Scaling and short-time corrections for random walks on two-dimensional exactly percolating clusters

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Random-walk simulations on square-lattice percolation clusters are performed for (a) all clusters at criticality; (b) the largest cluster at nominal criticality; and (c) the largest cluster at exact criticality for each realization (new method). The short-time correction-to-scaling exponent is obtained: $\omega=-0.48$ (for $N<10^3$ Monte Carlo steps). The scaling exponent appears to be in better agreement with the recent Aharony-Stauffer conjecture for the spectral dimension ($d_s=1.309$) than with the Alexander-Orbach-Rammal-Toulouse conjecture ($d_s=1.333$).

I. INTRODUCTION

The problem of establishing fractal, or fracton, behavior in binary lattices of several dimensionalities has been dealt with by many authors[1–9] from different disciplines over the last year, utilizing a variety of methods, thus showing an unusually high interest in its nature and potential applications. In particular, after the original conjectures of universal critical exponents,[1–4] several authors[5–7,10,11] used Monte Carlo simulation techniques to test the hypothesis that these exponents really exist as well as derive their values. This is still a very active field of research.[8]

For binary lattices fractal behavior can be observed in a self-similar structure which is realized only at the percolation threshold, where other critical properties have also been observed in the past, such as the correlation length, the average size of a cluster, etc. For several static properties exponents such as ν, γ, β, etc., have been derived and their values have been tested by numerical simulation.[12] The fractal dimension is[8] $D=d-\beta/\nu$, where d is the embedding Euclidean dimension. For $d=2$, one has[8] $\beta=\frac{5}{36}$, $\nu=\frac{4}{3}$, and thus $D=\frac{91}{48}$. Work on dynamic properties in these structures, such as those described by random walks, only began recently. The random walk is characterized by a spectral (fracton) dimension d_s, which *inter alia* relates the mean number of distinct sites visited S_N to the number of random steps N via $S_N\sim N^{d_s/2}$. While originally it was conjectured[1,2] that $d_s=\frac{4}{3}$, it has later been suggested[8] that $d_s=2D/(D+1)=\frac{182}{139}$, which is about 2% lower. Also of interest is the transition from the critical point to a regular lattice characterized by full translational symmetry, something often termed as the crossover[3,6,10,11] from fractal-to-Euclidean behavior.

We calculate here a correction-to-scaling exponent ω for short-time behavior. At the same time we optimize the scaling exponent d_s. We use three approaches to the Monte Carlo simulation, one of them is new. Our results are consistent with a negative derivation from $\frac{4}{3}$ for the scaling exponent d_s. They also support one previous simulation result for ω, based on the simulation of the mean-square displacement, but seem to disagree with another previous simulation based, like ours, on S_N.

In this study we provide a new method of generating *exactly percolating clusters*, described below. Consequently, dynamical simulations are performed on such clusters. We calculate several random-walk properties using this method, as well as two previous ones, and establish again here the fractal behavior of these critical structures. Finally, we applied these results to the short-time behavior of a random walk on a percolating cluster and established the deviations from the asymptotic limit. We find that these deviations dominate in the region up to 1000—2000 steps whereas the long-time behavior seems to dominate from that point on.

II. METHOD OF CALCULATIONS

In all calculations up to now no exact realization of a percolating cluster has been attained, but several indirect approximations were used. In most cases, a lattice was nominally assigned the critical percolation concentration P_c, but in the actual numerical computation, due to statistical fluctuations, no exact realization of the P_c value can be attained, with the result that some realizations are well above the percolation threshold while others have not percolated at all. For these cases only the average value of this threshold in a large number of realizations can be achieved, thus making it more difficult to establish fractal behavior. To compensate for the above problem some indirect approaches were used. Realizations that were found to start on small finite clusters were excluded[13] from the averaging process and thus some partial improvement could be attained. However, the basic problem remained.

Unlike all previous studies,[5,7,13,14] all binary lattices here are generated in a new manner. A lattice has two types of sites with identities: 1 (allowed or open sites) and 0 (blocking, nonallowed or closed sites). All random

walks are performed on the terrain of sites having the identity 1, and no steps are allowed on sites of nature 0. Randomness is introduced by allowing all 0's and 1's to occupy sites as dictated by a random-number generator. In all work up to now, a relative ratio (or concentration) is specified for each realization. The new method consists of the following: Initially the value of 0 is assigned to all sites. Then we change the identity of only one site from 0 to 1. The location of this site is chosen at random. We then perform the cluster distribution, we isolate the largest cluster, and ask whether it has percolated or not. The criterion that we use for percolation is as follows. Sites belonging to this maximum cluster must be present at both ends of the lattice, i.e., either at the right and left boundaries or at the upper and lower boundaries. If the lattice has not percolated we change another 0 site to 1 and repeat the same process. Right at the point where percolation occurs we stop and store this particular lattice in the computer memory. All subsequent work is done using this lattice.

In this method we do not need to nominally specify the overall relative concentration ratio, as was done in the past. We have the advantage of generating clusters that are exactly at the percolation threshold, permitting us to perform each individual realization of a random walk (and not just the average) at precisely the proper point.

The cluster distribution is performed by using a new, very efficient algorithm based on the cluster-multiple-labeling[15] technique (CMLT), and it is extremely fast compared to all previous work. The computer-time costs are higher due to the repeated calculation of cluster distributions, but the improved cluster-multiple-labeling technique has made it feasible. As a rough estimate, the costs now are about three times as much as the conventional methods, such as the cluster-growth technique. It now takes typically 15 sec of CPU time on the Digital Equipment Corporation VAX11/750 computer with 550 Mbytes ($10^6 \times 8$ binary digits) of memory to perform one run with parameters as in Fig. 3 (see below).

III. RESULTS

The following figures contain our results. In Fig. 1 we plot S_N as a function of N. For comparison purposes we use three different approaches. Case (a): A square lattice with nominal concentration $P_c = 0.5931$, where a random walk may originate at *any* allowed (open) site in the lattice with equal probability. This calculation is done using the cluster-growth technique reported elsewhere,[10,14] and, for all practical purposes, the lattice can be thought of as having an infinite size. Case (b): A square lattice with a nominal concentration $P_c = 0.5931$, with a size of $300 \times 300 = 9 \times 10^4$ sites where the random walker originates on the largest percolating cluster only. Cyclic boundary conditions are used, and if the lattice for a particular realization has not percolated then it is rejected. Case (c): A square lattice, using the method described in the preceding section. The actual average concentration was found to be 0.5947 (compared with the nominal value of 0.5931). The size was $200 \times 200 = 4 \times 10^4$ sites, and cyclic boundary conditions were employed.

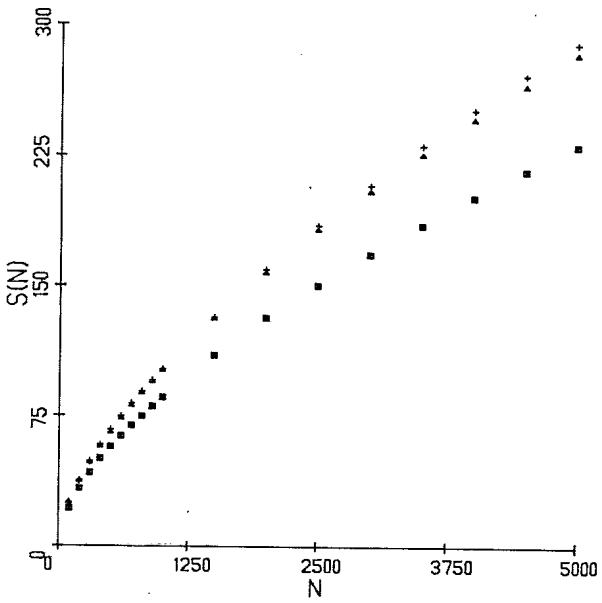

FIG. 1. Plot of S_N vs N for three different types of calculations at the critical percolation threshold: case (a), squares, 5000 runs; case (b), triangles, 5000 runs; case (c), crosses, 10 000 runs; see text for discussion. The topology is that of a square lattice.

We observe that case (a) differs considerably from case (b). This is expected because in case (a) the contributions from walks that start in small finite clusters tend to lower the overall S_N value, but are excluded from case (b). It gives[9] a scaling power $d_s' = d_s(2-d/D)$. There is only a small difference between cases (b) and (c) that shows above $N = 100$, and progressively increases. This is also expected because both cases involve random walks on the

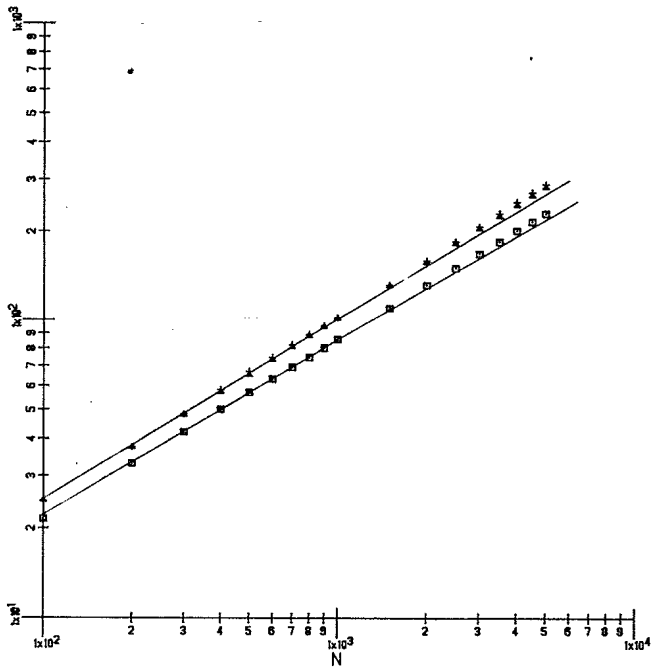

FIG. 2. Similar to Fig. 1 but in log-log scale. The point designation is also the same. The continuous lines are straight lines to show the deviation of the points from linearity.

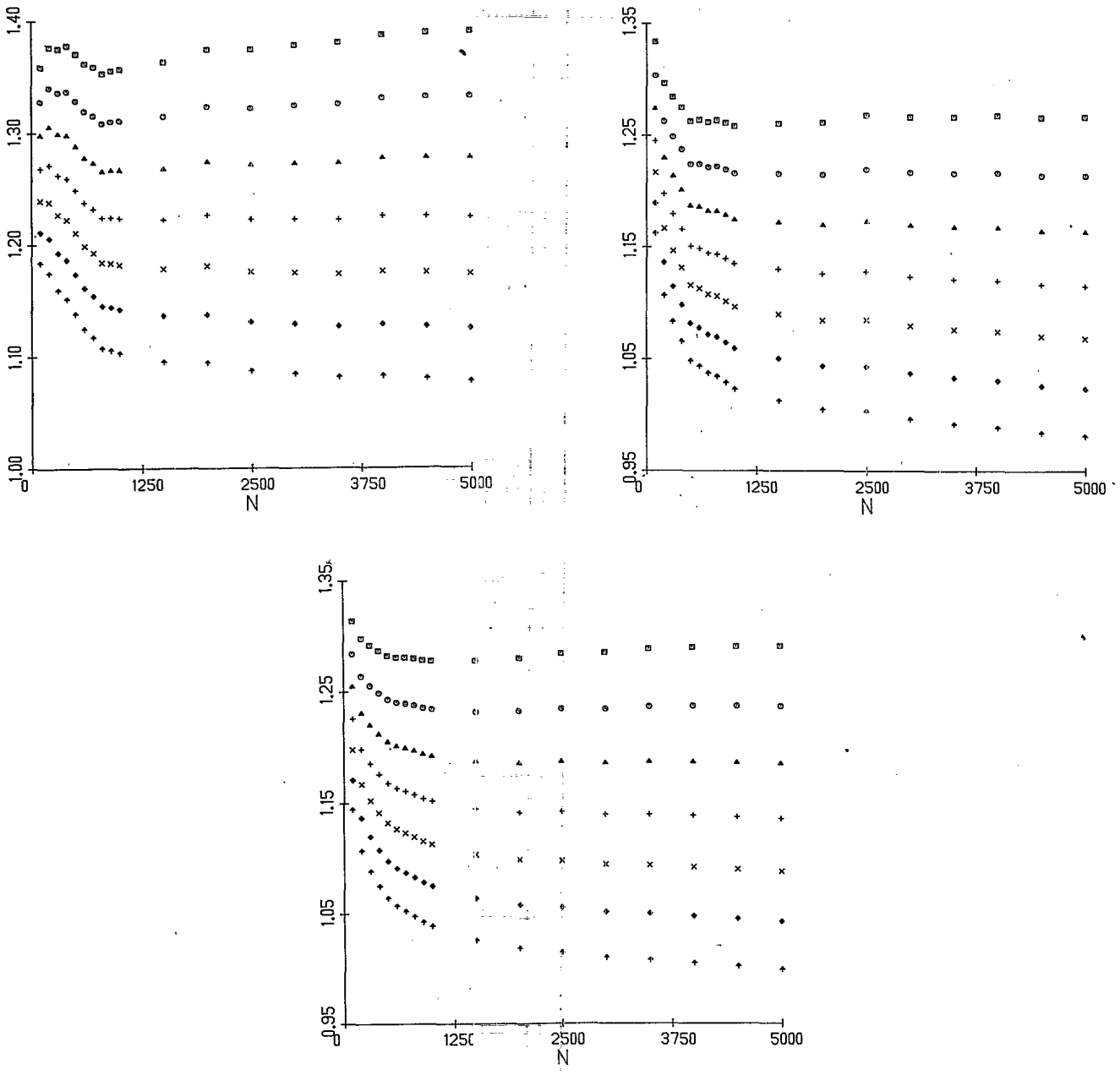

FIG. 3. Plot of S_N/N^f vs N. (a) Case (a) of text with $2f'=1.20$, 1.21, 1.22, 1.23, 1.24, 1.25, and 1.26 (top to bottom). (b) and (c) Cases (b) and (c) of text, respectively, with $2f=1.27$, 1.28, 1.29, 1.30, 1.31, 1.32, and 1.33 (top to bottom).

largest percolating cluster only.

To test the validity of the asymptotic conjecture,

$$S_N \sim N^{d_s/2}, \quad N \to \infty \tag{1}$$

we plot the following: $\ln S_N$ versus $\ln N$, Fig. 2. We observe that the data are almost fit on a straight line, but there are certainly apparent deviations observed for the range examined. It has actually been hypothesized[5,16,17] that Eq. (1) is valid only in the asymptotic limit of large N, and that correction terms to the scaling law are necessary to describe the short-time behavior. We believe that the deviations from a straight line in Fig. 2 are due to this effect.

To further elucidate this point we now plot S_N/N^f as a function of N, where $f=d_s/2$ is given a range of possible values for the largest cluster walks, and similarly $f'=d_s'/2$ for walks on *all* clusters. The results are given in Fig. 3. In Fig. 3(a), for case (a), we see that at N (where $S_N/N^{f'}$ is supposed to be a constant of N) the best value for $2f'$ is between 1.23 and 1.24 (lines nearest to horizontal). In Figs. 3(b) and 3(c) we find, likewise, for cases (b) and (c), that $2f \cong 1.29$, with case (c) showing a smoother behavior. The Alexander-Orbach-Rammal-Toulouse conjecture gives $2f=\frac{4}{3}$ and $2f'=1.260$, while the Aharony-Stauffer conjecture gives $2f=1.309$ and $2f'=1.237$. Our results clearly agree better with the latter conjecture. We believe that our case (a) simulations are statistically the best, because they are not sensitive to the exact location of

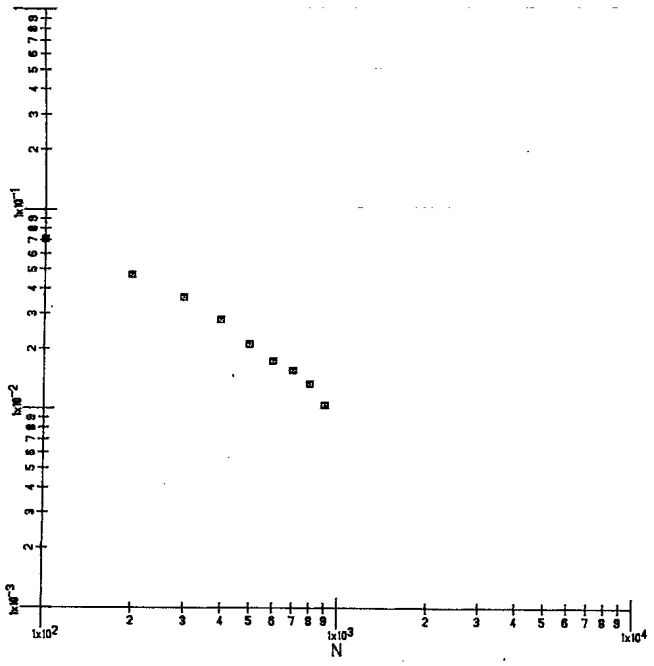

FIG. 4. Plot of $(S_N/N^f - a)$ vs N, where $2f = 1.29$ and $a = 1.184$ for the points of curves in Fig. 3(c). The slope (giving the exponent ω) is taken from a straight line drawn at small N.

the percolation threshold. The case (b) simulations are quite sensitive to this point while the case (c) simulations should be less sensitive to it. We note here that from independent simulations[18] on *all* clusters for long times ($N = 2\times 10^5$) we obtained $2f' = 1.235$, in excellent agreement with our present results (and with the Aharony-Stauffer conjecture). The $2f$ values there are obtained by a different approach ("discarding method"), giving $2f = 1.30$, also in very good agreement.

We also see from all three cases [Figs. 3(a)—3(c)] that for $N > 10^3$, the long-time behavior seems to have been approached, while for $N < 10^3$, the short-time corrections to scaling are very important. We now focus on the short-time regime and try to derive the correction to scaling. It has been assumed recently that these correction terms are included in the universal relation by the following formula:

$$S_N \sim N^f(1 + AN^{\omega}) , \tag{2}$$

where ω is a negative number, so that the contribution of the second term in parentheses goes to zero for large N. Rewriting Eq. (2),

$$\frac{S}{N^f} \sim 1 + AN^{\omega} \tag{3}$$

or

$$\frac{S}{N^f} - a = bN^{\omega} , \tag{4}$$

where a and b are constants. Here a represents the constant S_N/N^f value for large N, which as seen from Fig. 3 has the value $a = 1.18$. Therefore, if we plot Eq. (4) directly in logarithmic form we will recover immediately the ω exponent. This is done in Fig. 4 using the data of Fig. 3(c). We consider the slope of the curve at early times, because this is where the correction term predominates. At the straight-line segment in Fig. 4 the slope is

$$\omega = -0.48 \pm 0.08 .$$

We note that forcing an exponent $2f = \frac{4}{3}$ gives $a = 0.99$ and $\omega = -0.47$, showing that ω is not as sensitive to f as, obviously, a is. This is in good agreement with the correction term reported recently by Pandey *et al.*,[5] giving $\omega = -0.45 \pm 0.05$ and $a = 0.99$ from the scaling of the $\langle R_N^2 \rangle$ calculation. Rammal[17] gives a value of $\omega = -\frac{1}{6}$, which is inconsistent with our simulations.

IV. CONCLUSIONS

For the mean number of distinct sites visited on a two-dimensional percolating cluster (square lattice), the scaling exponent (spectral dimension) is 1.30 ± 0.03, which is in much better agreement with the Aharony-Stauffer conjecture (1.309) than with the Alexander-Orbach-Rammal-Toulouse conjecture ($\frac{4}{3}$). The short-time correction to scaling is about -0.48, in good agreement with the Pandey-Stauffer-Margolina-Zabolitzky work. For these short-term simulations the new method of simulating random walks on the largest cluster at exact criticality for each realization appears to be superior to the conventional method of simulation at nominal criticality.

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