic lattice. The exchange coupling between spins at sites i and j takes the value J_s if both spins are nearest neighbours within the surface layers, $J_\perp$ if it is between a spin on the surface and its nearest-neighbour in the next layer, and the value J_b, for nearest-neighbour 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-neighbour pair interactions. The strength of the J_{ij} is assumed to be positive (ferromagnetic). $\vec{S}_i$ is the operator of spin at site i of length $\vec{S}$, where $\bar{S}^2 = S(S+1)$. The correlation functions between spins at sites i and j, in powers of β [10]:

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

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

In our case, we have to deal with nearest-neighbour coupling J_{ij}. The coefficient α_l may be expressed for each topological graph as [11]:

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

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. [12] and $k_1, k_2, ..., k_w$ represent the sites surrounding the sites i and j. Here HTSE method is developed for the magnetic susceptibility $\chi(T)$ with arbitrary exchange interaction couplings J_S, J_b and $J_\perp$, up to order 6 in β. For the simple cubic and face centred cubic lattice ferromagnetic semi-infinite film, we obtain the following function:

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

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 with the condition $p + q \leq n$.

The nonzero coefficients $a(p,q,n)$ are computed till order $n = 6$, for two cases: first case magnetic susceptibility in the surface $\chi(L=0)$ and in the bulk $\chi(L=1)$ is available on request for two structures for the Heisenberg model. The coefficients of Ising and XY models are deducted by the transformation of the coefficients of Heisenberg model, using [12]. The values of $[\alpha_l]$ (Eq. (3)) are depending only on the dimension ν of the spin (i.e.: $\nu = I$ for Ising type, $\nu = XY$ for XY type and $\nu = H$ for the Heisenberg type). We use the well-known *Padé* approximants method [13] to estimate the reduced critical 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 magnetic susceptibility in the surface $\chi(L=0)$. To introduce the dilution x in the magnetic susceptibility at the surface $\chi(L=0)$, 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-neighbour layer and in the bulk. The interaction is between the nearest-neighbour 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 no contribution. The obtained results for the simple cubic lattice (see reference [14]) are:

$$J_s(x) = (x^5 - 3x^4 + 3x^3)J_s .$$
$$J_b(x) = (-4x^7 + 15x^6 - 20x^5 + 10x^4)J_b . \qquad (6)$$
$$J_\perp(x) = xJ_\perp .$$

and the obtained results of the face centered cubic lattice are:

$$J_s(x) = (x^5 - 3x^4 + 3x^3)J_s .$$
$$J_b(x) = (210x^{13} - 1386x^{12} + 3850x^{11} - 5775x^{10} + 4950x^9 - 2310x^8 + 462x^7)J_b \qquad (7)$$
$$J_\perp(x) = (x^5 - 3x^4 + 3x^3)J_\perp$$

III. Discussions and conclusions:

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 interaction R_1 and R_2 for semi-infinite film with a simple cubic lattice and face centered cubic lattice of for different film thickness. $\tau_c(\nu)$ is determinate from the divergence of the magnetic susceptibility in the surface $\chi(L=0)$. For

example *Figs* 1 and 2 shows the variations of $\tau_c(\nu)$ with R_2 for $L=0$ and $L=1$ with $R_1 = R_2$ for Heisenberg model.

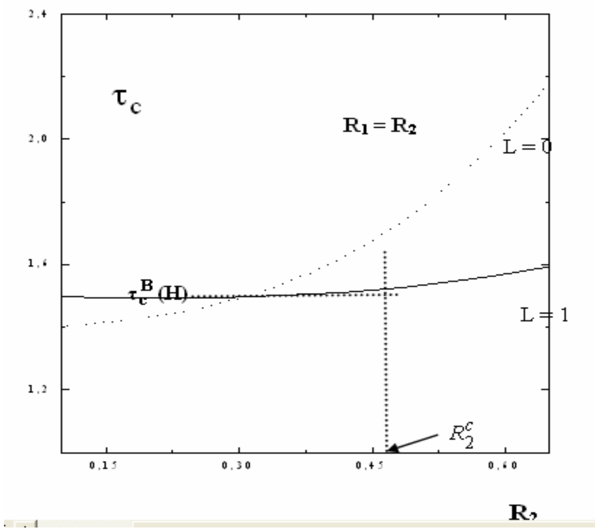

Fig. 1: The reduced critical temperature τ_c as a function of the ratio R_2 in the case of the simple cubic lattice (for the case where $R_1 = R_2$) for Heisenberg model (H).

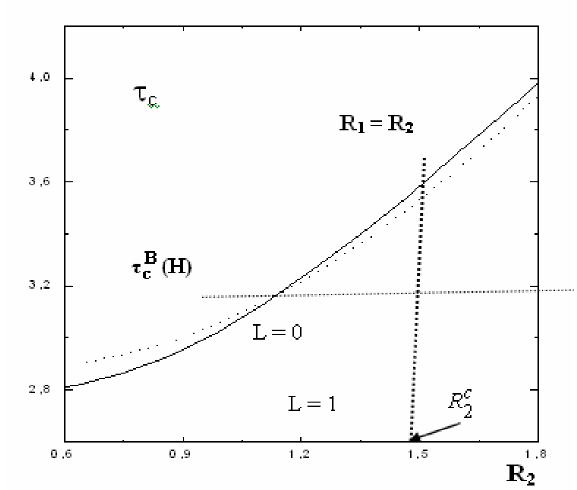

Fig. 2: The reduced critical temperature τ_c as a function of the ratio R_2 in the case of the face centred cubic lattice (for the case where $R_1 = R_2$) for Heisenberg model (H).

We see that for a given model the curves intersect at the abscises $R_2^c(I) = 0.291$, $R_2^c(XY) = 0.30$, $R_2^c(H) = 0.303$ and ordinate point: $\tau_c(I) = 4.483$, $\tau_c(XY) = 2.244$ and $\tau_c(H) = 1.498$ with a simple cubic lattice. The obtained values for a face centered cubic lattice are $R_2^c(I) = 0.817$, $R_2^c(XY) = 0.819$, $R_2^c(H) = 0.823$ (see Fig. 1) and ordinate point: $\tau_c(I) = 4.79$, $\tau_c(XY) = 2.386$ and $\tau_c(H) = 1.594$ (see *Fig.* 2). At those points $\tau_c(\nu)$ is independent on the film thicknesses and becomes similar to three-dimensional infinite bulk film. The results shows that the film exhibits two phases: a semi infinite ferromagnetic film phase where both bulk and surface are magnetized, and a semi infinite film paramagnetic phases where both bulk and surface are disordered. Hence we observe in the phase diagrams is the existence of a special coupling R_2^c at which all the semi-infinite film have a unique critical temperature $\tau_c(\nu)$ for an arbitrary thickness L. This special point separates the ordinary from the extraordinary transitions in the semi infinite system. We have also studied the influence of the dilution x on the reduced critical temperature $\tau_c(\nu)$. In figures.3a and 3b we present the magnetic phase diagrams of the semi infinite film in $(\tau_c(\nu); x)$ plane for the cases $R_1 = R_2 = R_2^c$ and $R_1 = R_2 = 5 > R_2^c$ for the three models for the simple cubic lattice.

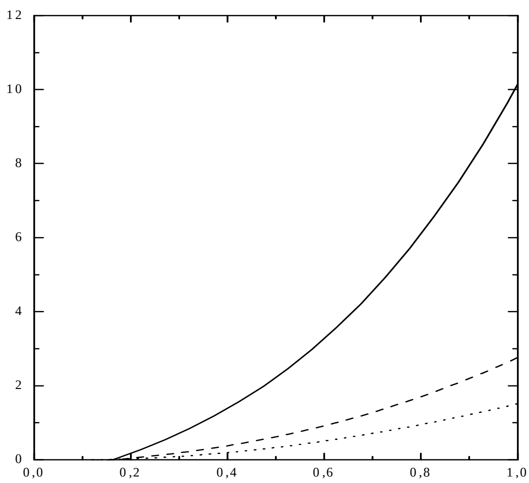

Fig. 3(a): Phase diagram, τ_c versus dilution x, for three models: Ising (I), XY and Heisenberg (H);: $R_1 = R_2 = R_2^c$

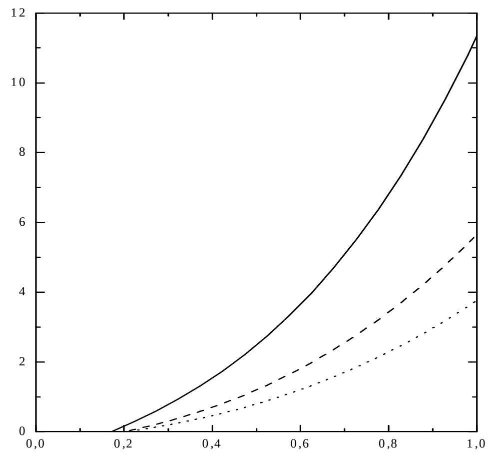

Fig. 3(b): Phase diagram, τ_c versus dilution x, for three models: Ising (I), XY and Heisenberg (H); : $R_1 = R_2 = 5 > R_2^c$ for $L = 0$ in the case of the simple cubic lattice in the surface

In Fig. 4a and 4b, we present the phase diagrams in ($\tau_c(\nu)$; x) plane of the semi infinite film for the cases $R_1 = R_2 = R_2^c$ and $R_1 = R_2 = 3$ for the three models for the face centred cubic lattice.

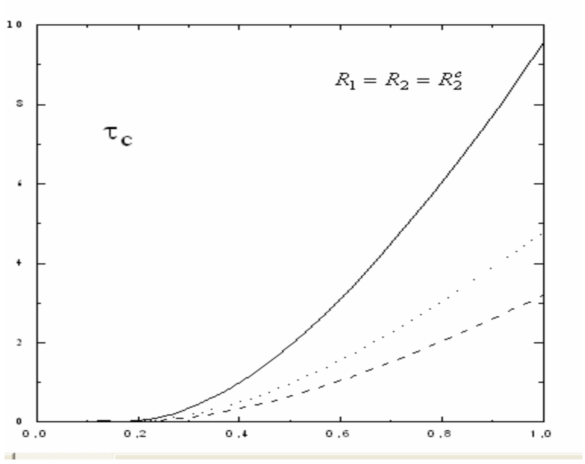

Fig. 4(a): Phase diagram, τ_c versus dilution x, for three models: Ising (I), XY and Heisenberg (H);: $R_1 = R_2 = R_2^c$ $R_1 = R_2 = 3 > R_2^c$ for $L = 0$ in the case of the face centred cubic lattice in the surface.

In thin spin-1/2 Ising film $T_c(I) \approx 7.203 J_b/k_B$ [14] with a simple cubic lattice, is superior to those found in the semi infinite film $T_c(I) \approx 5.073 J_b/k_B$ [15]. In thin spin-1/2

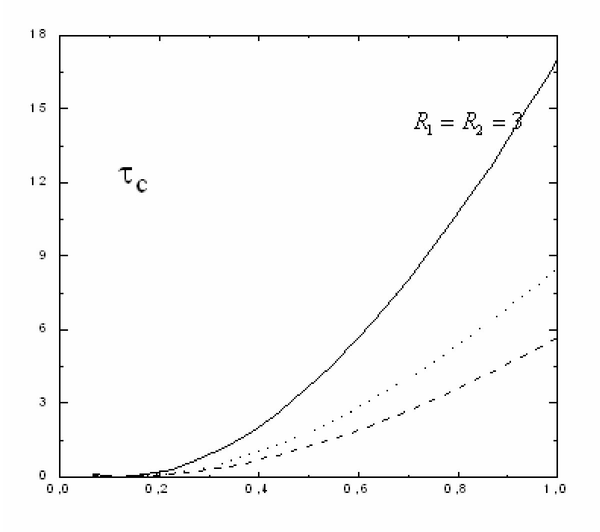

Fig. 4(b): Phase diagram, τ_c versus dilution x, for three models: Ising (I), XY and Heisenberg (H): $R_1 = R_2 = 3 > R_2^c$ for $L = 0$ in the case of the face centred cubic lattice in the surface.

Ising film $T_c(I) \approx 9.828 J_b/k_B$ [16] with a face centered cubic lattice (fcc) is superior of our result $T_c(I) \approx 7.32 J_b/k_B$ found in semi infinite film with the fcc lattice. Our value is slightly smaller than those found by the high-temperature expansions for spin-1/2 Ising $T_c(I) \approx 9.83 J_b/k_B$ [17]. The characteristic property of the curves, as indicated in the two figures, is an increase of the $\tau_c(\nu)$ when the dilution x increases. We know, on physical grounds, that if the magnetic concentration falls below the percolation concentration (for a given lattice), the spin correlation length will reduce to zero. Consequently the critical temperature vanishes. The percolation threshold is now defined as the concentration x_p at which $\tau_c = 0$. The obtained value is $x_p \approx 0.2$ for the two case $R_1 = R_2 = R_2^c$ and $R_1 = R_2 = 5$ for $L = 0$ in the simple cubic lattice and $x_p \approx 0.2$ in the case of face centred cubic lattice for the two case $R_1 = R_2 = R_2^c$ and $R_1 = R_2 = 3$ for $L = 0$.

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