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MONTE CARLO SIMULATIONS OF A DISORDERED BINARY ISING MODEL

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A disordered binary Ising model, with only nearest-neighbor spin exchange interactions $J > 0$ on the square lattice, is studied through Monte Carlo simulations. The system consists of two different particles with spin-1/2 and spin-1, randomly distributed on the lattice. We found the critical temperatures for several values of the concentration x of spin-1/2 particles, and also the corresponding critical exponents.

Keywords: Monte Carlo simulation; disordered binary magnetic model; critical exponents.

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1. Introduction

Magnetic properties of random systems, including diluted and binary site-substitutionally disordered Ising models, have been the subject of considerable attention from both theoretical and experimental point of view (see, for instance, Stinchcombe[1]). In the binary disordered case, two different types of magnetic ions (denoted by A and B) are randomly distributed on a lattice representing a magnetic binary alloy A_xB_{1-x}, which is suddenly frozen from high temperatures (liquid state) to low temperatures (solid state). Much of the theoretical work has assumed the two magnetic ions having the same spin-1/2 value. Such models have then been investigated by mean-field approaches[2–4] and Monte Carlo simulation.[5] On the other hand, less attention has been given to binary random-site models where the constituents have different spin values. Therefore, it is interesting to investigate a system as the binary random-site Ising model with one of the constituents having spin-1 and the other one having spin-1/2. Such systems have already been investigated by mean-field theories[6–8] and Monte Carlo simulation[9] (in the latter Ref. 9, however, only the $x = 1/2$ case was treated).

In this work, we consider the mixed-spin Ising model for a binary alloy which may be described by the following Hamiltonian

$$\begin{aligned}\mathcal{H} = -J\sum_{\langle i,j\rangle}\{&c_i c_j \sigma_i \sigma_j + (1-c_i)(1-c_j)S_i S_j \\ &+ c_i(1-c_j)\sigma_i S_j + c_j(1-c_i)S_i\sigma_j\},\end{aligned} \tag{1}$$

where the spin variables assume the values $S_i = \pm 1, 0$ and $\sigma_j = \pm 1/2$, and the nearest-neighbor interaction is ferromagnetic, $J > 0$ (one can also consider different interactions depending on the ions type like $A-A, A-B$ and $B-B$, however, similar results should be expected). We associated to each site i of the lattice an occupation variable c_i, so that $c_i = 1$, if the site is occupied by a particle with spin $\sigma = 1/2$ and $c_i = 0$, if it is occupied by a particle with spin $S = 1$. The sites are occupied independently by the two particles, with a probability distribution defined as

$$P(c_i) = (1-x)\delta_{c_i,0} + x\delta_{c_i,1}, \quad i = 1, 2, \ldots, N, \tag{2}$$

where x is the concentration of spin-1/2 and $(1-x)$ is the concentration of spin-1.

2. Simulations and Results

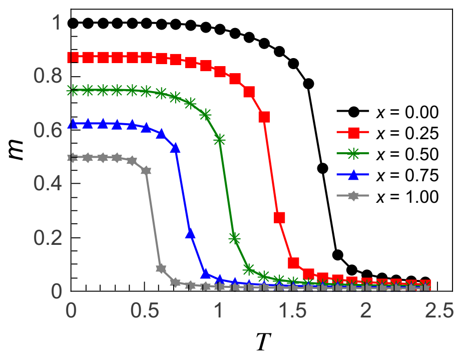
We computed the magnetization $m_L = [\frac{1}{N}\langle|\sum_{i=1}^{N}\{(1-c_i)S_i + c_i\sigma_i\}|\rangle]$, the energy $E_L = \frac{1}{N}[\langle\mathcal{H}\rangle]$, the susceptibility $\chi_L = N/T\big([\langle m_L^2\rangle] - [\langle m_L\rangle^2]\big)$, the specific heat $c_L = N/T^2\big([\langle E_L^2\rangle] - [\langle E_L\rangle^2]\big)$, and the fourth-order Binder cumulant $U_L = 1 - [\langle m_L^4\rangle]/3[\langle m_L^2\rangle^2]$. In the above expressions $[\cdots]$ denotes average over the samples of the system, and $\langle\cdots\rangle$ denotes the thermal average. $N = L^2$ is the total number of particles of the finite lattice with linear dimension L.

We used the theory of finite-size scaling[10,11] to estimate the static critical exponents β and γ at the critical point of the system from

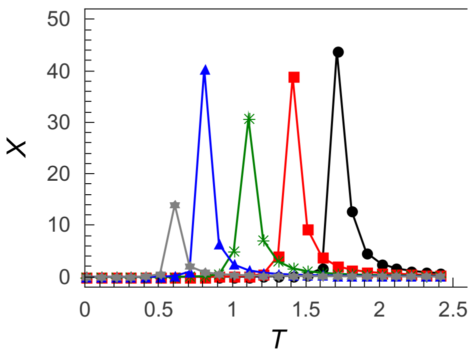
$$m_L(T_c) = L^{-\beta/\nu} m_o(0), \quad \chi_L(T_c) = L^{\gamma/\nu}\chi_o(0), \tag{3}$$

where T_c is the critical temperature and $m_o(0)$ and $\chi_o(0)$ are constants.

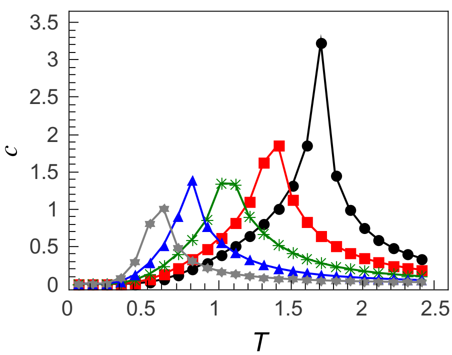
We consider values of L ranging from $L = 12$ to $L = 48$ with periodic boundary conditions. We prepared the system with the spins randomly distributed on the lattice with fixed x. However, each spin-1/2 can have as its nearest-neighbor spins of the type spin-1/2 or spin-1 and vice versa. Each trial to change a spin state on the lattice is accepted according to the Metropolis prescription.[12] To reach the equilibrium state we take at least 1×10^6 MCs (Monte Carlo steps) for all the lattice sizes we studied. Then, we take more 5×10^5 MCs to estimate the average values of the quantities of interest. Here, 1 MCs means L^2 trials to change the state of a spin. The average over the disorder was done by using 100 independent samples for lattices in the range $12 \le L \le 48$. All the results of the simulations presented here were realized for $x = 0, 0.25, 0.50, 0.75$ and 1.0. In Fig. 1, for $L = 48$, we display the behavior of the magnetization (Fig. 1(a)), susceptibility (Fig. 1(b)), specific heat (Fig. 1(c)), and



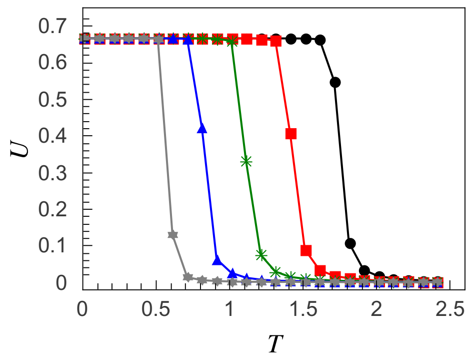
(a)



(b)



(c)

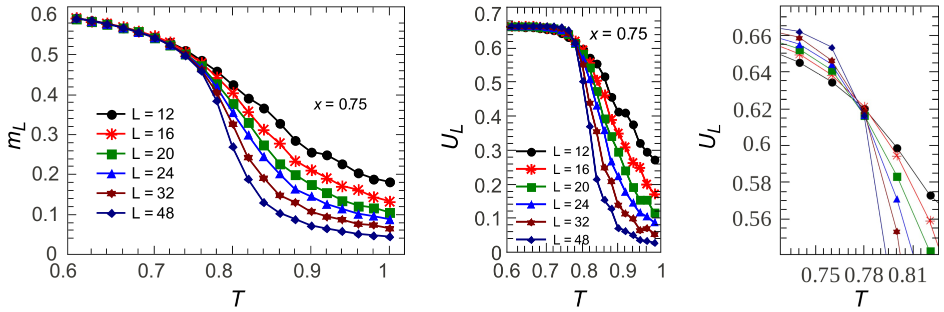


(d)

Fig. 1. (Color online) (a) Magnetization m, (b) susceptibility χ, (c) specific heat c, and (d) fourth-order Binder cumulant U as a function of temperature T for several values of the concentration x. The temperature is measured in units of J/k_B.

fourth-order Binder cumulant (Fig. 1(d)) as a function of temperature T, for several values of the concentration x. For $x = 0$, we have the critical behavior of the Blume−Capel model with the term of anisotropy equal zero ($D = 0$),[13,14] and for $x = 1.0$, we have the case of the pure Ising model. We can observe that the magnetization vanishes with the increase of temperature T. When the concentration x increases ($x \to 1$) the magnetization vanishes at different values of critical temperatures T_c. The critical temperature decreases with the increase of x which can be clearly observed by the shifting in the susceptibility and specific heat peaks.

The finite-size effects of the magnetization as a function of temperature were studied for the concentration $x = 0.75$, and for various system sizes L, and are shown in Fig. 2(a). We can observe from this figure that the magnetization m_L vanishes with the increase of temperature T, indicating indeed the existence of a phase transition.

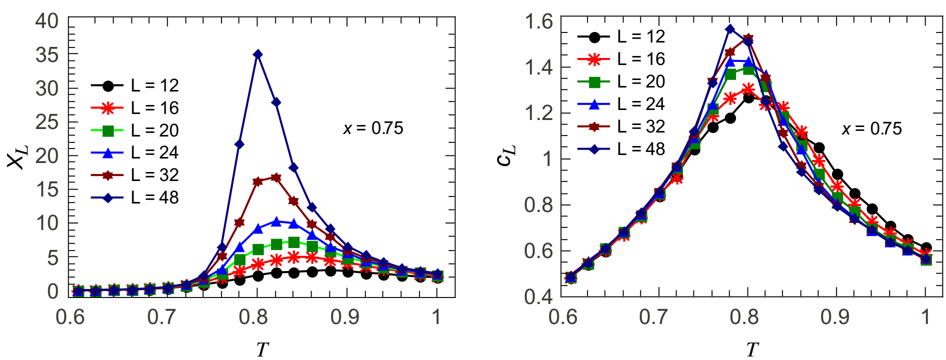


(a) (b) (c)

Fig. 2. (Color online) (a) Magnetization m_L and (b) fourth-order cumulants U_L as a function of temperature T for various lattice sizes L as indicated in the figure. Viewing expanded of the cumulants intersection point is shown in (c).

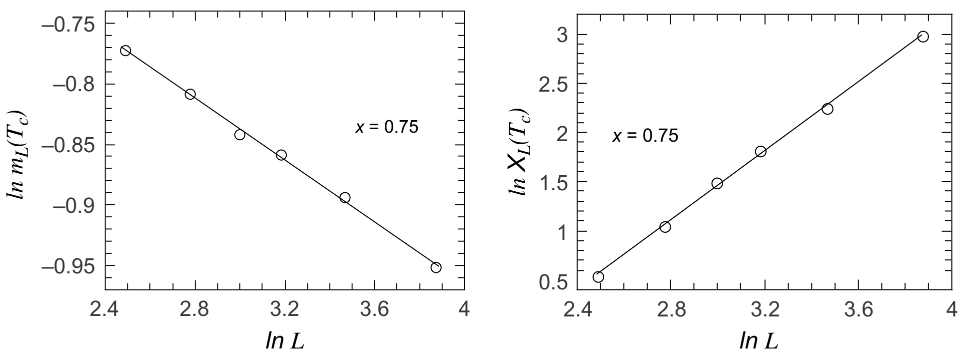
In order to study the phase transition in more details, we used the fourth-order Binder cumulants U_L intersection method to determine the value of temperature at which the transition occurs. To find the critical temperature, we also display in Figs. 2(b) and 2(c) the cumulants $U_L(T)$ vs temperature T, for several system sizes L and for $x = 0.75$. Our estimate for the dimensionless critical temperature is $T_c = (0.777 \pm 0.003)J/k_B$.

The susceptibility χ_L as a function of temperature T is shown in Fig. 3(a). For finite systems χ_L presents a peak around the critical temperature T_c, which grows in height with the increase of the system size. In Fig. 3(b), we also present the measurements of the specific heat. The peak observed in the curves of the specific heat exhibit a weak system size dependence compared to the susceptibility peak. The position of the specific heat and of the susceptibility peaks can be taken as a pseudocritical temperature $T^{\max}(L)$, which approaches T_c when $L \to \infty$.



(a) (b)

Fig. 3. (Color online) (a) Susceptibility χ_L and (b) specific heat c_L as a function of temperature T for various lattice sizes L as indicated in the figure.



(a) (b)

Fig. 4. Log−log plots of the (a) order parameter m_L and (b) the susceptibility χ_L as a function of the linear lattice size L, at the critical point T_c. The straight lines are the best fit to the data points. The error bars are smaller than the symbol sizes.

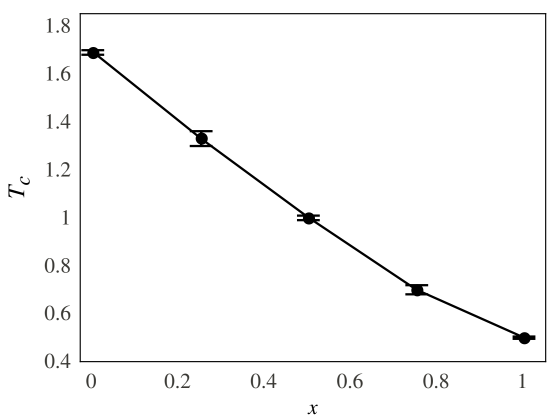


Fig. 5. Critical temperatures T_c in units of J/k_B as a function of the concentration x.

From the Monte Carlo simulations, we calculated the critical exponents of the model. For instance, in Fig. 4 we display the log−log plot of m_L and χ_L as a function of the linear size L at the critical point for $x = 0.75$. The best fit to the data points gives us $\beta/\nu = 0.127 \pm 0.003$ (Fig. 4(a)) and $\gamma/\nu = 1.76 \pm 0.03$ (Fig. 4(b)). From the weak dependence of the specific with the linear size we should have an α exponent close to zero. Similar results for the critical exponents are obtained for other values of the concentration x. Then, we can see that we have strong indications that this quenched random mixed-spin Ising model belongs indeed to the same universality class of the pure Ising model. This very same result has already been observed in the diluted Ising model in two dimensions.[15]

We have also obtained the critical temperature T_c for different values of x, as it can be seen in Fig. 5. For $x = 0$ (pure spin-1), we found $T_c = (1.69 \pm 0.01)J/k_B$, which is the critical temperature of the Blume−Capel model with $D = 0$ and comparable to the values $T_c = 1.681(5)$ and $T_c = 1.6935$ from Refs. 16, 17, respectively. On the other hand, for $x = 1.0$ one has $T_c = (0.565 \pm 0.003)4J/k_B$ which is agrees to the exact critical temperature of the two-dimensional Ising model $T_c = 0.567$. When $x = 0.50$ the critical temperature is $T_c = (1.00 \pm 0.003)J/k_B$, therefore, the result is not according to the one of the Ref. 9. The general features of the phase diagram show that the critical temperature change when concentration varies $0 < x < 1.0$, with the same exponents as the pure model.

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