Microcanonical simulation of the site-diluted three-dimensional Ising model

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We use a microcanonical simulation to obtain the phase diagram in the temperature-concentration space of the three-dimensional site-diluted Ising model, for concentrations of magnetic atoms in the range $1 \geq p \geq 0.4$. The temperature and concentration dependence of the magnetization, internal energy, and specific heat are calculated on $32 \times 32 \times 32$ lattices. The resulting phase diagram agrees well with recent Monte Carlo simulations and extends the numerical estimates up to the regime of strong dilution.

I. INTRODUCTION

In this paper we report the results of microcanonical simulations of the site-diluted simple cubic Ising model with nearest-neighbor interactions, having quenched and randomly distributed magnetic atoms. The simulations were performed on lattices of size $L = 32$ with periodic boundary conditions, and for various magnetic concentrations between $p = 0.4$ and $p = 1$. For each value of p our procedure allows a simultaneous simulation of 32 samples at the same energy. The system Hamiltonian is

$$H_S = -\sum_{\langle i,j \rangle} J\epsilon_i\epsilon_j\sigma_i\sigma_j, \tag{1}$$

where $\sigma_i = \pm 1$ are the Ising spin variables and the configurational (random) variables ϵ_i can take values one, with probability p, and zero, with probability $(1-p)$. The sum is over all nearest-neighbor pairs of sites, and $J > 0$ is the ferromagnetic exchange interaction.

Most of the numerical simulations of the model system (1) were based on Monte Carlo (MC) algorithms, and were centered on the investigation of the effects of disorder in critical phenomena. In particular, for the three-dimensional Ising model, where the specific heat exponent of the pure system is positive, the theoretical picture[1] of sharp transitions with varying critical exponents has been supported by previous Monte Carlo calculations.[2–8] On the contrary, there only exist a few attempts at using deterministic algorithms to simulate quenched site-dilute models.[9] These works were mainly motivated by the effects of dilution on the nature of the phase transitions of q-state Potts models.[10] The authors of Ref. 9 used the multilattice microcanonical simulation technique[11] to determine the energy-temperature curve and locate the tricritical point induced by dilution.

The multilattice microcanonical simulation (MLMS) method consists in applying the multilattice technique[12] to the Creutz algorithm.[13] The characteristic feature of the MLMS method is to simultaneously simulate many model systems at the same energy. Within Creutz's proposal the system is not isolated at all, but it can exchange energy with a much smaller system called a "demon." The demon works as a local heat bath and it travels around the system trying to change its dynamic variables. The energy that the demon can carry is bounded, and the change is accepted if the demon either can absorb the energy released or has enough energy to supply the amount of energy required by the system. Hence, the total energy of the system plus the demon remains constant.

The application of the Creutz algorithm to the three-dimensional site-diluted Ising model has not yet been reported in the literature. In the present work we use the MLMS technique to study the thermodynamic properties of such a disordered system in a wide range of temperature (energy) and concentration. Section II describes briefly the computational procedure. In Sec. III we present our results, and make a comparison with previous Monte Carlo data for both the critical temperature and the critical energy. Our conclusions are presented in Sec. IV.

II. THE SIMULATION PROCEDURE

In order to generate an ensemble of configurations microcanonically distributed of the Hamiltonian (1) we used the Creutz algorithm.[13] In the present implementation we follow the suggestion of Wilson and Vause,[11] which consists in simultaneously simulating multiple lattices. This kind of approach is particularly useful when quenched disorder comes into play, since each lattice system represents an independent sample and the relevant configurational averages are automatically carried out.

The occupation (static) variables ϵ_i of all the 32 systems are stored in an array of length 32^3 (the number of sites in the simple cubic lattice), in which the bits are

independently set with probability p. The corresponding spin (dynamic) variables σ_i are stored in another array of length 32^3. In both arrays, all bits of the same order within a computer word are associated to only one sample. From an arbitrary magnetic configuration, e.g., all samples in a ground-state configuration, we put them in independent configurations with a previously specified energy by frustrating an appropriated number of bonds. The demon states are stored in three computer words (see below), with each demon and its respective sample corresponding to the same bit position in a word. The demons are initialized to zero energy.

According to the Creutz algorithm, each demon travels around its respective lattice trying to flip the spins. A flip is accepted only if $\Delta H_S + \Delta H_D = 0$, where H_S and H_D are the system energy and the demon energy, respectively. During the flip procedure the simple cubic lattice is divided into two interpenetrating sublattices and the demon visits sequentially the sites of a given sublattice. A new configuration is generated after the demon has visited all sites of both sublattices: This corresponds to one MLMS step.

For the simple cubic randomly dilute Ising model with first neighbor interaction, Eq. (1), $\Delta H_S/J$ is an even integer ranging from -12 to $+12$. Therefore, a convenient choice for the demon energy is

$$H_D = 2J\delta, \tag{2}$$

where $2J$ is the smallest possible variation of the system energy, and $\delta = 0, 1, \ldots, \delta_{\max}$. It follows that the new demon state is specified by

$$\delta' = \delta + 2n_f - z, \tag{3}$$

where n_f is the number of frustrated nearest-neighbor bonds in the old configuration and z the number of nearest-neighbor sites occupied by magnetic atoms. Further we should have $0 \leq \delta' \leq \delta_{\max}$; otherwise, the flip is rejected. We have chosen $\delta_{\max} = 7$ in order to accommodate the demon energy into only three computer words, and still allow all possible changes in the system energy. This also saves computer time since the overall procedure is accomplished by logical operations.

Another function of the demon is to provide a means to probe the temperature of the system. By noting that during the simulation each demon state occurs a number of times proportional to its Boltzmann factor, we have sampled the $\delta = 0$ and $\delta = 1$ states to calculate the temperature.[14]

III. RESULTS

By employing the multilattice microcanonical simulation (MLMS) technique we have done extensive simulations of site-diluted simple cubic Ising models of size $32 \times 32 \times 32$, and with periodic boundary conditions. For a given value of concentration, the configurational averages were obtained from the data of simulations on 32 independent samples with random distribution of impurities. The errors are standard deviations of the mean values. For each value of energy, we ignored the first 100 configurations, which represent 10% of the 1000 equilibrium configurations per sample considered in the microcanonical averages. Therefore, our final results included a total of 32×10^3 equilibrium configurations.

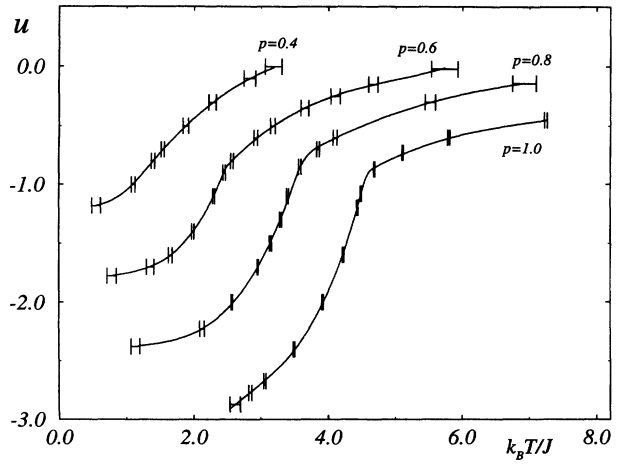

FIG. 1. Temperature dependence of the internal energy per magnetic site of the site-diluted simple cubic Ising model, for various concentrations p of magnetic sites. The curves are cubic spline fit to the numerical data.

In Fig. 1 we plotted the specific internal energy $u = E/Np$ as a function of the temperature for some values of the magnetic concentration p, where Np is the effective number of magnetic sites. The curves were obtained by making a cubic spline fit to the numerical data. In order to estimate the system temperature from the data of simulation at a given energy, the demon states were sampled after visiting 100 sites. However, for energies $u \ll u_c$ and $u \gg u_c$, where u_c is the critical energy, we sampled the demon states at intervals of five to ten visits, since we notice in these limit cases that the errors in the calculated temperatures are systematically larger than those for intermediate energies. In fact, this reflects the difficulty of simulating the system at even higher and lower energies (temperatures), and it may also be seen as an evidence of lack of ergodicity of the Creutz's algorithm.

In Fig. 2 we display the magnetization $m = \langle\langle|\Sigma_i \epsilon_i \sigma_i|\rangle\rangle/Np$ plotted against the temperature, where now we have statistical errors in both axes. The data for $p = 0.4$, 0.7, and 1.0 plotted against the reduced temperature $T/T_c(p)$ show that (see inset), for energies above the critical energy u_c, the finite size effects are enhanced for those systems with smaller values of concentration.

The dependence of the critical energy on the concentration $x = 1 - p$ of nonmagnetic impurities is shown in Fig. 3, where we plot our results (open symbols) for $u_c = u(x, T_c)/u(x, T = 0)$. The value for the critical energy in the pure ($x = 0$) system was taken from our previous work.[14] In the present paper, both the critical energy values and the error bars were obtained from the corresponding values for the critical temperatures shown in Table I, where we used the relation for $u(x, T)$ according to the fitting curves of Fig. 1. Comparing our results with those of previous MC calculations (dashed

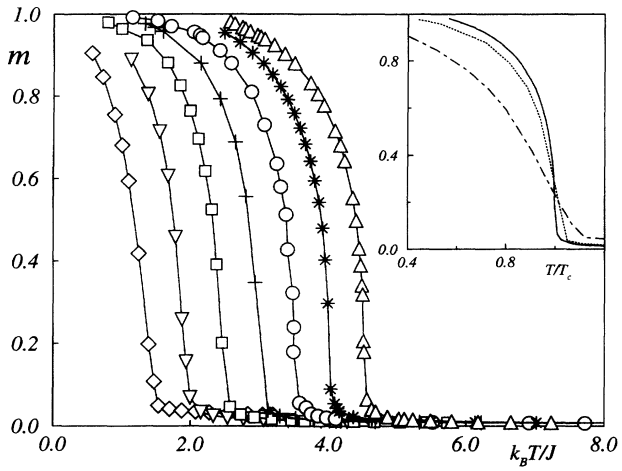

FIG. 2. Temperature dependence of the magnetization for values of p=0.4, 0.5, 0.6, 0.7, 0.8, 0.9, and 1.0 (curves from left to right). The inset shows the magnetization plotted against the reduced temperature $T/T_c(p)$, for $p = 0.4$ (dashed line), 0.7 (dotted line), and 1.0 (solid line).

line),[2,16] one notices a complete agreement in the region of low dilution $x \leq 0.2$, whereas, except for the most diluted system with $x = 0.6$, the observed deviations are within error bars. We also show the experimental results (solid symbols) (Ref. 15) on the diluted antiferromagnet $Co_{1-x}Zn_xCs_3Cl_5$, along with the curve (solid line in Fig. 3) for $u_c(x) = 0.269/(1-x)$ expected for Ising bcc models which follows closely the experimental data. We conclude that the MC data on simple cubic lattices (see also Refs. 2 and 16) cannot be directly compared with the experimental results shown in Fig. 3. Furthermore, the present analysis suggests that a simulation of the site-diluted bcc Ising models, with coordination number $z = 8$, is required.

The temperature and concentration dependence of the specific heat, calculated from the numerical derivative of

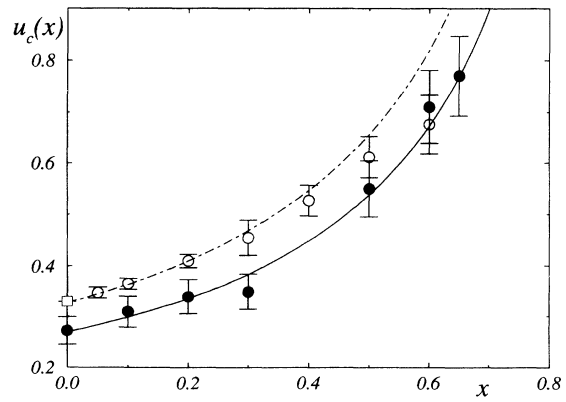

FIG. 3. The reduced critical energy as a function of the concentration x of non-magnetic impurities. The symbols are the following: open circles (this work), open square (Ref. 14), and solid circles (Ref. 15). The dashed line $u_c(x) = 0.328/(1-x)$ follows from the Monte Carlo data of Refs. 2 and 16, whereas the solid line corresponds to the experimental results of Ref. 15 (see text).

TABLE I. Critical temperature $T_c(p)$, for the three-dimensional site-diluted Ising model.

p	$T_c(p)$		
	This work	Ref. 17	Ref. 3
1.00	4.514(15)	4.5115(1)	4.511(6)
0.95	4.259(16)	4.2622(4)	4.263(6)
0.90	4.01(2)	4.0108(5)	4.030(6)
0.80	3.50(2)	3.4992(5)	3.505(6)
0.70	2.98(5)	—	3.045(6)
0.60	2.41(4)	2.4220(6)	2.509(6)
0.50	1.86(6)	—	1.968(6)
0.40	1.37(10)	—	1.449(11)

the specific internal energy (curves shown in Fig. 1), present a well-defined peak even for magnetic concentrations down to $p = 0.5$, indicating that the phase transition remains sharp for all systems with $p \geq 0.5$. The critical temperature for a given concentration, $T_c(p)$, was determined from the position of the peak (maximum for $p = 0.4$) in the corresponding specific heat curve. In Table I we display our results together with those of Heuer[17] and Chowdhury and Stauffer.[3] Note that we assumed for the quoted value of $T_c(1)$ given by Ref. 3 to be the same as that of Ref. 17.

A quite good agreement between our results and those of Ref. 17, may be observed spite of the much smaller CPU time spent in the present calculation. (In fact the work of Ref. 17 is mainly concerned with accurate evaluations of concentration-dependent exponents.) Except for the most diluted system simulated, $p = 0.4$, where one might expect a stronger dependence on the number of samples and on their effective sizes, all other estimates for $T_c(p)$ have error bars which are smaller than 7%. The observed linear dependence of the critical line with dilution, for all values of concentration considered in this work, indicates a rapid decrease in $T_c(p)$ in the interval between 0.4 and 0.33 (the percolation concentration).

IV. CONCLUSION

In this paper, we have employed the multilattice microcanonical simulation technique to study the thermodynamic behavior of the simple cubic Ising model having quenched (site-diluted) distribution of nonmagnetic impurities. Except in the extreme cases of lower and higher energies (temperatures), where we found some evidence of lack of ergodicity of the Creutz algorithm, our results for the magnetization and the internal energy on the $32 \times 32 \times 32$ lattice spin systems show a smooth variation with dilution. This fact should encourage further works on disordered systems using microcanonical simulation methods.

We have also calculated the concentration dependence of both the critical energy and the critical temperature. Our results for $u_c(x)$ and $T_c(x)$ agree reasonably well with previous Monte Carlo calculations. We recall that in the present work, the values of $T_c(x)$ are determined from the location of the peaks of the specific heat. Accordingly, a precise determination of the critical energy

is strongly dependent on this naive method of obtaining the critical temperature. We conclude that the estimated errors in these quantities reflect such a methodology rather than the statistical quality of our data. A direct method of analysis of the critical behavior, which we are not concerned here, consists in obtaining the critical energy without knowledge of the critical temperature, and vice versa.[14] Work in this direction is in progress.

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