Treelike percolation

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Several loopless percolation models are described, and low-density series are developed for Stephen's treelike percolation model. Analysis of these indicates that the two-dimensional bond and site models do not have an infinite cluster present at finite dilution.

I. TREELIKE PERCOLATION AND OTHER LOOPLESS PERCOLATIONS

Treelike percolation is concerned with connectedness and other properties of the ensemble of graphs on a lattice which contain no closed loops. The problem was first posed by Stephen.[1] He defined the treelike percolation problem in terms of a Potts model for s states with interaction energy $-sJ$ for neighboring sites in the same state. He showed that in the limit $s \to 0$ the graphs with loops vanish more rapidly than the tree graphs, so that for a lattice of N sites

$$\lim_{s\to 0}[Z(\beta,s)/s^N]=Q_N(z)=\sum_n z^n T_n \ , \tag{1}$$

where $z(\beta,s)$ is the partition function for the Potts model, T_n is the number of graphs of n bonds with no closed loops that can be drawn on the lattice, and

$$z=\lim_{s\to 0}(e^{sJ\beta}-1)/s=J\beta \ . \tag{2}$$

In this ensemble every tree graph with the same number of bonds occurs with equal probability. This ensemble is the principle subject of this paper. It has been previously discussed by Wu[2] and by Braswell, Family, and Straley.[3] The goal of this paper is to learn more about the behavior near the transition by use of expansion methods.

Other ensembles have been defined, generally due to a faulty analogy with ordinary percolation theory. Looplessness entails a correlation among bonds on the lattice, and while it is possible to define bond and site densities, it is erroneous to think of these as the probabilities that a given bond or site will be present, independent of the context. As examples of the ways this assumption can inadvertantly enter, three other ensembles will be described. These alternate ensembles are well defined, albeit not well characterized, and it is certainly possible to study any one of them. However, it is essential that they not be confused with each other; it is quite possible that these different ensembles differ from each other as much as the percolation problem differs from other bond models, such as the parking model[4,5] or the Ising model.

(i) Straley[6] proposed attempting to add bonds to an initially empty lattice at randomly chosen positions, rejecting the attempt whenever the chosen bond was already in place or when its addition would form a loop. The resulting ensemble does not contain all tree graphs with equal weight: at any intermediate stage, some graphs will contain compact clusters such that many links are constrained not to be present, whereas other graphs will predominately contain extended ones to which any bond can be added. Then there are more possible progeny of the "extended" graphs, with the result that any particular outcome is less likely. In this ensemble, graphs having compact subgraphs will tend to dominate. The extension of this construction to a site model runs into the further difficulty that the highest density graphs have a correlated structure that cannot in general be obtained by placing particles at random, as in the parking model.

(ii) Another construction scheme would be to start from the ensemble of close-packed trees, and delete bonds at random. Every deletion is legal, but the ensemble is again skewed in distribution, because the progeny graphs are not uniquely derived. The two clusters formed by deletion of a single bond can be rejoined in many ways, especially if each is large and they are extensively intercalated. The number of ways a graph can be formed by deletion is the number of ways a bond can be legally added; thus large, rough clusters are more likely to occur than any particular graph having small clusters.

(iii) Tzschichholz, Bunde, and Havlin[7] recently proposed a loopless percolation based on a growth process in which sites are added to the perimeter of an existing cluster with probability P provided that so doing does not form a loop, and that the site has not already been considered. They show that there is a critical value of P, above which the cluster grows indefinitely, and that the clusters at criticality resemble clusters for ordinary percolation at the percolation threshold in having a similar radial density profile and radius of gyration about the origin. However, it must be observed that these clusters will be highly inhomogeneous: to the extent that the clusters grow symmetrically, they will only be connected in the radial direction; at points distant from the origin of the cluster the circumferential correlation length will be much shorter than the radial one. Random walks that start at points distant from the origin will display an unsurprising one-dimensional behavior, as will all random walks at long times. It should also be noted that even for $P=1$ this construction scheme will not build clusters of close-packing density. In this respect the comparison with the parking problem[4,5] is quite apt.

These alternate construction algorithms are growth processes, for which the probability of occurrence of a

given graph is dependent on how it has been constructed and is not readily computed from the form of the graph itself. Under these circumstances one must be careful in the application of concepts from equilibrium statistical mechanics.

Uniformly sampling the ensemble of treelike graphs is not simply achieved. In principle this can be done by adding bonds at random to an empty lattice, and only accepting the results if a loop is never formed. Of course, the success rate would be extremely low. A more efficient algorithm has been described by Braswell, Family, and Straley;[3] it is still much slower than the construction of uncorrelated percolation clusters.

II. THE PERCOLATION THRESHOLD

At close packing, there is only one tree present, and the system obviously percolates. It is less clear whether there will ever be an infinite cluster present at finite dilution.

The bond problem on the square lattice does not percolate at finite dilution, according to an argument of Wu,[2] based on a duality relationship for the bond percolation problem in two dimensions. The dual transformation relates low-temperature properties of a Potts model to high-temperature properties of another Potts model defined on the dual lattice (which is also a square lattice). The critical temperature of the general Potts model can be located as the one temperature that is mapped into itself.[8] Reformulating this argument to the treelike percolation problem, Wu found that the critical fugacity is $z=\infty$, which implies that the transition occurs at close packing.[3] This argument only applies to the two-dimensional bond problem, and even there is slightly problematic, since the dual to a tree graph is a graph which contains only infinite linked clusters; the tree graphs have this property only at close packing.

It is a general property of treelike percolation that the percolation threshold will be close to the close-packing limit. Any tree graph at finite dilution can be generated by randomly deleting a finite fraction q of the elements from a close-packed tree, and the graphs built this way are composed only of finite clusters (there is only one path joining any pair of sites in the close-packed tree, and the probability that this path survives the deletion process is exponentially small). This argument seems to imply that the tree percolation and close-packing densities must coincide; however, the ensemble of bond graphs built this way is skewed, and it is possible (and consistent with the discussion above) that this has led to an improper estimate of the probability of an infinite cluster being present.

The close-packing limit of tree graphs is readily determined from geometrical considerations. At the close-packing limit there will be only one cluster present. In the bond percolation problem every site will belong to this cluster, and the number of occupied bonds B_o will be given by Euler's theorem

$$S=B_o+1 \ , \tag{3}$$

from which we may immediately conclude that the bond density per site is unity at close packing for treelike bond percolation. (It is more common to use the bond density per lattice bond in bond percolation problems. The number of bonds on the lattice is $zS/2$, where z is the coordination number, because z bonds meet at each site, and each bond is shared by two sites. Then the close packing bond density per lattice bond is $2/z$. However, in what follows, all quantities will be quoted on the per site basis.)

In the site problem, the sites of the lattice are classified as being occupied (o), constrained (c), or free (f), where the constrained sites are those whose addition would form a loop, and the free sites are those that are neither occupied nor constrained. The state of a bond is determined by the sites that it joins; they may be classified as oo, oc, of, etc. At close packing there are no free sites. Euler's theorem relates S_o to B_{oo} as before [Eq. (3)]; the bond-counting relationship now relates the number of occupied sites to the bonds internal to the cluster and bonds between occupied and constrained sites

$$zS_o=2B_{oo}+B_{oc} \ . \tag{4}$$

Bond counting around the constrained sites gives

$$zS_c=B_{oc}+2B_{cc} \ . \tag{5}$$

The constrained sites have at least two neighboring sites that belong to the cluster, and may have as many as z in loose-packed structures. In this latter case, B_{cc} is zero, and combining these three equations gives

$$\frac{S_o}{(S_o+S_c)}=\frac{z}{(2z-2)} \ . \tag{6}$$

Configurations which achieve this density are readily constructed for the quadratic, honeycomb, and simple cubic lattices.[9] Accomplishing this relatively high density requires that the vacant sites be multiply constrained (occupying the site would form more than one loop); then there are also configurations of lower density which still have no free sites, and cannot be obtained by deleting sites from the close-packed configurations.

III. LOW-DENSITY EXPANSIONS

Since the region of interest is the high-density limit, an expansion about this limit would be preferable. However, the high-density configuration is not unique, and in fact there is a finite entropy per bond.[10]

Low-density expansions are quite straightforward. Two problems were considered: treelike graphs of bonds (for which the bond set for each graph is specified explicitly) and treelike graphs of sites (for which the sites of the graph are specified, and neighboring sites in this set are always connected). The goal is to determine the number T_n of graphs of n bonds that can be drawn on a lattice of N sites. According to Eq. (1), these determine the partition function as a power series in z. The number of elements per site belonging to finite clusters is

$$p=\frac{z}{N}\frac{d\ln Q_N}{dz} \ , \tag{7}$$

which in the Potts language is the internal energy density.

For a finite cluster, such as a $L \times M$ rectangle of sites, the partition function is a polynomial P_{LM}. A transfer matrix can be defined which describes the effect of adding one row of sites to such a rectangle, and in this way the polynomials P_{2L}, P_{3L}, and P_{4L} were determined for the bond problem, and in addition the P_{5L} and P_{6L} were found for the site problem. Following Enting,[11] a "reduced" series R_{LM} corresponding to each rectangle is constructed by dividing the polynomial for the rectangle by the polynomials for all enclosed rectangles. For example, the nine-site square has the polynomial P_{33}; R_{33} is computed by dividing by $P_{11}^9 P_{21}^{12} P_{22}^4 P_{32}^4$ representing the 9 sites, 12 bonds, 4 squares, and 4 rectangles it contains. Each series is of the form $1-C_K z^K$, where K is the number of elements in the smallest nondecomposable graph that contains a loop and that fits into the rectangle but not into any smaller rectangle; C_K is the number of such graphs.

The site and bond problem differ in that the smallest bond polynomial is P_{21} for a single bond, whereas for the site problem it is P_{11}. They both have the value $1+z$.

Bond graphs having free ends or loops joined at a single point are decomposable, and K is the perimeter $2L+2M-4$ of the rectangle; the set of graphs that contribute to the leading term of the series are formed from the rectangular loop by turning in its corners. The number of such graphs is simply determined; in this way it was determined that $R_{55}=1-1110z^{16}$. This made it possible to determine the first 16 terms of all R_{LM}: for large L and M all terms are zero, and for small L and M the reduced series have been constructed explicitly or generated by this combinatorial method.

For the site problem, loops that share one point are not decomposible, and $K=2(L-M)+3M+1$ (assuming L is greater than M); for $L=M$, $C_M=-(-1)^M 2$, because the minimal nondecomposable graph is a diagonal series of corner-sharing squares. Thus, in particular $R_{77}\approx 1-2z^{19}+Dz^{20}$, where D is approximately 150. Except for the small uncertainty in the value of C_{20}, this determines the first 20 terms of all R_{LM} for the site problem.

The leading terms of the polynomial for a very large rectangle of N sites can now be computed from the reduced series R_{LM}, since every rectangle is contained N times (to order N). Thus the partition function is the product of the Nth powers of all the reduced series

$$Q_N=\prod_{LM} R_{LM}^N \ . \tag{8}$$

Taking the Nth root of both sides we obtain the "partition function per site" Q_1 and N drops out of the problem.

The coefficients of the series for Q_1 derived in this way are given in Table I. If there were a percolation threshold at which an infinite cluster forms for finite z, there would be a corresponding singularity in these series. However, Padé analyses of the series for Q_1, the series for p, and the logarithmic derivatives of these series indicate no poles on the positive real axis for the bond problem, and only a few scattered occurrences for the site problem, indicating that in both cases the transition is at close packing ($z=\infty$).

These series can be inverted to give z as a series in powers of p (or $p/2$ in the bond problem). These series

TABLE I. Coefficients of low-density series.

	$Q(z)$		$z(p/2)$	$z(p)$
n	Bonds	Sites	Bonds	Sites
0	1	1	0	0
1	2	1	1	1
2	1	0	1	1
3	0	0	1	1
4	−1	−1	3	5
5	2	3	3	5
6	−5	−4	9	−7
7	16	2	11	43
8	−54	−8	33	71
9	184	64	45	−355
10	−628	−220	73	497
11	2136	434	399	2749
12	−7229	−626	−357	−10 703
13	24 378	1612	2715	−149
14	−82 185	−7236	−1619	114 223
15	278 276	25 246	2715	−281 109
16	−951 192	−64 493	32 109	−509 937
17		149 603		4 378 279
18		−435 820		−5 598 677
19		1 358 526		−34 309 333
20		−5 103 194[a]		152 066 419[a]

[a]These coefficients assume $R_{77}=1-2z^{19}+150z^{20}$. The uncertainty in the coefficient of z^{20} gives a corresponding uncertainty in $Q(z)$.

are also given in Table I. The Padé analysis of these series showed a singularity near the close-packing density, as did the Padé analysis of the series for

$$\frac{p}{z}\frac{dz}{dp}=\frac{d\ln z}{d\ln p} .$$

The poles and residues for selected Padé approximants to the logarithmic derivative series are given in Table II. They clearly indicate a reciprocal square-root singularity at close packing for the bond model. The site model results indicate the present of a singularity of the form $z\approx(0.6-p)^{-0.8}$. This failure to correctly identify the close-packing density may be a consequence of the greater degree of positional correlations in the site model.

A check on the bond model results can be obtained by determining the degeneracy of close packing. For a finite cluster at close packing define

$$S=\frac{1}{N}\ln T_N . \tag{9}$$

Wu[10] has shown that the $N\to\infty$ limit of S exists and has determined its value to be $S=1.16624\ldots$ for the square bond lattice. This quantity can be calculated from the series in the following way. First note

$$\lim_{z\to\infty}\ln Q_N\approx\ln z^N T_N , \tag{10}$$

thus

$$S=\lim_{z\to\infty}[\ln Q_1-\ln z]$$
$$=\lim_{z\to\infty}\left[\int_0^z\frac{p}{z}dz-\ln z\right] , \tag{11}$$

where Eq. (7) has been used to evaluate the partition function. Changing variables in the integration,

TABLE II. Pole positions and residues of selected Padé approximants to $d\ln z(p)/d\ln p$.

Approximant	p	Residue
	Bond problem	
[8/6]	0.9964	−0.5306
[7/7]	0.9818	−0.4735
[6/8]	0.9819	−0.4737
[7/6]	0.9452	−0.3739
[6/7]	0.9810	−0.4709
[6/6]	1.000 69	−0.5338
	Sites problem	
[10/8]	0.5931	−0.7752
[9/9]	0.5965	−0.8162
[8/10]	0.5977	−0.8328
[9/8]	0.5939	−0.7843
[8/9]	0.5876	−0.6962
[8/8]	0.5567	−0.2777
[8/8]	0.6628	−0.7407
[8/7]	0.5946	−0.7920
[7/8]	0.5881	−0.7036

$$S=\int_0^{p(z)}\frac{d\ln z}{d\ln p}dp+\int_{p(z)}^{\infty}\frac{p-1}{p}\frac{d\ln z}{d\ln p}dp-\ln z , \tag{12}$$

where z is an arbitrary number and $p(z)$ is the corresponding value, which can be accurately determined if z is chosen to be small. The logarithmic derivative in the integrands was represented by the [6/6] Padé approximant, and the factor $(p-1)$ was replaced by $(p-1.000\,69)$ so that the critical pole in the approximant was accurately removed; then the integrals could be done numerically, giving $S=1.21$. This is comparable to Wu's value; the 6% error is consistent with the residue of the approximant being 0.53 rather than 0.5.

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