Critical behavior of the simple cubic Ising model with quenched site impurities

D. P. Landau
Department of Physics and Astronomy, University of Georgia, Athens, Georgia 30602
(Received 11 February 1980)

The thermal and magnetic properties of the simple cubic Ising model with random, quenched, site impurities have been determined by Monte Carlo calculations. The transition appears to remain sharp, and the critical temperature decreases monotonically towards zero as the impurity concentration is increased towards the percolation limit. No clear evidence is found for any change in the critical exponents away from the pure lattice values. These results are discussed in terms of Harris's predictions for the critical behavior of impure systems.

I. INTRODUCTION

Substantial interest in the effects of impurities on phase transitions has existed for many years. It is now known that the critical behavior of systems with annealed (mobile) impurities is related to the corresponding pure lattice behavior through a set of renormalized critical exponents.[1,2] The behavior of systems with quenched (fixed) impurities is both more varied and less well understood. Early series expansion studies[3–5] yielded estimates for the dependence of T_c on impurity concentration but did not shed any light on possible alteration of critical exponents. McCoy and Wu[6] showed that the transition in an Ising square lattice with random bonds between successive rows is smeared out. Later work on the square lattice with quenched, periodic impurities showed[7] that the transition was shifted in temperature but that critical exponents were essentially unchanged. Using general arguments Harris suggested[8] that the sharpness of the phase transition in a system with random, quenched impurities is unchanged if the specific-heat exponent α of the system is negative. If α is positive the asymptotic critical behavior is expected to change as the critical temperature is approached. The problem of an m-component continuous-spin model with random, quenched impurities has been studied using renormalization-group theory.[9–15] These calculations are quite complex and show that for positive α a new "random" fixed point is stable. The critical exponents may then change, however, ϵ-expansion results[11–13] are available only up to $O(\epsilon)$ and it is thus unclear if the exponent estimates are reliable. Monte Carlo simulations[16–18] for two-dimensional Ising models find no evidence for changes in critical behavior. However, for these models $\alpha = 0$ and it is unclear if any change should be expected. We have previously reported preliminary results[19] for the simple cubic Ising model (for which $\alpha \approx 0.12$) with small impurity concentrations. Ono and Matsuoka[20] estimated the variation of T_c with concentration from computer simulations but did not study the critical behavior. In Sec. II we shall describe the details and our simulations, and shall present results in Sec. III. In Sec. IV we shall analyze the critical behavior obtained for a wide range of impurity concentrations. Section V will summarize our conclusions.

II. MODEL AND METHOD

We have studied $L \times L \times L$ simple cubic Ising lattices containing random, quenched, nonmagnetic site impurities. The Hamiltonian for this model is

$$H = -J \sum_{\mathrm{NN}} \sigma_i \sigma_j \xi_i \xi_j \ , \tag{1}$$

where $\sigma_i, \sigma_j = \pm 1$ and $\xi_i = 1$ if site i is occupied by a magnetic ion and $\xi_i = 0$ if site i is occupied by a nonmagnetic impurity. Systems with ferromagnetic nearest-neighbor (NN) coupling J ($J > 0$) and periodic boundary conditions were studied for $6 \leq L \leq 30$. Up to $x = \langle \xi \rangle = 0.8$ of noninteracting impurities were distributed in the lattices at random, and for each value of x, data were obtained for at least two different distributions of impurities. We used an importance sampling Monte Carlo method which has already been described elsewhere.[21–23] Between 500 and 5000 MCS (Monte Carlo steps/spins) were kept for each data point; averages were usually obtained over data from at least two different starting configurations. Final values for each value of L and T were then determined by averaging over all data taken with different impurity distributions and from different starting configurations. Simulations were performed for several values of purity $p = 1 - x$ above the percolation limit[24] $p_c \sim 0.31$ as well as one value, $p = 0.2$, which shows no long-range order.

III. RESULTS

A. Thermal properties

The data obtained were qualitatively similar to those found for the pure simple cubic lattice.[22] The specific heat is shown for several concentrations in Fig. 1. Note that these data as well as those shown in the following figures are plotted per lattice site and not per magnetic site. For comparison we also show some of the pure lattice data taken from Ref. 22. The general characteristics are the same for $p > 0.4$. A relatively sharp specific-heat peak appears but it is shifted to lower temperature as the impurity concentration increases. In all cases the effect of decreasing the lattice size is to depress the peak. For a given value of L the peak value decreases quite rapidly with increasing impurity content. For $p = 0.2$ we find a very small, broad specific-heat peak with absolutely no sign of any sharp peak. Since $p = 0.2$ is below the percolation limit, no long-range order can occur. Even all completely ordered clusters are too small to span the entire lattice. For $p = 0.4$ the specific heat is quite rounded, even for $L = 20$ but the presence of a very shallow peak is still consistent with the data. Interpretation of these data becomes difficult since variations between different impurity distributions (see Fig. 2) become pronounced.

The internal-energy data shown in Fig. 3 also reflect the changes due to the addition of impurities. As the impurity concentration increases, the inflection points (corresponding to the peaks in the specific heat) shift to lower temperature and the ground-state internal energy approaches zero. The ground-state energy depends upon the number of "broken" bonds and hence both the distribution and number of impurities play a role. Finite-size effects are significant only very close to $T_c(p)$.

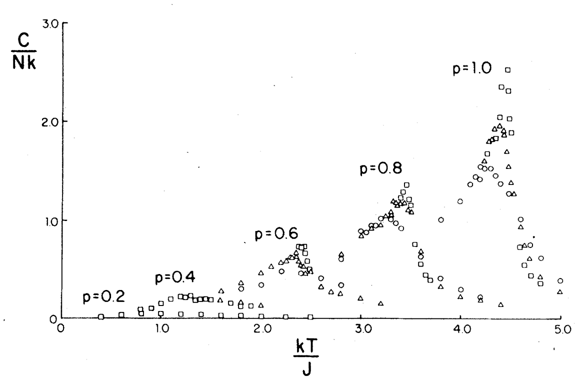

FIG. 1. Temperature dependence of the specific heat for various concentrations p of magnetic sites. Data are shown only for (O) $L = 6$, $L = 10$, and (□) $L = 20$. Data for $p = 1$ are from Ref. 22.

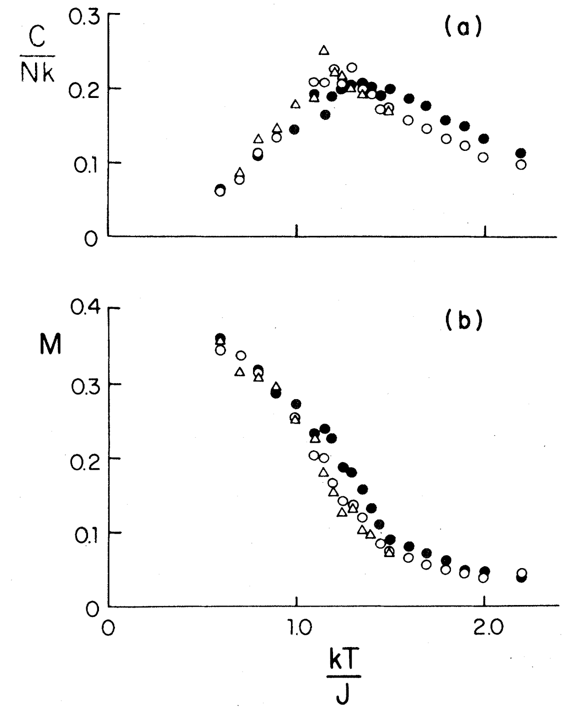

FIG. 2. Temperature dependence of: (a) specific heat; (b) spontaneous magnetization, for three different impurity distributions with $p = 0.4$ and $L = 10$.

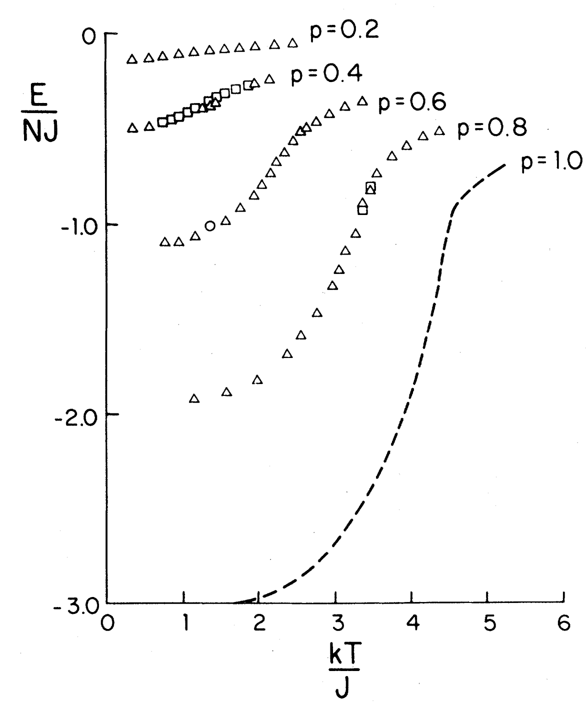

FIG. 3. Temperature dependence of the internal energy for various concentrations p of magnetic sites. Only results for (Δ) $L = 10$, and (□) $L = 20$ are shown. The dashed line is the $L = \infty$ curve (see Refs. 22 and 32).

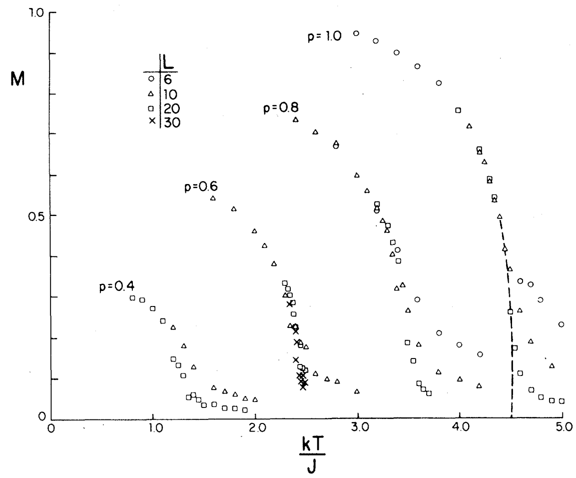

FIG. 4. Temperature dependence of the spontaneous magnetization for various concentrations p of magnetic sites. Data for $p=1$ are from Ref. 22.

B. Magnetic properties

The behavior of the order parameter (spontaneous magnetization) is shown in Fig. 4 for several purity values. In all cases the order parameter shows a rapid decrease near the location of the specific-heat peak and finite-size "tails" at higher temperatures. The shapes of the curves are very much the same except they tend to p rather than to 1 at absolute zero. For $p=0.2$ only a small, weakly temperature-dependent value of $M(\sim 0.05)$ was observed. Since $p=0.2$ is below the percolation limit $M=0$ for an infinite lattice, the observed value of M must then be a finite-size effect.

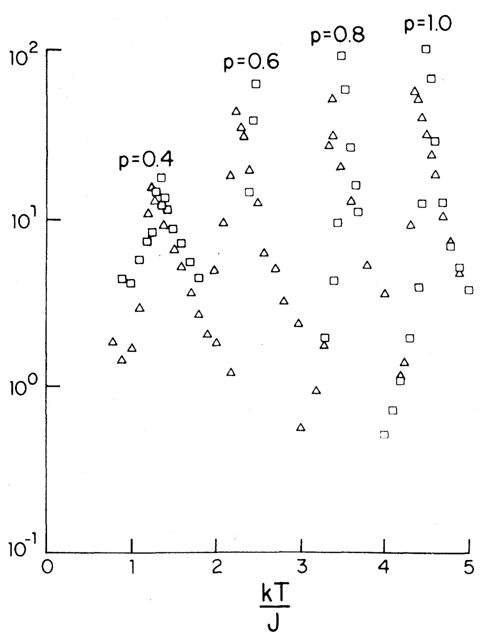

FIG. 5. Temperature dependence of the susceptibility for various concentrations p of magnetic sites. Only results for (Δ) $L=10$, and (□) $L=20$ are shown. The data for $p=1$ are from Ref. 22.

The susceptibility showed sharp peaks for all impurity concentrations with $p > p_c$. The data shown in Fig. 5 indicate that finite-size effects are important and that the location of the peak shifts to lower temperature with increasing impurity content. The finite lattice-peak values appear to be surprisingly insensitive to the impurity content (at least for $p \geqslant 0.6$). For $p=0.4$ quite noticeable differences appear between results for different impurity distributions and the effects of finite size alone are pronounced over a wide temperature range. For $p=0.2$ the susceptibility continues to increase as $T \rightarrow 0$ and shows no peak.

IV. ANALYSIS AND DISCUSSION

A. Critical temperatures

The determination of the critical temperature $T_c(p)$ for an impure system is nontrivial. Real-space renormalization-group studies[25] of several bond-impure models as well as experimental results[26] on a physical site diluted pseudo-XY model on a simple cubic lattice suggest that the specific-heat anomaly associated with long-range order may become very narrow and be superimposed on the low-temperature shoulder of a larger, broad peak produced by short-range order. A comparison of our specific-heat data with the susceptibility and order-parameter results leads us to believe that the observed specific-heat peaks locate the critical point within experimental error. We cannot exclude the possibility that two peaks exist and that we simply do not have sufficient resolution to separate the two. Analogous details in the critical behavior of the order parameter and susceptibility might also be unresolved. However, experimental measurements[27] on $Co_pZn_{1-p}Cs_3Cl_5$, which rather closely approximates a diluted, $S=\frac{1}{2}$, simple cubic antiferromagnet, also show no indication of two peaks in the specific heat. (The results certainly suggest differences in the behavior of the impure-XY and Ising models.) We shall therefore proceed to analyze our data using the specific-heat peaks to locate T_c. Finite-size scaling theory[28] predicts that the infinite-lattice critical temperature $T_c(p)$ is related to the finite-lattice pseudocritical temperature $T_c^L(p)$ by

$$T_c(p) = T_c^L(p) + aL^{-1/\nu} \quad . \tag{2}$$

We can use Eq. (2) to extrapolate our results to $L=\infty$ although additional error is of course introduced due to the uncertainty in ν for impure lattices.

We shall see in the next section that there is no evidence for any impurity dependence of exponents. We therefore believe that the added error is less than the uncertainty due to scatter in the data and differences for different impurity distributions. Our final estimates for $T_c(p)$ are shown in Fig. 6. These values lie systematically slightly below those obtained by Ono and Matsuoka[20] particularly for $p < 0.7$.

The observed variation of the critical temperature with impurity concentration $x = 1 - p$ could have several origins. Any analysis, however, will be complicated by the fact that x and T are not the proper scaling axes since the critical curve does not approach $T_c(x=0)$ along a path which is parallel to either x or T axes. A set of axes such as that shown in Fig. 6 would be suitable since μ_2 approaches $T_c(x=0)$ asymptotically tangent to the critical curve. In this coordinate system we might expect that[29]

$$\mu_{1c} \propto \mu_{2c}^{1/\phi} \ , \tag{3}$$

where ϕ is a characteristic exponent. If the critical behavior is unchanged by the presence of impurities, we might expect the generalized form of the scaling hypothesis of Fisher and Au-Yang[7] to hold. In terms of x this yields a variation of the critical temperature

$$\delta T_c = [T_c(x=0) - T_c(x)]/T_c(x=0)$$
$$= a_1 x + a_2 x^{2-\alpha} \ . \tag{4}$$

However, if the critical exponents do change, then Eq. (3) must be used and ϕ becomes the crossover exponent describing the approach to the pure lattice

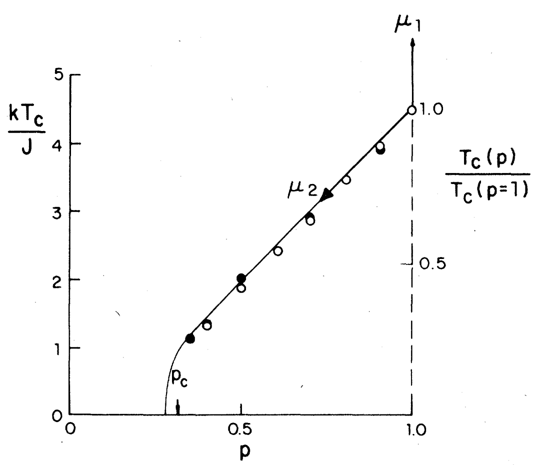

FIG. 6. Concentration dependence of the critical temperature. Monte Carlo results are given by open circles, the experimental results (Ref. 27) for $Co_pZn_{1-p}Cs_3Cl_5$ [in reduced units $T_c(p)/T_c(p=1)$] are shown by filled circles. The solid curve shows the variation of $T_c(p)/T_c(p=1)$ obtained from renormalization-group theory (Ref. 15). The estimate for the percolation limit p_c is obtained from Ref. 24. Optimum scaling axes μ_1 and μ_2 are shown by arrows.

behavior. Unfortunately the variation of T_c with x is consistent with either Eq. (3) with $a_1 = 1.09 \pm 0.02$ and $a_2 = 0.14 \pm 0.03$ or Eq. (4) and an extremely wide range of ϕ. To further complicate matters we expect that the large-x critical points will be affected by crossover to the percolation transition[30] at $T=0$, $p > p_c$. Since we do not have sufficient data near p_c we do not know what portion of the critical curve is dominated by this crossover and what portion can be used to study the approach to $T_c(x=0)$.

A real-space renormalization-group treatment of this model has been reported recently.[15] Although the results in absolute units [i.e., $kT_c(p)/J$] are not very good, the reduced estimates $T_c(p)/T_c(p=1)$ lie only slightly above our values (see Fig. 6).

B. Critical behavior

Harris[8] predicted that the addition of impurities to systems which had an $\alpha > 0$ in the pure case should produce altered critical exponents. He also argued, however, that the width of the "impure" critical region should vary as $x^{1/\alpha}$. We have therefore attempted to analyze the critical behavior over as wide a range of x as possible.

Since the specific-heat data show only a very weak peak it is not possible to do a direct analysis in terms of a power-law divergence

$$C = At^{-\alpha} + B \ , \tag{5}$$

where $t = [T - T_c(x)]/T_c(x)$. Instead we have used finite-size scaling theory[28] to interpret the finite-lattice data. The maximum value of the specific heat $C_{\max}$ is expected to vary as

$$(C_{\max} - B) \propto L^{+\alpha/\nu} \tag{6}$$

as $L \to \infty$ where B is a "background" term. Since we have no independent information regarding the concentration dependence of B, we have simply plotted the raw data, i.e., have set $B = 0$ for all x, and show the result in Fig. 7. The pure lattice data (taken from Ref. 22) show that the asymptotic form is reached for $L \gtrsim 20$. For small impurity concentration the size dependence is quite similar to that of the pure lattice except that the amplitude is reduced. For $p \lesssim 0.6$, however, the peak values appear to increase more slowly. Two very different explanations may be given: (i) the critical exponents change with p; or (ii) the asymptotic size dependence is reached only for lattices which are larger than those studied here. (In addition it is possible that the background term B changes substantially.) Harris[8] predicted that the specific-heat peak should become finite with a maximum value which varies as x^{-1}. If we assume that the peak is finite and choose reasonable maximum values which are consistent with the large-L data

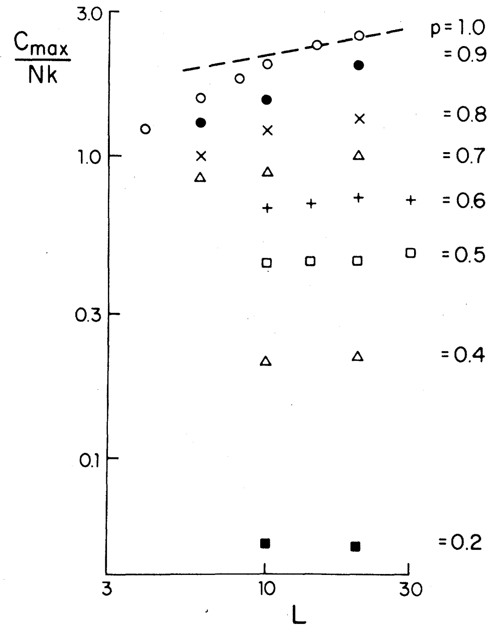

FIG. 7. Size dependence of the maximum specific heat. Data for $p = 1.0$ are from Ref. 22. The dashed line has slope $\alpha/\nu = 0.195$.

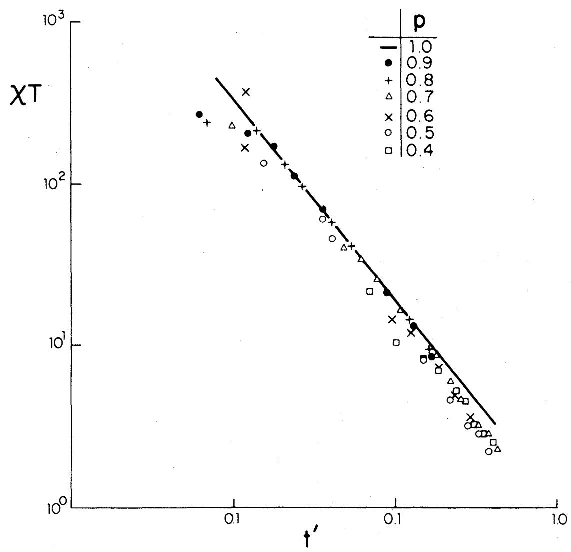

FIG. 9. Critical behavior of the high-temperature susceptibility for various concentrations p of magnetic sides. The solid line shows the asymptotic pure latice ($p = 1$) behavior (see Refs. 22 and 32).

shown in Fig. 7 (at least for $p < 0.7$) we obtain a much faster variation with impurity content. Harris's prediction, however, was made for small x and may not be valid for such large impurity content.

The order parameter M and high-temperature susceptibility x data were analyzed in terms of the usual power laws:

$$M = Bt^{\beta} \quad , \tag{7a}$$

$$\chi T = Ct'^{-\gamma} \quad , \tag{7b}$$

where $t = [T_c(x) - T]/T_c(x)$ and $t' = [T - T_c(x)]/T$. The data showed finite-size rounding near $T_c(x)$ and we therefore eliminated much of the small lattice data from the log-log plots of the order parameter (Fig. 8) and the high-temperature susceptibility (Fig. 9). To within experimental error all of the order-parameter data are consistent with the pure lattice value[31] of $\beta = 0.31$. Only data for $p = 0.4$ seem even to suggest a different value but this may be due to error in the choice of T_c and/or finite-size effects. The concentration dependence of the critical amplitude B is $\approx p^{1.3}$. The analysis of the high-temperature-susceptibility data is shown in Fig. 9. The data for all values of p can be fitted by the pure lattice exponent $\gamma = 1.25$. The critical amplitude C is virtually independent of concentration. The concentration dependence of the critical amplitudes may also be affected by crossover[30] to the percolation transition.

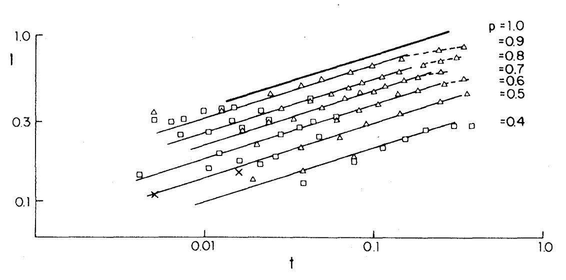

FIG. 8. Critical behavior of the spontaneous magnetization for various concentrations p of magnetic sides. The solid line shows the asymptotic pure lattice ($p = 1$) behavior (see Refs. 22 and 32).

V. SUMMARY AND CONCLUSIONS

The results of our Monte Carlo study describe the behavior of the quenched, site impure simple cubic Ising model over a wide range of temperature and impurity content. Two different types of "rounding" are observed. First, the addition of impurities tends to decrease the relative size of the peaks with respect to the background; and second, finite-size effects clearly round off peaks and produce high-temperature finite-size tails in the order parameter. Although effects due to the addition of impurities are clearly seen, we find no clear evidence of a change in critical behavior. Harris has estimated[8] that the width of the "impure" critical region should vary as $\sim x^{1/\alpha}$, and for the present model, since α is small, this would imply that new critical behavior would be observable only near $T_c(p)$. Recent preliminary work by Novotny and Landau[32] on the Baxter-Wu model ($\alpha = \frac{2}{3}$!) indicates that the addition of impurities does alter the critical behavior. Hence, it is probable that none of our "unrounded" data have penetrated the "impure" critical region. Prohibitively large lattices would probably be needed for us to penetrate closely enough to $T_c(p)$ to see changes in critical behavior. The best hope of observing "impure" critical behavior would appear to lie in the investigation of other models with larger values of α which should then lead to larger "impure" critical regions.

ACKNOWLEDGMENTS

This research was supported in part by the National Science Foundation. We are indebted to Professor M. Wortis and Dr. M. A. Novotny for valuable discussions and suggestions.

---

[1]I. Syozi, Prog. Theor. Phys. 34, 189 (1965).
[2]H. Garelick and J. W. Essam, Proc. Phys. Soc. London 92, 136 (1967).
[3]G. S. Rushbrooke and D. J. Morgan, Mol. Phys. 4, 1 (1961).
[4]D. J. Morgan and G. S. Rushbrooke, Mol. Phys. 4, 291 (1961).
[5]R. J. Elliott and B. R. Heap, Proc. R. Soc. London 265, 264 (1962).
[6]B. M. McCoy and T. T. Wu, Phys. Rev. 176, 631 (1968).
[7]M. E. Fisher and H. Au-Yang, J. Phys. C 8, L418 (1975); Phys. Rev. B 13, 1238 (1976); H. Au-Yang, *ibid.* 13, 1266 (1976).
[8]A. B. Harris, J. Phys. C 7, 1671 (1974).
[9]A. B. Harris and T. C. Lubensky, Phys. Rev. Lett. 33, 1540 (1974).
[10]T. C. Lubensky, Phys. Rev. B 11, 3573 (1975).
[11]G. Grinstein and A. Luther, Phys. Rev. B 13, 1329 (1976).
[12]D. E. Khmelnitskii, Zh. Eksp. Teor. Fiz. 68, 1960 (1975).
[13]C. Jayaprakash and H. J. Katz, Phys. Rev. B 16, 3987 (1977).
[14]A. Aharony, Y. Imry, and S.-K. Ma, Phys. Rev. B 13, 466 (1976).
[15]R. B. Stinchcombe, J. Phys. C 12, 4533 (1979).
[16]W. Y. Ching and D. L. Huber, Phys. Rev. B 13, 2962 (1976).
[17]E. Stoll and T. Schneider, in *Magnetism and Magnetic Materials—1975*, edited by J. J. Becker, G. H. Lander, and J. J. Rhyne, AIP Conf. Proc. No. 29 (AIP, New York, 1976), p. 490.
[18]R. Fisch and A. B. Harris, in *Magnetism and Magnetic Materials—1975*, edited by J. J. Becker, G. H. Lander, and J. J. Rhyne, AIP Conf. Proc. No. 29 (AIP, New York, 1976), p. 488.
[19]D. P. Landau, Physica (Utrecht) 86-88B, 731 (1977).
[20]I. Ono and Y. Matsuoka, J. Phys. Soc. Jpn. 41, 1425 (1976).
[21]D. P. Landau, Phys. Rev. B 13, 2997 (1976).
[22]D. P. Landau, Phys. Rev. B 14, 255 (1976).
[23]For a general review, see Monte Carlo methods in *Statistical Physics*, edited by K. Binder (Springer, Berlin, 1979).
[24]J. Hoshen, D. Stauffer, G. H. Bishop, R. J. Harrison, and G. D. Quinn, J. Phys. A 8, 1285 (1979).
[25]C. Jayaprakash, E. K. Riedel, and M. Wortis, Phys. Rev. B 18, 2244 (1978).
[26]M. A. Algra, L. J. Jongh, and W. J. Huiskamp, Physica (Utrecht) 86-88B, 737 (1977).
[27]E. Lagendijk and W. J. Huiskamp, Physica (Utrecht) 62, 444 (1972).
[28]M. E. Fisher, in *Proceedings of the International Summer School "Enrico Fermi," Varenna, Italy, 1970,* edited by M. S. Green (Academic, New York, 1971).
[29]E. K. Riedel and F. J. Wegner, Z. Phys. 225, 195 (1969).
[30]D. Stauffer, Z. Phys. B 22, 161 (1975).
[31]See, C. Domb, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1973), Vol. 3.
[32]M. R. Novotny and D. P. Landau, J. Magn. Magn. Mater. 15-18, 247 (1980).