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LETTER TO THE EDITOR

Diffusion on percolation clusters at criticality

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Abstract. The concept of fractal dimensionality is used to study the problem of diffusion on percolation clusters. We find from Monte Carlo simulations that the fractal dimensionality of a random walk on a critical percolation cluster in three-dimensional space is $D = 3.3 \pm 0.1$ where the size of the cluster is restricted to be larger than the span of the walk, and is $D' = 3.9 \pm 0.1$ for a walk on clusters not subject to this restriction. For two-dimensional space we find $D \simeq D' \simeq 2.7 \pm 0.1$. The exponent D (and D') is related to the scaling of the average length R of N steps via $R^D \propto N$. The *fracton* dimensionality which is related to the density of states was found to be $\bar{\bar{d}} = 1.26 \pm 0.1$. These results are in good agreement with the predictions of Alexander and Orbach.

The geometrical structure of percolation clusters has recently been the subject of considerable interest (Stauffer 1979, 1980, Mandelbrot 1982). In particular, at present two different models exist for the geometrical structure of the backbone at percolation: the node and links picture (de Gennes 1976, Skal and Shklovskii 1974, 1975) and the self-similarity picture with fractal dimensionality (Gefen *et al* 1981, Alexander and Orbach 1982).

In this Letter we present a numerical and theoretical study of diffusion on fractals and on percolation clusters. Our results strongly support the diffusion model presented very recently by Alexander and Orbach (1982) (hereafter referred to as AO) based on the fractal picture of the percolation cluster (Gefen *et al* 1981). It is shown numerically, as predicted by AO, that the relevant dimensionality appearing in the density of states for fractals is the *fracton* dimensionality $\bar{\bar{d}}$ (defined by AO) which is related to the diffusion exponent D (the fractal dimensionality of the walk) and the fractal dimensionality $\bar{d}$ of the percolation cluster. We have measured, numerically, the fractal dimensionality of the diffusion walk, D, as well as the fracton dimensionality $\bar{\bar{d}}$ appearing in the density of states. The numerical values obtained for these quantities are in good agreement with the predictions of AO.

The early work regarding diffusion on percolation clusters which was used as a powerful tool in the study of transport properties (de Gennes 1976, Mitescu *et al* 1978) considered mostly the region of non-anomalous diffusion, where $R^2 \propto N$. As Mitescu *et al* (1978) recognise, and as we show elsewhere (Havlin and Ben-Avraham 1982a), this region occurs only for sufficiently long walks in systems above the percolation threshold. However, we are interested in properties at the threshold where anomalous behaviour associated with fractal dimensionality of the clusters can be expected for all lengths of walk.

In a recent Letter we presented (Havlin and Ben-Avraham 1982b) a method of measuring the fractal dimensionality of a walk. We defined the concept of local fractal dimensionality (LFD) as

$$D(N) = \ln[(N+1)/N]/\tfrac{1}{2}\ln(\langle R^2_{N+1}\rangle/\langle R^2_N\rangle) \tag{1}$$

where $\langle R^2_N\rangle$ is the mean square length for an ensemble of walks, of *all* sections consisting of N steps. If $D(N) = D$ constant, $\langle R^2_N\rangle^{D/2} \propto N$ and D is the fractal dimensionality of the walk.

We first examine diffusion on an exact fractal with $\bar{d} = \ln 3/\ln 2$, the triangular Sierpinski gasket (Gefen *et al* 1981). For this system the walks starting at a symmetry point and ending after N steps were enumerated exactly for $N \leqslant 250$. We find that diffusion on this fractal is anomalous ($D \neq 2$), with $\langle R^2_N\rangle^{D/2} \propto N$ where $D = 2.32 \pm 0.01$. The value of D was obtained from the best fit of $\ln N$ against $\ln R_N$ shown in figure 1. This is in excellent agreement with the result $D = \ln 5/\ln 2 = 2.322$ predicted by AO.

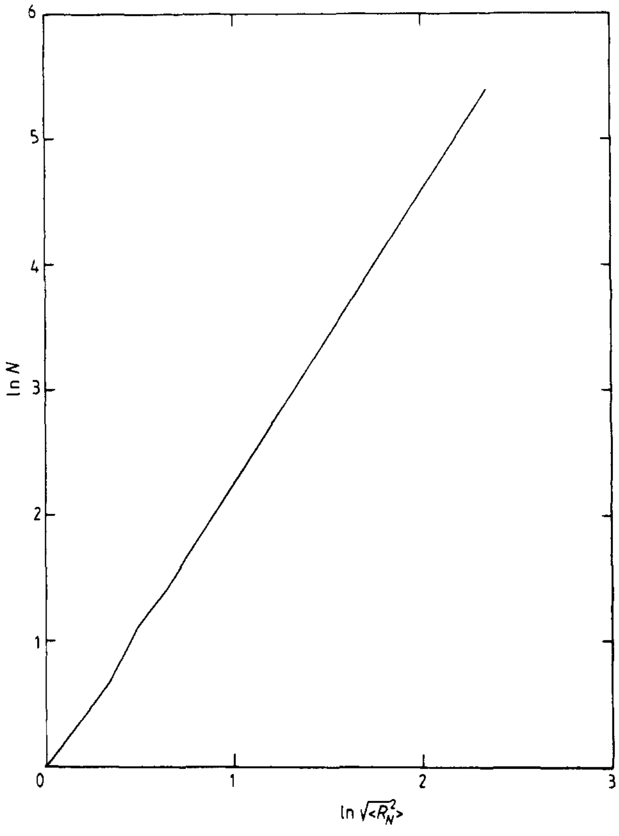

Figure 1. Plot of $\ln N$ as a function of $\ln\sqrt{\langle R^2_N\rangle}$ averaged on all walks up to 200 steps traced on a triangular Sierpinski gasket.

In the following we present the results of Monte Carlo calculations of diffusion on percolation clusters in two- and three-dimensional space at critical site percolation. The results are consistent with the assumption that such clusters have a statistical self-similarity property, i.e. that they are statistical fractals.

Very recently AO, using this assumption, have developed a theory of diffusion on critical percolation clusters, as well as the density of states for these clusters. Their main results are

$$\langle R_N^2 \rangle^{D/2} \propto N \tag{2}$$

with

$$D = 2 + \bar{\zeta} = 2 + (t - \beta)/\nu \tag{3}$$

where ν, β and t are the critical exponents for the correlation length, order parameter and conductivity respectively. They also find that the probability that a walk returns to the origin after N steps is

$$P_0(N) \sim V(N)^{-1} \sim R(N)^{-\bar{d}} \sim N^{-\bar{d}/D} \sim N^{-\tilde{d}/2} \tag{4}$$

where $V(N)$ is the total volume available on the fractal cluster within the diffusion distance, $\bar{d}$ is the fractal dimensionality of the percolation cluster and $\tilde{d}$ is the fracton dimensionality, i.e. the critical index governing the density of states on fractals.

In order to check the theory we simulated critical clusters on square and cubic lattices ($d = 2, 3$). A random walk was generated on these clusters. The clusters were chosen to be much larger than the span of the walks so as to avoid end effects. The LFD of the walks was measured and found to be nearly constant with N as shown in figure 2. The best fits of $\ln N$ against $\ln \langle R_N \rangle$ and $\ln P_0(N)$ against $\ln N$ are shown in

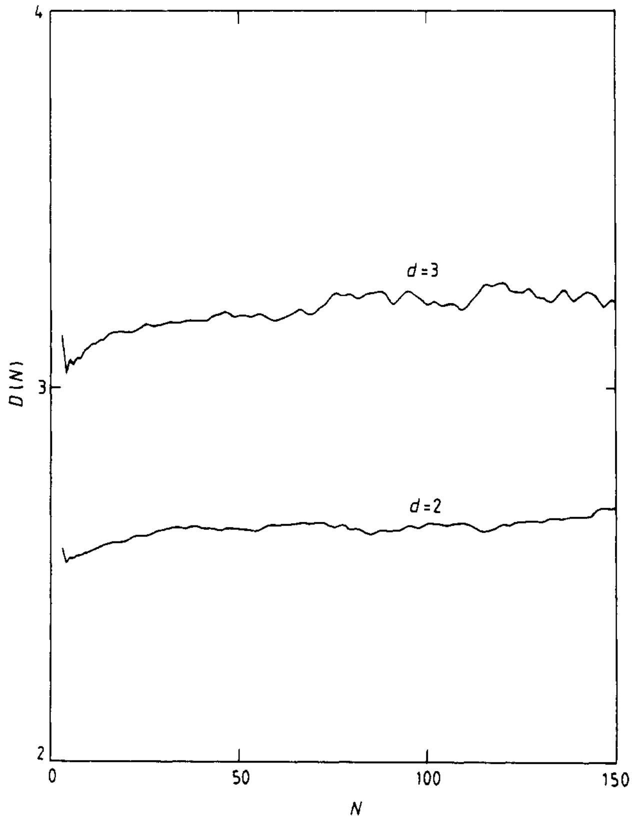

Figure 2. Plot of LFD $D(N)$ as a function of N for a set of 2×10^4 walks of 320 steps traced on 200 site percolation clusters restricted to be larger than the span of each walk.

figures 3 and 4 respectively. The results for diffusion are presented in table 1. A best fit yields $D=2.68\pm0.05$ or $\bar{\zeta}=0.68\pm0.05$ for $d=2$ and $D=3.3\pm0.1$ or $\bar{\zeta}=1.3\pm0.1$ for $d=3$. For both $d=2$ and $d=3$, the best fit for the slope of $\ln P_0(N)$ against $\ln N$ is $\frac{1}{2}\bar{d}=0.63\pm0.05$ giving $\bar{d}=1.26\pm0.10$. These results confirm that irregular exponents exist for diffusion on percolation clusters. The numerical values of the exponents are somewhat lower but in overall good agreement with the predictions of AO, as calculated from equation (3), with the numerical values given by Stauffer (1979). For $d=2$, $D=2.8$ and $\bar{d}=1.36$; for $d=3$, $D=3.55$ and $\bar{d}=1.42$. The small deviations from the theoretical predictions are apparently due to higher-order terms (corrections to scaling) which affect the results at small N, as seen in figures 3 and 4.

Diffusion on percolation clusters of unrestricted size is also of interest. We simulate diffusion on critical clusters taking into account all the clusters generated, without eliminating those smaller than the span of the walks. The fractal dimensionality D' describing diffusion in this case is different from D found above. Our results are presented in figure 5. A best fit yields $D'=2.76\pm0.05$ for $d=2$ and $D'=3.9\pm0.1$ for $d=3$. This deviation can be explained by the following simple arguments. The clusters were generated by a cluster-growth method (Leath 1976, Alexanderowicz 1980) so that the distribution for clusters of mass S is

$$P(S)\sim S^{1-\tau}. \tag{5}$$

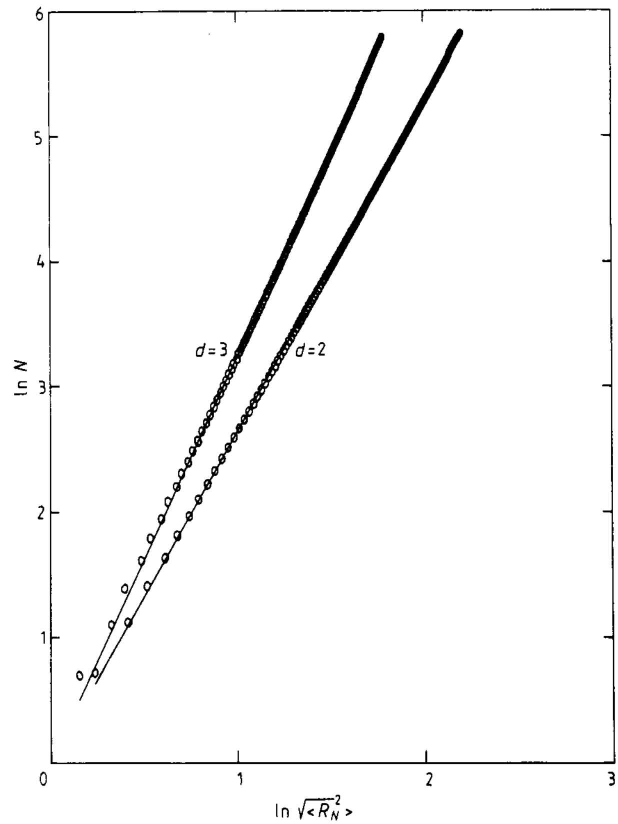

Figure 3. Plot of $\ln N$ as a function of $\ln\sqrt{\langle R_N^2\rangle}$ for the same walks described in figure 2. The open circles are the numerical data and the straight line is the best fit.

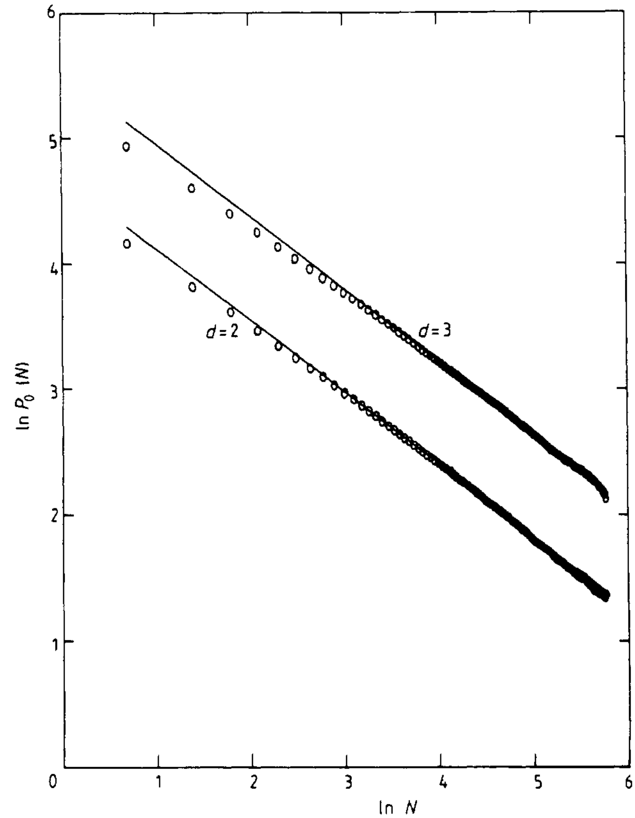

Figure 4. Plot of ln $P_0(N)$ against ln N for the same walks described in figure 2. The open circles are the numerical data and the straight line is the best fit.

Table 1. Diffusion exponents calculated in the present work.

d	D (present work)	D(AO)	$\bar{d}$ (present work)	$\bar{d}$(AO)	D' (present work)
2	2.68±0.05	2.8	1.26±0.10	1.36	2.76±0.05
3	3.3 ±0.10	3.55	1.26±0.10	1.42	3.9 ±0.10

It is reasonable to expect that the mean square distance of N steps on our S cluster is $\langle R_N^2\rangle_S$ where

$$\langle R_N^2\rangle_S \sim \begin{cases} N^{2/D} & \langle R_N^2\rangle_S \leqslant R_S^2 \\ R_S^2 & \langle R_N^2\rangle_S > R_S^2. \end{cases} \tag{6}$$

Here R_S^2 is the average squared size of an S cluster:

$$R_S^2 \sim S^{2/\bar{d}}. \tag{7}$$

Using (5), (6) and (7) the mean $\langle R_N^2\rangle$ (on all clusters) can be calculated and we find

$$\langle R_N^2\rangle_{P=P_c} \sim \sum_S S^{1-\tau}\langle R_N^2\rangle_S \sim \sum^{S_N} S^{1-\tau+2/\bar{d}} + \sum_{S_N} S^{1-\tau}N^{2/D} \sim S^{2-\tau+2/\bar{d}} + S_N^{2-\tau}N^{2/D}. \tag{8}$$

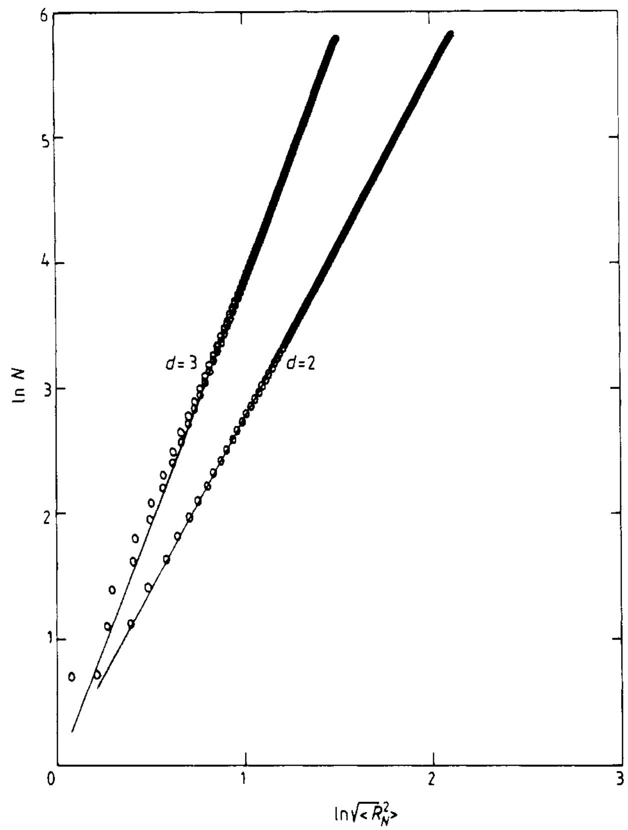

Figure 5. Plot of $\ln N$ against $\ln \sqrt{\langle R_N^2\rangle}$ for 2×10^4 walks of 320 steps traced on 2×10^4 site percolation clusters with no restrictions on the size of the cluster. The open circles are the numerical data and the straight line is the best fit.

The quantity S_N is the limiting mass in equation (6), i.e.

$$S_N^{2/\bar{d}} \sim \langle R_N^2\rangle_{S_N} \sim N^{2/D}. \tag{9}$$

Thus the two contributions in equation (8) are of the same order of magnitude and

$$\langle R_N^2\rangle \sim N^{2/D+(2-\tau)\bar{d}/D} \sim N^{2/D'} \tag{10}$$

or

$$D/D' = 1+\tfrac{1}{2}\bar{d}(2-\tau) = 1-\beta/2\nu, \tag{11}$$

where the last equation in (11) is derived from scaling laws. We find from our measurements (see table 1) that $(D/D')_2 = 0.97\pm0.05$ yielding $\tau_2 = 2.03\pm0.05$ and $(D/D')_3 = 0.85\pm0.05$ yielding $\tau_3 = 2.13\pm0.05$ where the subscripts 2 and 3 denote the dimension. These results are in good agreement with known results (Stauffer 1979).

We conclude that our direct Monte Carlo measurements of the fractal dimensionality of a random walk on a percolation cluster and of the fracton dimensionality confirm the predictions of AO. The anomalous values obtained for the fractal dimensionality of the diffusion walk and for the fracton dimensionality, which are in good agreement with theory, strongly support the basic assumption of the model concerning the fractal nature of the percolation cluster.

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