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FINITE CLUSTER APPROXIMATION STUDY OF FRUSTRATION IN THE SEMI-INFINITE ISING MODEL *

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ABSTRACT

The influence of frustration on the phase transitions of a semi-infinite three-dimensional Ising model is investigated. Temperature-concentration phase diagrams for fixed values of the ratio of surface and bulk interactions can exhibit five different types of phase transition.

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Various approximate methods have been used to study a semi–infinite Ising model with the nearest neighbours reduced coupling constant at the surface (S) allowed to be different from the corresponding bulk value (K) [1,2]. Some of these methods give a critical value $R_c(R = K/S)$. However, if R is greater than R_c the sytem orders at the bulk ferromagnetic transition temperature. This is the ordinary phase transition. If R is less than R_c, the system exhibits two successive transitions. The surface orders at a temperature higher than that of the bulk, and as the temperature is lowered, in the presence of the ordered surface, the bulk orders at the bulk transition temperature. These two phase transitions are, respectively, the surface and the extraordinary transition. If $R = R_c$ the system orders at the bulk transition temperature, but in this case the critical exponents differ from those of the ordinary transitions. This is the special phase transitions.

In the present work we study the semi–infinite frustrated Ising model using a finite cluster approximation (F.C.A.) [3]. However, frustration due to competitive interaction and disorder are characteristic features of spin glass systems. In a certain range of concentration C, such system exhibits two successive phase transitions. A first transition from the paramagnetic phase to the ferromagnetic phase takes place followed at a lower temperature by a second transition from the ferromagnetic phase to a disordered phase which is interpreted as a spin glass phase.

For three–dimensional systems the existence of a stable spin glass phase is still controversial but it seems clear now that such a phase does not exist at finite temperature for two–dimensional systems [4]. On the other hand, we cannot have this phase, spin glass, with the F.C.A. neither in two nor in three–dimensional systems. Thus, we discuss only the transition para–ferro and para–antiferro.

Consider a semi–infinite simple cubic ferromagnetic Ising model described by the effective Hamiltonian:

$$-BH = \sum_{<ij>} S_{ij}\, \sigma_i \sigma_j + \sum_{<k,\ell>} K_{k\ell}\, \sigma_k \sigma_\ell\,, \qquad (1)$$

where $\sigma_i = \pm 1$ are the Ising spins. The summation runs over all nearest neighbour pairs. S_{ij} and $K_{k\ell}$ are assumed to be random variables with probabilities distributions:

$$P(S_{ij}) = c\delta(S_{ij} + S) + (1 - c)\,\delta(S_{ij} - S) \qquad (2a)$$

$$P(K_{ij}) = c\delta(K_{ij} + K) + (1 - c)\,\delta(K_{ij} - K)\,, \qquad (2b)$$

where S is the reduced coupling constant between neighbouring spins, located on the two–dimensional surface of the system and K is the reduced coupling constant between remaining neighbouring spins.

If $< \sigma_0 >_c$ denotes the mean value of σ_0 for a given configuration c of all other spins, i.e. when all other spins $\sigma_i (i \neq 0)$ have fixed values, we have

$$< \sigma_0 >_c = \frac{\underset{o}{Tr}\, \sigma_0\, e^{-BH}}{\underset{o}{Tr}\, e^{-BH}}\,. \qquad (3)$$

The zero below Tr (i.e. the trace) indicates that the trace is performed over σ_0 only. For a spin σ_{0S} located on the surface and another one for a spin σ_{0B} located in the bulk, Eq.(3) gives (Fig.1):

$$< \sigma_{0S} >_c = \tanh(S_{01}\sigma_1 + S_{02}\sigma_2 + S_{03}\sigma_3 + S_{04}\sigma_4 + K_{05}\sigma_5) \quad (4a)$$

$$< \sigma_{0B} >_c = \tanh(K_{01}\sigma_1 + K_{02}\sigma_2 + K_{03}\sigma_3 + K_{04}\sigma_4 + K_{05}\sigma_5 + K_{06}\sigma_6) \quad (4b)$$

The magnetizations per site $m_S(m_B)$ is given by:

$$m_S = < \overline{\tanh(S_{01}\sigma_1 + S_{02}\sigma_2 + S_{03}\sigma_3 + S_{04}\sigma_4 + K_{05}\sigma_5)} > \quad (5a)$$

$$m_B = < \overline{\tanh(K_{01}\sigma_1 + K_{02}\sigma_2 + K_{03}\sigma_3 + K_{04}\sigma_4 + K_{05}\sigma_5 + K_{06}\sigma_6)} > . \quad (5b)$$

Averaging the right–hand side of Eqs.(4a) and (4b) over all spin configurations (denoted by angular brackets) and then over the random interactions (denoted by a bar). For the first step we use the following theorem:

The set of all bounded real functions f of $\sigma_1, \sigma_2, \ldots, \sigma_z$ is a 2^z dimensional Euclidean space; the set $\{1, \sigma_1, \ldots, \sigma_z, \sigma_1\sigma_2 \ldots, \sigma_1\sigma_2 \ldots \sigma_z\}$ which contains all the products of different spins · is an orthonormal basis for the inner product defined by:

$$< f_1 | f_2 > = \frac{1}{2^z} \underset{\sigma_1,\ldots,\sigma_z}{Tr} f_1(\sigma_1, \sigma_2, \ldots, \sigma_z) f_2(\sigma_1, \sigma_2, \ldots, \sigma_z) .$$

For the second step we use the probabilities given by (2a) and (2b). Then we can have the equations of state of the frustrated three–dimensional semi–infinite model with the F.C.A.

$$m_S = 4\overline{A}_1\, m_S + \overline{B}_1\, m_B + 4\overline{C}_1\, m_S^3 + 6\overline{D}_1\, m_S^2\, m_B + \overline{E}_1\, m_S^4\, m_B . \quad (6a)$$

$$m_B = 6\overline{A}_2\, m_B + 20\overline{B}_2\, m_B^3 + 6\overline{C}_2\, m_B^5 . \quad (6b)$$

The bars over the coefficients indicate that they have been averaged over disorder. To determine temperature–concentration phase diagrams for fixed values of the ratio R of the interactions, we need only the expressions for $\overline{A}_1$ and $\overline{A}_2$. These phase diagrams are given by:

$$1 = 4\overline{A}_1\,(c, K, \Delta) \quad (7a)$$

$$1 = 6\overline{A}_2\,(c, K) , \quad (7b)$$

where

$$\overline{A}_1 = \frac{1}{16}(1-2c)[\tanh S(4+R) + \tanh S(4-R) + 2\tanh S(2+R) + 2\tanh S(2-R)]$$

$$\overline{A}_2 = \frac{1}{32}(1-2c)[\tanh 6RS + 4\tanh 4RS + 5\tanh 2RS] .$$

Our estimate $R_c = 0.59$ represents an improvement on the mean field results ($R_c = 0.8$) and compares well with $R_c = 0.62$ from a series expansion [5] and $R_c = 0.67$ from Monte Carlo results [6]. The critical ferromagnetic C_F and antiferromagnetic concentrations C_{AF} are obtained for square lattice ($C_F = .167$ and $C_{AF} = .833$) and simple cubic lattice ($C_F = .233$ and $C_{AF} = .767$).

Typical temperature-concentration phase diagrams for $R < R_c$ and $R > R_c$ are represented in Fig.2a and Fig.2b respectively. The five types of phase transition in the ferromagnetic case ($c < 0.5$) can be founded in the antiferromagnetic case ($c > 0.5$).

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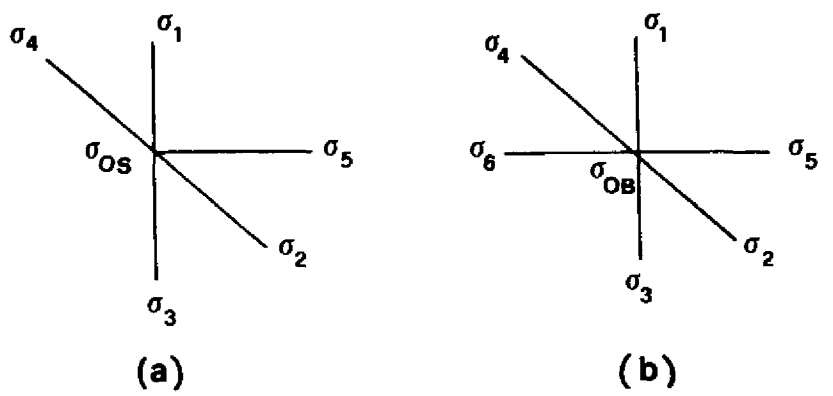

Fig.1

Fig.1 (a) Nearest neighbours of spin σ_{0S} located on the surface.

(b) Nearest neighbours of spins σ_{0B} located on the bulk.

σ_{0S} and σ_{0B} are assumed not to have neighbours in common.