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Diffusion on treelike clusters

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We present a general relationship between the diffusion exponent d_w and the fractal exponents of trees (i.e., clusters without loops), $d_w=(d_f/d_l)(2+d_l-d_l^s)$. The exponents d_f, d_l, and d_l^s are the fractal dimension, the intrinsic dimension of the tree, and the intrinsic dimension of its skeleton, respectively. This new result is supported by scaling arguments and numerical data.

Transport properties of random systems, such as diffusion, elastic response, and electrical conductivity, currently are being intensively studied.[1-5] Considerable effort has been devoted to finding relations between static and dynamical properties of cluster aggregates.[1,3-5] Recently, the static intrinsic dimension[6] d_l has been recognized as being useful for characterizing the dynamic properties of lattice animals.[7] In this Rapid Communication we argue that the general relationships between dynamical exponents and static exponents for trees (clusters without loops) are

$$d_w^l=2+d_l-d_l^s,\quad d_w=(d_f/d_l)(2+d_l-d_l^s)\ ,$$
$$\bar{d}=2d_l/(2+d_l-d_l^s)\ , \tag{1}$$

where d_w is the diffusion exponent, d_w^l is the chemical diffusion exponent,[6] and $\bar{d}$ is the fracton dimensionality.[4] The exponents d_l and d_l^s are the intrinsic dimensions of the cluster and its skeleton, respectively; they relate the cluster mass M or skeleton mass M_s to the chemical size l as $M\simeq l^{d_l}$ and $M_s\simeq l^{d_l^s}$. The chemical distance l is the shortest path of occupied sites linking two points on a cluster. The skeleton of a cluster whose chemical radius L is defined as the subcluster, which contains only sites belonging to the shortest paths from a chosen site to its Lth chemical shell (see Fig. 1). This definition implies that all dead ends, except those terminating at the Lth shell, do not belong to the skeleton.

The results given in Eqs. (1) can be obtained from the following arguments. We define $\rho_{\text{tot}}(l)$ as the total resistance between a chosen site A on the tree and all the sites in the lth shell surrounding that site, and define the resistivity exponent, $\bar{\zeta}_l$, by $\rho_{\text{tot}}\simeq l^{\bar{\zeta}_l}$. Let $\rho_1(l)$ be the resistance between site A and *one* site in the lth shell. Then $\rho_{\text{tot}}(l)$ can be related to $\rho_1(l)$ by

$$\rho_{\text{tot}}(l)\simeq\rho_1(l)/l^{d_l^s-1}\simeq l^{\bar{\zeta}_l}\ . \tag{2}$$

The quantity $l^{d_l^s-1}$ represents the effective number of paths connecting the origin A to shell l. We next make use of the relationships

$$d_w^l=\tilde{\nu}d_w,\quad d_l=\tilde{\nu}d_f,\quad \bar{\zeta}_l=\tilde{\nu}\bar{\zeta}\ , \tag{3}$$

where the exponent $\tilde{\nu}$ is the exponent which expresses the radius of gyration of a cluster in terms of its chemical size, i.e., $R\simeq l^{\tilde{\nu}}$. Thus, we obtain from the Einstein relation,[8,9] $d_w=d_f+\bar{\zeta}$, the equivalent expression in l space,

$$d_w^l=d_l+\bar{\zeta}_l\ . \tag{4}$$

Since there are no loops in a tree (by definition), it follows that $\rho_1(l)\simeq l$ and, from Eq. (2), one finds $\bar{\zeta}_l=2-d_l^s$. Then, by using Eqs. (3) and (4) and the definition[4,6] of the fracton dimension $\bar{d}=2d_f/dw=2d_l/d_w^l$, we obtain Eqs. (1).

The results given in Eqs. (1) are general for diffusion on trees. For the special case of finitely ramified trees, for which $d_l^s=1$, we obtain the results

$$d_w^l=d_l+1,\quad d_w=d_f(1+1/d_l),\quad \bar{d}=2d_l/(1+d_l)\ .$$

These results were applied recently[7] to lattice animals, which are assumed to be finitely ramified since they can be generated from percolation clusters.[10]

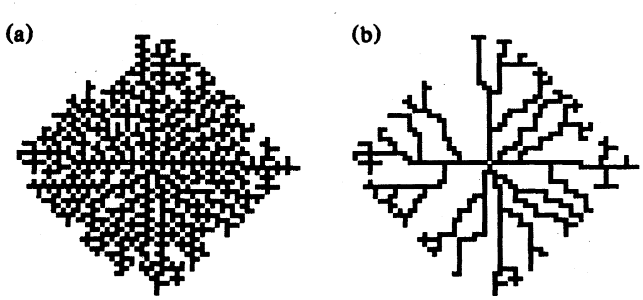

FIG. 1. (a) Example of a tree generated by a cluster growth model (Ref. 11) (see text). (b) The skeleton of the tree shown in (a). For clarity of illustration we have chosen a small tree ($L=30$), but much larger trees ($L=400$) were used when determining the exponents described in the text (see Fig. 2).

In the following we present two examples of trees for which these laws may be shown to be valid.

(i) Trees without dead ends. A model for trees without dead ends can be constructed as follows. Let $p(l)$ be the probability that a bond in shell $l-1$ will grow to two bonds in shell l, and let $1-p(l)$ be the probabilty that it will grow into only one. Thus, the expected number of bonds that grow from a bond in the $(l-1)$th shell is given by $2p(l)+1[1-p(l)]=1+p(l)$, and the total number of bonds $B(l)$ in the lth chemical shell will be

$$B(l)=\prod_{l'=1}^{l}[1+p(l')] \ . \tag{5}$$

If we choose $p(l')\simeq\alpha/l'$, we obtain

$$B(l)\simeq l^{\alpha} \ , \tag{6}$$

from which it follows that the mass $M(l)$ is given as

$$M(l)=\sum_{l'=1}^{l}B(l')\simeq l^{\alpha+1}\simeq l^{d_l} \ . \tag{7}$$

As a result of the way they have been constructed, these trees do not have dead ends. They can be embedded in any spatial dimension $d\geq d_l$.

We now show that, for this model, $d_w^l=2$. The probability that a random walker at the lth shell will, on a given step, move to shell $l+1$ rather than $l-1$ is

$$\frac{B(l+1)}{B(l+1)+B(l)}=\frac{1}{2}\left[1+\frac{B(l+1)-B(l)}{B(l+1)+B(l)}\right]\equiv\frac{1}{2}+\epsilon(l) \ . \tag{8}$$

From our definition of the present model we see that, conditional on $B(l)$, the random variable $B(l+1)$ has a binomial distribution with the properties

$$\begin{aligned}&\langle B(l+1)\rangle=B(l)(1+\alpha/l) \ ,\\&\langle B^2(l+1)\rangle-\langle B(l+1)\rangle^2=B(l)(\alpha/l)(1+\alpha/l) \ .\end{aligned} \tag{9}$$

An analysis based on the binomial distribution indicates that, to lowest order in l,

$$\langle\epsilon(l)|B(l)\rangle\simeq\alpha/4l \ . \tag{10}$$

In order to calculate $\langle l_n^2\rangle$, where $l_n=\mathbf{u}_1+\mathbf{u}_2+\cdots+\mathbf{u}_n$ is the sum of the individual steps, we have

$$\langle l_n^2\rangle=n+2\sum_{i\neq j}\sum\langle\mathbf{u}_i\cdot\mathbf{u}_j\rangle \ , \tag{11}$$

since each step is of unit length. Let us next evaluate a typical term in this sum by saying that the ith step starts from shell l' and the jth step starts from shell l''. By using an argument similar to that which led to Eq. (10), it may be shown that, for large l' and l''

$$\langle\mathbf{u}_i\cdot\mathbf{u}_j\rangle=4\langle\epsilon(l')\epsilon(l'')\rangle\simeq\alpha^2/4l'l'' \ , \tag{12}$$

so that the second term on the right-hand side of Eq. (11) can be at most of the order of $2\alpha^2(\ln n)^2$. But this implies that $d_w^l=2$.

The result $d_w^l=2$ is consistent with Eqs. (1), since for this model $d_l=d_l^s$. (Owing to the absence of dead ends, the skeletons of the trees are identical to the trees themselves.)

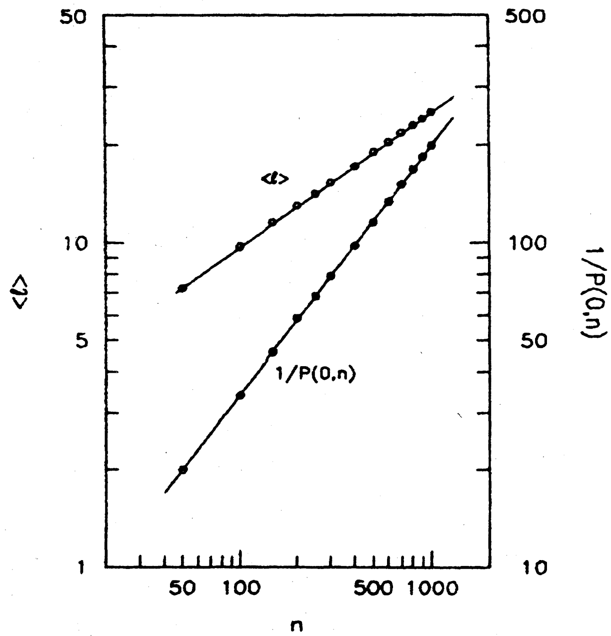

FIG. 2. The expected chemical distance $\langle l\rangle$ traveled by a random walk of n steps (open circles) on a tree of size $L=400$, which was generated according to the rules described in the text (Ref. 11). Also shown is $1/P(0,n)$, where $P(0,n)\sim n^{-\bar{d}/2}$ is the probability of returning to the origin after n steps.

It is interesting to note that, for this case, Eqs. (1) can be written as

$$d_w^l=2, \quad d_w=2d_f/d_l, \quad \bar{d}=d_l \ . \tag{13}$$

These equations are a generalization of the case of diffusion on linear chains,[4] which are obtained when one substitutes $d_l=1$ in Eq. (13). Also, note that the fracton dimension[4] $\bar{d}$, in this case, is equal to the intrinsic dimension d_l.

(ii) Trees with dead ends. A cluster growth model[11] was used to generate trees which have dead ends. We chose the origin on a square lattice to be the seed of a tree. The first nearest neighbors of the seed, representing the shell $l=1$, were chosen randomly to grow or be blocked. A similar procedure was used for successive shells. For any given value of d_l, the number of sites grown in a shell was determined by $B(l)\simeq dM/dl\simeq l^{d_l-1}$. Only those sites which would not create loops were allowed to grow. After thus choosing the occupied (growing) sites, the remaining nearest-neighbor sites were blocked.

The exponent d_w^l had been calculated by performing exact enumeration[9,12] of random walks on trees, with $d_l=1.9$. We found $d_w^l=2.48\pm0.05$ and $\bar{d}/2=0.75\pm0.03$ (see Fig. 2). The intrinsic exponent d_l^s of the skeleton of these trees was calculated and found to be $d_l^s=1.30\pm0.05$. These results are in very good agreement with Eqs. (1).

In conclusion, we have presented general relationships between dynamic exponents and static geometric exponents for systems for which $d_l^s\geq1$, i.e., which are infinitely ramified. It would be interesting to study the intrinsic dimension of the skeleton for aggregation models such as diffusion-limited aggregation and cluster-cluster aggregates.

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