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MONTE CARLO STUDY OF A SITE-BOND CORRELATED ISING MODEL

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Abstract. — The site-bond correlated Ising model for randomly diluted magnets is studied by Monte Carlo technique. Simulations are performed on two-dimensional square lattice with periodic boundary conditions, and the critical lines in temperature-concentration space are obtained for stronger correlation. We also present some thermal and magnetic properties of the model.

1. Introduction

The purpose of this paper is to report the results of Monte Carlo studies of the thermal and magnetic properties, as well as the phase diagram in the temperature-concentration \((T, p)\) space, of a randomly site-bond correlated (SBC) Ising model recently proposed by de Aguiar et al. \cite{1, 2}. The simulations were carried out on \(80 \times 80\) two-dimensional square lattices with periodic boundary conditions, and for various concentrations \(p\) of magnetic atoms.

The model Hamiltonian we consider is

\[
H = \frac{1}{2} \sum_{i, \delta} J_{i, i+\delta} \sigma_i \sigma_{i+\delta},
\]

where \(\sigma_i = \pm 1\) and \(\delta\) is a nearest-neighbor vector. The exchange interaction \(J_{i, i+\delta}\) is given by \cite{1}:

\[
J_{i, i+\delta} = J \epsilon_i \epsilon_{i+\delta} \left[ (1-\alpha) \epsilon_{i-\delta} \epsilon_{i+2\delta} + \alpha \right],
\]

where \(J > 0\) and the random variables \(\epsilon_i\) can take values one, with probability \(p\), and zero, with probability \((1-p)\). The parameter \(\alpha\) correlates the interaction between sites \(i\) and \(i+\delta\) with the magnetic occupancy of site \(i-\delta\) and \(i+2\delta\).

Earlier mean-field calculations \cite{1} have considered the phase diagram in the \((T_c, p)\) space, for several values of the correlation parameter \(\alpha\) and for Ising spins on the square lattice. More recently, the \((T_c, p)\) critical lines for a related site-bond correlated \(D\)-vector model on the Bethe lattice have been reported by Coutinho et al. \cite{3}. In the present Monte Carlo calculations we have restricted our attention to the most interesting case of stronger correlation that corresponds to consider \(\alpha = 0\) in the above model. For \(\alpha = 0\) the strength of the exchange interaction between a pair of magnetic atoms vanishes if at least one of the nearest-neighbor active sites is occupied by a nonmagnetic atom, and the model exhibits a percolation threshold \cite{1, 4} that is greater than the usual site percolation concentration \cite{5}.

2. Monte Carlo simulation

In order to simulate the model system describe by the above Hamiltonian, we proceed in the following way: initially \(N_p\) sites \((N = 80^2)\) chosen at random on a square lattice of size \(80 \times 80\) are occupied by magnetic atoms \((\epsilon_i = 1)\) and the remaining \(N (1-p)\) sites by nonmagnetic atoms \((\epsilon_i = 0)\). The corresponding quenched bond configuration is then specified by equation (2) with \(\alpha = 0\). This simulates a “sample” for a given magnetic concentration \(p\). Starting from an infinite temperature state, the spin system is let to evolve towards equilibrium at a given finite temperature \(T\) according to the standard Monte Carlo spin-flip technique \cite{6}. Typically the first \(1000-2000\) Monte Carlo steps per spin (MCS) were discarded and the followings \(2 \times 500-5000\) MCS were averaged, with the longest runs in the critical region. For each concentration \(p\) calculations were made with five samples.

3. Results and conclusion

In figures 1, 2 we display the results of our simulations for lattices \(80 \times 80\), with periodic boundary conditions, for the temperature and concentration dependence of the internal energy and the specific heat. In each case we include the Onsager’s exact result (full lines). For the disordered system the curves show the same qualitative behaviour with increasing quenched impurity concentration as observed for usual \(\alpha = 1\) site dilution. However the shift of the “critical region”
Fig. 2. - Specific heat of the SBC Ising model with $\alpha = 0$. The dashed curves are the temperature derivative of the spline fit to the energy data in figure 1. The inset shows a comparison between the exact result and the MC data for the pure system.

To lower temperatures with increasing dilution is much more pronounced for the $\alpha = 0$ model of disorder considered here. We also obtained a stronger dependence on dilution for the ground-state energy per spin which, for $\alpha = 0$, decreases approximately with $p^3$ instead of $p$ for $\alpha = 1$.

In figure 3 we show the phase diagram that follows from our simulation and the corresponding mean-field result of reference [1]. To determine the critical temperature for a given concentration, $T_c(p)$, we first looked for the best agreement between the specific heat MC data and the numerical derivative of the internal energy (dashed curves in Fig. 2) that follows from a cubic spline fit to the energy MC data (curves shown in Fig. 1). Then the corresponding value of $T_c(p)$ was estimated from the maximum in the resulting specific heat curve. This criteria [7] allows us to estimate the critical temperature within an accuracy that is better than that one which use a “guide to the eye” curve to fit (and locate the maximum of) the specific heat data. Except for the most diluted samples analysed, $p = 0.8$, where there is a noticeable spreading reflecting the smearing of the transition probably due to a stronger dependence on the number of samples, as well as their effective sizes, all other estimates for $T_c(p)$ support error bars which are smaller than the symbols in figure 3.

To summarize, we presented the first Monte Carlo analysis of the site-bond correlated (SBC) Ising model for quenched, randomly diluted magnetic systems in the limit of stronger correlation, in two-dimensions. Our results for the energy and the specific heat show the main features of the model. In particular the MC critical line obtained in this work is in reasonable agreement with previous mean-field calculation [1] for small dilution, and, since the percolation concentration for this model is $\sim 0.75$ [4] this indicate in analogy with the MF curve a rapid decrease in $T_c(p)$ in the interval between 0.80 and 0.75 (see dashed line in Fig. 3).

We hope that this work will be followed by further Monte Carlo studies of the SBC model in what concern both the simulation of more realistic experimental realizations, such as for three-dimensional lattices and/or Heisenberg systems, and the analysis of the static and dynamic properties of the model.

The calculations take $\sim 200$ hours in a VAX-750. This research was partially supported by CNPq, CAPES and FINEP.

Fig. 3. - Reduced critical temperature as a function of magnetic concentration of the SBC Ising model with $\alpha = 0$. The symbols for the MC data are: circles (●) (this work), and square (■) (Ref. [4]). The MF curve is the mean-field result in reference [1], whereas the MC curve (dashed line) is only a eye-guided to the MC results.