Random walk on percolation clusters

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Random-walk simulations at and above the percolation threshold were performed for two- and three-dimensional lattices. The number of distinct sites visited on the percolating cluster at threshold obeys the "superuniversality" relation, showing a fractal spectral (fracton) dimensionality of $\frac{4}{3}$. We also observe fractal-to-Euclidean crossovers with time and with increased concentration (above threshold). The mean-squared displacement (from the origin) shows a similar behavior and its critical exponents are compared with previous work.

How relevant are fractal dimensions to condensed-state dynamics? Much work and speculation have been dedicated recently to this question. In addition to the embedding Euclidean dimension (1,2,3, ...) we have now (see Mandelbrot[1]) the fractal (Hausdorff) dimension d_f and the spectral (fracton) dimension (see Alexander and Orbach[2]) d_s characterizing self-similar spaces (see Rammal and Toulouse[3]), i.e., "fractals." The spectral dimension d_s has been applied to disordered solids such as glasses and polymers (see Orbach[4]), to conductivity in alloys (Geffen, Aharony, and Alexander[5]), and to exciton trapping in isotopic mixed crystals (de Gennes[6]). The link to fractals has been made via percolating clusters (see Stauffer[7,8]). Rammal and Toulouse[3] have suggested that at the percolation threshold the number S_N of distinct sites visited during an N-step random walk on an infinite cluster varies asymptotically as

$$S_N \sim N^f, \quad f \equiv d_s/2 \approx \tfrac{2}{3} \tag{1}$$

in all Euclidean dimensions.

Here we are reporting our simulation investigations of random walks on percolating clusters. Our aim was to check out the above conjecture [Eq. (1)] as well as the interesting resulting *crossovers* from fractal to Euclidean behaviors. Similar tests have been carried out before on the quantities d_s and D by Ben-Avraham and Havlin.[9] They simulated the mean-square displacement $\langle R_N^2 \rangle$, related to D, and the probability of a walker returning to the origin $P_0(N)$, related to d_s, but only at criticality (the percolation threshold). We note that the relations among the above three measures of the random walk on clusters, S_N, $\langle R_N^2 \rangle$, and $P_0(N)$ have been discussed (see Webman[10]), and compared to random walks on Euclidean lattices (see Montroll and Weiss[11] and Weiss and Rubin[12]). We investigated here S_N and $\langle R_N^2 \rangle$, both at criticality and above it.

The present work uses the same techniques as our previous work on random and correlated walk visitation efficiencies for two- and three-dimensional percolation systems (see Argyrakis and Kopelman[13]). We monitor several properties as a function of the number of steps N, i.e., the number of distinct sites visited S_N, the mean-squared displacement $\langle R_N^2 \rangle$, the first passage time, etc. All lattices employed are of a size large enough so that the boundaries are *never* crossed. We thus avoid artificial revisitations. The location of the sites as well as the direction of motion are determined using a pseudorandom number generation routine. The initial point of origin is chosen at random, so that each walk may or may not start at the largest (percolating) cluster.

Calculations that involve small numbers of steps, of the order of 1000, are repeated and averaged after 3000 runs. For long walks, up to 200 000 steps, we performed 500–700 runs. Further work is in progress. We performed two types of averages: First we averaged all the walks simulated, regardless of their origin, thus including walks on the largest percolating cluster and also walks on smaller finite-size clusters. Secondly, we averaged only the walks that start in the largest cluster. We report both averages. In the short walks reported we give d_s and D every 10 steps. In the long walks we do the same every 2000 steps. As an example, Fig. 1 shows the variation of d_s as a function of N for the first 1000 steps. In other words, Fig. 1 shows the effective dimension d_s' as a function of effective time (N), with the concentration C (often called p) as parameter, from just above the critical concentration $C_C = 0.5931$ (see Hoshen and co-workers[14,15]) to pure square lattice ($C = 1$). Here d_s' is *defined* by the relationship

$$\langle S_N \rangle \sim N^{d_s'/2} . \tag{2}$$

We note that the values of d_s' are between 1.2 and 1.8. However, *longer random-walk runs* ($N = 2 \times 10^5$, 700 runs each) result in the values of d_s' given in Table I.

The *crossover* behavior between fractal (heterogeneous) and Euclidean (homogeneous) behavior[5,10] is evident from Fig. 1 and Table I. For instance, for $C = 0.70$, $d_s' = 1.3$ at low-N (Fig. 1) but 1.8 at high-N values (Table I). In principle, the location (in N) of the crossover is a measure of the correlation length which, close to the threshold, goes as

$$\xi \propto |C - C_C|^{-\nu}, \quad \nu = \tfrac{4}{3} \text{ for } d = 2 \tag{3}$$

(the value of ν has been tested by simulation[8,15]). The crossover behavior itself is also predicted[5,10] from scaling arguments, but we reserve discussion on this point for the future.

In trying to extract d_s from the Fig. 1 data one encounters several difficulties: (1) The definition of d_s is only valid as an asymptotic expression, i.e., for long times ($N \to \infty$); (2) for long times ($N \to \infty$) one expects a homogeneous ("classic") behavior rather than a fractal one; (3) the simulations of Fig. 1 include contributions from finite clusters as well as from the "infinite" cluster; (4) if one attempts to discard the random-walk runs pertaining to the miniclusters

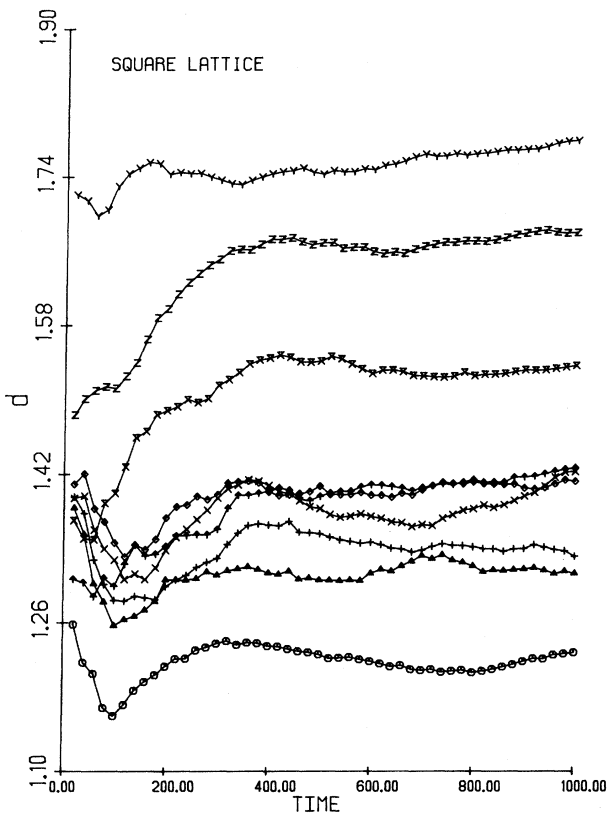

FIG. 1. Effective fracton dimension $d \equiv d_s'$ vs "time" $(=N)$, for the square lattice. The percent guest (occupied site) is (top to bottom at long time) 100, 80, 70, 65, 63,64, 62, 61, 60. Note that percolation is at (Ref. 15) 59.31% and that these figures are averages over about 1000 runs (3000 for 60%), including runs on finite clusters (whose probability is significant only for the 60% case). Note the crossovers (or incipient crossovers) for the 65%, 70%, and 80% lattices.

one does *not* want to discard runs on large finite clusters with size $M \geq N$.

To overcome the above problems we applied corrections for cases where the site percolation probability ($\bar{P}_\infty$) and the average minicluster size ($I_{\rm av}'$) are small . Noting the actual values (Hoshen *et al.*[14]) it appears that the only regime where such corrections are necessary is close to C_C. We have appropriately corrected our runs for certain values of C and obtained the results shown in Figs. 2 and 3.

The corrected runs (Table I and Fig. 2) give d_s' values that are surprisingly close to the conjecture $d_s = \frac{4}{3} = 1.333\,33$. Specifically, for $C = 0.60$, i.e., 0.7% above C_C, one gets $d_s = 1.29$ from the short runs (see Fig. 2) and 1.331 from the long runs (see below). The values for D, where $\langle R_N^2 \rangle \sim N^{2/D}$, are also listed in Table II.

Figure 3 gives the results for three-dimensional (simple cubic) runs, for both corrected and uncorrected simulations. Again, close to C_C $(=31.17)$, the value of d_s is very close to $\frac{4}{3}$. For values of d_s and D, see Table II. Long runs are in progress.

The corrections for the inclusion of finite-cluster contributions can be dealt with in a number of ways. For instance, at C_C, the probability of the walker being on a cluster size N or larger is about

$$P_N = N^{-\epsilon}, \quad \epsilon = \beta/(\gamma+\beta) = \delta^{-1} \tag{4}$$

(compare the equivalent expression for trapping, $P = S^{1/\delta}$ of Hoshen *et al.*[14]). We note that, for $C \geq 0.6$, $P_N \approx \bar{P}_\infty$. However, $P_N(C_C) = P_N(C=0.6)$ while $\bar{P}_\infty(C_C) << \bar{P}_\infty(0.6)$. Thus correction (exclusion) of runs according to the above formula, i.e., excluding $(1-P_N)$ runs, is equivalent to the exclusion of $1-\bar{P}_\infty$ runs for the square lattice. This works because, for the square lattice, the average finite-cluster size falls very sharply above percolation as

$$I_{\rm av} \propto |C - C_C|^{-\gamma} \tag{5}$$

and[14,15] $\gamma = 2.39$. However, for the cubic lattice[14,15] $\gamma \approx 1.6$ and the corrections can be made safely only at higher C (see Fig. 3). Another approach is to retain the finite-cluster random-walk contributions and to correct[6,10] Eq. (1):

$$S_N \propto N^{f(1-\epsilon)}, \quad f = d_s/2 \ . \tag{6}$$

As ϵ is $\frac{5}{91} \approx 0.055 \approx 5.5\%$ for two dimensions (i.e., square lattice), the correction is relatively small, giving for the exponent

$$d_{s\,\rm eff} = d_s(1-\epsilon) = \tfrac{4}{3}\tfrac{86}{91} = 1.260 \ .$$

This number is in very good agreement with our uncorrected value just above percolation (1.23 ± 0.03). However, above percolation we expect this correction to be valid only for short runs (see below). We emphasize that our values are derived from the random-walk visitation efficiency and not from $P_0(N)$, i.e.,

$$\mathscr{E} \equiv S_N/N \propto N^f/N = N^{f-1}, \quad f = d_s/2 \ . \tag{7}$$

We notice that $\mathscr{E} \propto t^{-1/3}$ for percolating clusters at C_C, and falls off steeper (with time) for finite clusters than for infinite clusters. For cubic crystals, $\epsilon \approx 0.2$ and thus the correction is larger, giving an effective d_s of the order of 1.1 at C_C. We get (Fig. 3) 1.19. Similar corrections have been applied[5,9] to the exponents D, giving $D = D'(1-\beta/2\nu)$. We note that Ben-Avraham and Havlin[9] report from short-run

TABLE I. Random-walk exponents from long runs (square lattice, $N = 2\times10^5$; 500–700 runs, no discards above 60%).

C	60%	65%	70%	80%	90%	100%
d_s'	1.331	1.720	1.775	1.820	1.837	1.840

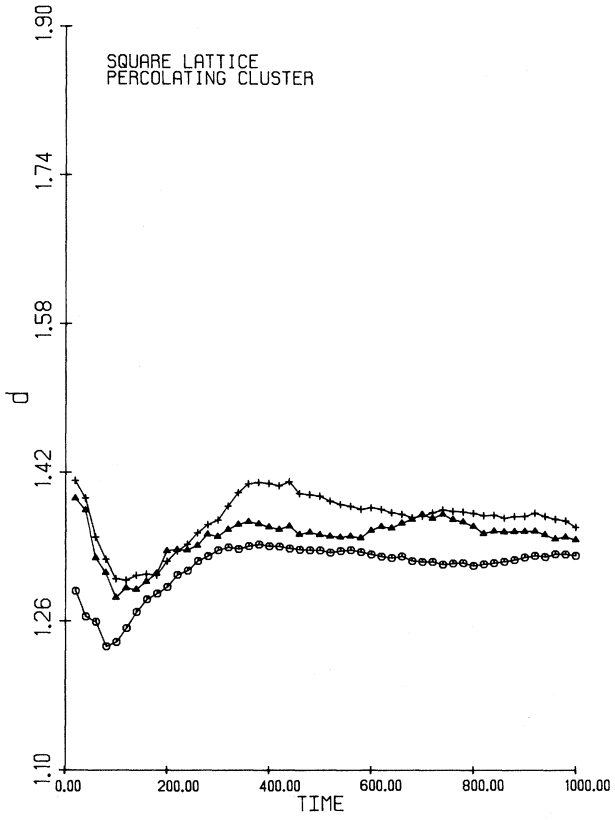

FIG. 2. Selected runs from Fig. 1, correcting for finite-cluster effects. Top to bottom: (1) 62% lattice, 905 of 1000 runs were retained, discarding the low efficiency tail (i.e., 95 least efficient runs); (2) 61% lattice, 890 of 1000 runs retained; (3) 60% lattice, 2290 of 3283 runs retained.

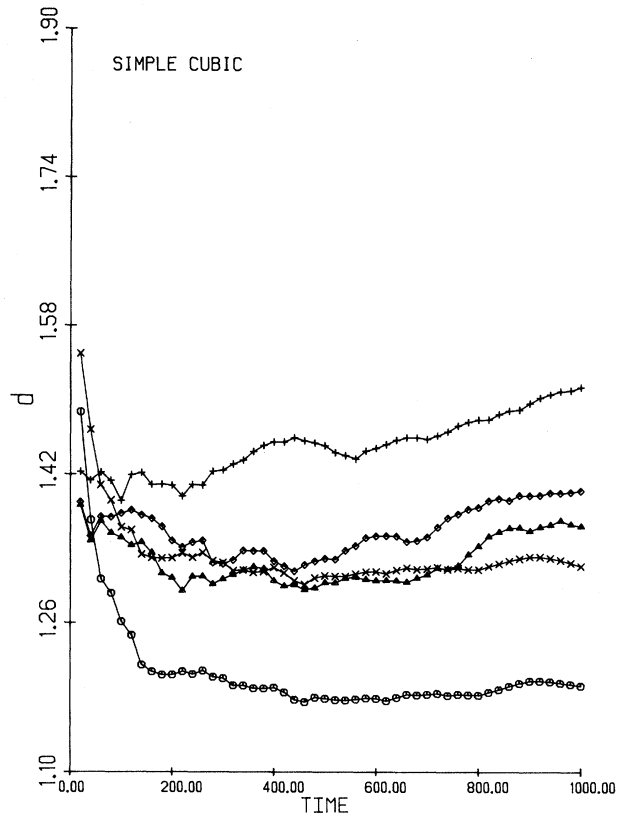

FIG. 3. Effective fracton dimension vs number of steps for simple cubic lattice. Top to bottom (long time): (1) 36% lattice, 1000 runs, none discarded; (2) 33% lattice, 747 of 1000 runs retained; (3) 34% lattice, 1000 runs, none discarded; (4) 32% lattice, 2130 of 3448 runs retained; (5) 32% lattice, 3448 runs, none discarded. Note that percolation is at 31.15%. Interestingly, while for a 36% lattice $d' = 1.51$ (classical value 2), $D' = 2.98$ (classical value 2).

simulations that $D' = 2.7 \pm 0.1$ and 3.9 ± 0.1 while our rougher values are 2.7 and 3.8, for $d = 2$ and 3, respectively (see also Fig. 3 caption).

The advantages of our method of simulation are as follows. (1) We use two uncorrelated random processes: (a) the creation of the lattice (cluster distribution) and (b) the random walk on the lattice or cluster. (2) We have *no* runs with boundary crossings, thus avoiding the complications involved in cyclic or other boundary conditions. (3) We do not simulate *at* criticality (0.5931 or 0.3117), where some configurations are bound to be *below* percolation, but slightly above it (0.60 or 0.32), where (a) all configurations have percolated; (b) there are no intermediate-size clusters left (especially in two dimensions[14]), only very small ones ("miniclusters") and one very large one ("maxicluster"), thus obviating some scaling corrections [see Eq. (6)], especially at *long* times (200 000 steps); and (c) the correlation length is still larger than the extent of the random walk. (4) Having lattices on the order of 4×10^6 sites we still avoid performing millions of steps, thus preventing scattering at boundaries and/or classical behavior due to effective translational symmetry (due to cyclic boundary conditions). We also note that our figures and Table II are based on comparing $S(t)$ to $S(t/2)$. Deriving the exponents from

TABLE II. Random-walk exponents from short runs. BH is Ben-Avraham and Havlin (Ref. 9); AO is Alexander and Orbach (Ref. 2). Our values are based here on short runs ($N = 10^3$) with partial discards (Figs. 2 and 3), for comparison with BH. Note that AO give asymptotic values.

d	d_s	d_s (BH)	d_s (AO)	D	D (BH)	D (AO)
2	1.29 ± 0.06	1.26 ± 0.10	1.33333	2.55 ± 0.5	2.68 ± 0.05	2.84
3	1.32 ± 0.06	1.26 ± 0.10	1.33333	3.53 ± 0.4	3.3 ± 0.1	3.55

the limiting behavior at long times we get $d_s/2=1.331$ (from the runs at 0.60), in excellent agreement with the conjecture of $\frac{4}{3}$. In addition, our long time $S(t)$ for the 100% lattice is within 0.1% of the analytical result.[16]

In summary, we show that the Rammal and Toulouse conjecture of $f=\frac{2}{3}$ for the asymptotic random-walk visitation on a percolating cluster at *percolation* (C_C) is very successful. It works even for relatively small N (10^2 to 10^3). This is similar to the success of the Euclidean (Montroll) asymptotic expressions at small N for one and three dimensions (but not two). On the other hand, the *crossover to "nonfractal" behavior* starts relatively early in time and especially in concentration, thus giving *effective exponents* $2f$ ranging from 1.3 to 1.9 for the square lattice and approaching the value $2f=2$ much quicker for the cubic lattice. Thus any general deductions about "fracton behavior" in disordered systems such as glasses and polymers should take into account the range $2f=1.3$ to 2, rather than expecting the "magic value" of $\frac{4}{3}$ to be all encompassing. Our simulations thus indicate both the potential successes and the potential pitfalls of the fractal (fracton) approach when applied to "real" disordered materials.[2-6]

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