# Critical behavior of the bond-dilute two-dimensional Ising model

D. Zobin*
*Department of Physics, Simon Fraser University, Burnaby, British Columbia, Canada V5A 1S6*
(Received 7 March 1978)

We have performed Monte Carlo calculations of the thermodynamic properties of the bond-dilute Ising model on the square lattice. The results are obtained for the magnetization, internal energy, specific heat, and susceptibility for several concentrations of missing bonds. The dependence of the Curie temperature on dilution is in good agreement with the results obtained by other methods. The phase transition is found to remain sharp with the same value of the susceptibility exponent as for the pure Ising model.

In the last few years, there has been growing interest in the critical properties of magnetic systems with quenched randomly distributed impurities. Recent remormalization-group calculations,[1,2] in general, confirm a heuristic argument of Harris[3] which predicts no change in the critical behavior of a disordered system if the specific-heat exponent $\alpha$ of the corresponding pure system is negative, and a possible change in the critical exponents of a disordered system if $\alpha_{\text{pure}} > 0$. However, the Harris criterion is not applicable to the two-dimensional disordered Ising model, since in this case $\alpha_{\text{pure}} = 0$. There have been a number of studies of this particular model, both near the percolation threshold $p = p_c$,[4] where the phase transition is "geometrically driven," and at low concentration of nonmagnetic impurities $p \lesssim 1$.[5] Most of the recent work is based on the use of position-space renormalization-group methods which apply directly to physical dimensionalities. In particular, Jayaprakash *et al.*[6] have employed a generalization of the Migdal-Kadanoff recursion relations to calculate the phase diagram, the critical and percolation exponents, and thermodynamic functions for the bond-dilute two-dimensional Ising model. They find that the critical region becomes narrower as $p$ decreases and that the critical behavior for $p > p_c$ exhibits pure-system exponents. There have also been a number of Monte Carlo calculations,[7-9] all performed for the site-dilute two-dimensional Ising model. Whereas Ching and Huber[7] and Stoll and Schneider[8] find a sharp transition with the pure-system susceptibility exponent $\gamma$ for $p > 0.7$ and $p > 0.9$, respectively, the results obtained by Fish and Harris[9] are less unambiguous.

In the present paper, we wish to report the results of Monte Carlo studies of the bond-dilute Ising model on the square lattice. To the best of our knowledge this is the first extensive Monte Carlo simulation of thermodynamic properties of a magnetic system with bond dilution.

The calculations were performed using the same Monte Carlo method as was applied to the pure[10] and site-dilute Ising models.[7] The Hamiltonian we consider is given by

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

where $\sigma_i = \pm 1$ are the Ising spins occupying the sites of the square lattice, and the sum is over all pairs of nearest neighbors. The exchange coupling constant $J_{ij}$ is 0 or 1 with probabilities $1-p$ and $p$, respectively. We have calculated the magnetization $M$, the internal energy $E$, the specific heat $C$, and the susceptibility $\chi$ using the following definitions of these quantities[10]:

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

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

$$C = \frac{1}{k_B T^2}\left(\langle E^2 \rangle - \langle E \rangle^2\right), \tag{4}$$

$$\chi = \frac{1}{k_B T}\left(\langle M^2 \rangle - \langle M \rangle^2\right). \tag{5}$$

Here, $N$ is the total number of atoms in the sample, and $\langle \cdots \rangle$ denotes the statistical-mechanical expectation value in the Monte Carlo sense.[10]

The calculations were carried out for $p = 1.0$, 0.9, 0.8, 0.7, and 0.6 using samples containing 1600 ($40\times40$) and 3600 ($60\times60$) atoms with periodic boundary conditions (i.e., the lattice is wrapped on a torus). The first 500 Monte Carlo steps were discarded and the averages were computed from the next 4000 steps per spin for $40\times40$ arrays, and from 2000 steps per spin for $60\times60$ arrays. The initial state at each temperature was chosen to be either the equilibrium state generated at a lower nearby temperature or the ferromagnetic ground state with all the $\sigma_i = +1$.[11]

 

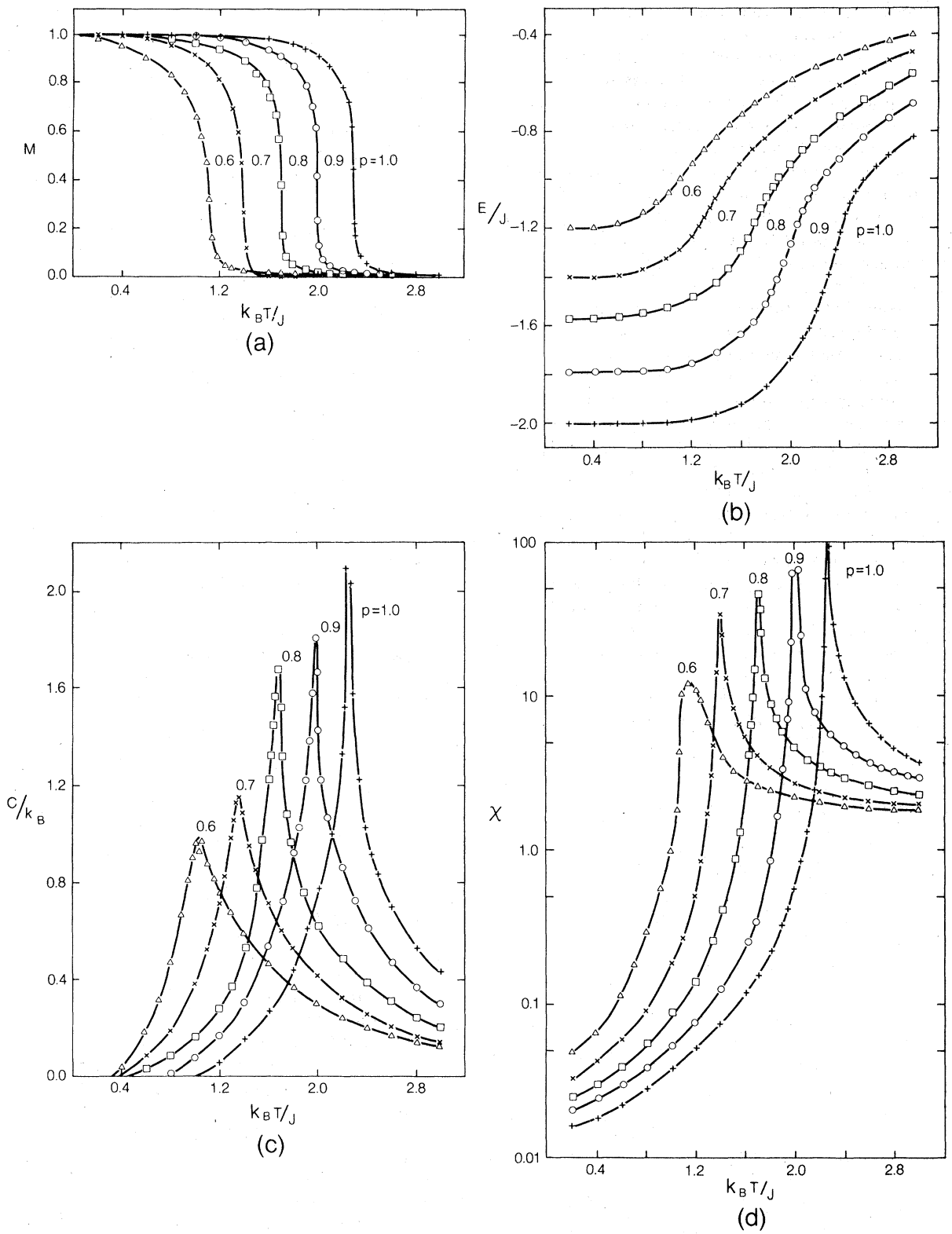


FIG. 1. Temperature dependence of the magnetization (a), internal energy (b), specific heat (c), and susceptibility (d) for five values of the concentration of ferromagnetic bonds—$p = 1.0$ (pure case), 0.9, 0.8, 0.7, 0.6. The data points have been obtained according to the procedure described in the text.

The results were obtained by averaging over six different distributions of exchange interactions—three for $40\times40$ samples and three for $60\times60$ samples. Averaging over the outcomes of the runs for lattices of two different sizes is a legitimate procedure in our case, because the error introduced by the difference in size is smaller than those due to intrinsic properties of the Monte Carlo technique such as the limited fraction of the total number of states which can be sampled.[12]

The results obtained for the thermodynamic functions are shown in Fig. 1. Our data for the pure lattice ($p=1$) are in good agreement with those reported by Landau.[10] Following Ching and Huber,[7] we identify the Curie temperature in the case of the magnetization and internal energy with the point of maximum slope, and in the case of the susceptibility and specific heat with the point where the corresponding function has a maximum. The values for the transition temperature obtained using this method are shown in Fig. 2. The slope of the $T_c(p)$ line is found to be $3.0\pm0.1$. This value is in good agreement with the exact result of Harris,[3] $\partial T_c(p)/\partial p = 3.016$, and with that calculated by Jayaprakash *et al.*[6] who find 3.108. It is, however, somewhat lower than the value of 3.33 obtained by Ching and Huber[7] in their Monte Carlo study of the site-dilute two-dimensional Ising model. Unfortunately, our calculations do not yield sufficient accuracy near the percolation threshold ($p_c=0.5$ for the square lattice). Therefore, we have not been able to determine the initial slope of percolation which is exactly calculable[13]

$$\frac{d}{dp}\exp[-2J/k_BT_c(p)]\Big|_{p=p_c=0.5} = 2\ln 2 \simeq 1.386 . \qquad (6)$$

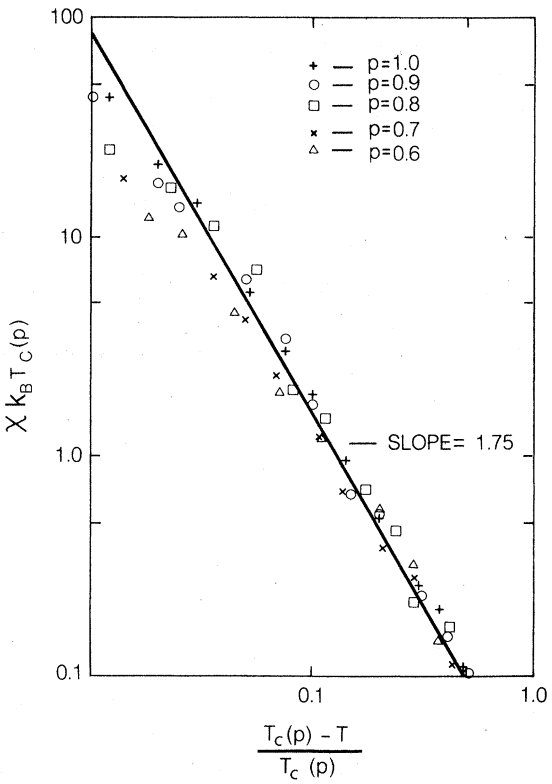


FIG. 3 Log-log plot of the temperature dependence of the isothermal susceptibility for five values of the concentration of ferromagnetic bonds. $T_c(p)$ is the temperature at which the susceptibility [Fig. 1(d)] has a maximum. Also plotted is a straight line with a slope of 1.75.

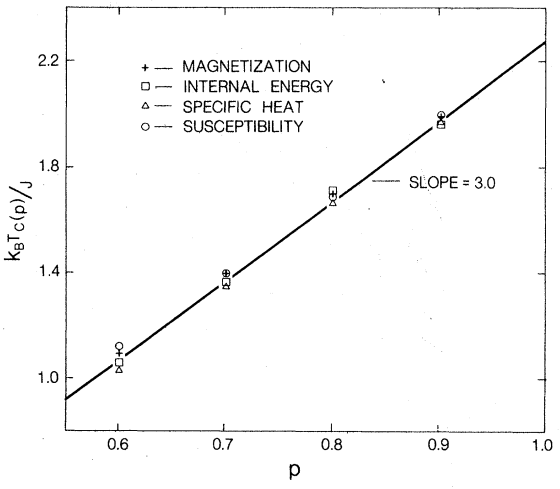


FIG. 2. Transition temperature as a function of the concentration of ferromagnetic bonds. The data points are taken from the temperature dependence of the thermodynamic functions plotted in Fig. 1. Also shown is a straight line with a slope of 3.0.

Finally, in Fig. 3 we have shown on a log-log plot $\chi T_c(p)$ as a function of $[T_c(p)-T]/T_c(p)$ for $p=1.0$, 0.9, 0.8, 0.7, and 0.6. Also shown in Fig. 3 is a straight line with a slope of 1.75, which is the value of the susceptibility exponent in the pure case. The data points are seen to lie very close to the straight line, at least above $[T_c(p)-T]/T_c(p)>0.02$. The deviations observed below this value are probably caused by the finite-size effects as well as the intrinsic Monte Carlo errors mentioned above.

In conclusion, we have performed Monte Carlo calculations for the bond-dilute Ising model on the square lattice. Our results indicate that for the

concentration of magnetic impurities $p \geq 0.6$ the phase transition is sharp and is characterized by the same value of the susceptibility exponent as for the pure system. This is in agreement with the results of various renormalization-group calculations and of the Monte Carlo simulation on the site-dilute two-dimensional Ising model.

ACKNOWLEDGMENTS

The author would like to thank Dr. M. Plischke for his support of this work and for several informative discussions. The National Research Council of Canada is gratefully acknowledged for financial support.

*Present address: Dept. of Physics, Queen's University, Kingston, Ontario, Canada K7L 3N6.

[1]T.C. Lubensky, Phys. Rev. B 11, 3573 (1975).
[2]G. Grinstein and A. Luther, Phys. Rev. B 13, 1329 (1976).
[3]A. B. Harris, J. Phys. C 7, 1671 (1974).
[4]Some of the recent papers are: A. P. Young and R. B. Stinchcombe, J. Phys. C 8, L535 (1975); H. E. Stanley, R. J. Birgeneau, P. J. Reynolds, and J. F. Nicoll, *ibid.* 9, L553 (1976); S. Kirkpatrick, Phys. Rev. B 15, 1533 (1977).
[5]D. C. Rapaport, J. Phys. C 5, 1830 (1972); M. Plischke and D. Zobin, *ibid.* 10, 4571 (1977).
[6]C. Jayaprakash, E. K. Riedel, and M. Wortis, Phys. Rev. B (to be published).
[7]W. Y. Ching and D. L. Huber, Phys. Rev. B 13, 2962 (1976).
[8]E. Stoll and T. Schneider, J. Phys. A 9, L67 (1976).
[9]R. Fisch and A. B. Harris, AIP Conf. Proc. 29, 488 (1976).
[10]D. P. Landau, Phys. Rev. B 13, 2997 (1976).
[11]The difference in the initial spin configuration was found to have a negligible effect on the equilibrium state in the temperature region of interest.
[12]Estimates of the corresponding errors can be obtained as follows: It is known from the exact calculations for the pure Ising model on finite square lattices with periodic boundary conditions [A. E. Ferdinand and M. E. Fisher, Phys. Rev. 185, 832 (1969)] that the values of various thermodynamic functions for $40 \times 40$ and for $60 \times 60$ lattices differ by less than 0.5%. On the other hand, in a truly stochastic process the standard deviation decreases as $M^{-1/2}$, where $M$ is the number of Monte Carlo steps. This puts a lower limit of $\sim 1\%$ on the accuracy of our calculations. However, near the transition temperature $T_c(p)$, where the critical fluctuations become significant, the standard deviation increases to about 5%.
[13]E. Domany, J. Phys. C 11, L337 (1978).