Single-cluster algorithm for the site-bond-correlated Ising model

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We extend the Wolff algorithm to include correlated spin interactions in diluted magnetic systems. This algorithm is applied to study the site-bond-correlated Ising model on a two-dimensional square lattice. We use a finite-size scaling procedure to obtain the phase diagram in the temperature-concentration space. We also have verified that the autocorrelation time diminishes in the presence of dilution and correlation, showing that the Wolff algorithm performs even better in such situations. [S0163-1829(97)06146-8]

I. INTRODUCTION

For randomly diluted magnetic systems the critical concentration where the magnetic order vanishes is of great interest. The dependence of the critical temperature on the concentration is ruled by the topological properties of the lattice and by the symmetry of the interaction Hamiltonian.

In the simplest description of a dilute magnet, the occupied lattice sites correspond to magnetic atoms and the empty sites are associated with the presence of nonmagnetic atoms (impurities). Interactions are short ranged, usually of the exchange interaction type. The strength of the exchange interaction is not affected by their neighbors. At $T=0$, the cluster structure is well described by the ordinary site percolation model.

However, it has been found experimentally that sometimes the *local environment* may modify the exchange coupling constant between two atoms or may even suppress their magnetic manifestations. This means that interactions involving more than two atoms are present in the system. To take these effects into account, two kinds of correlations were proposed: the long- and the short-ranged correlation models. The bootstrap percolation model[1] is a good example for the former and the site-bond-correlated model[2,3] for the latter. Long-ranged correlation may change the critical exponents or even the order of the transition of its corresponding uncorrelated model. In contrast, the short-ranged correlation seems to be unable to cause such drastic effects. Anyway, for these systems, dilution as well as correlation plays an important role.

An analysis of ^{19}F NMR linewidths in the randomly diluted magnetic system $KNi_xMg_{1-x}F_3$ and in the isostructural compound $KMn_xMg_{1-x}F_3$ (where x is the concentration) show remarkable differences in their properties.[2,4] For instance, the concentration and percolation thresholds where the magnetic order ceases are different. Further, the former displays an upward curvature in the temperature-concentration plane which is absent in the latter. In order to explain these facts, Aguiar *et al.*[2] proposed a dilution model where the exchange coupling constant of two ions Ni^{2+} depends directionally on the magnetic attributes of their nearest-neighbor atoms. That is, the magnetic spins are correlated. In a subsequent work,[3] a parameter α was introduced which is a measure of the correlation strength. When $\alpha>0$ or $\alpha<0$ we have *ferro-* or *antiferromagnetic correlation*, respectively. Due to the presence of both ferro- and antiferromagnetic coupling constants, the antiferromagnetic correlation brings competition to the system and a spin-glass behavior is expected.

The thermal properties of the site-bond-correlated (SBC) Ising model was investigated using several approaches: mean field,[3] Honmura-Kaneyoshi effective field,[5] renormalization group,[6,7] and Monte Carlo renormalization group.[8] Any of these techniques lead to almost the same physical scenario with the exception of the SBC model defined on the Bethe lattice.[9] Here there are some unexpected features which seem to be due to the pathological geometry of the Bethe lattice. Also SBC cluster characteristics have been studied in connection to the percolation problem. For the square lattice, it is now well established that there are two kinds of percolations: the usual site percolation with threshold $p_c\sim0.592$ when $0<\alpha\leqslant1$ and a *correlated* percolation with threshold $p_c\sim0.740$ at $\alpha=0$.[10] There are now strong indications that both percolations belong to the same universality class.[11,12]

As far as we know, Ref. 13 is the only work which treats the thermal properties of the SBC model by using the Monte Carlo technique. In that paper, the parameter α is restricted to be null. Everyone knows that it is very difficult to simulate near phase transitions due to the emergence of the critical slowing down phenomenon. In the SBC model this becomes even worse since dilution together with correlation conspires to weaken the Metropolis technique. Fortunately, for the so-called *cluster algorithms* the dilution makes these algorithms even more robust.[14] In the Ising model (diluted or not) the Metropolis algorithm is a local Monte Carlo method where only one spin is flipped each time. For the *cluster algorithms*, however, the entire cluster can be flipped. Indeed, there are actually two kinds of cluster algorithms: the single-cluster algorithm like the Wolff[15] algorithm and those involving multiple clusters as the Swendsen-Wang[16] and the invaded cluster[17] algorithms.

In spite of the great interest critical slowing down received during the last decades, it is still a hard question to find under what conditions it can be reduced. Two independent strands of thought contributed to enlightening the problem. The first was the search for the so-called ''physical cluster'' of the Ising model. The idea is to find a percolation

problem in absolute harmony with the thermal problem: The temperature where the percolation threshold occurs (T_p) must coincide with the critical temperature (T_c) and also their corresponding critical exponents need to be the same. The ''geometrical cluster,'' i.e., those clusters formed by grouping all nearest neighbors up (or down) spins, were discarded since in three dimensions they neither have $T_p = T_c$ nor are their exponents the same. An explicit construction of ''physical clusters'' was proposed by Coniglio and Klein.[18] Parallel to this research line, Kasteleyn and Fortuin[19] introduced the random cluster model. They proved that the susceptibility of the Ising model is equal to the mean cluster size of the random cluster model on the right side. Gathering these ideas, Swendsen and Wang[16] developed an algorithm for the Potts model. In this algorithm, clusters of spins in the same states are grown and flipped. Thus, a number of spins are updated in a single move and the correlation time is reduced.

In 1989, a *single-cluster* Monte Carlo algorithm was introduced by Wolff[15] for the $O(N)$ spin models as a variation on the Swendsen-Wang scheme for the Ising model and has proven to be even more effective. In the Wolff algorithm only one cluster is formed and flipped with probability 1, whereas in the Swendsen-Wang dynamics all percolation clusters are formed and flipped with probability 1/2. According to Tamayo *et al.*[20] the main reason for a better performance of the Wolff algorithm is that the mean size of the clusters flipped is significantly larger than in the Swendsen-Wang case.

In this paper we generalize the Wolff algorithm to include correlation. Our results are used to construct the SBC phase diagram for many concentrations and for the correlation α in the interval $[0,1]$. We also determine the behavior of the autocorrelation time with both dilution and spatial correlation included in the model. With *augmented* dilution or spatial correlation, our generalized cluster algorithm becomes even better, exhibiting a *decreasing* autocorrelation time. This is a nice and different result, since for *local* algorithms, dilution and correlation always reduce enormously their efficiency.

II. MODEL

In the SBC model the presence of nonmagnetic impurities in the neighborhood of a given pair of nearest-neighbor magnetic atoms can modify the strength of the exchange interaction between the two atoms. Moreover, in the limit of strong correlation α, the correlation can even suppress the relevant exchange interaction.

The model Hamiltonian is the following:

$$H = -\sum_{i,\delta} J_{i,i+\delta}(\sigma_i \sigma_{i+\delta} - 1), \tag{1}$$

where $\sigma_i = \pm 1$ and δ denotes an elementary lattice vector. The exchange interaction $J_{i,i+\delta}$ is given by

$$J_{i,i+\delta} = J\varepsilon_i \varepsilon_{i+\delta}[(1-\alpha)\varepsilon_{i-\delta}\varepsilon_{i+2\delta} + \alpha], \tag{2}$$

where $J > 0$. The random variables ε_i can take values 1 with probability C and 0 with probability $1-C$, where C is the concentration of magnetic atoms. The parameter α correlates the interaction between sites i and $i+\delta$ with the magnetic occupancy of the sites $i-\delta$ and $i+2\delta$. The uncorrelated dilute Ising model is reobtained in the limit $\alpha = 1$. For $0 < \alpha < 1$, the bond between i and $i+\delta$ is only weakened by the absence of a magnetic atom at $i-\delta$ or $i+2\delta$. The limit $\alpha = 0$ corresponds to the maximum correlation, i.e., two magnetic first-neighbor sites are connected by an active bond only if their nearest-neighbor sites along the line joining them are also present.

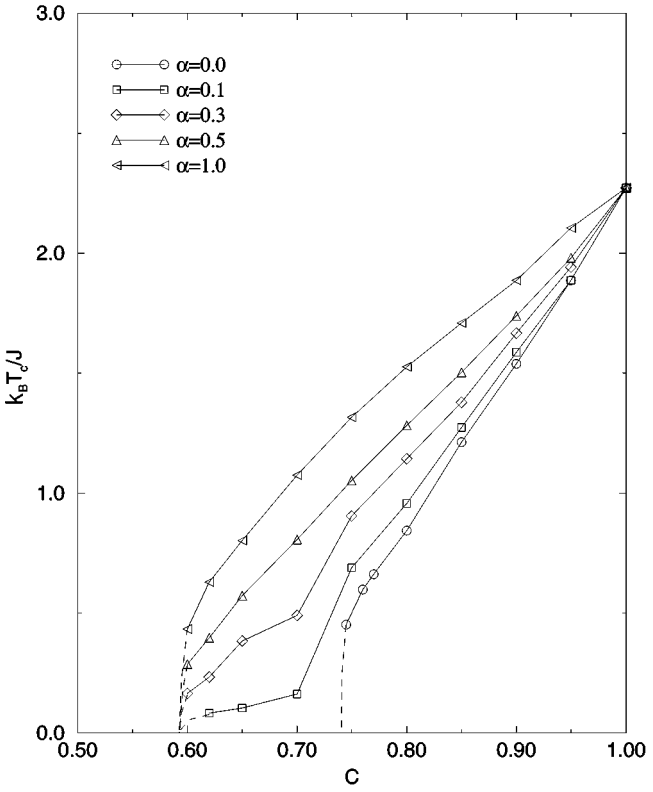

FIG. 1. The SBC Ising model phase diagram for many values of α. The percolation thresholds are 0.740 and 0.592 for $\alpha = 0$ and $0 < \alpha \leqslant 1$, respectively. The dashed lines are only a guide to the eye.

III. FORTUIN-KASTELEYN MAPPING

In the Wolff algorithm for the pure Ising model, first a site is randomly chosen in the lattice. A nearest-neighbor site will be added to the cluster with an activation probability $p = 1 - e^{-2K}$ (where $K = J/K_B T$) if it is in the same spin state. This procedure is repeated until no more sites can be incorporated to the cluster. The whole cluster is then flipped. Following Fortuin and Kasteleyn,[19] we derive the bond activation probability,

$$p_{i.i+\delta} = 0 \quad \text{if} \quad \sigma_i \neq \sigma_{i+\delta},$$

$$p_{i.i+\delta} = 1 - e^{-2K} \quad \text{if} \quad \sigma_i = \sigma_{i+\delta} \quad \text{and} \quad \varepsilon_{i-\delta}\varepsilon_{i+2\delta} = 1,$$

$$p_{i.i+\delta} = 1 - e^{-2\alpha K} \quad \text{if} \quad \sigma_i = \sigma_{i+\delta} \quad \text{and} \quad \varepsilon_{i-\delta}\varepsilon_{i+2\delta} = 0,$$

TABLE I. Range of the number of samples, N_s, and number of iterations, N_i, used in this work. The numbers N_s and N_i are increased for small α (strong correlation) and C (strong dilution).

L	N_s	N_i
50	20−150	3000−5000
100	05−50	3000−5000
150	05−50	3000−5000
300	05−50	3000−10000

between sites i and $i+\delta$. The definition of these activation probabilities guarantees correctly the applicability of the cluster dynamics and constitutes the Fortuin-Kasteleyn mapping for the SBC model.

IV. PHASE DIAGRAM

We simulate the SBC model for various values of correlation (α) and concentration (C) on a square lattice of size $L=50$, 100, 150, and 300. A random uniformly distributed magnetic sites configuration (or simply *sample*) is generated with an occupation probability C. Over this quenched (geometric) configuration, an *initial* spin configuration is chosen with half of the spins up. One Wolff's cluster is then constructed using the activation probabilities just described. The entire cluster is then flipped and the new magnetization is determined. We call the sequence: cluster construction+ flipping+magnetization measure *one* iteration or Monte Carlo step. Our first 1000 iterations were discarded while the system achieves thermal equilibrium. The remaining iterations were used to measure the mean magnetization and its fluctuation—the magnetic susceptibility. On these quantities, another average over the samples was necessary in order to anneal the geometric influence (always present in diluted systems). Finally, we scan the coupling K to find $K_{\max}$ where the susceptibility is maximum. In Table I we show the number of iterations and realizations necessary to reduce the error of $K_{\max}$ to ~ 0.01. Of course, they depend on the values of α and C.

The determination of $K_{\max}$ was done for fixed values of α, C, and L and then extrapolated to the thermodynamic limit $L\to\infty$ through the BST algorithm.[21] The BST is a useful algorithm to extrapolate physical quantities that converge obeying a power law $F(L)=F(L=\infty)+AL^{-\Theta}$. It allows a reliable determination of critical parameters in the limit $L\to\infty$ and its versatility becomes more pronounced if there are only very short sequences available (see Fig. 1).

TABLE II. The number of samples, N_s, and number of iterations, N_i, used to get the autocorrelation time.

L	N_s	N_i
16	400	40000
32	300	50000
64	200	80000
128	200	80000

V. AUTOCORRELATION TIME BEHAVIOR

Before we come to our results, it is appropriate to define the statistically relevant quantities necessary to obtain the system dynamical properties. The normalized autocorrelation function $\rho(t)$ and the integrated autocorrelation time $\tau_{\rm int}$ are given by

$$\rho(t)=\frac{\langle O_j O_{j+t}\rangle-\langle O\rangle^2}{\langle O^2\rangle-\langle O\rangle^2}, \tag{3}$$

$$\tau_{\rm int}=\frac{1}{2}\sum_{t=-\infty}^{\infty}\rho(t)=\frac{1}{2}+\sum_{t=1}^{\infty}\rho(t), \tag{4}$$

where O_j is the value of an observable (here, the magnetization) in the configuration j. The brackets mean averages made on the configurational space. The mean autocorrelation time $\langle\tau_{\rm int}\rangle$ was estimated after a sample average. Since one Wolff step has a computational cost of the cluster size $|S|$, we need to rescale $\langle\tau_{\rm int}\rangle$,[15]

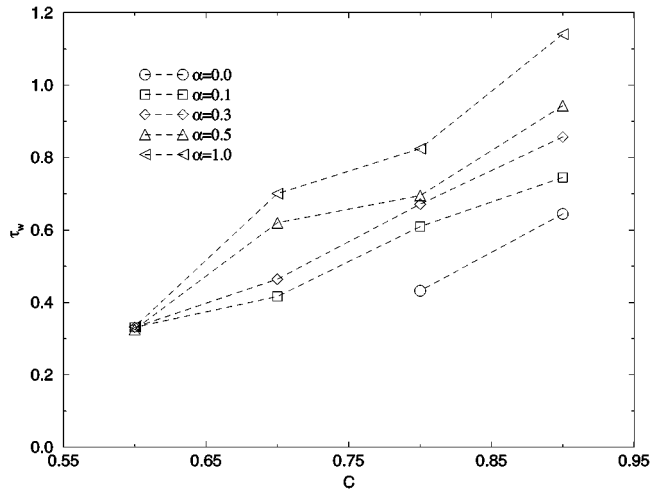

FIG. 2. Dependence of the autocorrelation time with the dilution for fixed lattice size $L=64$.

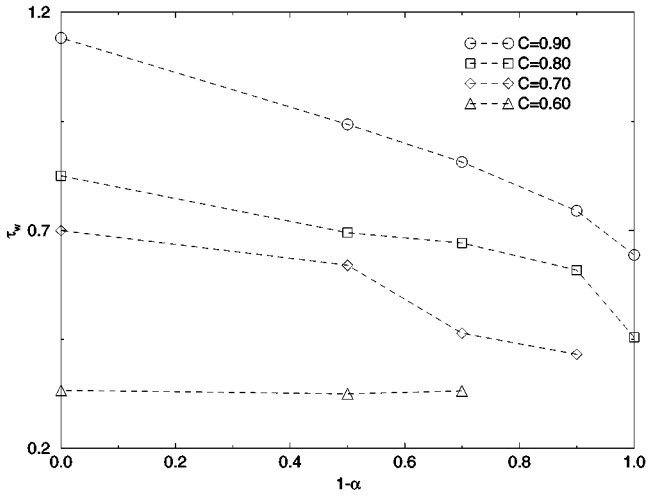

FIG. 3. Plot of the autocorrelation time versus the correlation for fixed lattice size $L=64$.

$$\tau_w = \langle \tau_{\rm int} \rangle \quad \frac{\langle |S| \rangle}{CL^d}, \tag{5}$$

where d is the lattice dimensionality. This is the correct rescaling for $\langle \tau_{\rm int} \rangle$ since the total magnetic mass of the dilute system is CL^d. In Table II we show the lattice sizes, the number of iterations and realizations necessary to reduce the error of τ_w up to 1% or 2%. A large number of samples is needed in order to diminish the geometric fluctuations present in diluted systems.

In Figs. 2 and 3, we plot the τ_w dependence on the dilution and correlation, respectively. The autocorrelation time decreases with the dilution for all values of the correlation α and with the correlation for all values of the concentration C. This behavior is completely opposite to that exhibited by *local* algorithms. For example, in the Metropolis algorithm the probability to flip one single spin depends exponentially on the ratio between the energy increment (produced by the spin flip) and the temperature. This means that a smaller critical temperature leads to a smaller acceptance rate for energetically unfavorable spin flips. On the other hand, for the cluster algorithms the presence of dilution and correlation has antagonistic effects. Indeed, the bond activation probability (see Sec. III) increases when the critical temperature is reduced. This simple argument works very well for the dilution aspect but it is not so straightforward concerning the correlation. In the last case there is a competition between the temperature and the correlation α. Both parameters appear in the exponent (see the bond activation formula in Sec. III) in the form $\sim \alpha/T_c$. If for a fixed concentration C we *augment* the correlation (i.e., diminish α), our results show that the critical temperature T_c decreases faster than α. So even in the case of stronger correlation, the Wolff algorithms performed very well.

VI. CONCLUSIONS

The phase diagram is shown in Fig. 1. The initial slope $(1/T_c)(dT_c/dC)$ at the pure $C=1$ case increases with the degree of correlation, which is supported by both experimental[2] and theoretical[3,5,13] data. At $T=0$, we obtain two distinct percolation thresholds: one for $\alpha=0$ and another for $\alpha \neq 0$. It can be seen in the figure that the curves for intermediate correlation $0<\alpha<1$ have an upward curvature (not present in the extreme cases $\alpha=0$ and $\alpha=1$) in agreement with the *experimental* results for the $KNi_xMg_{1-x}F_3$ compound.[2] Our results show this behavior in a more clear way than previous work.[6] Further, our localization of the critical concentration (at $T=0$) is more precise than those obtained using other techniques[3,5] and it is in good agreement with earlier results in the context of the percolation theory.[12]

From Figs. 2 and 3 we conclude that the Wolff algorithm performs even better in the presence of both dilution and correlation. This means that for diluted systems, the Wolff algorithm should be preferred to single-spin-flip algorithms. The more delicate question about the dynamical universality class requires an exhaustive computational effort and is now under investigation.

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