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Breakdown of Alexander-Orbach conjecture for percolation: Exact enumeration of random walks on percolation backbones

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We carry out the first exact enumeration studies of random walks on the percolation backbone. Using a relation between the backbone and the full cluster, we find for the $d=2$ conductivity exponent $t/\nu=0.970\pm0.009$, which means that the Alexander-Orbach conjecture for percolation can hold *only* if our error bars were multiplied by a factor of 3. We also perform the first calculations of the chemical length exponent $\bar{d}_l$ that measures the dependence on l of the number of *backbone* sites within a chemical distance l; we find $\bar{d}_l=1.44\pm0.03$.

Considerable recent interest has focused on how the laws of diffusion are modified when the diffusion takes place on a random fractal instead of in d-dimensional Euclidean space.[1-7] It is becoming clear that Fick's law connecting the rms displacement with the number of steps of a random walk, $N\sim R^2$, must be replaced by a more general power-law relation $N\sim R^{d_w}$. Here, d_w is the random-walk dimensionality, since it relates the number of objects (steps) N to the characteristic distance (range) of the walk. One finds for percolation fractals that d_w is a strong function of d, varying from 2 for $d=1$ to 6 for $d=6$.

If we are to understand dynamics fully, it is clearly of importance to learn which features of the fractal determine the diffusion exponent d_w. Therefore, considerable interest arose when Alexander and Orbach (AO) made the remarkable numerical discovery that to within the accuracy of calculation, $d_w=\frac{3}{2}d_f$, for $d\geq 2$.[1] Here, d_f is the fractal dimension of the substrate, $M\sim R^{d_f}$, which in percolation increases from $\frac{91}{48}$ for $d=2$ to 4 for $d=6$. Much effort has gone into testing this conjecture for percolation, and into finding out whether it applies to other classes of fractals as well.[6,7] However, all determinations thus far of d_w and d_f have had an accuracy in the range of 4%–8%, and so have not provided a sufficiently searching test.[5] Clearly it is of importance to determine d_w and d_f to an accuracy of 1%–2% in order to put the AO conjecture to as stringent a test as possible. Here, we use a new exact enumeration procedure to calculate random walks on the backbone, *which has less fluctuation than the full percolation cluster.* As a by-product, we will calculate a new topological exponent $\bar{d}_l$.

Our work is based on two new ideas. The first of these is to enumerate random walks not on a percolation cluster but rather on the *backbone;* the backbone between two points on a percolation cluster is the set of bonds carrying current between these two points. We find considerably less statistical fluctuation when considering random walks on the backbone only, because the dangling ends are excluded. Combining the relation[1] connecting the conductivity exponent t/ν to d_w-d_f with a recent identity[8] connecting the *percolation* exponents d_w and d_f with the corresponding *backbone* exponents $\bar{d}_w$ and $\bar{d}_f$, we find for $d=2$ that

$$t/\nu=d_w-d_f=\bar{d}_w-\bar{d}_f \ . \tag{1}$$

Hence, the AO conjecture for percolation, $t/\nu=\frac{1}{2}d_f$, can be tested by calculations *on the backbone fractal alone.*

The second new idea is to enumerate the random walks *exactly* for a given backbone configuration which was generated by a Monte Carlo method.[9] Normally, in percolation problems, we enumerate random walks by a Monte Carlo sampling procedure. However, it is possible to analytically solve for the statistics exactly, once the origin is chosen for a given cluster configuration (see Fig. 1). The advantage of exact enumeration is evident if one realizes that the total number of random walks of N steps on a square lattice is 4^N and N is typically of order 10^3–10^4, so any Monte Carlo procedure can enumerate only a minute fraction of the total number of walks.

The chemical distance l between two sites is the minimum number of bonds that link the two sites.[10] Our simulations are carried out in the "constant-l" ensemble, which consists of clusters that contain only sites with chemical distance smaller than $l_{\max}$ from the origin of the walk. This renders the calculation far more efficient because it provides a criterion for the minimum size cluster needed for an N-step

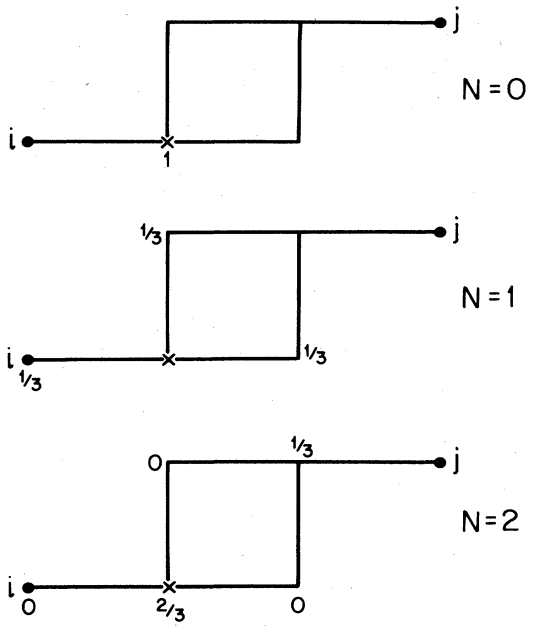

FIG. 1. Illustration of how one calculates *exactly* the weights for a random walk on a very small backbone fractal connecting sites i and j. Shown are three successive times and the *exact* probability $P_N(r)$ for the last step to be at site r. The origin of the walk has a cross.

walk (thus, avoiding edge effects). We found the same value for $\bar{d}_w$ and $\bar{d}_f/\bar{d}_w$ to six decimal places for $l_{\max}=150$ as for $l_{\max}=400$ for 2000-step walks, so we set $l_{\max}=150$ in this work. This value of $L_{\max}=150$ corresponds to an effective radius $r_g=100$ of the cluster. Specifically, we have calculated two quantities (Table I): (i) the rms displacement

$$R(N)\sim(\langle r^2\rangle)^{1/2}\sim N^{1/\bar{d}_w} , \tag{2a}$$

and (ii) the probability of the walk being at the origin after N steps,

$$P_0(N)\sim N^{-\bar{d}_f/\bar{d}_w}\sim N^{-\bar{d}_s/2} . \tag{2b}$$

Our goal is thus to obtain accurate estimates for both exponents in (2a) and (2b), since we can then use (1) to obtain $d_w-d_f=t/\nu$ for the full percolation cluster and, hence, test the AO conjecture. To accomplish this goal, we first note that since our enumerations of random walks are exact, the quantities $R(N)$ and $P_0(N)$ vary extremely smoothly with the number of steps in the walk, N. Thus, methods of extrapolation previously reserved for series expansions can be utilized. For example, from (2a) we want to find the limiting slope, as $N\to\infty$, of the log-log plots of R vs N. There is a weak curvature in this plot, as in all critical phenomena plots, due to the presence of corrections to the leading scaling behavior. Hence, one can analyze the sequence of "successive slopes" obtained by joining a line segment between successive pairs of points. Geometrically, this corresponds to calculating the *local* random-walk dimensionality[11]

$$[\bar{d}_w(N)]^{-1}=\log[R(N+1)/R(N)]/\log[(N+1)/N] , \tag{3a}$$

$$\bar{d}_s(N)=2\log[P_0(N+1)/P_0(N)]/\log[(N+1)/N] . \tag{3b}$$

The local fractal dimensions corresponding to Eqs. (2a) and (2b) [Figs. 2(a) and 2(b)] vary smoothly with N, so it is straightforward to substitute in (1) to obtain

$$\bar{d}_w(N)-\bar{d}_f(N)=\bar{d}_w(N)[1-\bar{d}_s(N)/2]$$

(see Fig. 3). We see that this function varies smoothly with N, is *nearly constant* for $N\geq 500$, and *is always considerably larger than the AO prediction* $d_w-d_f=\frac{1}{2}d_f=\frac{91}{96}=0.9479$; the data used for calculating $\bar{d}_w(N)-\bar{d}_f(N)$ in Fig. 3 (the central value) were obtained from averaging $\langle r^2\rangle_N$ and $P_N(0)$ over 3200 configurations. We also calculated $\bar{d}_w(N)-\bar{d}_f(N)$ for each set of 50 configurations for which smooth curves were obtained, representing the effect of correlations

TABLE I. Results for (i) $[R(N)]^2$ and its standard deviation $\Delta(R^2)$ for 3200 realizations, (ii) $P_N(0)$ and its standard deviation $\Delta[P_N(0)]$, and (iii) $\bar{d}_w(N)-\bar{d}_f(N)$ and its standard deviation $\Delta[\bar{d}_w(N)-\bar{d}_f(N)]$.

N	$[R(N)]^2$	$\Delta(R^2)$	$P_N(0)$	$\Delta[P_N(0)]$	$\bar{d}_w(N)-\bar{d}_f(N)$	$\Delta[\bar{d}_w(N)-\bar{d}_f(N)]$
100	41.420	0.446	0.038 83	0.000 54	0.982 78	0.012 80
200	71.409	0.817	0.025 35	0.000 32	0.972 84	0.015 01
300	97.965	1.101	0.019 70	0.000 25	0.969 40	0.012 96
400	122.482	1.370	0.016 46	0.000 22	0.968 98	0.010 58
500	145.580	1.643	0.014 32	0.000 20	0.969 39	0.008 78
600	167.602	1.916	0.012 78	0.000 18	0.969 68	0.008 00
700	188.767	2.182	0.011 60	0.000 16	0.970 27	0.008 04
800	209.222	2.437	0.010 67	0.000 15	0.970 62	0.008 04
900	229.077	2.682	0.009 91	0.000 14	0.970 71	0.008 97
1000	248.412	2.915	0.009 28	0.000 13	0.970 79	0.009 32
1100	267.291	3.138	0.008 74	0.000 12	0.970 44	0.009 42
1200	285.764	3.350	0.008 27	0.000 11	0.970 47	0.009 45
1300	303.873	3.554	0.007 87	0.000 11	0.970 54	0.009 32
1400	321.651	3.751	0.007 51	0.000 10	0.970 32	0.009 02
1500	339.126	3.939	0.007 19	0.000 10	0.970 55	0.008 68
1600	356.323	4.122	0.006 91	0.000 10	0.970 39	0.008 18
1700	373.262	4.298	0.006 65	0.000 09	0.970 69	0.007 59
1800	389.960	4.468	0.006 41	0.000 09	0.970 28	0.007 29
1900	406.435	4.634	0.006 20	0.000 09	0.971 22	0.006 91
1980	422.698	4.795	0.006 04	0.000 09	0.970 96	0.006 23

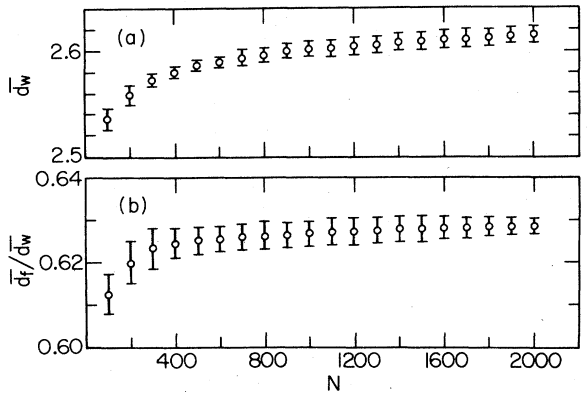

FIG. 2. Successive estimates for exponents (a) $\bar{d}_w$ and (b) $\frac{1}{2}\bar{d}_s = \bar{d}_f/\bar{d}_w$ calculated from the local slopes of the log-log plots of $\langle r^2 \rangle$ vs N and $P_0(N)$ vs N, respectively. Walks were enumerated exactly on a total of 3200 distinct backbone configurations. The error bars were obtained by calculating the standard deviations for each N between the results obtained from ensembles of 50 configurations.

between successive points. The error bars reflect the fluctuation of these curves and, therefore, are not effected by the correlation between the individual points in the same curve. We estimate the limiting value of $\bar{d}_w(\infty) - \bar{d}_f(\infty)$ by the following procedure.

(i) We consider the usual functional form

$$\bar{d}_w(N) - \bar{d}_f(N) = a + bN^{-\omega} \ , \tag{4a}$$

where ω is the leading correction to scaling exponent. For each trial value $\omega = \omega_{\text{trial}}$, we fit the best straight line to the points $x_N = N^{-\omega}$ and $y_N = \bar{d}_w(N) - \bar{d}_f(N)$ in Eq. (4a). The quality of fit is measured by

$$x^2(\omega_{\text{trial}}) = \sum_N (y_N - a - bx_N)^2 \ .$$

The value $\omega = \omega_{\text{trial}} = 0.81$ corresponds to the minimum in $x^2(\omega_{\text{trial}})$, for which $a = \bar{d}_w(\infty) - \bar{d}_f(\infty) = 0.969 \pm 0.008$ and $b \cong 0.4$; the error bar is obtained by taking into account the effect of the error bars of all successive points using the usual least-squares-fit method.

(ii) The second way of analyzing our data is to consider

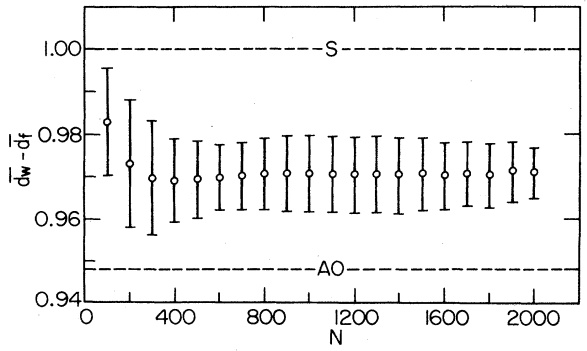

FIG. 3. Successive estimates of $\bar{d}_w - \bar{d}_f = d_w - d_f$. Here, $\bar{d}_f$ was obtained from $\frac{1}{2}\bar{d}_s = \frac{1}{2}\bar{d}_f/\bar{d}_w$ [Fig. 2(b)] while $\bar{d}_w$ was obtained directly [Fig. 2(a)]. The Straley and AO conjectures—1 and $\frac{1}{2}d_f = 0.9479$, respectively—are indicated by dashed lines.

an analytic correction in Eq. (4a). Then we take the functional form

$$\bar{d}_w(N) - \bar{d}_f(N) = a + \frac{b}{N} + cN^{-\omega} \ . \tag{4b}$$

But, here analytic correction term b/N can be eliminated by forming new effective exponents $\bar{d}_w(N)$ and $\bar{d}_f(N)/\bar{d}_w(N)$:[12]

$$\bar{d}_w = [(R_{N+1} - R_N)(R_N - R_{N-1})]/[R_N^2 - (R_{N+1}R_{N-1})]$$
$$= d_w(N) + D/N^{\omega} \ . \tag{4c}$$

The same technique can be utilized for $\bar{d}_f/\bar{d}_w$. The same analysis used in procedure (i) yields $\bar{d}_w(\infty) - \bar{d}_f(\infty) = 0.970 \pm 0.008$ with $\omega \cong 3.07$. Thus procedures (i) and (ii)—even though they assume different functional forms for the correction to scaling—result in the same final estimate, which we take to be

$$t/\nu = \bar{d}_w - \bar{d}_f = 0.970 \pm 0.009 \ . \tag{5}$$

Thus, our error bars would have to be multiplied by a factor of 3 to encompass the AO conjecture. Our result is also *not consistent with the Straley conjecture*[13] *for* $d = 2$, $t/\nu = 1$.

Since we used the chemical distance l in fixing the "ensemble of clusters," it is natural to consider this variable in more detail. For example, we can calculate the exponent $\bar{d}_l$ defined by[10]

$$M(l) \sim l^{\bar{d}_l} \ , \tag{6}$$

where $M(l)$ is the number of sites within a chemical distance l. Alternatively, if we imagine that sites are "burned" successively starting from some origin,[14] then $M(l)$ is the number of sites burned after time $t = l$. For the backbone, we found (Fig. 4)

$$\bar{d}_l = 1.44 \pm 0.03 \ . \tag{7}$$

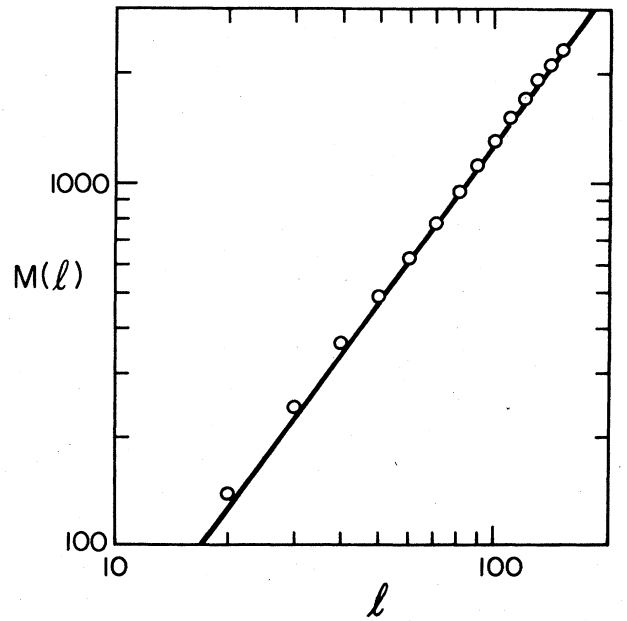

FIG. 4 Dependence of mass on chemical distance l; the slope of the straight line, $\bar{d}_l = 1.44 \pm 0.03$, is the chemical exponent defined in (6).

This number was confirmed by two other computations. First we calculated the dependence of the radius of gyration R_g of backbone sites on l, $R_g \sim l^{\tilde{\nu}}$, where clearly $\tilde{\nu} = \bar{d}_l/\bar{d}_f$. Second we calculated the dependence on N of the rms value chemical distance traveled by the walker, $\langle l^2 \rangle^{1/2} \sim N^{1/\bar{d}_w^l}$, where $\bar{d}_w^l/\bar{d}_w = \bar{d}_l/\bar{d}_f = \tilde{\nu}$. Our values $\tilde{\nu} = 0.87 \pm 0.02$, $d_w = 2.69 \pm 0.04$, and $\bar{d}_w^l = 2.34 \pm 0.04$ are consistent with the direct estimate (7). We note that $\tilde{\nu}$ for backbone has the same value as for percolation clusters.[10] This can be understood from scaling arguments.

In summary, we have used the identity (1) to provide a way of obtaining information about the fractal properties of percolation clusters by studying the percolation backbone—a far simpler fractal from the point of view of random walks since there are no dangling ends. We have carried out exact enumerations of random walks on 3200 configurations and find results that vary smoothly with the number of steps N for N up to 2000. Our results fall midway between the AO conjecture and the Straley conjecture, and exclude the possible validity of both.

We recently learned of parallel work by three other groups, each using a completely independent technique. At Universität Köln, phenomenological renormalization has been used to calculate t/ν,[15] while at Saclay the same technique has been used to calculate the superconductivity exponent s, which is equal to t for $d = 2$.[16] At Harvard University, the large-cell, position-space renormalization-group approach was used for cells of up to 200×200.[17] All three groups obtain the same basic result: the AO conjecture fails by about 3% for percolation in $d = 2$.

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