Monte Carlos studies of critical and dynamic phenomena in mixed bond Ising model

Journal of Physics: Conference Series **249** (2010) 012038 doi:10.1088/1742-6596/249/1/012038

Monte Carlos studies of critical and dynamic phenomena in mixed bond Ising model

J. B. Santos-Filho[1], N. O. Moreno[1], Douglas F. de Albuquerque[2]

[1]Departamento de Física, Universidade Federal de Sergipe, 49100-000, São Cristovão, SE, Brasil

[2]Departamento de Matemática, Universidade Federal de Sergipe, 49100-000, São Cristovão, SE, Brasil

E-mail: nomoreno@fisica.ufs.br

Abstract. The phase transition of a random mixed-bond Ising ferromagnet on a cubic lattice model is studied both numerically and analytically. In this work, we use the Metropolis and Wolff algorithm with histogram technique and finite size scaling theory to simulate the dynamics of the system. We obtained the thermodynamic quantities such as magnetization, susceptibility, and specific heat. Our results were compared with those obtained using a new technique in effective field theory that employs similar probability distribution within the framework of two-site clusters.

1. Introduction

The study of the effects of disorder in magnetic systems has been an object of intense investigations during the last five decades.

The Monte Carlo technique is an useful tool which in many cases, gives better results regarding other methods from analytical approximations. The influence of quenched, random disorder on phase transitions is of great importance in a large variety of fields [1]. For pure systems exhibiting a continuous phase transition, Harris [2] derived the criterion that random disorder is a relevant perturbation when the exponent of the specific heat of the pure system is positive, $\alpha > 0$. In this case one expects that the system falls into a new universality class with critical exponents governed by a disordered fixed point. For $\alpha < 0$ disorder is irrelevant, and in the marginal case $\alpha = 0$ no prediction can be made.

Since for the three-dimensional (3D) Ising model it is well known that $\alpha > 0$, quenched, random disorder should be relevant for this model. In three dimensions (3D) most of the computer simulation studies have concentrated mainly on the site-diluted Ising model [3, 12].

In this work, we study the Ising model with mixed-bond by using of Monte Carlo simulation, applying the algorithm cluster of Wolff [5].

2. Model and Simulation Setup

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

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

where the sum extends over all pairs of neighboring sites on a cubic 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 $K_{ij} = K \equiv J/k_BT$ and 0. The interactions are assumed to be independent random variables with the probability distribution

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

where p is the concentration of magnetic bonds in the system bonds such that $p = 1$ corresponds to the pure case and λ is the competition parameter with $|\lambda| \leq 1$.

The simulations were performed on a set of following lattice sizes L = 10, 16, 20, 26, 30, 36, 40 with periodic boundary conditions. The aim of the first set of simulations is to estimate the critical temperature of the model at different L. Due to the finite-size scaling theory [6], the finite system of linear size L will demonstrate an evidence of a critical behavior at a certain temperature $T_C(L)$ which differs from the critical temperature of the infinite system $T_C(\infty)$ [7].

$$T_C(L) = T_C(\infty) + \alpha L^{-1/v} + ..., \tag{3}$$

where the correction-to-scaling terms have been omitted.

The static thermodynamic quantities of interest include the average magnetization M and the magnetic susceptibility χ

$$M = \frac{1}{n}\sum_{i=1}^{n}\sigma_i, \tag{4}$$

$$\chi = \frac{1}{k_BT}[\langle M^2\rangle - \langle M\rangle^2]. \tag{5}$$

The phase diagram is obtained numerically from the maxima 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 [8, 9]. Thus, the error in this quantity is larger than for the susceptibility. To get an accurate determination of the maxima of the susceptibility, we used the histogram reweighting technique with 2500 Monte Carlo sweeps (MCS) and between 2500 and 5000 samples of disorder. The number of Monte Carlo sweeps is justified by the increasing behavior of the energy autocorrelation time, τ_E, and we chose for

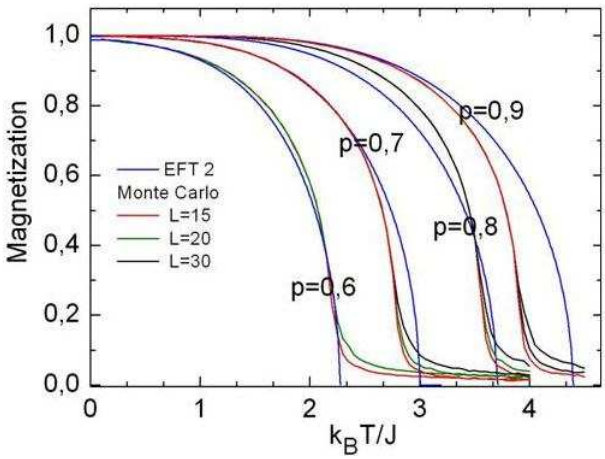

Figure 1. Magnetization vs. k_BT/J for the Ising model with L = 15, 20 and 30 in a cubic lattice with $\lambda = -0.1$.

each size at least 250 independent measurements of the physical quantities ($N_{MCS} > 250\ \tau_E$). The choice of N_{MCS} is justified by the 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 z is the dynamical critical exponent

3. Results

The figure 1 displays curves of magnetization versus temperature through computational simulation for $\lambda = -0.1$ and $L = 15$, 20 and 30. The critical temperature obtained when $p = 1$ was $T_C = 4.510$ it is close of the expected value $T_C = 4.51$.[10] We observe that the curves keep the same behavior, in spite of in the proximities of the critical point they move away each other. The critical point was estimated of the inflection of the curve. It can be notice that increasing the lattice size, i.e. the value of L, we get more precision to estimate the critical temperature. For comparison we have drawn, however, a simple effective-field approximation estimate of the temperature dependence of magnetization for several p-values, it gives very good agreement with the simulated transition line over the full temperature range.

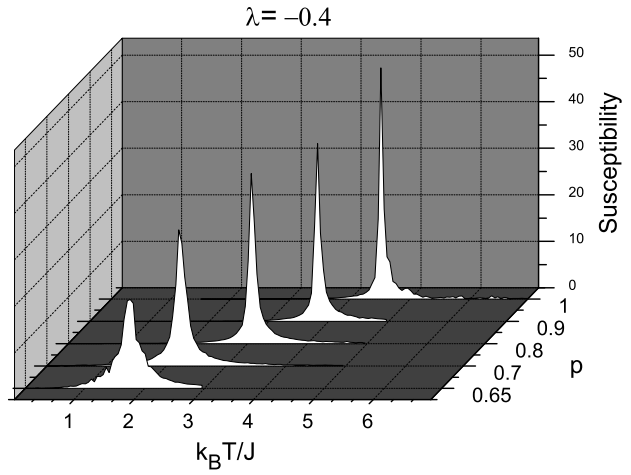

Figure 2. χ vs. k_BT/J for the Ising model with $\lambda = -0.4$ and L = 40 for several concentrations p.

The magnetic susceptibility as a function of temperature for different p values and for $\lambda = -0.4$ and L = 40 is shown in Fig. 2. The peaks are sharper for lower p values. In order to $p < 0.65$ and $\lambda = -0.4$ the susceptibility does not displays the peak associate with the magnetic transition due to competitions of the exchange interactions. When $\lambda \geq 0$ the system presents always ferromagnetic long range order. We used the histogram reweighting technique with 2500 Monte Carlo sweeps (MCS) and between 2500 and 5000 samples of disorder to get an accurate determination of the maxima of the susceptibility.

The phase diagram obtained from the location of the maxima of the susceptibility for the largest lattice size (L = 40) as a function of the concentration of magnetic bonds is shown in Fig. 3 for λ=0, 0.1, 0.2, 0.5, -0.2 and -0.4. Solid lines are the predictions of the effective field approximation. A very good agreement with the simulated transition line is obtained.

The reduced fourth-order Binder cummulants[11] supply an alternative method to estimated critical points that can be determined from the crossing point of the cumulants for different lattice sizes. It is calculated by using

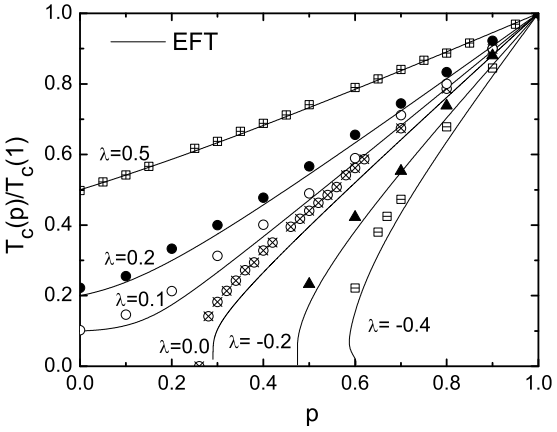

Figure 3. Phase diagram of the 3D mixed-bond Ising model compared with the effective field approximation.

$$U_4 = 1 - \frac{[\langle m^4 \rangle]}{3\left[\langle m^2 \rangle^2\right]},$$

where [...] denotes the average over disorder and $\langle ... \rangle$ refers at the thermal average. As an example, we show in Fig 4 the Temperature dependence of the reduced fourth-order Binder cummulant for $p = 1$ and for various lattice sizes. Critical temperature obtained from this figure is in agreement with those obtained of the maxima of the magnetic susceptibility.

The peak locations of the maxima susceptibility for each L are plotted versus $L^{-1/\nu}$, where the value of ν is determined of the linear fit of log-log plot $\frac{\partial U_L}{\partial T}$ vs L (not shown here). The critical temperature can be estimated from an infinite-size extrapolation in according with Eq.(3). We illustrate this procedure in Fig 5 for $\lambda = 0.5$ and $p = 0.4$, the linear fit gives $T_C = 3.1065(3)$.

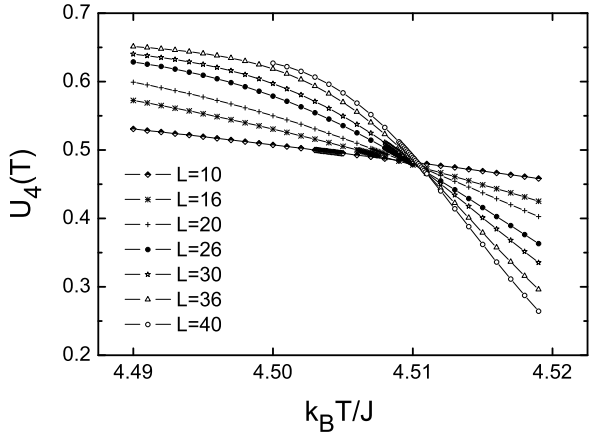

Figure 4. Fourth-order Binder cumulant U_4 vs. k_BT/J, for different lattice sizes as indicated in figure.

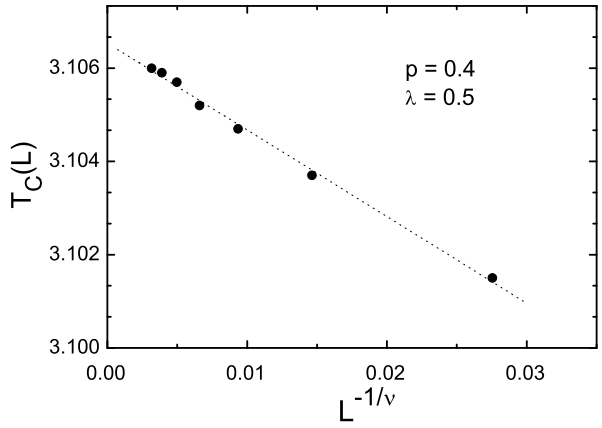

Figure 5. Size-dependent critical temperature $T_C(L)$vs. $L^{-1/\nu}$, for $\lambda = 0.5$ and $p = 0.4$.

Table 1. Critical exponents for three dilutions and $\lambda = 0.5$.

p	1	0.8	0.6	0.4
$1/\nu$	1.591(7)	1.68(7)	1.63(4)	1.56(3)
β/ν	0.4920(5)	0.49(1)	0.50(13)	0.496(5)
γ/ν	2.008(6)	2.06(3)	1.950(6)	2.001(6)

The average magnetization m and the magnetic susceptibility χ scale with the lattice size as:

$$m \sim a_m L^{-\beta/\nu}, \quad \chi \sim a_\chi L^{\gamma/\nu,} \tag{6}$$

here a_m and a_χ are non-universal amplitudes. From these power-laws we extracted the exponents β and γ plotting in logarithm scale the lattice size dependence of the susceptibility and average magnetization. The critical exponents obtained to $p = 0.4$, 0.6, 0.8 and $\lambda = 0.5$ are listed in Table I. The critical exponents oscillate without having an apparent correlation with the dilution. One can note that they are pretty close of those obtained for disordered Ising model [12]

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 $|\lambda| \leq 1$.

Satisfactory results are obtained using the algorithm of Wolff and showed that this technique is appropriated to treat the Mixed-bond problem. On the other hand, the Monte Carlo technique results gives very good agreement with the effective field theory data.

The critical behavior of the mixed-bond model is governed by the same universality class as the site-diluted model and pure Ising model.

ACKNOWLEDGMENT

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

[1] R. Folk, Y. Holovatch, T. Yavorskii: Physics Uspiekhi **173** (2003) 175.
[2] A. B. Harris: J. Phys. C **7**(1974) 1671.
[3] S. Wiseman and E. Domany, Phys. Rev. Lett. **81**, (1998) 22.

[4] H.G. Ballesteros, L.A. Fernández, V. Martín-Mayor, A. Muñoz Sudupe, G. Parisi, J.J. Ruiz-Lorenzo, Phys. Rev. B **61**, (2000) 3215.
[5] U. Wolff, Phys. Rev. Lett. **62** (1989) 361.
[6] M. N. Barber Finite-size scaling. In: Phase Transitions and Critical Phenomena, eds. C.Domb and J.Lebowitz, Academic, New York, 1983, vol.8
[7] A. M. Ferrenberg, D.P. Landau, Phys. Rev. B **44** (1991) 5081.
[8] J. T. Chayes, L. Hayes, D. S. Fisher, T. Spencer, Phys. Rev. Lett. **57** (1986) 2999.
[9] L. E. Zamora, G. A. Pérez Alcázar, A. W. Bohórquez, A. A. Rivera and J. A. Plascak, Phys. Rev. B **51** (1995) 9329.
[10] C Domb and M. S. Green, 1976. Phase Transitions and Critical Phenomena, ed. por C. Domb e M. S. Green, (Academic, London)
[11] K. Binder and D. W. Heermann, Monte Carlo Simulation in Statistical Physics. An Introduction, 3rd ed. (Springer, Berlin, 1997).
[12] H. G. Ballesteros, *et al*, Phys. Rev. B **58** (1998) 2740.