Percolation at a surface: The surface fractal dimension

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It is shown that the fractal dimension which characterizes the intersection of percolation clusters with the lattice surface at the critical point may be expressed in terms of the bulk fractal dimension and critical exponents γ, ν, and γ_1 at the ordinary transition. Estimates of this quantity are obtained from exact enumeration data for the triangular and fcc lattices.

The concept of a fractal dimensionality has, in recent years, assumed considerable importance, in part because of the large number of naturally occurring structures which can be characterized by one or more fractal dimensions.[1] The importance of this concept in critical phenomena and its relation to conventional critical exponents was first pointed out by Stanley,[2] who applied the concept to percolation[3] clusters. In the case of percolation the fractal dimension d_f is equivalent to the field renormalization-group exponent y_h,

$$d_f = y_h \ . \tag{1}$$

d_f here is defined by

$$S \propto l^{d_f} \ , \tag{2}$$

where S is the number of sites belonging to a dominant cluster,[4] contained in a box of side l. The equality (1) follows immediately if it is assumed that a renormalization-group transformation which preserves the generating function

$$G = \sum_s e^{-sh} P_s \tag{3}$$

for the probability that a cluster of exactly s sites occurs, P_s, can be constructed (G is the analog of the free energy and h the analog of the external field in magnetic systems[3]). At their fixed-point values the parameters which determine P_s are invariant under the transformation and the preservation of G_s then implies

$$h's' = hs \tag{4}$$

(where primed quantities are those obtained after the transformation). If the length-rescaling factor of the transformation is b, then (2) implies

$$S' = S/b^{d_f} \ . \tag{5}$$

From (4) and the definition of y_h,

$$y_h = \ln(\partial h'/\partial h)/\ln b \ , \tag{6}$$

one obtains (1). [The derivatives in (6) are evaluated at the fixed point with $h=0$.]

The above argument is now extended to the case of percolation in a semi-infinite system.[5] In this case the generating function is written

$$G_1 = \sum_{s,s_1} e^{-hs - h_1 s_1} P_{s,s_1} \ , \tag{7}$$

where P_{s,s_1} is the probability of a cluster with exactly s sites, s_1 of which are in the surface. h_1 may be interpreted as an external field that couples only to the surface sites. We assume that the way the number of surface sites of a dominant cluster scale with the side of the box containing them is determined by a surface fractal dimension d_s such that

$$S_1 \propto l^{d_s} \ . \tag{8}$$

Following the same argument used to obtain (1) and evaluating the surface renormalization group exponent[5]

$$y_{h_1} = \ln(\partial h_1'/\partial h_1)/\ln b \ , \tag{9}$$

we obtain

$$y_{h_1} = d_s \ . \tag{10}$$

To relate d_s and d_f we note that y_h and y_{h_1} are related to the correlation-length exponent ν, bulk gap exponent Δ, and surface gap exponent Δ_1 at the ordinary transition by[4,5]

$$y_h = \Delta/\nu \ , \tag{11a}$$

$$y_{h_1} = \Delta_1/\nu \ . \tag{11b}$$

The two surface mean-cluster-size exponents γ_1 and γ_{11} are related to the gap exponents by[5]

$$\gamma_1 - \gamma_{11} = \Delta - \Delta_1 \tag{12}$$

and to the bulk mean-cluster-size exponent γ by

$$\gamma + \nu = 2\gamma_1 - \gamma_{11} \ . \tag{13}$$

Combining Eqs. (10)—(13) and Eq. (1) one obtains

$$\frac{\gamma-\gamma_1}{\nu}=(d_f-1)-d_s \ . \tag{14}$$

The significance of (14) is that it gives a direct geometrical interpretation to the difference between the exponent γ_1 which characterizes the divergence of the mean size of clusters attached to the surface as the critical point is approached and its bulk (clusters not in contact with the surface) counterpart. We see from (14) that the difference in these two exponents is a measure of the difference between the surface fractal dimension d_s and d_f-1, two geometric properties which would be equal if the percolation clusters were compact structures with the Euclidean dimensions of the space in which they are embedded.

If the bulk properties γ, ν, and d_s are known, it remains only to determine γ_1. Previously, estimates of γ_1 have been based on exact enumeration data[6] for the triangular and face-centered-cubic (fcc) lattices.

Here we give improved estimates for γ_1 for bond percolation on the triangular and fcc lattices. The improvements come from extensions of the low-density series for the surface mean cluster size

$$\chi_1=\sum_n C_n p^n \ , \tag{15}$$

by one term ($C_{11}=812\,716$) for the triangular lattice and two terms ($C_8=36\,992\,550$, $C_9=318\,618\,041$) for the fcc lattice, and the use of the Baker-Hunter[7] method of analysis to allow for confluent singularities. [p in (15) is the probability that a lattice bond is occupied.]

χ_1 is expected to diverge as p approaches its critical value from below according to

$$\chi_1\sim(p_c-p)^{-\gamma_1}(1+\cdots) \ . \tag{16}$$

In recent years several authors have demonstrated that confluent singularities due to nonanalytic corrections [contained in the ellipses of (16)] must be allowed for in analyzing series of this type.[8] The Baker-Hunter[7] method constructs an auxiliary function from χ_1 which has a simple pole at $1/\gamma_1$ and in which the remaining confluent singularities in χ_1, only gives rise to poles further removed from the origin. $1/\gamma_1$ may then be estimated from a Padé approximant analysis of the auxiliary function.

The value of p_c is required as input in the Baker-Hunter method. Since this is not known exactly for the fcc lattice, we used a number of trial values in the range $p_c=[0.1185,0.1205]$. As for other series analyzed by this method[9,10] the higher-order approximants show an improved convergence for a relatively small range of p_c values (Fig. 1). Estimating p_c from this region of best convergence we obtain

$$p_c=0.11965^{+0.000\,10}_{-0.000\,10} \quad \text{(fcc)}$$

in good agreement with the estimate $p_c=0.1196^{+0.0001}_{-0.0002}$ obtained from an analysis of the corresponding bulk series for which one more term is available.[10]

The corresponding estimate of γ_1 for the fcc lattice is

$$\gamma_1=1.28\pm0.03 \quad \text{(fcc)} \ ,$$

where the error bounds represent only the variation over the approximants shown in Fig. 1 and include the variation due to the uncertainty in p_c.

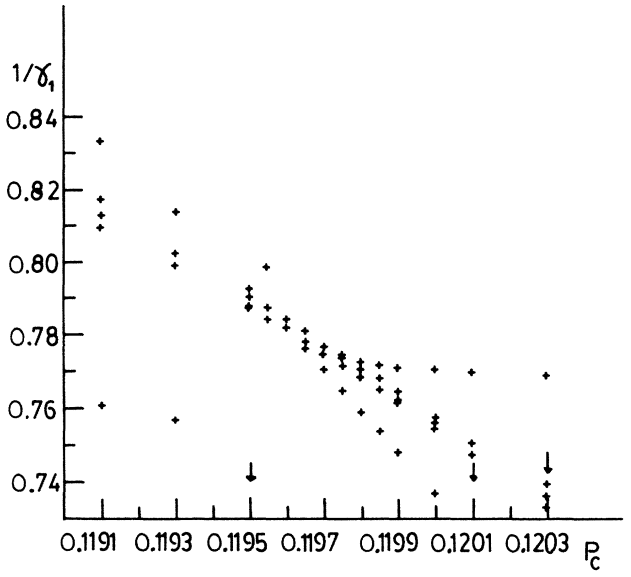

FIG. 1. Estimates of $1/\gamma_1$, for various trial values of p_c, from $[N/M]$ Padé approximants with $8\leq N+M\leq 9$. Arrows indicate that a Padé approximant pole lies outside the range of the diagram.

In the case of the triangular lattice p_c is known exactly[11] to be

$$p_c=2\sin\frac{\pi}{18}\approx 0.3473 \quad \text{(triangular)} \ .$$

Using this value of p_c in the Baker-Hunter method, we estimate

$$\gamma_1=2.07\pm0.03 \quad \text{(triangular)} \ .$$

In an attempt to test the method by which p_c was determined for the fcc lattice, we varied the value of p_c for the triangular lattice around its exact value. However, there is no significant change in the degree of convergence for the trial values of p_c in the range [0.3469,0.3476]. A similar result was found for the bulk series for this lattice. This may indicate that longer series for this lattice are required to obtain convergent results from the Baker-Hunter method and, hence, the rather wide error bounds on γ_1 (which again reflect only the variation over the higher-order approximants used) despite p_c being known exactly.

We now return to the calculation of d_s. For two-dimensional systems the exponents γ, ν, and γ_1 have been calculated by methods which assume invariance properties of the model under a conformal transformation, but are otherwise exact.[12] These methods give

$$\gamma_1=\tfrac{25}{12}, \quad \gamma=\tfrac{43}{18}, \quad \text{and} \quad \nu=\tfrac{4}{3} \ .$$

Our present results for γ_1 are consistent with these values as are previous estimates of γ (Ref. 10) and ν (Ref. 13), and we adopt them to calculate d_s. It is well known that using the above values of γ and ν, the scaling relation

$$\Delta=(d\nu+\gamma)/2 \ , \tag{17}$$

where d is the dimension of the space in which the clusters are embedded, and Eqs. (1) and (11), one obtains the bulk fractal dimension for $d=2$

$$d_f=\tfrac{91}{48} \quad (d=2) .$$

Using this value of d_f and the above values of γ, γ_1, and ν in Eq. (14) gives the surface fractal dimension for $d=2$

$$d_s=\tfrac{2}{3} \quad (d=2) .$$

For the case $d=3$ we use the estimate obtained from our analysis for γ_1 and previous estimates of γ for the fcc lattice[10]

$$\gamma=1.74\pm0.03$$

and ν for $d=3$ (Ref. 14),

$$\nu=0.88\pm0.02 .$$

From these values of γ and ν we obtain the bulk fractal dimension

$$d_f=2.49^{+0.03}_{-0.04} \quad (d=3) ,$$

Our estimate of γ_1 and these values for the bulk quantities gives

$$d_s=0.97\pm0.11 \quad (d=3) .$$

In conclusion, we have estimated the fractal dimensionality d_s which characterizes the intersection of percolation clusters close to criticality (at the ordinary transition) and the surface of the semi-infinite Euclidean space in which they are embedded for $d=2$ and 3. In addition, it is trivial to show that for $d=1$, $\gamma_1=\gamma=1$ and, hence, $d_s=(d_f-1)=0$. At $d=6$ we expect γ, ν, and γ_1 to achieve their mean field values[15] so that at $d=6$, $d_s=(d_f-1)-1$, and first-order corrections in $\epsilon=(6-d)$ to this mean-field result can be calculated from the ϵ expansion for these exponents[16,17]

$$(d_f-1)-d_s=1-\epsilon/7 .$$

These results, together with the above estimates for $d=2$ and 3, indicate the difference between d_f-1, and d_s increases with d for $1\le d\le 6$. In fact, this reduction in d_s below (d_f-1) is due purely to the reduction in the connectivity when the space is cut by a surface which cannot be penetrated by the percolation clusters. To see this consider a $(d-1)$-dimensional plane which passes through the bulk space. Such a plane passes through the clusters but does not disconnect the parts of the bulk clusters it intersects. This is the special plane problem of Ref. 5 (with $p_1=p$) and in this case $\gamma_1=\gamma$. Thus the intersection of a bulk cluster with a $(d-1)$-dimensional plane (which does not disconnect the two parts of the cluster which it passes through) is (d_f-1) for any Euclidean dimension d (in the special plane problem γ_1 is the exponent for the mean size of clusters which are in contact with the special plane).

Note added: Since submitting this manuscript for publication, the authors have learned of a paper by Christou and Stinchcombe[18] in which they discuss the surface fractal dimension for percolation. These authors express the surface fractal dimension in terms of the high-density exponents β and β_1, and conclude that there is no numerical work available to confirm their qualitative conclusions about the importance of the surface as lattice dimensionality increases. However, the relationship for the surface fractal dimension given by these authors is easily shown to be equivalent to our Eq. (14) by using the scaling relations of Ref. 5. (The high-density surface exponent β_1 referred to in Ref. 18 has been estimated by Monte Carlo methods in two dimensions.[19])

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