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Monte Carlo Studies of Percolation Phenomena for a Simple Cubic Lattice

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The site-percolation problem on a simple cubic lattice is studied by the Monte Carlo method. By combining results for periodic lattices of different sizes through the use of finite-size scaling theory we obtain good estimates for p_c (0.3115 ± 0.0005), β (0.41 ± 0.01), γ (1.6 ± 0.1), and ν (0.8 ± 0.1). These results are consistent with other studies. The shape of the clusters is also studied. The average "surface area" for clusters of size k is found to be close to its maximal value for the low-concentration region as well as for the critical region. The percentage of particles in clusters of different sizes k is found to have an exponential tail for large values of k for $p < p_c$. For $p > p_c$ there is too much scatter in the data to draw firm conclusions about the size distribution.

KEY WORDS: Site percolation; Monte Carlo method; percolation threshold; critical exponents; finite-size scaling.

1. INTRODUCTION

Percolation processes, first discussed by Broadbent and Hammersley,[1] occur in diverse physical systems (for recent reviews see Refs. 2 and 3). Consider a disordered binary alloy in which each site of a lattice can be occupied by an A or a B particle independently with probabilities p and $1 - p$, respectively. The probability $P(p)$ that a given site (in the infinite lattice) is part of a

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connected cluster of A-type particles of infinite size is nonzero only if p is greater than a critical concentration p_c, the percolation threshold for the site-percolation process. A cluster of size k is defined as a group of k A-type particles connected by nearest neighbor bonds and not connected to other A particles. It is also possible to consider processes where the bonds are chosen at random to be in two different states, the so-called bond-percolation problem, but we shall not discuss that here.

The percolation phenomenon has been studied in detail for the Bethe lattice (infinite Cayley tree) by Fisher and Essam.[4] More recently other authors[5] have extended this method to interacting systems. Fisher and Essam showed that the percolation threshold in this case is given by $p_c = 1/\sigma$, where σ is the branching ratio of the lattice. They also showed that as p approaches p_c from above, $P(p)$ goes to zero linearly. The mean square cluster size $S(p)$ was found to have a simple pole at p_c. Numerical estimates of p_c have also been obtained for a number of common lattices by series expansion[6–9] and Monte Carlo calculations.[10–15]

Recent interest in the percolation problem[16–23] has been stimulated partly by Fortuin and Kasteleyn's observation that this problem can be related to the critical behavior of the one-component Ashkin–Teller–Potts model. In particular the behavior of $P(p)$ and $S(p)$ near p_c, written in the form $P(p) \sim \tau^\beta$ and $S(p) \sim |\tau|^{-\gamma}$, where $\tau = p/p_c - 1$, makes β and γ correspond to the critical exponents usually associated with the spontaneous magnetization and susceptibility, respectively. Harris *et al.*[17] and Young and Stichombe[19] carried out computations of critical exponents using the renormalization group technique, while Kirkpatrick[21] obtained Monte Carlo estimates for the exponents β and γ for hypercubical lattices of different dimensionalities (2–6). From the work of the latter author it is found that the Bethe lattice results are in good agreement with those of the hypercubical lattice of dimensionality six.

Our interest in this problem stems from our investigations, by means of computer simulations, of the time evolution of a model binary alloy (A–B) system which is quenched (cooled suddenly) from a high temperature to a low temperature.[24,25] At very high temperatures A and B atoms are randomly distributed over different lattice sites, while at low temperatures ($T < T_c$) the equilibrium state of the system is (for suitable interactions and concentrations) one of segregation into two phases. The study of clusters in the high-temperature regime, e.g., in the random system corresponding to $T = \infty$, is therefore of importance for understanding the coarsening (segregation into phases) occurring by means of nucleation of droplets or other processes after the system is quenched and particles on nearest neighbor sites are permitted to exchange positions according to a certain transition probability.

We are particularly interested in the shape and distribution of clusters in the random system at various concentrations of A particles to see the extent to which these are modified after the quench. In particular we wish to understand the relationship (if any) between the (more compact) clusters at lower temperatures and physical "droplets." These questions are of course of interest also in Fisher's "droplet model" used for investigating critical exponents and other phase transition phenomena.[26–28] We have therefore analyzed the average "surface area" (number of broken bonds) $\bar{s}_k$ of clusters of size k as well as the size distribution of the clusters. We find, as expected, that $\bar{s}_k \sim Ak$ ($A \simeq 3.7$) at all values of p studied, i.e., the clusters, even the large ones, are very loose or "ramified."[27] The size distribution appears to behave exponentially in k for $p < p_c$.

2. ESTIMATION OF PERCOLATION PARAMETERS

Let Λ be a cubical lattice with periodic boundary conditions containing $N = L^3$ sites. The computer simulation consists in choosing, at random, N_A sites in Λ and placing A-type particles (or just particles) there. We identify N_A/N with p, the probability that a site chosen at random is occupied in the "grand canonical" or independent site problem. (We do not expect this difference from the independent site problem to be of importance for our considerations.) Let us call $\Lambda_A \subset \Lambda$ the set of sites chosen; the sites not occupied by the A particles $\Lambda - \Lambda_A = \Lambda_B$ are occupied by the B particles (or are just vacant). The set Λ_A will consist of a union of clusters C_α. Each cluster C_α will be characterized by k, the number of sites in the cluster, and s, the surface area, which is defined as the number of A–B bonds incident on C_{ks}, i.e., we count *all* the bonds emanating from all $r_i \in C_{ks}$ that are not A–A bonds. This definition of s is different and always greater than or equal to b, the number of B sites (empty sites), which form the perimeter of cluster.[27,28] Our definition corresponds, for nearest neighbor interactions, to the (suitably normalized) energy of the cluster C_{ks}. Let n_{ks} be the number of clusters having the same value of k and s present in the system. We have programmed the computer to list n_k, the total number of clusters of size k ($n_k = \sum_s n_{ks}$), and s_k, the total surface area of all the clusters of size k ($s_k = \sum_s n_{ks}s$).

We note here that the probability that a given occupied site in Λ belongs to a cluster of size k with surface area s is given by

$$P(k, s:p) = kn_{ks}/pN \tag{1}$$

since there are altogether kn_{ks} lattice sites in such clusters. Similarly,

$$P(k:p) = \sum_s P(k, s:p) = kn_k/pN \tag{2}$$

We also have

$$P(k, s:p) = p^{k-1} \sum_{b} M(k, s, b)(1 - p)^b \tag{3}$$

where $M(k, P, b)$ is a geometrical factor equal to the number of clusters containing the given site of size k, surface area s, and border (neighboring sites occupied by B particles) b. Clearly, for all k

$$s/2d \leqslant b \leqslant s, \qquad K_1 k^{2/3} \leqslant s_k \leqslant K_2 k \tag{4}$$

The factor $M(k, s, b)$ is, for fixed arguments, independent of L, the size of the lattice, for sufficiently large L. There is thus no problem, in principle, in determining any quantities relating to clusters of fixed size from Monte Carlo computations on sufficiently large systems. The same is, however, not true for percolation properties. These are, in an intrinsic way, a property of the infinite system and their extraction from computations on finite systems requires some care. We shall define the "percolation probability" $P_L(p)$ for a lattice of size L^3 as the ratio of the number of particles present in the largest cluster to the total number of sites in the lattice.[21] We expect that $P_L(p) \to_{L\to\infty} P(p)$ whenever (as is usually assumed) there is only one infinite cluster present. Our result for $P(p)$ for $L = 50$, averaged over ten different random configurations, is shown in Fig. 1. The recent results of Kirkpatrick[21] for a much larger lattice ($L = 144$) are also shown in the figure. We note that because of the finite size of the system, $P_L(p)$ is nonzero even if $p < p_c$. The question as to how a sharp transition grows out of a smoothed-out transition of a finite-sized system as the size of the system grows larger and larger (and eventually becomes infinite) has received a great deal of attention in ordinary critical phenomena. Adopting Fisher's "finite-size scaling theory"[29] to the problem of site percolation, we assume[5] that the behavior of $P_L(p)$ near the percolation threshold can be described in the form

$$P_L(p) \sim L^{-\beta/\nu} X_1(\tau L^{1/\nu}) \tag{5}$$

where $\tau = (p - p_c)/p_c$, ν is the correlation length exponent [$\xi(p) \sim \tau^{-\nu}$], and X_1 is a scaling function.

We have plotted $L^{\beta/\nu} P_L(p)$ against $\tau L^{1/\nu}$ for various values of p_c, β, and ν, for $L = 30, 40, 50, 80, 100$, to look for a set of values of p_c, β, and ν for which the results for the different lattices fall on one and the same curve, which gives the form of the scaling function X_1. The range of p_c and the critical exponents for which the finite-size scaling theory holds approximately (as discerned by the eye) are shown in Table I. As can be seen from Table I, our results are in good agreement with those of other authors. The plots were

[5] The same assumption was made by Levinshtein *et al.*[15] Their method of obtaining p_c and the critical exponents, however, is different from ours.

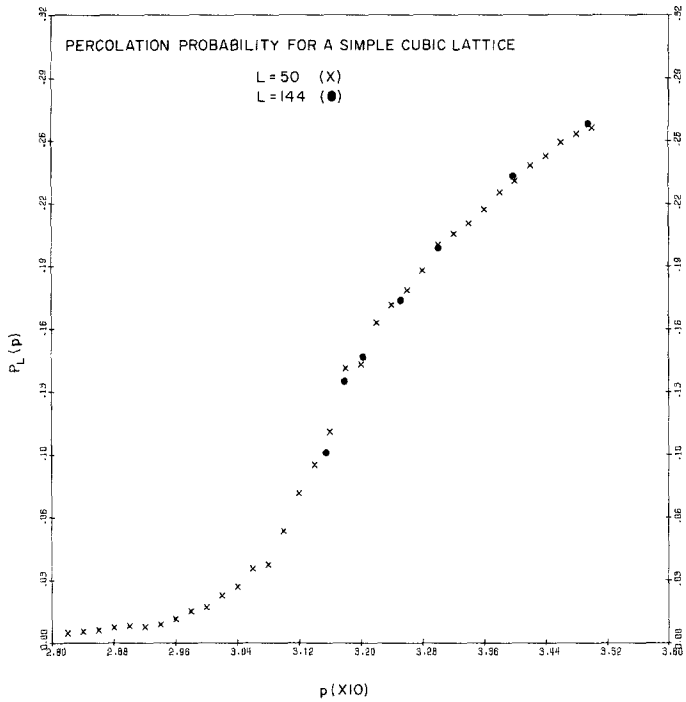

Fig. 1. Percolation probability $P_L(p)$ for a simple cubic lattice of size L^3 for $L = 50$ (×). The corresponding results of Kirkpatrick[21] for $L = 144$ are also shown (●).

Table I. Critical Exponents for Percolation[a]

		Other authors	
	Present result	Monte Carlo	Series
p_c	0.3115 ± 0.0005	0.312 ± 0.001[21]	0.307 ± 0.01[6–9]
β	0.41 ± 0.01	0.39 ± 0.02[21]	
		0.35 ± 0.05[15]	
γ	1.6 ± 0.1	1.80 ± 0.05[21]	
		1.69 ± 0.03[15]	
ν	0.8 ± 0.1	0.9 ± 0.05[15]	

[a] Percolation threshold and critical exponents for site percolation on a simple cubic lattice as obtained by the Monte Carlo method. Results of previous studies are also shown.

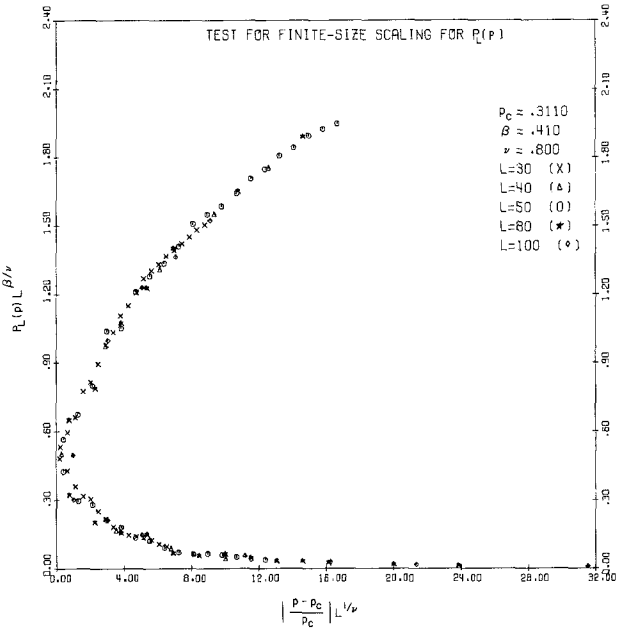

Fig. 2. Test for finite-size scaling for $P_L(p)$. The results for $L = 40$ are taken from Dean and Bird.[12]

found to be very sensitive to p_c, which enables us to prescribe a rather narrow range for p_c. A typical plot is shown in Fig. 2.

The mean square cluster size $S(p)$,

$$S(p) = \langle \sum k^2 n_k \rangle / \langle \sum k n_k \rangle = \langle \sum k^2 n_k \rangle / pN \tag{6}$$

is expected to diverge at p_c with an exponent γ. We have studied $S(p)$ only for $p < p_c$. For $p > p_c$ the statistics are poor because one has to take out the largest cluster from the sums in (2). We assume that $S_L(p)$ has the form

$$S_L(p) \sim L^{\gamma/\nu} X_2(\tau L^{1/\nu}) \tag{7}$$

where X_2 is another scaling function. Following exactly the same procedure as that for $P_L(p)$, we find that the finite-size scaling theory holds for a rather narrow range of γ, while p_c and ν are consistent with those obtained from our study of the percolation probability. Our estimate for γ is shown in the third row in Table I. It should be noted that the Josephson scaling relation $d\nu = 2\beta + \gamma$ holds approximately for our range of values of β, γ, and ν. The prediction of Harris *et al.*[17] for $d = 3$ is, however, not consistent with our results, which is not so surprising, considering the rather large value of their expansion parameter, $6 - d = 3$, for this case.

3. SHAPE OF CLUSTERS

The shape of the large clusters that arise in the percolation problem has been studied by several authors.[22,23,30,31] The degree of compactness of typical clusters appearing in the system, especially at finite temperatures, is of both physical and mathematical interest.[26,32] A measure of this compactness may be obtained by considering the behavior of $\bar{s}_k$, equal to the average value of s over all clusters of size k.

In order to find the asymptotic behavior of $\bar{s}_k$, we grouped the clusters in bands of gradually increasing width. The average values of $\bar{s}_i$, $\bar{k}_i$, and $\bar{n}_i$ for the ith band are then defined (other definitions are also possible) as follows:

$$\bar{k}_i = \frac{\langle \sum_{k\in I_i} k n_k \rangle}{\langle \sum_{k\in I_i} n_k \rangle}; \qquad \bar{s}_i = \frac{\langle \sum_{k\in I_i} s_k \rangle}{\langle \sum_{k\in I_i} n_k \rangle}; \qquad \bar{n}_i = \frac{\langle \sum_{k\in I_i} n_k \rangle}{k^i_{\max} - k^i_{\min}} \tag{8}$$

where the set I_i is given by $I_i = \{k \mid k^i_{\min} \leqslant k \leqslant k^i_{\max}\}$. We then plotted $\bar{s}/\bar{k}$ against $1/\bar{k}$ for different values of p, disregarding, however, the largest cluster for $p \geqslant p_c$. We find that for all values of p we have studied, $p \lesssim 0.35$, $\bar{s}/\bar{k}$ can be very well approximated by the linear relation $\bar{s}_k/\bar{k} = A + B/\bar{k}$. The value of A is very close to 4 (decreasing gradually from about 3.8 for low concentrations to about 3.7 for the critical region), which is the value of $\bar{s}/\bar{k}$ for the Bethe lattice of coordination number six. This shows that our clusters are very "ramified" indeed.[27] (Our value of A is considerably larger than Domb's[33] values of $\bar{b}_k/k$ for $k \approx 15$. This suggests that typical clusters have many bends in them.) A scatter plot of $\ln(s_k/k)$ vs. $\ln k$ (excluding the largest cluster) obtained from ten independent runs is shown in Fig. 3 for $p = 0.322$ ($> p_c$). The horizontal line corresponds to $\ln A$ for this case. This shows the consistency of our averaging procedure.

The size distribution of the clusters is also of interest. In order to have a reasonable statistic, we have studied the fraction of A-type particles that are in clusters of size k,

$$p_k = \bar{k}\bar{n}_k/N_A \tag{9}$$

where $\bar{k}$ and $\bar{n}_k$ are defined in Eq. (8). This is essentially $P(k{:}p)$ defined in Eq. (2). For small values of k, say $k \lesssim 10$, $p(k{:}p)$ can be obtained[34] from Eqs. (2) and (3). For monomers and dimers, n_{ks} is the same for both the simple cubic lattice and the Bethe lattice of coordination number six. We have checked that our result for the $50 \times 50 \times 50$ lattice, averaged over ten runs, is in very good agreement with the expected values. We find that $-\log(p_k)/k \to \alpha$ for large value of k, where α decreases with p as the concentration is increased to about 25%, although for higher concentrations there are considerable fluctuations (scatter) of our data. For concentrations above p_c, this scatter is rather large and it is difficult to draw any firm conclusions for the behavior of p_k for large values of k.

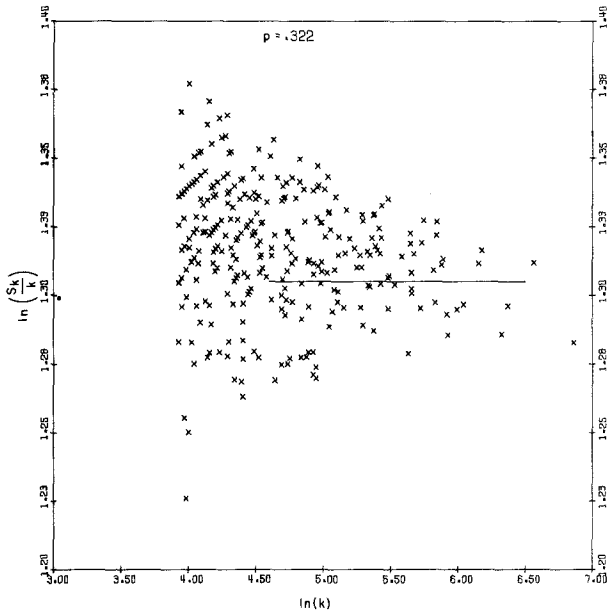

Fig. 3. Scatter plot of $\ln(s_k/k)$ vs. $\ln k$ above the percolation threshold ($p = 0.322$).

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