Monte Carlo studies of the critical behavior of site-dilute two-dimensional Ising models*

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The results of Monte Carlo studies of the critical properties of finite site-dilute two-dimensional spin-1/2 Ising models are reported. Numerical values are obtained for the magnetization, internal energy, specific heat, and susceptibility. The dependence of the Curie temperature on dilution is determined and compared with predictions from series analysis. Possible power-law behavior in the susceptibility is also discussed.

The purpose of this paper is to report the results of Monte Carlo studies of the critical behavior of site-dilute two-dimensional spin-$\frac{1}{2}$ Ising ferromagnets. The calculations were carried out on 40×40 arrays with periodic boundary conditions for relative (average) fractions of magnetic atoms p equal to 0.7, 0.8, and 0.9. We present graphs displaying the temperature dependence of the magnetization, internal energy, specific heat, and susceptibility. Estimates are obtained for the dependence of the critical temperature on dilution and compared with the results of series calculations for the plane triangular lattice.[1] Possible power-law behavior in the susceptibility is also discussed.

Since the use of Monte Carlo techniques to study critical phenomena in Ising systems has been reviewed by Landau[2] and Binder[3] we will not go into detail on the mathematical techniques other than to state that each run involved up to 4000 Monte Carlo steps per spin, with the longest runs in the vicinity of the Curie point. For each value of p calculations were carried out with five different distributions of magnetic atoms. The outcomes of the various runs were then averaged together, giving the data shown in Fig. 1.

The calculations were based on the Hamiltonian

$$H=-\sum_{i,j} J_{ij}\sigma_i\sigma_j, \tag{1}$$

where the sum is over nearest-neighbor pairs, and $\sigma_i=\pm 1$. The exchange integral $J_{ij}=1$, if i and j are both magnetic atoms, and zero, otherwise. In Fig. 1 we display our data for the magnetization S, the internal energy U, the specific heat C_H, and the susceptibility χ. These functions are defined by the equations

$$S=\frac{1}{N}\sum_i \langle\sigma_i\rangle, \tag{2}$$

$$U=-\frac{1}{N}\sum_{i,j} J_{ij}\langle\sigma_i\sigma_j\rangle, \tag{3}$$

$$C_H=\frac{1}{NT^2}\sum_{i,j}\sum_{k,l} J_{ij}J_{kl}\,(\langle\sigma_i\sigma_j\sigma_k\sigma_l\rangle-\langle\sigma_i\sigma_j\rangle\langle\sigma_k\sigma_l\rangle), \tag{4}$$

$$\chi=\frac{1}{NT}\sum_{i,j}(\langle\sigma_i\sigma_j\rangle-\langle\sigma_i\rangle\langle\sigma_j\rangle), \tag{5}$$

where the sums are over the N magnetic atoms, T is the temperature in units of J_{ij}, and $\langle\ \rangle$ denotes a thermal average in the Monte Carlo sense.[2,3] In each case the functions are plotted against the scaled temperature $T/T_C(1)$, where $T_C(1)$ is the Curie temperature of the infinite lattice with $p=1$, 2.269, ...

Our data are to be compared with the corresponding results for the pure ($p=1$) lattice reported by Landau.[2,4] The "critical region" in each graph is seen to shift to lower temperatures with increasing dilution. In the case of the magnetization we identify the Curie temperature with the point of maximum slope, whereas in the case of the susceptibility and specific heat it is the point where the corresponding function is a maximum. Our values for the transition temperature obtained by the use of these criteria are shown in Fig. 2, where we have plotted $T_C(p)/T_C(1)$ vs p.

It is apparent that the various values of $T_C(p)/T_C(1)$ are close to one another for $p=0.9$ and 0.8. In the case of $p=0.7$ there is a noticeable spreading which reflects the relative smearing of the transition indicated in Fig. 1. Also shown in Fig. 2 is a straight line with slope 1.47, which passes close to the center of gravity of the cluster of points at $p=0.9$. From the data we infer an initial slope in $T_C(p)/T_C(1)$ equal to 1.47 ± 0.05, which is very close to the value for the plane triangular lattice, 1.45 ± 0.05, reported in Ref. 1. The values of T_C for $p=0.7$ fall unexpectedly near the line. Since the critical percolation concentration for this lattice is 0.59,[5] this would indicate a rapid decrease in $T_C(p)$ in the interval between 0.59 and 0.7.

In Fig. 3 we have plotted $\ln[T_C'(p)\chi]$ vs $\ln|T/T_C'(p)-1|$, $T_C'(p)$ being the temperature of the maximum in χ. In this plot we have drawn parallel straight lines in the regions of maximum slope to emphasize similarities in the behavior for the different concentrations. As expected, the magnitudes of the slopes are extremely sensitive to the choice of $T_C'(p)$. Taking $T_C'(0.9)$ to be smaller by about 2% leads to curves with slopes which are the same above and below T_C, with the common value 1.78, which is close to 1.75, the value for $p=1$. A decrease in the effective value of $T_C(p)$ may be at least partly attributed to finite-size effects. For $p=1$ $T_C(N=40)$ is about 0.8% above $T_C(N=\infty)$.[6]

The insensitivity of the slope to p is in contrast

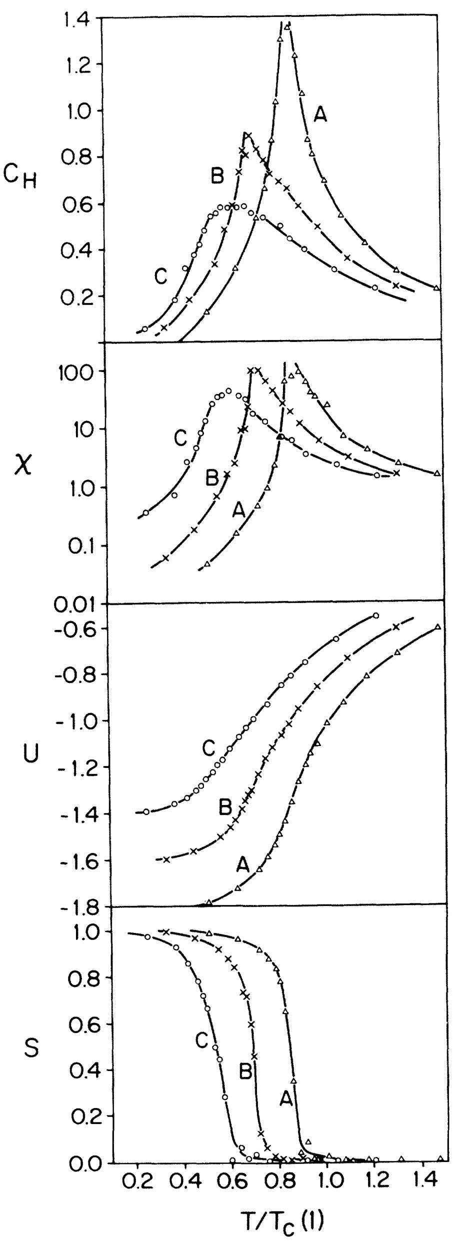

FIG. 1. Specific heat C_H, susceptibility χ, internal energy U, and magnetization S vs $T/T_C(1)$ for different concentrations p of magnetic atoms. A: $p=0.9$; B: $p=0.8$; C: $p=0.7$. The data points are the averages of five runs with different configurations of magnetic atoms. The curves are drawn as a guide to the eye.

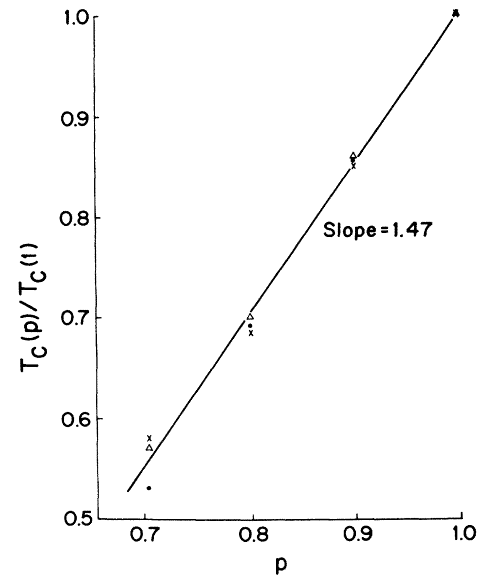

FIG. 2. Transition temperature vs p. The solid circles, crosses, and triangles correspond to values of $T_C(p)$ determined from the magnetization, specific heat, and susceptibility data, respectively.

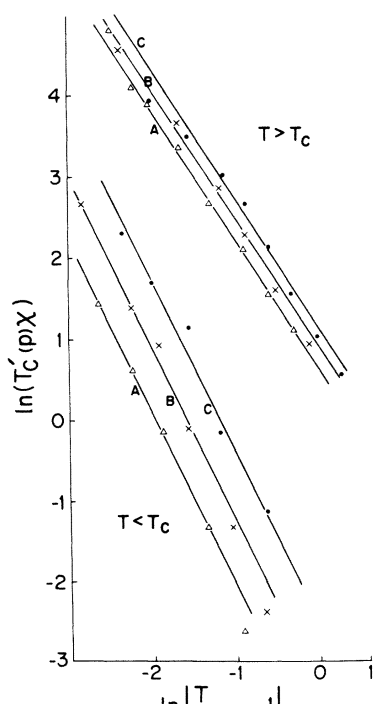

FIG. 3. $\ln[T_C'(p)\chi]$ vs $\ln|T/T_C'(p)-1|$. A (triangles): $p=0.9$; B (crosses): $p=0.8$; C (solid circles): $p=0.7$. The data points are the averages of five runs with different initial configurations. The straight lines are drawn to emphasize similarities in behavior for different p.

to the (physically implausible) results of series analysis on site-dilute systems.[1,7,8] These studies indicate a rapid increase in $\gamma(p)$ with decreasing[9] p [$\gamma(p) > 2.5$ for $p < 0.8$ in the plane triangular lattice[1]]. Unfortunately our results are not sufficiently accurate to test current heuristic[10] and renormalization-group[11–13] arguments which predict no change in the critical exponents of disordered systems when the specific-heat exponent of the corresponding ordered system is negative[14] (apart from possible logarithmic corrections when $\alpha = 0$, which is the value appropriate to the two-dimensional Ising model).

In summary, we have demonstrated that Monte Carlo techniques can be used to provide information about the critical behavior of disordered magnets. It is hoped that this work will lead to further Monte Carlo studies of both the static and the dynamic properties of these systems.

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[6]D. P. Landau (private communication). After submitting this manuscript we received an unpublished report of calculations by E. Stoll and T. Schneider on site-diluted 110×110 lattices with $p \geq 0.9$. Their value for $T_C(0.9)$ is slightly below ours [$T_C(0.9) = 0.836\, T_C(1)$, as opposed to our estimate, $T_C(0.9) = 0.853\, T_C(1)$]. Since finite-size effects are expected to be somewhat less important in the larger lattice, their results are consistent with our explanation for the different slopes shown in Fig. 3. Using their value of $T_C(0.9)$ we obtain susceptibility exponents $\gamma = \gamma' \approx 1.75$. Also, R. Fisch and A. B. Harris have studied a site-diluted 64×64 lattice with $p \geq 0.8$. Their value for the initial slope in $T_C(p)/T_C(1)$ is 1.5 ± 0.1. The work by Stoll and Schneider and by Fisch and Harris is reported in papers 6 D-1 and 6 D-2, respectively, which were presented at the Twenty-First Annual Conference on Magnetism and Magnetic Materials, Philadelphia, December, 1975 (unpublished).

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