Revista Mexicana de Física S **58** (2) 210–212 DICIEMBRE 2012

Critical Concentration of Mixed-Bond Ising Model

J.B. Santos-Filho[a], D.F. de Albuquerque[b], and N.O. Moreno[c]
[a]*Departamento de Física, Universidade Federal de Minas Gerais, 31270-901, Belo Horizonte, MG, Brazil.*
[b]*Departamento de Matemática, Universidade Federal de Sergipe, 49100-000, SE, Brazil,*
e-mail: douglas@ufs.br
[c]*Departamento de Física, Universidade Federal de Sergipe, 49100-000, SE, Brazil.*

Recibido el 25 de junio de 2010; aceptado el 22 de febrero de 2011

The study for critical concentration of mixed-bond Ising model with competitive interactions it is obtained by using a differential operator technique in the effective field theory. In this work, we obtained the phase diagram to bi- and three-dimensional lattices and our results show a correlation between lattice coordination number and the critical concentration. On the other hand, there are a finite number of critical concentrations which depend of method employed.

Keywords: Monte Carlo; effective field; Ising model.

El estudio de la concentración crítica en el modelo de Ising de enlaces mixtos con interacciones competitivas se estudia mediante el uso de la técnica del operador diferencial en la teoría de campo efectivo. En este trabajo, se obtuvo el diagrama de fase de redes bi y tridimensionales, y nuestros resultados muestran una correlación entre el número de coordinación y la concentración crítica. Por otra parte, hay un número finito de concentraciones críticas que dependen del método empleado.

Descriptores: Monte Carlo; campo efectivo; modelo de Ising.

PACS: 02.50.Ng; 75.10.Nr; 75.40.Cx

1. Introduction

The experimental discovery of re-entrance which occur in some compound, as example the insulator $Eu_pSr_{1-p}S$, has been predict theoretically by mean-field theory of mixed-bond Ising models. This compound showed behavior re-entrance in a range of concentration p, upon lowering the temperature the successive phases are paramagnetic, ferromagnetic and spin glass [1]. There have been a number of letters in the literature [2] that claim to provide either a rather simple explanation of re-entrant behavior or claim to demonstrate that reentrance occurs very generally in short-range disordered systems, in particular, simple random Ising models with short-range interactions. Some of these letters are based in the existence of a single critical concentration. However results of numerical transfer matrix calculations and Migdal-Kadanoff renormalization group studies on a random nearest-neighbour Ising model in two and three dimensions has been show the existence of a critical concentration as function of competition parameter. On the other hand, results obtained by employing effective field approximation (EFA) suggest that a denumerable group of critical concentrations exists for that model [3]. In this work, we investigated the result of EFA for cluster with one (EFA-1) and two spins (EFA-2) for mixed-bond Ising model on square, simple cubic, body centered cubic and face centered cubic lattices.

2. Model and simulation setup

We study the spin-$1/2$ ferromagnetic Ising mixed-bond model defined by Hamiltonian

$$-\beta H = \sum_{\langle i,j\rangle} K_{ij}\sigma_i\sigma_j, (\sigma_i = \pm 1)\,, \tag{1}$$

where the sum extends over all pairs of neighboring sites on a d dimensional lattice of linear size L with periodic boundary conditions, $\beta = 1/k_BT$ and the exchange couplings K_{ij} are allowed to take two different values $K_{ij} \equiv J_{ij}/k_BT$ and 0. The interactions are assumed to be independent random variables with probability distribution given by

$$P\left(K_{ij}\right) = p\delta\left(K_{ij} - K\right) + (1-p)\,\delta\left(K_{ij} - \lambda K\right), \tag{2}$$

where p is the concentration of magnetic bonds such $p = 1$ corresponds to the pure case and λ is the competition parameter with $|\lambda| \leqslant 1$, By applying the operator differential technique and the Suzuki-Callen [4] identity, ones get

$$m_1 = \left\langle \prod_{j\neq 1} e^{K_{1j}\sigma_i D_x} \right\rangle f\left(x\right)|_{x=0},$$

$$m_2 = \left\langle \prod_{k\neq 2} e^{K_{ik}\sigma_k D_x} \prod_{k\neq 1} e^{K_{2k}\sigma_k D_y} \right\rangle g\left(x,y\right)|_{x=0,y=0}, \tag{3}$$

where the product is taken over all first neighbors. The functions $f(x)$ and $g(x,y)$ are given by

$$f\left(x\right) = \tanh x,$$

$$g\left(x,y\right) = \frac{\sinh\left(x+y\right)}{\cosh\left(x+y\right) + e^{-2K_{12}}\cosh\left(x-y\right)}. \tag{4}$$

The phase diagram is obtained numerically when $m_1 \approx 0$ to find EFT1 and $m_2 \approx 0$ for EFT2.

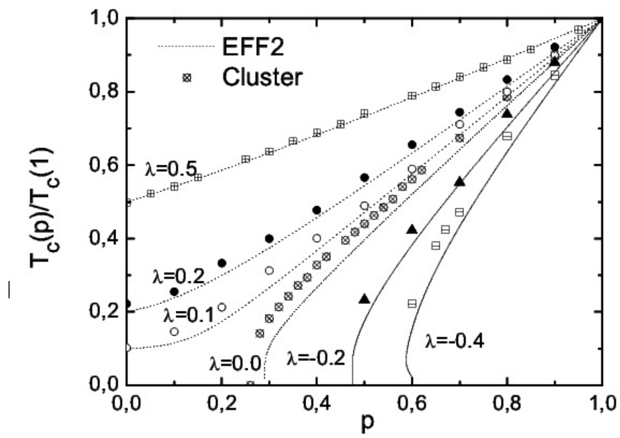

FIGURE 1. Phase diagram of the 3D mixed-bond Ising model for lattice cubic for λ = 0, 0.1, 0.2, 0.5,-0.2,-0.4. Solid lines are the predictions of the effective field approximation and the points are results of Monte Carlo simulation.

3. Results

In order to analyze the results obtained by effective field approximation (EFA) based in the introduction of a differential operator, we study the system also by Monte Carlo (MC) simulation. The phase transition diagram obtained by employing the differential operator technique and one obtained by computer simulation are presented in Fig. 1, where the points presented is obtained numerically from the peak of a diverging quantity. Here we choose the magnetic susceptibility, since the stability of the disordered fixed point implies that the specific heat exponent is negative in the random system [5,6]. Thus, the error in this quantity is larger than for the susceptibility. To get an accurate determination of the peak of the susceptibility, we used the histogram reweighing technique with 10000 Monte Carlo sweeps (MCS) and between 2500 and 5000 samples of disorder. The number of MCS is justified by increasing behavior of the energy autocorrelation time, τ_E, and we choice for each size at least 250 independent measurements of the physical quantities ($N_{\text{MCS}} > 250\tau_E$). On the other hand, the adjust of N_{MCS} is justified by increasing behavior of the energy autocorrelation time τ_E as a function of p and L. At the critical point of a second-order phase transition one expects a finite-size scaling (FSS) behavior $\tau_E \propto L^Z$, where here $z$is the dynamical critical exponent. Although the two techniques show good coincidence to high temperatures to near freezing temperatures, the technique of Monte Carlo simulation does not produce satisfactory results, because the spins were frozen, and requires much computational time. Such facts make that operator technique is used in percolation. There is evidence that the results generated by employing operator technique when $T \to \infty$ are failures of the approach.

Figure 2 shows the results of the critical concentration p_c vs λ obtained by $m \approx 0$ when $T \to \infty$, where we observed that the critical concentration depends of λ, unlike the mean

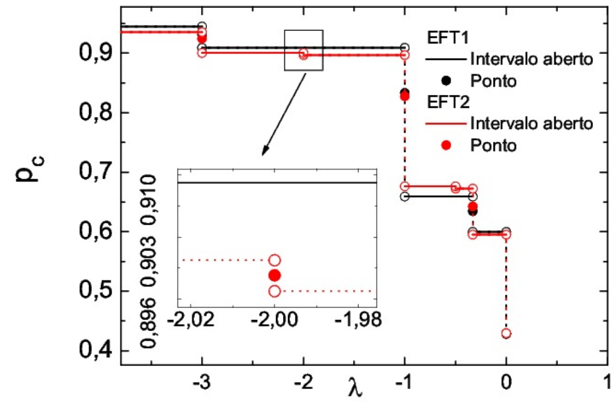

FIGURE 2. Critical concentration vs. λ for square lattice. Open circles represent the limits of an open interval.

field technique whose critical concentration is a constant. However, we observed which critical concentration does not changes continuously with variation of λ, but there is a discrete variation, and the number of intervals increases when we considers two spins on the approach Eq. (3-b), that suggests which number of intervals it is related to the number of terms in the equation describing the system. Thus the exact solution with infinite terms would infinite intervals and thus the critical concentration would vary continuously with the competition parameter λ competition.

In Fig. 3 the results of the critical concentration p_c vs λ for body-centered cubic lattice (bcc), shows the most critical concentration ranges. The larger number of intervals, greater the number of terms in the equation describing the system. As the body-centered cubic lattice has a larger number of nearest neighbors, so it has a greater number of intervals.

4. Conclusion

We carried out Monte Carlo simulations for study the influence of bond dilution on the critical properties of the Ising Model applied for cubic lattice. We obtained thermodynamic parameters for $|\lambda| \leqslant 1$. Results satisfactory are obtained by

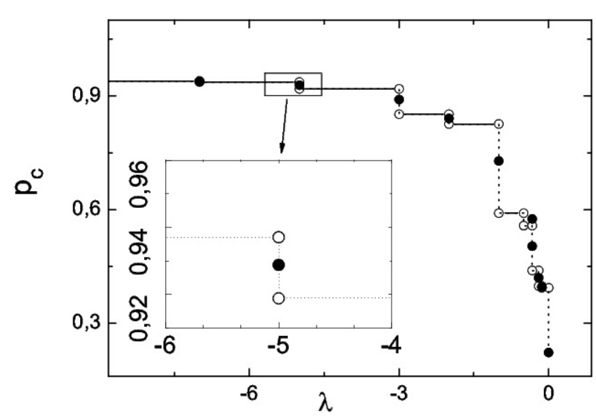

FIGURE 3. Critical concentration vs. λ for bcc lattice. Open circles represent the limits of an open interval.

using the Wolff algorithm and we showed that this technique is appropriated to approach the mixed-bond problem. The MC simulations give similar results to the obtained ones by the effective field theory. The critical behavior of the mixed-bond model is governed by the same universality class as the site-diluted model and the pure Ising model.

Acknowledgements

N.O. Moreno is partially supported by FAPITEC-SE and CNPq Brazilian agencies. J. B. Santos Filho acknowledge financial support by CAPES.

1. N. Benayad N, A. Benyoussef, and N. Boccara , *J. Phys. C: Solid St. Phys.* **20** (1987) 2053.
2. J.D. Reger and A P Young, *J. Phys.: Condens. Matter* **1** (1989) 915.
3. J. Santos-Filho, N.O. Moreno, D.F. Albuquerque, and A.S. de Arruda, *Physica B* **398** (2007) 294.
4. H.B. Callen, *Phys. Lett.* **4** (1963) 161; H. Suzuki, *Phys. Lett.* **19** (1965) 267.
5. J.T. Chayes, L. Hayes, D.S. Fisher, and T. Spencer, *Phys. Rev. Lett.* **57** (1986) 2999.
6. L.E. Zamora, G.A. Pérez Alcázar, A.W. Bohórquez, A. Rosales-Rivera, and J.A. Plascak, *Phys. Rev. B* **51** (1995) 9329.
7. H.G. Ballesteros, *et al*, *Phys. Rev. B* **58** (1998) 2740.
8. W.F. Wolff, J.J. Zittartz, *Magn. Magn. Mater* **144** (1986) 54.