Exact-enumeration approach to random walks on percolation clusters in two dimensions

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We present a useful method for the study of random walks on disordered systems, and apply it to the problem of diffusion on percolation clusters at criticality. The method is based on the exact enumeration of *all* possible random walks of a certain size on a given cluster. In particular, we calculate the mean-square end-to-end distance, the probability of return to the origin, and a diffusion chemical exponent d_w^l (that describes the chemical distance traveled by the random walker) as functions of the number of steps. Also we present for the first time data showing clearly the difference between the myopic and blind ants, and find much more rapid convergence for the blind ant.

The study of diffusion laws in disordered systems has recently attracted a great deal of attention, in part because of the immediate physical importance of the problem, and more recently because of the remarkable Alexander-Orbach (AO) discovery[1] that the fracton dimension $d_s = 2d_f/d_w \cong \frac{4}{3}$ on percolation clusters independent of dimension. Here, d_f is the fractal dimension of the substrate and d_w is the exponent describing the rms distance traveled by a random walker after taking N steps (i.e., $N \sim R^{d_w}$).

Previous studies of diffusion on percolation clusters have been confined to the conventional Monte Carlo simulation method,[2-7] where a small fraction of all possible, very long (N steps) random-walk configurations are generated and the averages then performed over this set of configurations. In the exact enumeration method to be described below, we enumerate exactly walks, typically $N = 5 \times 10^3$ steps for each cluster configuration, and average these over typically 1000 different clusters. For example, on the triangular lattice at the percolation threshold ($p_c = 0.5$), we can assume the average number of nearest neighbors of a site to be $0.5 \times 6 = 3$; then we enumerate all possible N-step walks exactly corresponding to 3^N configurations. For $N \sim 10^3$ this represents much more "information" than obtained by Monte Carlo methods. We shall see that this exact enumeration procedure reduces the error bars considerably compared to Monte Carlo[2] calculations using a comparable amount of computer time (Fig. 1).

Method. Before proceeding to describe the exact enumeration method we note that for the ant in a labyrinth problem, one can have two different types of ants: a blind ant and a myopic ant.[6]

The difference is simple to state in operational terms. Consider, for concreteness, a square lattice in which a fraction of the sites are open and the remainder blocked. For the blind ant, at each time step a coin with *four* possible outcomes is tossed. If the outcome corresponds to an allowed possibility, the ant moves; otherwise it remains at its present position. For example, suppose the outcome is north and the site on the north is open: then the ant moves one step north. Suppose, however, that the outcome is east and the site on the east is blocked. Then the ant stays at its present site and one unit of time is said to elapse.

The myopic ant is not so "blind": it realizes that not all four paths are open, in general, and chooses among only the open sites. For example, if the sites on the north and south are open, and the other two are blocked, then the ant throws a coin with only two possible outcomes. Thus, the myopic ant moves at every time step.

In Figs. 2(a) and 2(b) we illustrate the exact time evolution of the probability distribution function for the blind ant
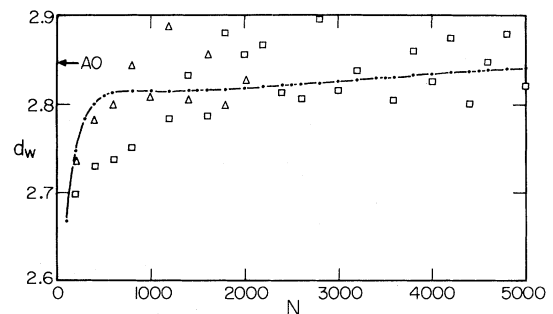

FIG. 1. Graph of d_w vs N comparing Monte Carlo data ($\triangle, \square$) with exact-enumeration data ($\bullet$). The triangles refer to diffusion on the triangular lattice, the squares to diffusion on the square lattice.
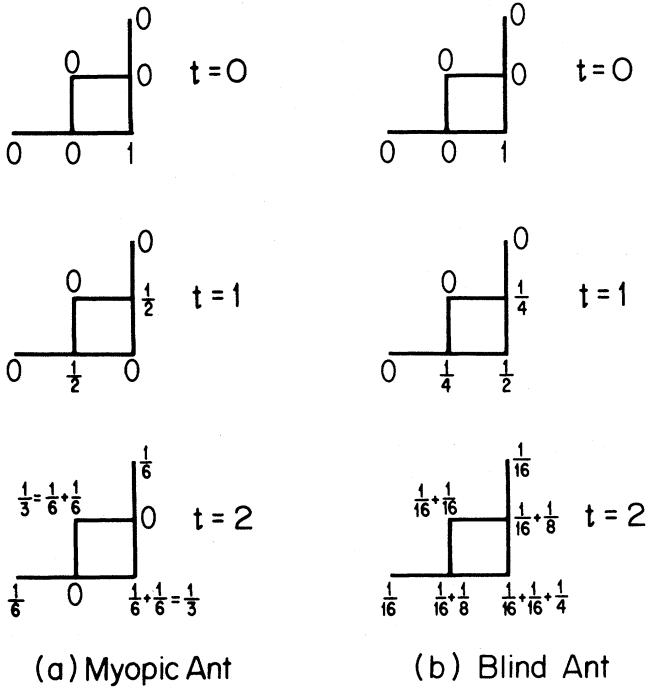
FIG. 2. Time evolution of the probability distribution function for three successive instants of time for the cases of (a) the myopic ant and (b) the blind ant.

and the myopic ant, respectively. The key to the above exact enumeration procedure is that the probability of the ant being at any site (j) at some time t is determined solely by the probabilities of being at the nearest neighbors of site (j) at time $t-1$.

An algorithm for the simulation of diffusion was developed. We first store the cluster in a matrix keeping track of the nearest neighbors of each site. To simulate the diffusion we have two matrices $M_t(j)$, $M_{t'}(j)$ that store the probability distribution function of the random walker at times t and t', where (j) represents the set of all sites in the cluster. Thus, given the distribution function at time t, $M_t(j)$, the distribution function at time $t+1$ is given by

$$M_{t+1}(j) = \sum_{i=1}^{z(j)} M_t(i) w(i,j) \ . \tag{1}$$

Here, i indexes the nearest neighbors of j [$z(j)$ can take on values from 1 to z, where z is the coordination number] and $w(i,j)$ is the probability of the walker coming to j from i. The $w(i,j)$ depend on whether we are simulating the blind ant or the myopic ant. Having obtained $M_{t+1}(j)$, we can go back and obtain the distribution function at time $t+2$ by

$$M_{t+2}(j) = \sum_i M_{t+1}(i) W(i,j) \ . \tag{2}$$

Once we have the probability distribution function at some time t, we may calculate various spatial averages, e.g., the mean-square end-to-end distance,

$$\langle r^2 \rangle_t = \sum_j M_t(j) [r(j)]^2 \ . \tag{3}$$

The probability of returning to the origin $P_t(0)$ is just

$M_t(j=0)$. This procedure may easily be continued to $t \sim 10^3$ steps for clusters of $\sim 10^3$ sites, computation time increasing linearly with the number of sites in the clusters. Specifically, on an IBM 3081 it takes approximately one minute of central processing unit (CPU) time to simulate a 1000-step walk on an 8000-site cluster.

Constant-l ensemble. The chemical distance l between two points is the minimum number of bonds that link the two points.[8,9] Its importance lies in the fact that clusters in the grand canonical ensemble may be characterized by either l (as measured from the origin) or s (the number of sites in the cluster).[8] In particular, for diffusion-related studies, it is plausible that the more natural choice of variable is l. Hence, we suggest that diffusion-related problems should be simulated at constant l, instead of fixing the number of sites in the cluster. We find that this renders the calculations far more efficient because it provides a criterion for the minimum size cluster needed for an N-step walk (avoiding end effects). This is an important observation and one that we employ consistently in our simulations, resulting in considerable savings in computation time. Our simulations were performed at $l_{max} = 220$. To see whether boundary effects are important we also performed several runs with $l_{max} = 300$ and obtained identical results to 10 significant figures. The chemical length exponent d_l is defined by $\langle s \rangle \sim l^{d_l}$; $\langle s \rangle$ is the average number of sites within a chemical distance l. The chemical diffusion exponent d_w^l is defined by[8] $\langle l \rangle \sim N^{1/d_w^l}$; $\langle l \rangle$ is the average chemical distance traveled by the random walker after N steps. Also, d_l and d_w^l are related to d_w and d_f by[8]

$$d_w^l / d_w = d_l / d_f \equiv \tilde{\nu} \ . \tag{4}$$

From our simulations we can calculate d_w^l by calculating the N dependence of $\langle l \rangle$ using

$$\langle l \rangle_t = \sum_j M_t(j,l) l \ , \tag{5}$$

where $M_i(j,l)$ is the probability of being at site j located at a chemical distance l from the origin.

Results. To calculate the diffusion exponents d_w, d_s, and d_w^l on percolation clusters at criticality, we enumerated exactly all walks up to 5000 steps long on each cluster (on the triangular lattice with $p_c = 0.50$ exactly; the cluster was grown by the cluster growth method,[10] omitting all small clusters), and averaged over 1000 different clusters. In particular we calculate $\langle r^2 \rangle_N$ and $\langle r^4 \rangle_N$ to determine d_w, $P_N(0)$, the probability of returning to the origin after N steps [which scales as $\sim N^{-d_s/2}$], to determine d_s directly, and $\langle l \rangle_N$ and $\langle l^2 \rangle_N$ to calculate d_l.

We can calculate all these exponents by the method of successive slopes which is used in series expansion methods. This procedure is equivalent to finding a local fractal dimensionality[4] D_N of some quantity A by the relation

$$D_N = [\ln(\langle A \rangle_{N+1} / \langle A \rangle_N)] / [\ln(N+1)/N] \ . \tag{}$$

In Fig. 1 we show results for d_w obtained by this method and compare with recent Monte Carlo simulation results.[4] The Monte Carlo data appear quite scattered in comparison with the exact enumeration data. The use of the exact enumeration method, therefore, renders the data sufficiently smooth that one can extract the true exponent by $1/N$ extrapolations customarily used in series expansion methods.
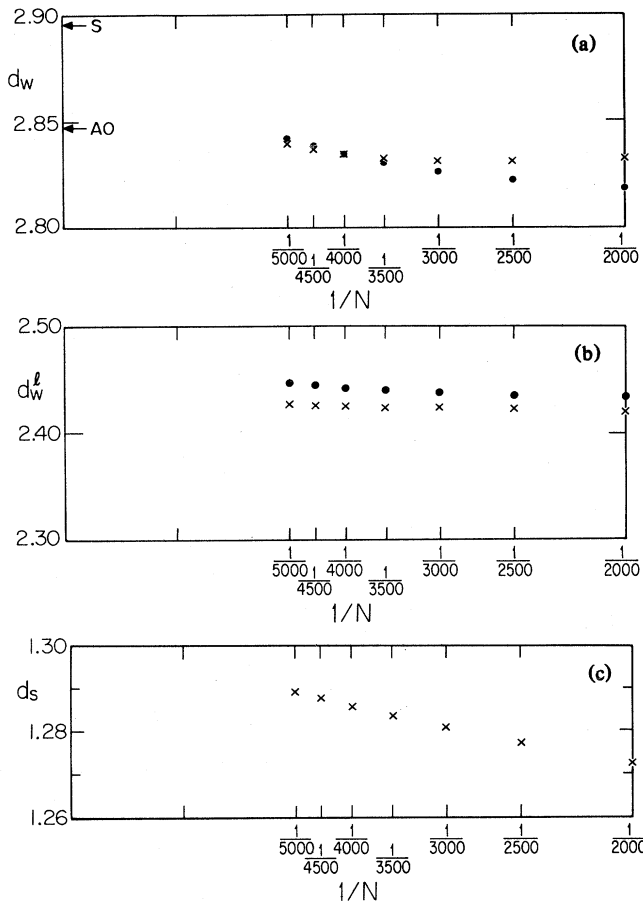
FIG. 4. Plot of d_w vs N comparing blind ant ($\times$) and myopic ant ($\bullet$).

FIG. 3. (a) Graph of d_w vs $1/N$, for 5000-step walks on the triangular lattice obtained from $\langle r^4 \rangle_N$ ($\bullet$) and $\langle r^2 \rangle_N$ ($\times$). The error bars associated with each point are ± 0.015 for $\langle r^2 \rangle_N$ and ± 0.011 for $\langle r^4 \rangle_N$. (b) Graph of d_w^l vs $1/N$ for 5000-step walks on the triangular lattice from $\langle l^2 \rangle_N$ ($\bullet$) and $\langle l \rangle_N$ ($\times$). Error bars associated with each point are ± 0.015. (c) Plots of d_s vs $1/N$ for 5000-step walks on the triangular lattice obtained from $P_N(0)$. Error bars associated with each point are ± 0.020.

Plots of the effective exponents d_w, d_w^l, and d_s vs $1/N$ are shown in Fig. 3. Typical error bars for points beyond 2000 steps are (a) $\langle r^4 \rangle$: ± 0.011 and $\langle r^2 \rangle$: ± 0.015 for d_w, (b) $P_N(0)$: ± 0.017 for d_s, and (c) $\langle l \rangle$: ± 0.015 and $\langle l^2 \rangle$: ± 0.015 for d_w.

Our extrapolated results are as follows:

$$\langle P_N(0) \rangle: \quad d_s = 1.31 \pm 0.02 \ , \tag{6a}$$

$$\langle r^2 \rangle: \quad d_w = 2.860 \pm 0.02, \quad \langle r^4 \rangle: \quad d_w = 2.875 \pm 0.02 \ , \tag{6b}$$

$$\langle l \rangle: \quad d_w^l = 2.44 \pm 0.02, \quad \langle l^2 \rangle: \quad d_w^l = 2.47 \pm 0.02 \ , \tag{6c}$$
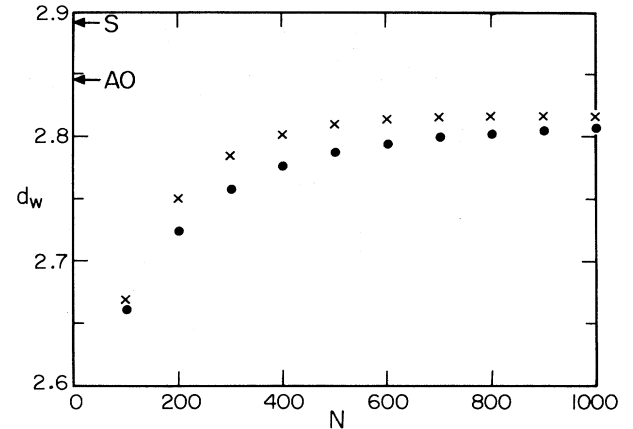
$$d_s = 2d_f/d_w = 1.32 \pm 0.01 \ . \tag{6d}$$

Note that d_s calculated from $2d_f/d_w$ is consistent with, but more accurate than, the value from $P_N(0)$.

As our final estimates we give $d_w^l = 2.460 \pm 0.025$, $d_w = 2.87 \pm 0.02$, and $d_s = 1.32 \pm 0.01$. Hence, even though these results seem to exclude the AO conjecture ($d_w = \frac{91}{32} = 2.845$; $d_s = \frac{4}{3} = 1.333 \ldots$) the subjective estimates of the error bars make it impossible in this case to rule out the AO conjecture convincingly. For the chemical length exponent d_l we find from $d_l = (d_f/d_w)d_w^l$ that $d_l = 1.63 \pm 0.02$, consistent with other recent estimates.[8,9]

Lastly, we note that the exact enumeration method presented above is sufficiently sensitive to distinguish between the blind ant and the myopic ant, at least for walks $\lesssim 1000$ steps long. Furthermore, although both converge to the same asymptotic behavior, it seems that the blind ant converges so more rapidly than the myopic ant (Fig. 4); we, therefore, chose to perform all our simulations for accurate determination of the exponents d_w, d_s, and d_w^l by using the blind ant algorithm.

In summary, we have introduced and applied an exact enumeration method of generating random walks on percolation clusters. Working in the constant-l ensemble, we obtain accurate estimates of the diffusion exponents d_s, d_w, and d_l. Also we present the first numerical data that indicate, at least for walks of $\lesssim 1000$ steps, the clear difference between the rate of convergence of exponents obtained from the myopic ant and the blind ant.

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