Spectral dimension of fractal trees

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We present in detail a calculation of the spectral dimension for a class of fractal trees called NT_D (i.e., "nice trees of dimension D," defined as trees whose branches are splitting in r every time the distance from the origin is doubled, where r is an integer greater than 1) which presents nonanomalous diffusion. This is performed by an analytical technique, related to an exact rescaling of the time variable, which can be extended to more general geometrical structures.

I. INTRODUCTION

In a recent Rapid Communication [1] we showed that for a particular class of fractal trees called NT_D ("nice trees of dimension D") in mathematical literature, since the spectral and the fractal dimension coincide, diffusion is not anomalous, as was commonly believed to happen on fractals. While the determination of the fractal dimension for these trees can be performed with standard arguments, the calculation of the spectral dimension, related to the solution of the random walk problem, requires the introduction of an alternative technique, leading to an exact implicit expression for the random-walk generating functions. Such an expression can be used to obtain asymptotic behavior at large times for the probability of returning to the origin of a random walker, which in turn defines the spectral dimension. More precisely one introduces on the given infinite and connected discrete structure a simple random walk, i.e., a nearest neighbor random walk with homogeneous jumping probabilities and discrete time steps, and, after choosing an origin point O from where the walker starts at time 0, one calculates the probability $P_O(n)$ of returning to the origin after n steps. The spectral dimension $\tilde{d}$ is then defined as [2]

$$\tilde{d} = -2 \lim_{n \to \infty} \frac{\ln P_O(n)}{\ln n}, \tag{1}$$

and such a definition can be shown to be independent of the particular origin point [3]. The time-rescaling technique that we will introduce in the following for the

specific case of NT_D is actually more general and can be applied to other discrete structures, even nonfractal ones, as we shall briefly discuss.

The paper is organized as follows: in Sec. II we will first deal with the determination of the fractal dimension of NT_D; in Sec. III we will obtain the exact implicit relation for the generating function of the probability of returning to the origin; and in Sec. IV the value of $\tilde{d}$ will finally be calculated. Section V is devoted to conclusions and discussions.

II. THE GEOMETRY OF NT_D

NT_D (see Fig. 1) can be recursively defined as follows [4]: an origin point O is connected to a point A by a link of length 1; from A, the tree splits in k branches of length 2 (i.e., consisting of two consecutive links); the ends of these branches split in k branches of length 4, and so on; each end point of a branch of length 2^n splits into k branches of length 2^{n+1}. The coordination number z_i is therefore 1 for the origin O, 2 on the branches, and $k+1$
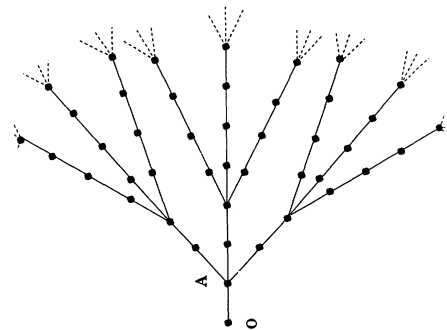
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FIG. 1. An NT_D with $k = 3$ [$D = d_F = \tilde{d} = 1 + \ln(3)/\ln 2$].

for the end points of each branch. Let us begin by computing the connectivity dimension of an NT_D. This quantity is defined [5] by introducing the growth function $N_i(r)$ that represents the number of points within a sphere of radius r centered in a point $i \in NT_D$, where r is given in terms of the chemical distance, i.e., the minimum number of links between two points:

$$d_C = \lim_{r \to \infty} \frac{\ln N_i(r)}{\ln r} \ . \tag{2}$$

Since it can be shown that d_C does not depend on i, for the sake of simplicity we will center the sphere in O. In this case the growth function is a step function, but it is easy to see that it satisfies the following inequalities:

$$ar^{1+(\ln k/\ln 2)} < N_O(r) < br^{1+(\ln k/\ln 2)} \ , \tag{3}$$

where a and b are positive constants. Relations (3) imply

$$d_C = 1 + \frac{\ln k}{\ln 2} \ . \tag{4}$$

The fractal dimension d_F [6] of an NT_D can be defined only after the tree has been embedded in an Euclidean space by

$$d_F = \lim_{R \to \infty} \frac{\ln \mathcal{N}_i(R)}{\ln R} \ , \tag{5}$$

where now $\mathcal{N}_i(R)$ is the number of points within a sphere of radius R centered in i and R is given in terms of the Euclidean distance. As for the d_C, the definition (5) is independent of i. The value of d_F obviously depends on the particular embedding. It is possible to choose a very natural embedding in a d-dimensional space $(d \geq d_C)$, where the points at a given chemical distance from the origin lie on a (hyper)spherical surface centered in the origin. In this case the distances l_n between the two subsequent spherical surfaces n and $n+1$ satisfy the conditions

$$0 < a < l_n < b < \infty \ . \tag{6}$$

The growth function then satisfies the following inequalities:

$$hr^{d_C} \leq N_O(r) \leq lr^{d_C} \ , \tag{7}$$

where h and l are two positive numbers. This immediately gives

$$d_C = d_F = 1 + \frac{\ln k}{\ln 2} \ . \tag{8}$$

Notice that this is an embedding in a continuous space and not in a lattice. The common value (8) is defined to be the dimension D of an NT_D [4].

III. RANDOM WALKS ON NT_D

We now turn to the determination of the spectral dimension of an NT_D. The computation is based on the analysis of the asymptotic behavior at large times of a random walker on an NT_D.

We define a transition matrix for the probabilities p_{ij} of

jumping from a site i at time n to a neighbor site j at time $n+1$. The jumps are chosen to be equiprobable:

$$p_{ij} = \frac{1}{z_i} \ . \tag{9}$$

We will now compute recursively the probability of coming back to the origin $P_O(n)$ after n steps of a random walker starting from the origin O at time $t = 0$, using the structure of the tree, applying well known relations between generating functions of probability in a random walk, and introducing an exact rescaling technique on the time variable, which is very useful in treating a wide class of infinite graphs.

First, let us consider the k subtrees that originate from the point A; we will call each of them SA. The first step will be the calculation of the probability $P_A(n)$ of coming back in n steps to the origin A of subtree SA. $P_O(n)$ and $P_A(n)$ are simply related, because the minimum path between two points is unique on a tree. If we consider the probability $F_O(n)$ of coming back to the origin of an NT_D for the first time after n steps, we have

$$F_O(n) = \frac{1}{k+1} P_A^{\mathcal{G}}(n-2) \ . \tag{10}$$

Two time steps have been used to cross forward and backward the link OA. $P_A^{\mathcal{G}}(n)$ is the probability of coming back to the origin A of the graph $\mathcal{G}$ obtained by removing O and the corresponding link from the NT_D, for a random walker with a decay probability $1/(k+1)$ on A. The probability of coming back to the origin A of an SA for the first time after n steps $F_A(n)$ is related to the corresponding quantity $F_A^{\mathcal{G}}(n)$ by

$$F_A^{\mathcal{G}}(n) = \frac{k}{k+1} F_A(n) \ . \tag{11}$$

This identity can be restated in terms of the corresponding generating functions of probability [we recall that the generating functional $\tilde{f}(\lambda)$ of $f(n)$ is defined to be $\tilde{f}(\lambda) = \sum_{n=0}^{\infty} f(n)\lambda^n$],

$$\tilde{F}_A^{\mathcal{G}}(\lambda) = \frac{k}{k+1} \tilde{F}_A(\lambda) \ . \tag{12}$$

We can now introduce the fundamental relation between generating functions of probabilities of return and probabilities of first return, holding for any random walker [7]:

$$\tilde{P}_A^{\mathcal{G}}(\lambda) = \frac{1}{1 - \tilde{F}_A^{\mathcal{G}}(\lambda)} \ . \tag{13}$$

Substituting (12) in (13) and inverting the corresponding relation for $\tilde{F}_A(\lambda)$ we finally obtain

$$\tilde{P}_A^{\mathcal{G}}(\lambda) = \frac{(k+1)\tilde{P}_A(\lambda)}{k + \tilde{P}_A(\lambda)} \ . \tag{14}$$

The relation (10) implies the corresponding relation for generating functions,

$$\widetilde{F}_O(\lambda) = \sum_{n=0}^{\infty} \lambda^n F_O(n)$$

$$= \frac{1}{k+1} \sum_{n=0}^{\infty} \lambda^n P_A^{\mathcal{G}}(n-2)$$

$$= \frac{1}{k+1} \lambda^2 \widetilde{P}_A^{\mathcal{G}}(\lambda) . \tag{15}$$

Substituting (14) in (15) we finally obtain the relation between the probability of coming back to the origin of an NT_D and the corresponding quantity on a subtree SA,

$$\widetilde{P}_O(\lambda) = \frac{\widetilde{P}_A(\lambda) + k}{(1 - \lambda^2)\widetilde{P}_A(\lambda) + k} . \tag{16}$$

Let us now consider in detail a single branch. The SA is not an NT_D because its adjacency matrix is different. Nevertheless, an interesting scale transformation on the time variable can be found, mapping the SA to an NT_D with given probabilities of staying on the sites.

Let us study the probability of coming back to the origin on a SA for even time steps $n' = 2n$,

$$P_A'(n) \equiv P_A(2n) . \tag{17}$$

With this rescaling, the subtree SA with simple nearest-neighbors jumping probabilities is mapped into an NT_D with a new definition for the jumping probabilities matrix. We will call this structure NT_D'. In particular, the new probabilities for a single jump between two nearest neighbors sites are given by

$$p_{ij}' = \frac{1}{2} \frac{1}{z_i} . \tag{18}$$

The other possibility is a sequence of two old steps forward-backward, which corresponds to the new walker staying in the site i,

$$p_{ii}' = \frac{1}{2} \frac{1}{z_i} z_i = \frac{1}{2} . \tag{19}$$

The staying probabilities can be described using a parameter s_i by

$$p_{ii}' = \frac{s_i}{z_i + s_i} = \frac{1}{2} . \tag{20}$$

From (20) it follows:

$$s_i = z_i . \tag{21}$$

If we now denote by asterisk the random walker following the new rules (19) and (20) for the jumping probabilities, we obtain the following relations:

$$P_A'(n) = P_A(2n) = P_O^*(n) , \tag{22}$$

where now $P_O^*(n)$ is the probability of return to the origin of an NT_D' with the new definition of the transition matrix. When applied to the generating functions of the corresponding probabilities, since $P_A(n) \neq 0$ only for even n, this relation gives

$$\widetilde{P}_A(\lambda) = \sum_{n=0}^{\infty} P_A(n)\lambda^n = \sum_{m=0}^{\infty} P_A(2m)\lambda^{2m}$$

$$= \sum_{m=0}^{\infty} P_O^*(m)(\lambda^2)^m = \widetilde{P}_O^*(\lambda^2) . \tag{23}$$

Let us now look for a very general relation between the generating functions for the probability of coming back to the origin of a given graph, with and without staying probabilities. In general, we will consider graphs with variable coordination number z_i and we will define the matrix $Z_{ij} = \delta_{ij} z_i$. The generating functional $\widetilde{P}_{ii}(\lambda)$ on a graph without staying probabilities can be then written as

$$\widetilde{P}_{ii}(\lambda) = [I - \lambda Z^{-1} A]_{ii}^{-1} . \tag{24}$$

If we now consider the graph described by the same adjacency matrix but with an additional probability of staying on the site, we can define the matrix $S_{ij} = \delta_{ij} s_i$ and obtain

$$\widetilde{P}_{ii}^S(\lambda) = [I - \lambda(Z+S)^{-1}(A+S)]_{ii}^{-1} = [(Z+S)^{-1}(Z+S) - \lambda(Z+S)^{-1}A - \lambda(Z+S)^{-1}S]_{ii}^{-1}$$

$$= \{[Z+S-\lambda A - \lambda S]^{-1}[Z+S]\}_{ii}$$

$$= [\{1 - \lambda[Z+(1-\lambda)S]^{-1}A\}^{-1}[Z+(1-\lambda)S]^{-1}(Z+S)]_{ii} . \tag{25}$$

In general the two matrices Z and S do not commute. Here from the relation (20) we know they are equal. We can therefore rewrite expression (25) as

$$\widetilde{P}_0^{S=Z}(\lambda) = [I - (2-\lambda)^{-1} Z^{-1} A]_{00}^{-1} \frac{2}{2-\lambda} \tag{26}$$

or, recalling (24)

$$\widetilde{P}_{0,S=Z}^*(\lambda) = \frac{2}{2-\lambda} \widetilde{P}_0 \left[\frac{2}{2-\lambda} \right] . \tag{27}$$

Substituting (27) in (16) and using (22) and (23) we easily obtain an implicit form for the generating functional of the probability of coming back to the origin of an NT_D, $\widetilde{P}_O(\lambda)$:

$$\widetilde{P}_O(\lambda) = \frac{\dfrac{2}{2-\lambda^2} \widetilde{P}_O \left[\dfrac{\lambda^2}{2-\lambda^2} \right] + k}{\dfrac{2-2\lambda^2}{2-\lambda^2} \widetilde{P}_O \left[\dfrac{\lambda^2}{2-\lambda^2} \right] + k} . \tag{28}$$

IV. THE SPECTRAL DIMENSION OF AN NT_D

The spectral dimension of the graph NT_D is defined by the asymptotic behavior of the probability of returning to the origin in n steps, when n becomes very large. Such a behavior can be obtained from the asymptotic expansion of the generating function in its first singularity from the origin of the complex plane, using Tauberian theorems [9].

In the preceding section we have obtained an implicit expression for the generating function. On the other hand, generating functions for the probability of returning to the origin for a random walker on a graph with finite connectivity dimension have a convergence radius equal to 1 [8]. So we will give an estimation of the asymptotic behavior of to $\tilde{P}_O(\lambda)$ for $\lambda \to 1-$ using relation (28) as a consistency condition.

Expanding (28) for $\epsilon \equiv 1 - \lambda \to 0+$ we find

$$\tilde{P}_O(1-\epsilon) \sim \frac{(2-4\epsilon)\tilde{P}_O(1-4\epsilon)+k}{(2-\epsilon)2\epsilon\tilde{P}_O(1-4\epsilon)+k} \ . \tag{29}$$

Let us now introduce the asymptotic expansion of the leading singular part of $\tilde{P}_O(\lambda)$ for $\lambda \to 1-$. First, let us consider the trial function

$$\tilde{P}_O(\epsilon) = c\epsilon^\alpha \ , \tag{30}$$

where c is a constant, and let us take $\alpha < 0$, corresponding to a recursive random walk.

Substituting (30) in (29) we obtain the following relation:

$$c\epsilon^\alpha \sim \frac{c2(4\epsilon)^\alpha + k}{c4\epsilon(4\epsilon)^\alpha + k} \ , \tag{31}$$

and equating the singular parts of the two sides we find

$$\alpha = \frac{1}{2}\left[\frac{\ln k}{\ln 2} - 1\right] \ , \tag{32}$$

which is consistent with the hypothesis $\alpha < 0$ only for $k < 2$. Relation (32) would give $\alpha = 0$ for $k = 2$; in this case (29) can be satisfied by introducing a multiplicative logarithmic correction to the trial function

$$\tilde{P}_O(1-\epsilon) = c \ln \epsilon \ . \tag{33}$$

If $k > 2$, the generating function converges for $\epsilon \to 0+$ and the divergence is carried by its derivatives. Namely, for $0 < \alpha < 1$,

$$\tilde{P}_O'(1-\epsilon) = c\alpha\epsilon^{\alpha - 1} \tag{34}$$

diverges as $\epsilon \to 0+$. Taking an explicit derivative with respect to λ in expression (28) and substituting the development (34), we obtain an alternative relation for the ex-

ponent α, from which it follows again:

$$\alpha = \frac{1}{2}\left[\frac{\ln k}{\ln 2} - 1\right] \ , \tag{35}$$

valid now for $2 < k < 4$. Reiterating the procedure for bigger values of k and α, we finally obtain the following asymptotic behavior for the singular part of the generating function $\tilde{P}_O(\lambda)$:

$$\text{sing}\tilde{P}_O(\lambda) \sim \begin{cases} (1-\lambda)^{(1/2)(\ln k/\ln 2 - 1)} & \text{if } k \neq 2^n \ , \\ (1-\lambda)^{(1/2)(\ln k/\ln 2 - 1)} \ln(1-\lambda) & \text{if } k = 2^n \ . \end{cases} \tag{36}$$

Now applying standard Tauberian theorems [9] to (36) we immediately obtain the asymptotic behavior of $P_O(n)$,

$$P_O(n) \propto n^{-(1/2)[1+\ln k/\ln 2]} \ . \tag{37}$$

The asymptotic law (37) gives the value of the spectral dimension of an NT_D,

$$\tilde{d} = 1 + \frac{\ln k}{\ln 2} \ . \tag{38}$$

This value coincides with the fractal and connectivity dimension. We point out that solutions (36) and (37) are unique up to corrections of lower order in $1-\lambda$, which do not affect the value of the spectral dimension, defined in (1).

V. CONCLUSIONS

In this paper we presented a time-rescaling method that allows us to solve exactly the random walk problem on NT_D. While the relevance and the implications of the result we obtained has already been discussed elsewhere [1], here we would comment on technical aspects of such a calculation. First of all, notice that a necessary condition for the application of time rescaling is the fact that NT_D are bipartite graphs, i.e., graphs without odd cycles. This implies that they can be divided in two subgraphs A and B, such that at even times the walker is always on A and at odd times it is always on B so that random walks at even time steps on NT_D can be mapped into random walks at generic time steps on A. The other fundamental feature of NT_D is that the new structure A coincides with the original NT_D, up to a finite number of points (actually one, in this case). Since these features are common to a wider class of graphs, the time-rescaling technique can be successfully applied also to other relevant discrete structures. Some of these possible applications will be discussed in more detail in a forthcoming paper [10].

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