Single Random Walker on Disordered Lattices[1]

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Random walks on square lattice percolating clusters were followed for up to 2×10^5 steps. The mean number of distinct sites visited $\langle S_N \rangle$ gives a spectral dimension of $d_s = 1.30 \pm 0.03$ consistent with superuniversality $(d_s = 4/3)$ but closer to the alternative $d_s = 182/139$, based on the low dimensionality correction. Simulations are also given for walkers on an *energetically disordered* lattice, with a jump probability that depends on the local energy mismatch and the temperature. An apparent fractal behavior is observed for a low enough reduced temperature. Above this temperature, the walker exhibits a "crossover" from fractal-to-Euclidean behavior. Walks on two- and three-dimensional lattices are similar, except that those in three dimensions are more efficient.

KEY WORDS: Fractal; energetic disorder; random walk; percolation; spectral dimension.

1. INTRODUCTION

Does a random walk on a substitutionally disordered binary lattice exhibit a fractal behavior? Does a random walk on an energetically disordered lattice exhibit a fractal behavior? A random walk on a random binary lattice at *criticality* has not only been claimed[1–18] to exhibit a "fracton" (spectral-fractal) dimension, but, moreover, is expected to show superuniversality i.e., the same spectral dimension $(d_s = 4/3)$ for all topological dimensions $d > 2$. We have thus performed refined Monte Carlo simulations for random walks on percolation clusters bracketing the critical point. The mean-squared displacement of the walk, $\langle R_N^2 \rangle^{1/2}$, did not exceed the correlation length. Data on the crossover from fractal-to-Euclidean behavior will be reported elsewhere[19] as well as data on long-range percolation clusters[20] and on early time corrections.[21] We also report here preliminary

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data on lattices with random energetic disorder[22] and nearest-neighbor hopping probabilities that depend on energy mismatches and temperature. These simulations are not only related to many experimental situations but are intended to probe whether the fractal (fracton) approach is indeed useful for such systems. The problem of the single random walker is also of much current interest because of its relation to the problems of trapping and binary reactions of random walkers in disordered media,[23-31] as well as the problem of interacting walkers.[32]

Our specific simulations involve the number of distinct sites visited S_N after N steps:

$$\langle S_N \rangle \propto N^f, \qquad f = d_s/2 \tag{1}$$

Here f is a "fractal exponent," which, on a genuine fractal, is given, asymptotically in terms of the spectral dimension d_s. Occasionally we also use the heterogeneity exponent[27] $h = 1 - f$. For the random binary lattice we find that $f = d_s/2$ agrees with the expectations from scaling arguments.[1-6] For the energetically disordered lattice we find that $f = f(T)$ is a function of *temperature*, and that Eq. (1) is a reasonable approximation.

2. METHODS

We use different approaches for the two different types of disorder. For the first case of binary lattices the details of calculations have been reported elsewhere.[26,33] Briefly, a lattice is made of two types of sites identified as open and closed. Their position is determined at random using a pseudo-random number generating routine. A random walker is introduced at a random point of origin and the direction of propagation is also determined at random at the end of each step. To avoid artificial results that depend on the particular structure of the lattice (for example its size) we use a small N/L ratio (where L is the size of the lattice and N implies the maximal number of steps), of the order of $N/L \sim 0.05$ for short- and long-time behavior. In this work we call the short-time limit the case of $N = 5000$ steps and the long-time limit $N = 200\,000$ steps. A square lattice topology (two dimensional) is employed but all work can be extended to other topologies with no difficulty.

For the energetically disordered lattice we use periodic boundary conditions with $L = 500 \times 500$ sites and $N = 100\,000$ steps in two dimensions and $L = 64 \times 64 \times 64$ sites with $N = 10\,000$ steps in three dimensions. The walker starts at the center of the lattice with $S_N = 1$ at $N = 0$. A uniformly distributed pseudo-random number generator, FUNIF, is used to move the walker to nearest-neighbor sites. As the walker moves, a random number from a separate uniform distribution is used to assign site

energies, E, which correspond to a normalized distribution of bandwidth W. The parameter of primary interest here is the unitless temperature $T'' \equiv kT/W$ used in assigning the jump probability, $P_i = z^{-1} \exp(-\Delta E/T'')$, for a move to a site of equal or higher energy; $P_i \equiv z^{-1}$ for a move to a site of lower energy. Hence, the microscopic transfer rates are not symmetric. The residual, $1 - \sum_{i=1}^{z} P_i$, is used to assign the probability of a walker remaining on the same site for two consecutive steps (z is the coordination number).

3. RESULTS

3.1. Binary Lattices

We have reported extensive simulations on such lattices for short and long times, covering the entire range from the critical percolation threshold, p_c, to the pure lattice.[18,33] We have shown that the effective spectral dimension d_s' lies in the range 1.2–1.8 for the square lattice topology.[18,33]
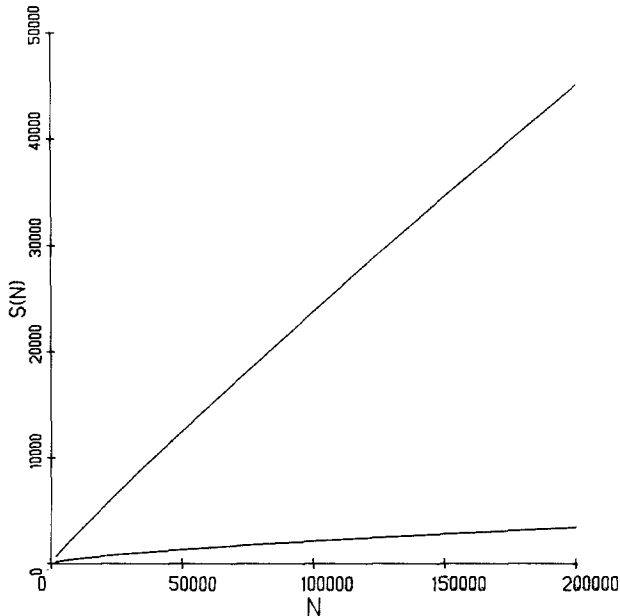

Fig. 1.   Mean number of distinct sites visited, $\langle S_N \rangle$, vs. number of steps, N. Lower curve: $p = 0.60$. Upper curve $p = 1.00$. Averages of 1000 runs using the cluster growth technique.[33] However, for $p = 0.60$, runs have been discarded if $S_{200\,000} - S_{100\,000} < 20$. This eliminates runs on finite clusters, leaving only runs on percolating clusters. Note: Lattice of 2000×2000, but boundaries were never crossed.

To investigate the conjectured asymptotic behavior of d_s we take the log of both sides of Eq. (1),

$$\log\langle S_N \rangle \propto \frac{d_s}{2} \log N \qquad (2)$$

and thus plot $\log\langle S_N \rangle$ versus $\log N$. Figure 1 shows a linear plot of $\langle S_N \rangle$ vs. N, while Fig. 2 is the same plot in logarithmic form. The lines in the linear plot of Fig. 1 are *not* straight, while the lines of the logarithmic plot of Fig. 2 are quite straight. From the slopes we obtain $d_s = 1.33$ to 1.36 for $p = 0.60$ but 1.28 to 1.33 for $p = 0.595$. This seems to agree better with Alexander's[16] formula $d_s = 2D/(D+1) = 1.31$, where $D = 91/48$ is the fractal dimension, than with Alexander and Orbach's superuniversality[1] ($d_s = 4/3$). We also obtain an effective $d_s = 1.84$ for $p = 1.00$. If we take into account random walks that do not necessarily originate on the largest cluster but on any point in a lattice at the critical percolation threshold $p_c = 0.593$, then we obtain $d'_s = 1.24$, in good agreement with the expected value,[18,19] $d'_s = 86/91 \, d_s$, if $d_s = 1.31$.

The following points are in order: The proposed critical behavior holds in the asymptotic limit of large N. For the range of the present study where
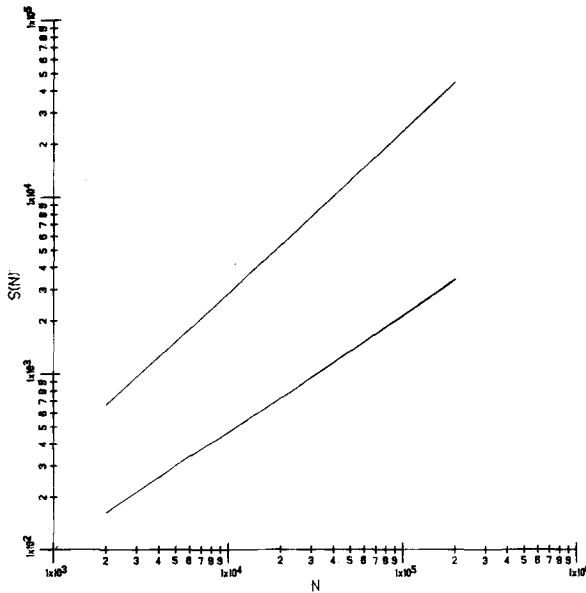

Fig. 2. $\text{Log}\langle S_N \rangle$ vs. log N. Lower curve: $p = 0.60$. Upper curve: $p = 1.00$. Same data as on Fig. 1.

N goes to 2×10^5 we are well within this limit. However, the short-time behavior is obscured in these figures. In a separate study[21] we cover this particular region and its behavior. In the region where the probability of open sites increases from the critical threshold value to the pure lattice limit one observes the crossovers from fractal-to-Euclidean behavior. This will be the scope of another study.[19,33]

3.2. Energetically Disordered Lattices

The parameter of primary interest here is the temperature; we use the unitless temperature T'' defined above. Monte Carlo simulations were performed on *square lattices* for $T'' = 0.05$, 0.08, 0.10, 0.20 and for the temperature-independent perfect lattice ($P_i \equiv z^{-1}$), as well as on *simple cubic lattices* for $T'' = 0.01$, 0.03, 0.05, and 0.10. The temperature-dependent analog of Eq. (1) for N steps is

$$\langle S_N \rangle = aN^{f(T'')}, \qquad f(T'') \equiv d'(T'')/2 \tag{3}$$

This is used to obtain the effective spectral dimension, $d'(T'')$, using a nonlinear regression. Results of the regression analysis are given in Table I. The statistics include data for $N = 2000$ to $100\,000$ for square lattices and $N = 0$ to $10\,000$ for cubic lattices, where each $\langle S_N \rangle$ used is an average over 100 realizations. Simulation results (symbols) and fitted curves of $\langle S_N \rangle$ as a function of N are plotted for square lattices in Figs. 3a and 3b, using linear coordinates and in Fig. 4 using log–log coordinates. The time dependence of

Table I.   Exponent *f* and Preexponent *a* for Energetically
Disordered Lattices

	Two dimensions				
	$T'' = 0.05$	$T'' = 0.08$	$T'' = 0.10$	$T'' = 0.20$	Perfect
$f(T'')$	0.32	0.66	0.84	0.91	0.92
a	1.2	0.11	0.037	0.15	0.62

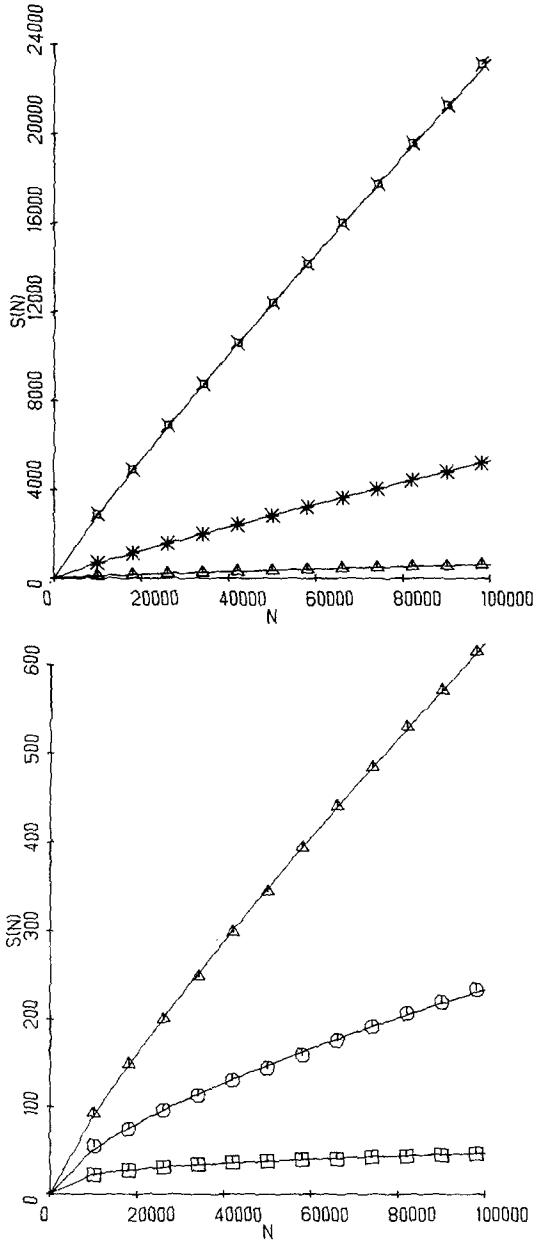|	Three dimensions			
	$T'' = 0.01$	$T'' = 0.03$	$T'' = 0.05$	$T'' = 0.10$
$f(T'')$	0.046	0.236	0.534	0.922
a	2.46	1.20	0.307	0.0876

Fig. 3.   (a) Mean number of distinct sites visited vs. N ($d = 2$), for the perfect lattice (top curve), $T'' = 0.2$ (middle curve) and $T'' = 0.10$ (bottom curve). The symbols are the simulation results and the solid curves are the fit to Eq. (3). (b) Same as in (a), but the top curve is $T'' = 0.1$; middle curve is $T'' = 0.08$; and the bottom curve is $T'' = 0.05$.
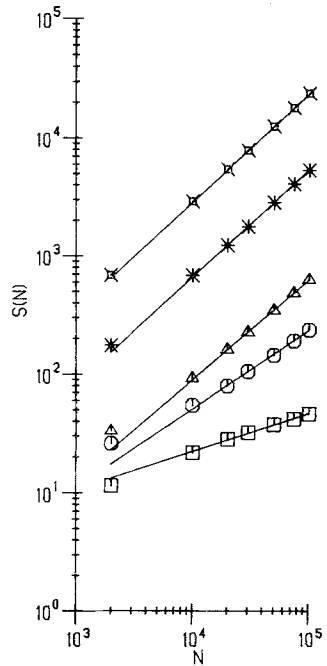
Fig. 4. Log–Log plot of $\langle S_N \rangle$ vs. N for $d = 2$, in order from top to bottom: perfect lattice, $T'' = 0.20$, $T'' = 0.10$, $T'' = 0.08$, and $T'' = 0.05$. The curves are the fit to Eq. (3) and the symbols are the simulation results.
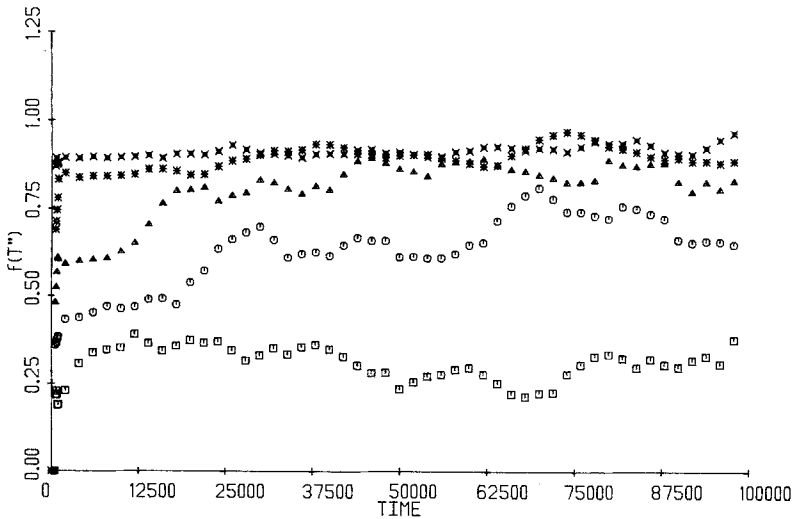

Fig. 5. Half the effective spectral dimension, $d'/2 = f(T'')$ vs. time (N). Top to bottom at long times: perfect lattice, $T'' = 0.2$, $T'' = 0.1$, $T'' = 0.08$, and $T'' = 0.05$, for $d = 2$.
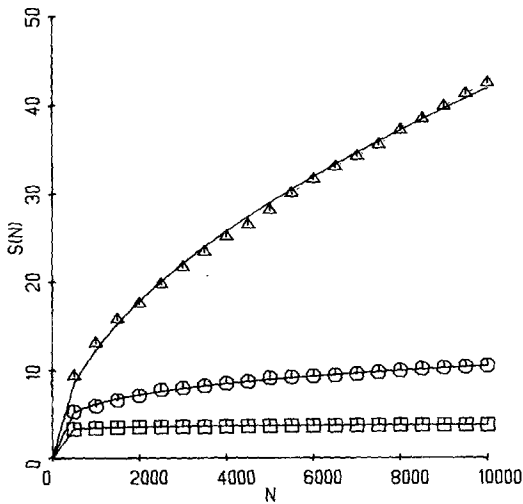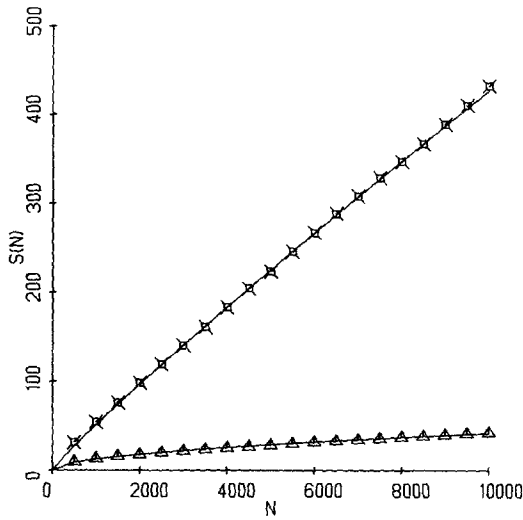
Fig. 6.   (a) Mean number of distinct sites visited, $\langle S_N \rangle$ vs. N $(d = 3)$. Upper curve $T'' = 0.1$.
Lower curve $T'' = 0.05$. The symbols are the simulation results and the solid curves are the fit
to Eq. (3). (b) Same as in (a), but the top curve is $T'' = 0.05$, the middle curve is $T'' = 0.03$,
and the bottom curve is $T'' = 0.01$. The symbols are the simulation results and the solid
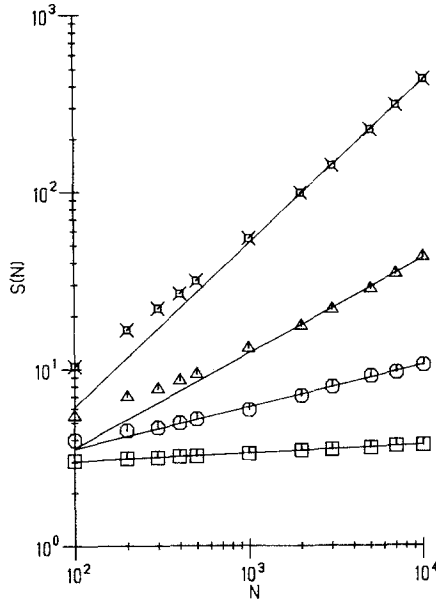curves are the fit to Eq. (3).

Fig. 7.   Log–Log plot of $\langle S_N \rangle$ vs. N for $d = 3$, in order from top to bottom: $T'' = 0.1$, 0.05, 0.03, and 0.01. The curves are the fit to Eq. (3) and the symbols are the simulation results.

the exponent f generated using finite differences of the log–log data is shown in Fig. 5 where we may see some effective crossover of fractal-like-to-Euclidean-like behavior at higher temperatures. At the temperature $T'' = 0.05$ we see that the curve is clearly separated from all other curves. Analogous results for simple cubic lattices are given in Figs. 6a, 6b, and 7.

   For the energetically disordered lattice, the temperature dependence is very important. As the temperature is raised the probability of moving to a site of higher energy increases; the mobility increases and the number of distinct sites visited is higher. As the temperature decreases, the walker moves primarily to sites of equal or lower energy, getting caught in small regions which act as traps. Trapping in these systems is only temporary. Nonetheless, the walker is restricted and the number of distinct sites visited is lowered. Note that for $T'' = 0.01$ (Figs. 6b and 7), the walker visits only three to four sites and is thus effectively trapped.

4. CONCLUSIONS

   The single random walker on a percolating cluster (in a binary lattice) shows the conjectured fractal behavior near the percolation threshold. The

spectral dimension is 1.30 ± 0.03. At higher concentrations the crossover to the classical regime is observed. The single random walker on an energetically disordered lattice shows a roughly analogous behavior. This may be related to the self-attracting interacting random walks studied very recently by Stanley et al.[32] In any event, at low temperatures the walk on an energetically disordered lattice is well characterized by a spectral dimension that is a function of the temperature and the local disorder. The implications for reacting random walkers are given in the following paper.[34]

NOTE ADDED IN PROOF

The just published paper by A. Aharony and D. Stauffer, *Phys. Rev. Lett.* **52**:2368 (1984), gives additional arguments in favor of $d_s = 2D/(D+1) = 1.31$ for two-dimensional percolating clusters. Our numerical results favor this result (rather than $4/3$): Our $d_s = 1.30 \pm 0.03$ for $p = 0.595$ provides an upper bound for d_s at p_c; also our $d_s' = 1.24 \pm 0.02$ obtained by interpolating between $p = 0.590$ and $p = 0.595$, agrees better with Aharony and Stauffer, while $d_s = 4/3$ (resulting in $d_s' = 1.26$) appears to be just at the upper end of the simulation error.

ACKNOWLEDGMENTS

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