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LETTER TO THE EDITOR

Diffusion and fracton dimensionality on fractals and on percolation clusters

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Abstract. We present simulations of diffusion on an exact fractal and on percolation clusters at criticality for two and three dimensions. The results for the fractal support the Rammal and Toulouse proposition that $\mathrm{d}S(N)/\mathrm{d}N \propto B(N)/S(N)$. The results for percolation are in excellent agreement with the Alexander and Orbach conjecture that the fracton dimensionality $\tilde{d} = \frac{4}{3}$.

The problem of the density of states on fractals and on percolation clusters has recently been intensively discussed (Alexander and Orbach 1982, Alexander 1983, Domany *et al* 1983, Rammal and Toulouse 1983, Ben-Avraham and Havlin 1982). Of particular interest is the Alexander and Orbach (1982) *conjecture* that the fracton dimensionality $\tilde{d}$ which describes the density of states has the same numerical value $\tilde{d} = \frac{4}{3}$ for percolation in any space dimensionality. Very recently, Rammal and Toulouse (1983) have proposed the following argument to support this conjecture. For diffusion on percolation clusters (at criticality) or on fractals, let $S(N)$ be the number of distinct sites visited by the diffusion after N steps, and let $B(N)$ be the number of boundary sites in $S(N)$, i.e. those sites with accessible neighbours outside $S(N)$. Then

$$\mathrm{d}S(N)/\mathrm{d}N \propto B(N)/S(N). \tag{1}$$

In order for the conjecture to be correct, it is required that

$$B(N) \propto S(N)^{1/2} \propto R(N)^{\bar{d}/2} \propto N^{\bar{d}/2D}, \tag{2}$$

where $\bar{d}$ is the fractal dimensionality and D is the exponent describing the diffusion length $R(N)^D \propto N$.

In the present letter, we present some numerical evidence which strongly supports the conjecture for percolation in $d = 2$ and 3. This is done by improved calculations of D (Ben-Avraham and Havlin 1982, Havlin *et al* 1983) achieved mainly by increasing N by one order of magnitude. Also, equation (1) is verified to high accuracy for an exact fractal. Moreover, we show conclusively that $B(N)$ does not behave like $R^{\bar{d}-1}$, as one might expect considering the boundary to be a sphere cut of the fractal (Alexander 1983).

We first consider an exact fractal with $\bar{d} = \ln 3/\ln 2 \simeq 1.585$ described in figure 1. The fracton dimensionality and the diffusion exponent are easily calculated exactly via the conductivity exponent μ by a method similar to that presented by Gefen *et al* (1981). The results are found to be $D = \ln(21/4)/\ln 2 \simeq 2.392$ and

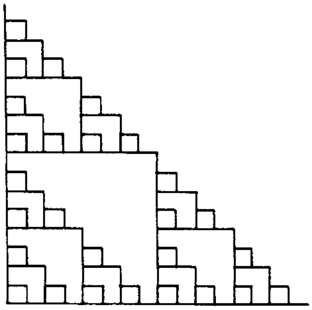

Figure 1. Fractal used in the text. The iteration process making the structure self similar should be continued indefinitely.

$\tilde{d} \equiv 2\bar{d}/D = 2\ln 3/\ln(21/4) \simeq 1.325$. We simulated about 40 000 diffusions on this fractal up to $N = 500$. From measurements of $S(N) \propto N^{\tilde{d}/2}$, we obtained $\tilde{d} = 1.32 \pm 0.01$, which is in excellent agreement with the theoretical value. In order to confirm equation (1), it is equivalent to show that

$$B(N) \propto S(N)^x, \qquad x = 2 - 2/\tilde{d}. \tag{3}$$

Indeed, results of the above simulations yield $x = 0.493 \pm 0.005$, which fits very well the prediction obtained from equation (1) that $x = 2 - 2/\tilde{d} \simeq 0.491$. The measurement of $B(N)$ was done by counting for each N-steps diffusion those sites which have at least one nearest neighbour site not visited previously. In figure 2, we present a plot of $\ln B(N)$ against $\ln S(N)$ which shows graphically the results of the simulations as compared with the theoretical prediction. We note that one can confidently reject the possibility that $B(N) \propto R(N)^{\bar{d}-1} \propto S(N)^{(\bar{d}-1)/\bar{d}}$. The distinction between $x = 2 - 2/\tilde{d}$ and $x = 1 - 1/\bar{d}$ is easy to see in this exact fractal, in contrast to the situation in percolation where these two predictions do not differ by very much (Alexander 1983). Indeed, $x = 1 - 1/\bar{d}$ gives the value of 0.369, which differs from the measured value of $x = 0.493 \pm 0.005$. Thus, we conclude that equation (1) holds while it is not true that the boundary of diffusions is like a sphere cut in the fractal.

In the following, we consider results for diffusion on percolation on square, triangular and cubic lattices at criticality. Using the same methods we presented previously (Ben-Avraham and Havlin 1982), we simulated about 10^4 random walks on each of two different ensembles of percolation clusters. In the first ensemble, we considered only those clusters whose size is larger than the span of the walks (large clusters). In the other ensemble, all clusters were taken into account (all clusters). Denote the diffusion exponent measured for large clusters by D, and that for all clusters by D'. The two exponents are related by $D' = D/(1 - \beta/2\nu)$ (Ben-Avraham and Havlin 1982, Havlin *et al* 1983, Gefen *et al* 1983). The main improvement of the present results is that walks were performed for up to 5 000 steps, which is an order of magnitude larger than previously (Ben-Avraham and Havlin 1982). Thus, it is possible to see from these new results that the exponents D and D' do not converge for $N \sim 500$. The results of diffusion on large clusters for percolation in $d = 2$ and $d = 3$ are presented in figure 3, where we plot $\ln N$ as a function of $\ln R(N)$. The slope of the resulting curve is the exponent D. It is seen that the slope changes with N, and it is smaller for smaller N. In figure 4, we plot the slope of the curve in figure 3, which is the local fractal dimensionality $D(N)$ (Havlin and Ben-Avraham

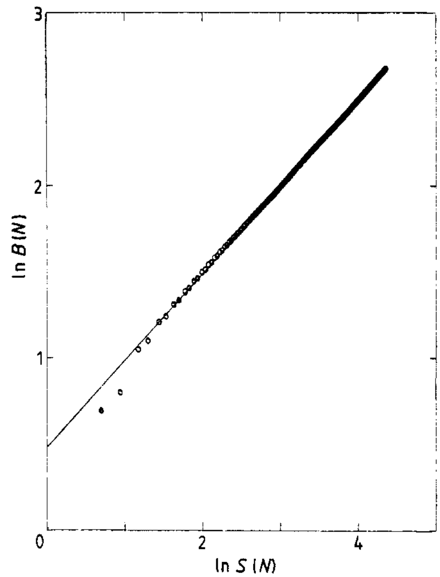

Figure 2. Graph of $\ln B(N)$ against $\ln S(N)$ for diffusion on the fractal described in figure 1. The circles represent the numerical data and the full line is drawn from equation (1).

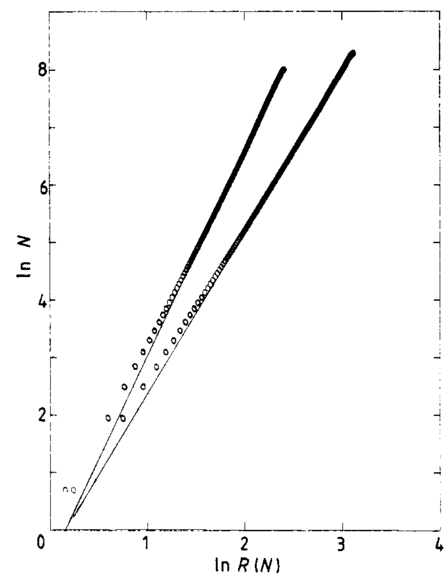

Figure 3. Graph of $\ln N$ against $\ln R(N)$ for diffusion on large clusters in $d=2$ and $d=3$. The circles represent numerical data and the full line is the extrapolated slope of the curve.

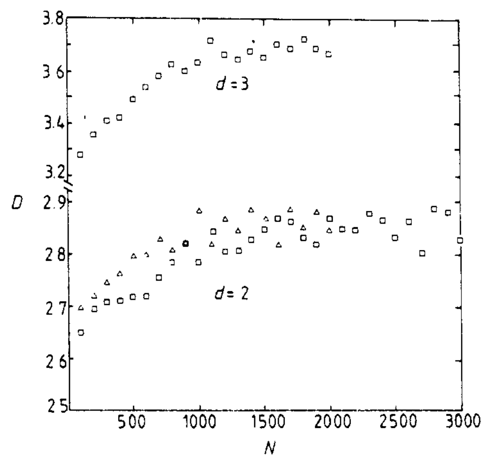

Figure 4. Graph of $D(N)$, the slope of the curve in figure 3. The squares represent the data for diffusion on percolation on a square lattice, and the triangles on a triangular lattice.

1982). In this figure we also present results for diffusion on percolation on a triangular lattice. It is seen that for $N \geqslant 10^3$ the results for the square and triangular lattices coincide while for $N \leqslant 10^3$, $D(N)$ for the triangular lattice is consistently higher than $D(N)$ of the square lattice. This indicates that the range below $N \sim 10^3$ (which corresponds to $R \sim 10$ lattice spacings) is affected by the lattice geometry which allows convergence only for very large N. The errors of $D(N)$ can also be determined from figure 4.

A similar analysis was performed for diffusion on all clusters and the results are presented in table 1. The result for the diffusion exponent D obtained from calculations using D' is somewhat smaller than the value of the directly measured D. This is probably because convergence for D' is affected not only by geometry but by the cluster distribution convergence as well. This is consistent with results of Pandey and Stauffer (1983) that D' converges for $N \sim 10^7$ (for $d = 3$). We used for the calculation of $\bar{d} = d - \beta/\nu$ the known values of β and ν for $d = 2$ and 3 (Stauffer 1979). The main result is in very good agreement with the Alexander and Orbach (1982) conjecture that $\bar{\bar{d}} = \frac{4}{3}$.

Table 1. Diffusion exponents and fracton dimensionality.

d	D	D'	$D = D'(1 - \beta/2\nu)$	$\bar{\bar{d}} = 2\bar{d}/D$
2	2.84 ± 0.05	2.95 ± 0.05	2.80 ± 0.10	1.33 ± 0.03
3	3.68 ± 0.05	4.90 ± 0.05	3.63 ± 0.10	1.34 ± 0.03

We also measured the fracton dimensionality $\bar{\bar{d}}$ from the above simulations on large clusters directly by

$$S(N) \propto R(N)^{\bar{d}} \propto N^{\bar{d}/D} \propto N^{\bar{\bar{d}}/2}. \tag{4}$$

The results for $\bar{\bar{d}}$ are 1.26 for $d = 2$ and 1.24 for $d = 3$. These values are lower than the conjectured value of $\frac{4}{3}$. The reason is that the clusters are limited to a frame, which causes $\bar{d}$ to be effectively smaller (finite-size effects). Indeed, we measured $\bar{d}$ via $S(N) \propto R(N)^{\bar{d}}$ and found $\bar{d} = 1.8$ instead of 1.9 for $d = 2$ and $\bar{d} = 2.3$ instead of 2.5 for $d = 3$. One should note, however, that the ratio $2\bar{d}/D$ gives excellent agreement with the directly measured $\bar{\bar{d}}$. The important fact is that the value of D for large clusters is not influenced by finite-size effects, since the random walk never reaches the limiting frame of the cluster. Therefore, in table 1 we calculated $\bar{\bar{d}}$ using known and reliable values of $\bar{d}$ and measured values of D, rather than directly measuring $\bar{\bar{d}}$.

In conclusion, we have presented simulations of diffusion on exact fractal and on percolation clusters at criticality in $d = 2$ and 3. The results strongly support both the Alexander and Orbach (1982) conjecture $\bar{\bar{d}} = \frac{4}{3}$ and the proposition of Rammal and Toulouse (1983) given in equation (1).

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