Classical Diffusion on Eden Trees

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We study an aggregation process which gives rise to compact clusters with no loops. A generalization of the node-counting theorem, applicable to such branched graphs (trees), is proved. This is used to determine the spectral dimension of these clusters on square and cubic embedding lattices by Monte Carlo simulations. The results are explained in terms of the geometric structure of these trees.

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The study of aggregation models is of relevance to a variety of nonequilibrium phenomena such as nucleation, gelation, polymerization, tumor growth, etc.[1] Here we examine a modification of the Eden aggregation process[2] which gives rise to clusters with *no* loops. These clusters presumably have an integral Hausdorff dimension, but because of their tenuous tree structure, diffusion on these clusters—called Eden trees (ET's)—is characterized by nontrivial exponents.

Classical diffusion on trees is also important in the study of transport processes in clusters, such as percolation clusters or Witten-Sander aggregates, as these are treelike on the large scale. The distribution of dead ends in such clusters determines the long-time behavior of a diffusing particle; ET's thus have a nontrivial spectral dimension which we determine using Monte Carlo simulations.

The node-counting theorem[3] is a powerful tool to study disordered one-dimensional harmonic systems. It proves that the mth eigenmode of such a system has precisely $(m-1)$ nodes. For trees with some branching symmetry, there are localized modes with all but a small number of sites having no displacement, and the counting of nodes is nontrivial. We prove a generalization of the node-counting theorem applicable to arbitrary tree networks.

The conventional Eden process is the model wherein starting from a single occupied site on a d-dimensional lattice, sequential growth occurs by additional occupation of one of the perimeter sites at each (discrete) time step. The perimeter is the set of vacant sites that neighbor occupied sites: At each step, one of these is occupied at random. A compact cluster results, with diameter (the maximum extent in any direction) varying as $N^{1/d}$ for large N, where N is the size of the cluster.[4]

Our present model involves the modification that any vacant site which neighbors two or more occupied sites *cannot* be occupied. Under this rule, the resulting cluster, while space filling, has no loops (Fig. 1). We find that the diameter still varies as $N^{1/d}$, and the structure is compact, although its average density is less than 1. The sites of an ET may be divided into two classes—those on the backbone of the tree and those on side branches. The backbone is the set of sites on paths connecting the origin to the perimeter.

To determine the spectrum of harmonic excitations on ET's, we solve the eigenvalue equation for the normal-mode frequencies of the system. For a set of unit masses on occupied sites, with neighbors connected by springs of force constant 1, these are

$$-\omega^2 U_i = \sum_j \{U_j - U_i\}, \tag{1}$$

where U_i is the scalar displacement at site i and the summation is over all nearest neighbors j of i. For each site i except the origin we define $F_i = U_i / U_{p(i)}$ [where $p(i)$ labels the predecessor site of i on the tree]. The F_i's satisfy the recursion relations

$$F_i = [1 - \omega^2 + \sum_j (1 - F_j)]^{-1}, \tag{2}$$

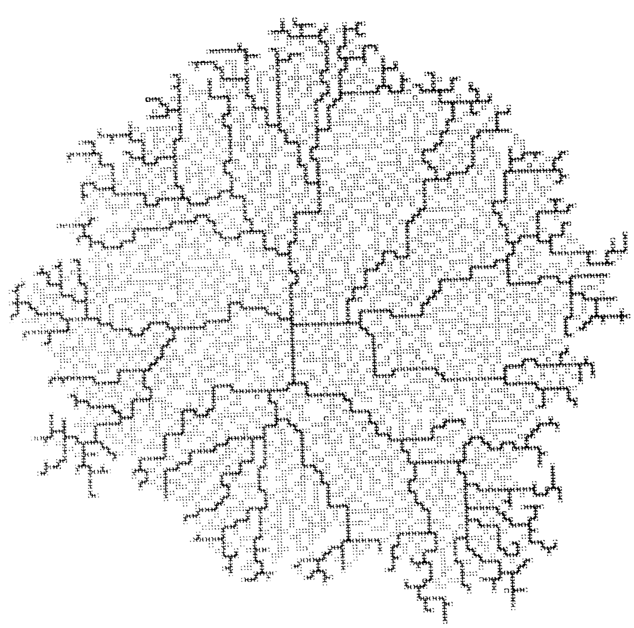

FIG. 1. An Eden tree on a square lattice. This cluster has 4000 sites; the backbone sites are marked by lines joining them.

where the sum is over all sites j that are successors of i. For a site i having no successors, $F_i = 1/(1-\omega^2)$, and all F_i's can be determined recursively starting from the end points of branches of the tree and using Eq. (2). By induction, F_i's are rational functions of ω^2, with $\partial F_i/\partial\omega^2 > 0$, except at the poles of F_i. Let $H(\omega^2)$ be the number of modes of frequency below ω and N_F be the number of negative F_i's. Then

$$H(\omega^2) = N_F + \theta[\omega^2 - \textstyle\sum_k (1-F_k)] \qquad (3)$$

where the summation is over nearest neighbors k of the origin, and θ is the Heaviside step function.

An outline of the proof is as follows: The equation holds if $\omega^2 = 0^+$, with $H(\omega^2) = 1$, $N_F = 0$, and $F_i = 1^+$ for all i. As ω^2 is increased, $H(\omega^2)$ increases by 1 each time the argument of the θ function crosses 0, preserving equality (3). If m (≥ 1) of the F_k's in Eq. (3) have a simultaneous pole at $\omega^2 = a^2$, as ω^2 is increased past a^2 these change from $+\infty$ to $-\infty$. Thus N_F increases by m, the θ function changes from 1 to 0, and the increase in $H(\omega^2)$ equals $m-1$, the number of independent eigenmodes with frequency a having a node at origin. Similarly, at singular points of F_j, where j is not a neighbor of the origin, if m of the F_j's in Eq. (2) have a simultaneous pole at b^2 ($m \geq 1$), then N_f increases by $m-1$ as ω^2 is increased past b^2, and there are exactly $m-1$ eigenmodes with a node at site i. This proves Eq. (3), which generalizes the node-counting theorem to arbitrary trees.

With use of this result, the integrated frequency spectrum $H(\omega^2)$ is numerically determined in a very efficient manner. Figure 2 shows the fractional integrated spectral density for ET's on a square lattice averaged over 90 trees containing approximately 10 000 sites each.[5] The asymptotic power law, $H(\omega^2)$, holds over four decades of ω^2 with the spectral dimension

$$\tilde{d} = 1.22 \pm 0.04. \qquad (4)$$

We note that the spectral dimension $\tilde{d}$ for $d=2$ in our simulations is significantly different from the values $\frac{4}{3}$ and $2d/(2+\theta)$ argued for recently by Leyvraz and Stanley and by Havlin *et al.*[6]

The spectral density for ET's grown on the simple-cubic lattice is also shown (averaged over eight trees of size 8000). There is a significant curvature at low frequencies due to finite-size effects, and a slightly higher value, $\tilde{d} = 1.30 \pm 0.12$, is obtained for the spectral dimension. (We cannot rule out the possibility that the spectral dimension for ET's on the square and cubic lattices is identical.)

As an alternative means of determining the spectral dimension, consider a random walk on an ET, "the ant in the labyrinth problem."[7] It is known[8] that after N steps, the probability of return to the origin is $P_0(N) \sim N^{-\tilde{d}/2}$. For $\tilde{d} \leq 2$, the average number S_N of distinct sites visited by the ant in N steps varies as the inverse of $P_0(N)$; hence $S_N \sim N^{\tilde{d}/2}$ and the variance of S_N, $\sigma_N \sim N^{\tilde{d}}$. For trees on a square lattice, results of Monte Carlo simulations, averaged over 100 trees of size 4000 and for 100 walks on each tree, are shown in Fig. 3. The value of $\tilde{d} = 1.19 \pm 0.03$ so obtained is in excellent accord with Eq. (4). Unlike random walks on some nontree fractals,[8] the exponent governing the

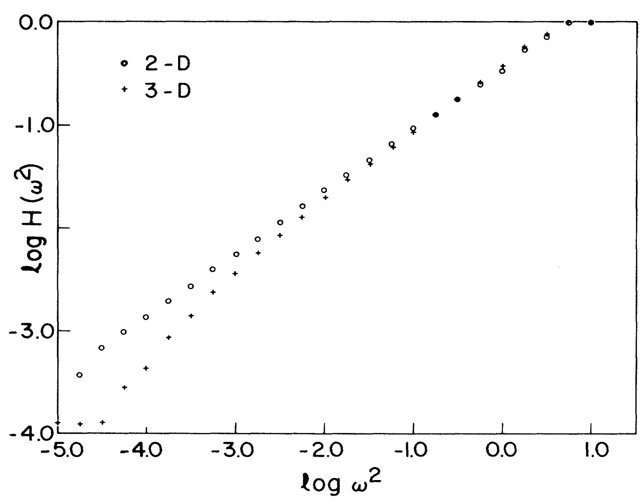

FIG. 2. $H(\omega^2)$, the fractional number of modes of frequency below ω for the square and cubic lattices.

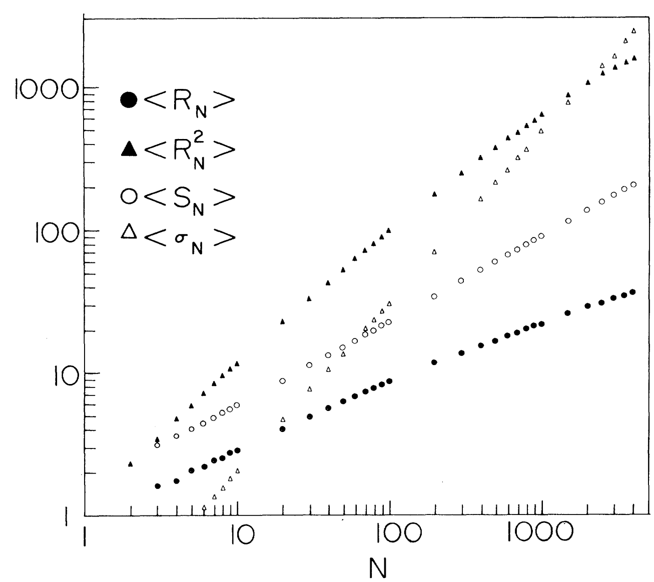

FIG. 3. Results of Monte Carlo simulations of diffusing ants on ET's grown on a square lattice. After N steps, $\langle S_N \rangle$ is the number of distinct sites visited, σ_N is the variance of S_N, and R_N is the distance measured along bonds, from the origin.

mean displacement is *not* $\tilde{d}/(2\bar{d})$. We observed that $\langle \sum_x R_x \rangle$ summed over all distinct sites x visited up to time N varies quite linearly with N. Since this quantity should vary as $\langle R_N \rangle \langle S_N \rangle$, we get $\langle R_N \rangle \sim N^{1-\tilde{d}/2}$, in agreement with the $N^{0.42 \pm 0.04}$ observed (Fig. 3). Similar simulations for $d = 3$ give an exponent for $\langle S_N \rangle$ in rough agreement with $\tilde{d}$ obtained from node counting. The behavior of $\langle R_N \rangle$ is harder to fit by a simple power law. However, a fit by the form $\langle R_N \rangle \sim V^{1/3} f(NV^{-\phi})$, where f is a scaling function, for different tree sizes V gives $\langle R_N \rangle \sim N^{0.44 \pm 0.04}$. The alternate prediction $\langle R_N \rangle \sim N^{\tilde{d}/2\bar{d}}$ is definitely ruled out by our data in both two and three dimensions.

We describe below a theoretical model to explain these results. The average number of sites in a side branch in an ET increases with the distance from the origin. Side branches tend to trap the random-walking ant and decrease its mean-square displacement at large times. Larger side branches have longer average trapping times and lead to an effective diffusion constant which decreases as a negative power of R for large R. Thus the trapping effect in the side branches leads to a nontrivial exponent for the mean-square displacement. (Such an effect in the presence of external fields has been studied earlier.[9])

Consider a continuous-time version of the random walk by an ant starting at the origin, with unit transition probability per unit time for each pair of occupied neighboring sites on an ET, and zero otherwise. Let $P(i,t)$ be the probability that the ant is at site i at time t. The probabilities satisfy the evolution equation

$$\partial P(i,t)/\partial t = \sum_j [P(j,t) - P(i,t)], \qquad (5)$$

where the summation over j extends to all nearest neighbors of i. Let the side branch attached to backbone site i at distance R_i from the origin have n_i sites. With use of Laplace transformation and elimination of variables in the side branch, Eq. (5) may be rewritten for $t >> n_i$ as

$$(1 + n_i)\partial P(i,t)/\partial t = \sum_j{}' [P(j,t) - P(i,t)]. \qquad (6)$$

The prime restricts the summation to neighbors j of i that lie on the backbone.

We approximate $P(i,t)$ and n_i by their mean values $P(R,t)$ and $\bar{n}_R$, respectively. (A more detailed theory could take into account spatial fluctuations, and the distribution of number of sites in the side branches.[10]) An ET is not homogeneous, and $\bar{n}_R$ depends on R. We assume that $\bar{n}_R \sim R^\theta$, where $\theta \geqslant 0$. Since the number of sites in the backbone as well as side branches within a distance R from the origin varies as R^d, the number of sites in the backbone within a distance R varies as $R^{d-\theta}$: The backbone has the Hausdorff dimension $\bar{d} = d - \theta$. Substituting the power-law behavior of $\bar{n}_R$ into Eq. (6), and taking the continuum limit, yields

$$R^\theta \frac{\partial}{\partial t} P(R,t) = \left(R^{-\bar{d}+1} \frac{\partial}{\partial R} R^{\bar{d}-1} \frac{\partial}{\partial R} \right) P(R,t),$$

where the operator in the large round brackets is the Laplacian operator on the $\bar{d}$-dimensional backbone fractal. By scaling, this implies that the mean distance traveled by the ant in time t scales as

$$\langle R_t \rangle \sim t^{1/(2+\theta)}.$$

For a typical long walk, the ant samples only order-one segments of the backbone. Hence the mean number of distinct sites visited varies as the number of sites in one segment of the backbone of length R_t and its side branches:

$$\langle S_t \rangle \sim t^{(1+\theta)/(2+\theta)}.$$

Had a typical walk sampled most of the sites within a distance $\langle R_t \rangle$ from the origin, we would have obtained[8] $\langle S_t \rangle \sim \langle R_t \rangle^d$. Note also that the finite-density constraint $\theta \leqslant d - 1$ gives us $\tilde{d} \leqslant 2d/(d+1)$, in agreement with Witten and Kantor.[11]

The value of N_R, the number of sites in the backbone at a distance R from the origin, averaged over 100 two-dimensional trees of approximate size 10 000 is plotted as a function of R in Fig. 4, from which the exponent $\theta = 0.54 \pm 0.04$ is obtained ($\theta \simeq \frac{1}{2}$ seems to be a good mnemonic). This value of θ is also consistent with the exponents for $\langle R_N \rangle$ and $\langle S_N \rangle$ observed in the Monte Carlo simulations (cf. Fig. 3).

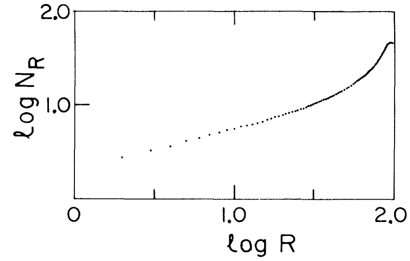

FIG. 4. N_R, the average number of backbone sites at a distance R from the origin, for ET's on a square lattice.

For ET's on the triangular lattice, the spectral dimension that we obtain is very close to the value seen for the square lattice. Presumably, the problems belong to the same universality class. On the other hand, Eden clusters with loops (obtained by allowing a perimeter site to neighbor two, but not three, perimeter sites), however, have the expected dimension $\tilde{d} = d$.

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[1]T. A. Witten and L. M. Sander, Phys. Rev. Lett. **47**, 1400

(1981); M. E. Cates, J. Phys. A **17**, L487 (1984); P. Meakin, Phys. Rev. Lett. **51**, 1119 (1983); M. Plischke and Z. Racz, Phys. Rev. Lett. **53**, 415 (1984); J. Vannimenus, B. Nickel, and V. Hakim, Phys. Rev. B **30**, 391 (1984).

[2]M. Eden, in *Proceedings of the Fourth Berkeley Symposium in Mathematics, Statistics and Probability,* edited by J. Neyman (Univ. of California Press, Berkeley, 1961), p. 233.

[3]J. Hori, *Spectral Properties of Disordered Chains and Lattices* (Pergamon, Oxford, 1968).

[4]See, however, G. Parisi and Y. C. Zhang, Phys. Rev. Lett. **53**, 1791 (1984).

[5]Computationally, it is convenient to work with dense trees that completely fill an $n \times n$ grid. In most simulations, we take $n = 129$.

[6]F. Leyvraz and H. E. Stanley, Phys. Rev. Lett. **50**, 77 (1983); S. Havlin, R. Nossal, B. Trus, and G. H. Weiss, to be published.

[7]P. G. de Gennes, La Recherche **7**, 916 (1976); C. D. Mitescu and J. Roussenq, Ann. Isr. Phys. Soc. **5**, 81 (1983).

[8]R. Rammal and G. Toulouse, J. Phys. (Paris), Lett. **44**, L13 (1983).

[9]T. Ohtsuki, J. Phys. Soc. Jpn. **51**, 1493 (1982); M. Barma and D. Dhar, J. Phys. C **16**, 1451 (1983).

[10]For percolation clusters, the distribution of dead-end sites is studied by T. Ohtsuki and T. Keyes, J. Phys. A **17**, L287 (1984).

[11]T. A. Witten and Y. Kantor, Phys. Rev. B **30**, 4093 (1984).