Surface fractal dimension for percolation clusters: A Monte Carlo study

T. Lookman

Department of Applied Mathematics, University of Western Ontario, London, Ontario, Canada N6A 5B7

K. De'Bell

Physics Department, Trent University, Peterborough, Ontario, Canada K9J 7B8

(Received 11 February 1992)

Monte Carlo methods have been used to determine the fractal dimension which characterizes the intersection of percolation clusters with the lattice surface at the critical point. A comparison is made with earlier exact enumeration results. In two dimensions surface scaling laws for cluster statistics have been directly verified.

I. INTRODUCTION

It has previously been shown that the difference between the fractal dimension d_s which characterizes the intersection of percolation clusters with a lattice surface, and the bulk fractal dimension d_f may be expressed in terms of the bulk critical exponents γ and ν and the surface critical exponent γ_1 by^{1,2}

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

In previous work we used estimates for γ_1 , γ , and v, obtained from exact enumeration data, to calculate $d_f - d_s$. (The difference in these fractal dimensions can also be expressed in terms of the bulk and surface order parameter exponents β and β_1 . Watson³ has estimated β_1 from Monte Carlo data.)

In this study we have generated large percolation clusters attached to a surface and hence obtained direct estimates of $d_f - d_s$ in two and three dimensions. This has allowed a more precise estimate of this difference in three dimensions than that obtained from exact enumeration data. By an analysis of the surface cluster data, we have verified the scaling form for surface cluster statistics in two dimensions.

II. SIMULATION AND ANALYSIS

A modified Leath⁴ algorithm was used for growing clusters. A point on the surface of the lattice was chosen as the seed point. During the growth process, sites in the perimeter of the growing cluster (which have not previously been visited) are visited and occupied with probability $p = p_c$. This growth process terminated when the list of sites to be visited was empty or the cluster reached another boundary of the lattice. Clusters that terminated in the latter manner were considered to have died unnaturally and were excluded from the cluster statistics. Small clusters (less than 1000 sites in two dimensions or 500 in three dimensions) were also excluded, since these do not have enough sites to allow a meaningful analysis of the fractal dimensions.

We expect that, for sufficiently large clusters, the total

number of sites in the cluster N and the number of cluster sites in the lattice surface N_s are related by

 $\langle N_{\rm s}/N \rangle = Ar^D$, (2)

where A is a constant,

$$
D = d_s - d_f \t{,} \t(3)
$$

and r is the root-mean-square distance from the seed. Since, in general, we do not expect two clusters to have exactly the same value of r , we binned clusters according to their value of r . The size of the bins was chosen so that each bin contained at least 50 clusters. The value of r used in the analysis was the average value of r in each bin and the corresponding average $\langle N_s/N \rangle$ calculated for each bin.

For each bin i we calculated

$$
D_i = \ln \langle N_s / N \rangle_i / \ln r_i \tag{4}
$$

The error E_i in D_i is

$$
E_i = \ln A / \ln r_i + \sigma_i \tag{5}
$$

where σ_i is the statistical error associated with bin *i*. The average (over bins) of D_i and its standard deviation was plotted as a function of 1/(minimum value of $\langle N \rangle_i$ in the bins used in the average). This procedure was chosen because for large clusters where the systematic error $(\ln A / \ln r_i)$ is small, the statistical error is large due to the relatively small number of clusters available for analysis. Figure ¹ shows typical plots of this type. The plot is extrapolated to infinite cluster size to obtain the final estimate for D. These are summarized in Table I.

TABLE I. Summary of results for two- and threedimensional lattices.

Lattice	Cluster size range	Number of clusters	$d_{\ell}-d_{\kappa}$
Triangular	1000-150000	6000	1.20 ± 0.05
Square	1000-150000	8500	1.18 ± 0.05
Simple cubic	$500 - 1250$	8500	1.34 ± 0.04

 (a) -1.15 $<$ D $>$ -1.20 -1.25 -1.30 θ 0.4 1.2 0.8 1.6 2.0 2.4 2.8 10^5S $\textbf{-}1.0$ (b) -1.1 -1.2 \langle D $>$ -1.3 -1.4 -1.5 -1.6 $\overline{0}$ 10 12 18 6 14 $16\,$

FIG. 1. The average (over bins) of D , $\langle D \rangle$, plotted against 10⁵S where $S = 1/(minimum$ value $\langle N \rangle$ in each bin) for (a) triangular and (b) simple cubic lattices. The dashed lines indicate the standard deviation.

 10^5S

III. SCALING ANALYSIS

Generalizing the standard scaling theory for bulk percolation,⁵ we expect the number of clusters of N sites, N_s of which are in the surface, to scale as

$$
n_{N,N_s} = N^{-\tau_s} \phi(\epsilon N^{\sigma}, \epsilon N_s^{\sigma_1}), \qquad (6)
$$

where

$$
\epsilon = p_c - p \t{,} \t(7)
$$

$$
\sigma/\sigma_1 = d_s/d_f, \tag{8}
$$

and

$$
\tau_s = \frac{(d-1)}{d_f} + 1 \tag{9}
$$

Hence, for $\epsilon = 0$ and N very large we expect

$$
n_{N,N_s} \sim N^{-\tau_s} \tag{10}
$$

FIG. 2. A plot of $\ln n_{N,N_s}$ against $\ln N$ for the triangular lattice. The slope gives the value for τ_s .

 10

 10.5

 $\mathbf{1}$

 11.5

 9.5

 $ln N$

ġ

We have been able to verify this form for the twodimensional lattices and obtain estimates

$$
\tau_{\rm s} = 1.48 \pm 0.06 \quad \text{(triangular)} \tag{11}
$$

$$
\tau_s = 1.53 \pm 0.06 \quad \text{(square)} \tag{12}
$$

from the data (see Fig. 2), consistent with the value of τ =1.53, obtained by using the scaling relation (9) and the exact value of $d_f = 1.89$. In three dimensions, due to a lack of data for sufficiently large clusters, there is too much curvature in the plots of $\ln n_{N,N_c}$ vs $\ln N$ to allow us to estimate τ_{s} .

IV. SUMMARY

The aim of this work has been to directly measure the geometrical properties of the intersection of large percolation clusters with a lattice surface. These properties are characterized by the difference $d_f - d_s$ (noting that $d_f - d_s = 1$ for a Euclidean object). Our estimates for $d_f - d_s$ in two and three dimensions are given in Table I. In two dimensions our results are consistent with the values obtained from conformal invariance theory and Eq. (1). In three dimensions our value is 1.34 ± 0.04 , lower than the value 1.53 ± 0.09 obtained earlier by using exact enumeration data and Eq. (1). The series result is based on a relatively small number of terms and, as such, the error estimate represents only the apparent convergence in the analysis. Therefore we consider the Monte Carlo estimate to be more reliable.

ACKNOWLEDGMENT

This work was supported in part by the National Sciences and Engineering Research Council of Canada.

 -1.10

¹K. De'Bell and T. Lookman, Phys. Rev. B 34, 4812 (1986).

²A. Christou and R. B. Stinchcombe, J. Phys. A 19, 757 (1986).

³B. P. Watson, Phys. Rev. B 33, 6446 (1986).

⁴P. L. Leath, Phys. Rev. B 14, 5046 (1976).

⁵D. Stauffer, *Introduction to Percolation Theory* (Taylor and Francis, London, 1985).