Treelike percolation in two dimensions

W. Danny Braswell
Department of Physics and Astronomy, University of Alabama, University, Alabama 35486

Fereydoon Family
Department of Physics, Emory University, Atlanta, Georgia 30322

Joseph P. Straley
Departments of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506 and University of Alabama, University, Alabama 35486*

(Received 20 July 1983)

The Metropolis Monte Carlo method is adapted to locate the phase transition for treelike percolation. The relationship between this problem and the $s \to 0$ limit of the Potts model is clarified.

INTRODUCTION

Treelike percolation is a problem concerning the statistics of bonds on a lattice which are constrained to form only clusters that are trees (i.e., no closed loops). This problem was originally proposed by Stephen,[1] who suggested the occurrence of a phase transition in such systems; namely, that there is a concentration of bonds such that the infinite lattice will contain an infinite cluster (with probability unity). The problem has been discussed subsequently by Wu[2] and Straley;[3] however, there has remained an inconsistency between the results obtained regarding the problem as a percolation problem and those which can be derived from its relationship to the Potts model. The purpose of this paper is to resolve this discrepancy; we will show that there were errors in methodology both in the theoretical discussions and in the efforts to provide numerical estimates of the percolation threshold.

I. CONNECTION WITH THE POTTS MODEL

The Potts model is a lattice model in which each site can be in any of s different states with an interaction energy $-Js$ if neighboring sites are in the same state, and zero otherwise (some authors—Ref. 1 in particular—omit the factor of s, which changes the temperature scale). In the first discussion[1] of treelike percolation, Stephen showed that the leading terms in s in the high-temperature expansion are due to treelike graphs, so that in taking the limit $s \to 0$ with temperature fixed, the partition function becomes the generating function for treelike graphs. Specifically, if we define a bond fugacity z by

$$zs = v = e^{sJ\beta} - 1 \tag{1}$$

(where $\beta = 1/kT$), then

$$Q(z) = \lim_{s \to 0} [Z(\beta, s)/s^N] = \sum_n z^n T_n \ , \tag{2}$$

where T_n is the number of graphs of n bonds with no closed loops that can be drawn on a lattice of N sites.

Unfortunately, Stephen confused the issue by asserting the relationship

$$z = p/(1-p) \ , \tag{3}$$

where p is the density of bonds present; the correct relationship on a hypercubic of coordination number $2d$ is

$$p = (NQd)^{-1} \sum_n n z^n T_n = (Nd)^{-1} z \frac{\partial \ln Q}{\partial z} \ , \tag{4}$$

which in the Potts model language is the internal energy. This definition is equivalent to (3) only if the bonds are random and uncorrelated. A study of simple examples (for example, the set of trees that can be drawn on a triangle) shows that in the latter definition p reaches close packing only at $z \to \infty$, whereas the former would give finite z at close packing.

In two dimensions, the dual transformation[4] determines the transition temperature for the s-state Potts model

$$e^{Js\beta} - 1 = s^{1/2} \ , \tag{5}$$

which implies that it goes to zero similar to the square root of s. Wu[2] attempted to apply this result to the treelike percolation problem, but used (4) to calculate the transition density. The correct result is that in two dimensions the phase transition takes place at infinite z, that is, at close packing ($p = \frac{1}{2}$).

The two-dimensional Potts model exponents have been given extensive discussion, and the consensus is[5]

$$\nu \simeq \pi/(3s^{1/2}) \tag{6}$$

for small s, which implies

$$\xi = \lim_{s \to 0} (1 - v/v_c)^{-\nu} = \lim_{s \to 0} (1 - s^{1/2} z)^{-\pi/(3s^{1/2})} = \exp(\pi z/3) \ . \tag{7}$$

For comparison with numerical work, we need to express ξ as a function of $p_c - p$, for which we need to know the analytical relationship between p and z for large z. Since the specific-heat exponent α is negative, the leading

dependence on z is not the "singular" part, but rather is determined by the background dependence (which theorists usually ignore). For a variety of simple models [e.g., Cayley trees, decorated trees (cactus models), and hierarchical lattices] we have found $p_c - p \simeq e^{-z}$; accepting this result as general we anticipate

$$\xi \simeq (p_c - p)^{-\pi/3} . \tag{8}$$

II. SIMULATING TREELIKE PERCOLATION

The percolation threshold for the square lattice must be at or below $p=0.5$ since trees close pack at this bond density: There can only be one infinite tree present in this case. In order to estimate the percolation probability we need an algorithm for constructing treelike graphs, which should fairly sample the possible set of graphs in the usual sense that a graph of N bonds is as likely to occur as any other graph of N bonds.

In a previous publication[3] a sequential algorithm was proposed: Choose possible bonds at random, and add them to the graph if the tree condition is not violated. At every step of this process, every bond of the lattice belongs to one of three categories: (1) It belongs to the graph; (2) it may not be added to the graph because it would introduce a closed loop; or (3) it may be added to the graph. On the basis of this algorithm, it was argued that p_c for treelike percolation must lie below p_c for ordinary percolation (for which $p_c = \frac{1}{2}$), because the sequential algorithm for ordinary percolation counts bond additions that do not change the number of sites in any cluster (namely the ones that connect sites belonging to the same cluster), whereas the treelike percolation algorithm only counts the bonds that join disconnected trees.

This conclusion is incorrect because there is a systematic bias in the algorithm. This bias comes about because the number of bonds that can be added legally to any given graph is graph dependent, and thus so is the probability that any particular graph will follow the given graph in the sequence. The result is that some graphs are favored over others in the construction algorithm; in the thermodynamic limit the favored graphs are overwhelmingly likely to occur. The sequential algorithm works for ordinary percolation because in that case the number of bonds that may be added to a graph depends only on the number that have been added already; all graphs of N bonds have the same probability of being constructed.

The bias can have an effect on the conclusion, as can be seen by consideration of another (equally faulty) algorithm: starting from a close-packed tree graph, delete a finite fraction q of the bonds. We can prove that the resulting graph does not percolate by considering any two sites of the graph. Initially the sites were connected by a single path having M steps. The probability that this path was not broken by the bond deletions is $(1-q)^M$, which is small for large M. Thus it is very unlikely that sites that are distant from each other are connected, and so all trees must be finite.

This algorithm also is biased (this is readily established by considering the subgraphs of the Wheatstone bridge). Since the arguments cannot both be correct, we must conclude that both are seriously faulty.

The difference between these algorithms is similar to the difference between percolation processes and growth processes.[6] Percolation is an example of an equilibrium process in which each distinct cluster is counted only once; whereas in growth models, a given cluster is constructed by successive addition of new elements to an existing cluster. Generally there are many ways of growing a given cluster, and so each distinct cluster can occur more than once. Monte Carlo simulations[6] and renormalization calculations[7] have shown that the scaling behavior of clusters in growth models is different from those generated in equilibrium models, owing to the different weights assigned to the clusters.

III. AN UNBIASED ALGORITHM

The Metropolis Monte Carlo method[8] suggests the following algorithm. Starting from an arbitrary tree graph of N bonds, iterate the two-step process: (1) delete a bond at random and (2) add a bond at random which does not violate the tree condition.

Defining $P_i(n)$ to be the probability that graph i occurs on the nth iteration, the process defines a transformation

$$P_j(n+1) = \sum_i T_{ji} P_i(n) . \tag{9}$$

To show that the iteration converges to an unbiased distribution, we need to show that $T_{ij} = T_{ji}$. Then the distribution $P_i = \text{const}$ is an eigenvector of T, and corresponds to the largest eigenvalue (unity). Then for arbitrary starting distribution, $P_i(n)$ converges to the uniform distribution.[9]

To prove that T_{ij} is symmetric, consider an arbitrary graph G of N bonds, the intermediate graph I generated from it by the deletion of a bond, and the graph G' generated from I by addition of a bond which does not form a closed loop. The probability that the two-step process will take this particular route is the product of the probability that the chosen bond will be deleted, which is just $1/N$, and the probability that the graph G' (and not some other

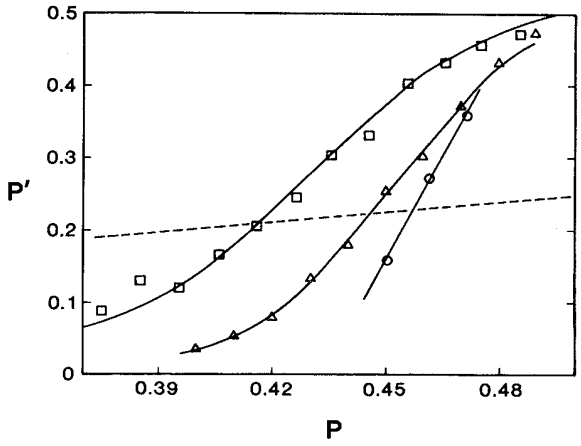

FIG. 1. Average probability p' that a graph percolates as a function of bond probability p, for various L (squares, $L=10$; triangles, $L=20$; circles, $L=40$). Dashed line is the locus $p'=p$.

graph) will be formed by the bond addition: This is the reciprocal of the number of graphs that could be formed, which is also the number of bonds that may be added to I without forming a closed loop. The graph G is also one of these graphs, and so it is equally likely that the second step will produce the graph G as it is that any particular graph G' will result.

Now consider the reverse process, which starts from G' and produces G. The probability of the first step is again $1/N$, and the probability of the second step is also the same, by the argument just given. This completes the proof that T_{ij} is symmetric, and that the algorithm is unbiased.

IV. SIMULATION RESULTS

The algorithm described in the preceding section was programmed in FORTRAN and run on the University of Alabama Univac 1100/60. Finite lattices of edge $L=10$, 20, and 40 were considered. Helical boundary conditions were employed, and the condition for percolation was that there be a site on the last row which is connected to a site on the first row. An important part of our algorithm is an array which determines which tree each site belongs to. The condition that a new bond not form a closed loop is easily implemented, by checking that distinct trees are being connected. The updating of this array after a bond is added is quite simple. However, after a bond is deleted, the sites of the tree involved must be sorted into the two new trees involved, and this proved to be a costly process when a large tree is cut. Of course these are also the cases which make possible a large scale reorganization of the graph. The consequences are that the data for the 40×40 lattices are based on Monte Carlo runs in which only 10 000 bonds were altered, i.e., six changes per site, but that these results may still be usable, since for the smaller lattices the fraction of percolating graphs stabilized within a few changes per site to an average value that did not change greatly thereafter. For the 20×20 and 10×10 lattices, 12 000 and 15 000 bonds (respectively) were altered.

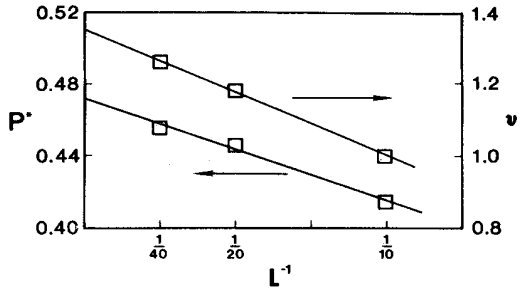

FIG. 2. L dependence of p_c^* and ν.

The results are shown in Fig. 1. Finite-size scaling and renormalization theory[10] assigns a size-dependent percolation threshold p_c^* by the rule $p=p'=p_c^*$; Fig. 2 shows how these values depend on lattice size. These results indicate that p_c is above 0.48, suggesting that the percolation threshold is exactly $\frac{1}{2}$.

The correlation length for treelike percolation is also given by finite-size scaling arguments; it is related to the slope of the curves in Fig. 1 by the rule

$$L^{1/\nu^*}=dp'/dp\,|_{p_c}\,, \tag{10}$$

where L is the lattice edge. The trend of the derived values for ν^* are also shown in Fig. 2; they suggest $\nu=1.35\pm0.1$.

ACKNOWLEDGMENTS

This work was supported by the National Science Foundation under Grants Nos. DMR-81-14767, 82-44366 (J.P.S.) and DMR-82-08051 (F.F.).

*Permanent address.

[1]M. J. Stephen, Phys. Lett. 56A, 149 (1976).
[2]F. Y. Wu, Phys. Rev. B 18, 516 (1978).
[3]J. P. Straley, Phys. Rev. B 19, 4845 (1979).
[4]R. B. Potts, Proc. Cambridge Philos. Soc. 48, 106 (1952).
[5]M. P. M. den Nijs, J. Phys. A: Math. Gen. 12, 1857 (1979).
[6]For a review of the scaling properties of growth models, see H. E. Stanley, F. Family, and H. Gould, J. Poly. Sci. (in press).
[7]H. Gould, F. Family, and H. E. Stanley, Phys. Rev. Lett. 50, 686 (1983).
[8]N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. 21, 1067 (1953).
[9]A. W. Goodman and J. S. Ratti, *Finite Mathematics with Applications* (Macmillan, New York, 1971), pp. 255–262.
[10]K. G. Wilson and J. Kogut, Phys. Rep. 12, 75 (1974).