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Scaling of the first-passage time and the survival probability on exact and quasi-exact self-similar structures

B Kahng and S Redner

Center for Polymer Studies and Department of Physics, Boston University, Boston, MA 02215, USA

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Abstract. We calculate the asymptotic behaviour of the moments of the first-passage time and survival probability for random walks on an exactly self-similar tree, and on a quasi-self-similar comb, by applying an exact decimation approach to the master equations. For the hierarchical comb, a transition from ordinary to anomalous diffusion occurs at $R=2$, where R is the ratio of teeth length in successive iterations of the structure. In the anomalous regime ($R>2$), the positive integer moments of the first-passage time, $\langle t^q \rangle$, scale as L^{τ_q}, with $\tau_q = 1+(2q-1)\ln R/\ln 2$, where L is the linear distance from input to output. The asymptotic behaviour of the survival probability is studied using both scaling theory and by a direct solution to the master equations. We find that the characteristic time, t^*, in the asymptotic exponential decay of the survival probability, $\exp(-t/t^*)$, scales as $t^* \sim L^{\tau^*}$, with $\tau^* = \ln R^2/\ln 2$, i.e. τ^* is distinct from τ_1. However, substantial corrections to this asymptotic form for τ^* exist, and these are needed to account for the recent simulation data of Havlin and Matan.

1. Introduction

Anomalous diffusion in random systems has been the focus of considerable attention. (see, e.g., [1-3]). One very useful line of investigation is the study of random walks of deterministic self-similar structures [3-6]. These systems have the advantage that they retain some of the features of diffusion on random structures, while being simple enough to permit analytical solutions of random walk processes. It is important, however, to determine which features of diffusion on deterministic structures carry over to more realistic models of random media. This leads us to investigate the similarities and differences between diffusion on exactly self-similar, and quasi-self-similar structures. A generic example of the latter case is the hierarchical comb (figure

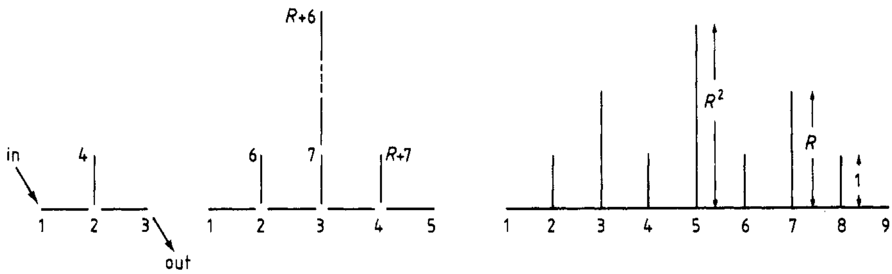

Figure 1. The first three iterations of the hierarchical comb. Branching occurs only from the main backbone.

1) [7-9], in which there are side branches with a hierarchical distribution of lengths, R^k ($k=1,2,\ldots$). Interest in this system has arisen because it mimics the backbone and dangling ends organisation of percolation clusters, and ultrametricity in spin glasses and related systems [10-15].

We study diffusion on an exactly self-similar hierarchical tree and a hierarchical comb in order to determine whether one, or more than one timescale characterises diffusion on these structures. For the tree, we find that a single timescale does account for the scaling properties of all the positive integer moments of the first-passage probability, as well as the characteristic time in the asymptotic exponential decay of the survival probability. However, the anisotropic nature of the comb leads to more than one timescale being needed to describe asymptotic properties.

In § 2, we outline a direct enumeration approach [16] to compute the first-passage time, $\langle t\rangle$. For the hierarchical comb, the first-passage time exhibits a dynamical transition at $R=2$. For $R<2$, $\langle t\rangle \sim L^2$, where L is the length of the backbone; i.e. normal diffusive behaviour occurs. However, when $R>2$, anomalous diffusion arises, as $\langle t\rangle \sim L^{\tau_1}$ where $\tau_1 = \ln 2R/\ln 2$. This value of τ_1 arises from the anisotropic scaling of the comb, wherein the length of the side branch increases by R, while the linear chain increases by 2 at each successive iteration of the structure. In §§ 3 and 4, we employ an exact decimation method to obtain the generating function for the first-passage probability on the hierarchical tree and on the hierarchical comb. Our approach should be applicable to any finitely ramified hierarchical structure [17].

In § 5, we compute the exponents τ_q associated with the scaling of the higher moments of the first-passage time on the comb, $\langle t^q\rangle$. We find $\langle t^q\rangle \sim L^{\tau_q}$, with $\tau_q = 1+(2q-1)\ln R/\ln 2$, when $R>2$. Thus there is a multifractality of the transit time moments, as $\tau_q \neq q\tau_1$, but only of a relatively trivial character that arises from the anisotropic scaling of the comb. In §§ 5 and 6, we also study the scaling behaviour of the survival probability, $S(t)$. Asymptotically, $S(t)$ decays as $\exp(-t/t^*)$ on any finite graph, and for the comb we show that this characteristic time scales as $t^* \sim L^{\tau^*}$, with $\tau^* = \ln R^2/\ln 2$. However, there are non-negligible corrections to this result which depend on the iteration order of the comb. These corrections are needed in order to help understand the recent numerical simulations of Havlin and Matan [9, 18]. The final section gives a brief summary and discussion.

2. Enumeration for the first-passage time

The mean first-passage time, $\langle t\rangle$, can be calculated simply by using enumeration, together with renormalisation group ideas. Consider the zeroth-order hierarchical comb in the left-hand part of figure 1. A random walk starts at an input site at one end of the structure, and is absorbed at an output site at the opposite end. At each step, the walk moves to any of its nearest neighbours with equal probability. Let T_x and T_y be the times to move between nearest-neighbour sites on the x and y axes, respectively, and let t_i be the mean first-passage time to reach the output starting from site i. Then the first-passage times obey the relations

$$t_1 = T_x + t_2 \tag{1a}$$

$$t_2 = \tfrac{1}{3}T_x + \tfrac{1}{3}(T_x + t_1) + \tfrac{1}{3}(T_y + t_3) \tag{1b}$$

$$t_3 = T_y + t_2. \tag{1c}$$

Eliminating t_3, (1b) can also be written as

$$t_2=\tfrac{1}{2}(T_x+t_1)+\tfrac{1}{2}T_x+T_y. \qquad (1b')$$

The term T_y can be interpreted as the waiting time associated with the presence of site 3, so that the corresponding equation in the absence of the side branch is $t_2=\frac{1}{2}(T_x+t_1)+\frac{1}{2}T_x$. Since the walk begins at site 1, t_1 coincides with the mean first-passage time for this structure and from (1) we find

$$t_1\equiv\langle t\rangle=2(2T_x+T_y). \qquad (2)$$

Now consider the first-order comb in which there are R sites on the longest side branch. The equations governing the first-passage times starting at any site are given in appendix 1. By decimating all the first-order sites to recover a renormalised zeroth-order structure, we can recast the transit time equations in a form analogous to (1), namely,

$$t_1^{(1)}=T'_x+t_2 \qquad (3a)$$

$$t_2^{(1)}=\tfrac{1}{2}(T'_x+t_1)+\tfrac{1}{2}T'_x+T'_y \qquad (3b)$$

with

$$T'_x=2(2T_x+T_y) \qquad (4a)$$

$$T'_y=2RT_y. \qquad (4b)$$

The mean first-passage time for this first-order comb is then given by $t_1^{(1)}\equiv\langle t\rangle_1=2(2T'_x+T'_y)$ and the mean first-passage time on the Nth order comb, $\langle t\rangle_N$, is $2(2T_x^{(N)}+T_y^{(N)})$. We compute $\langle t\rangle_N$ by 'diagonalising' this recursion relation. We define $u\equiv T_x+\lambda T_y$, which obeys

$$T'_x+\lambda T'_y=4[T_x+\tfrac{1}{2}(1+\lambda R)T_y]. \qquad (5)$$

Thus choosing λ such that $\lambda=\frac{1}{2}(1+\lambda R)$, i.e. $\lambda=(2-R)^{-1}$, yields $u'=4u$. Then for N iterations, $u^{(N)}=4^Nu$, while (4b) gives $T_y^{(N)}=(2R)^NT_y$. Therefore the first-passage time for the Nth-order structure is

$$\begin{aligned}\langle t\rangle_N&=2(2T_x^{(N)}+T_y^{(N)})\\&=2[2u^{(N)}+(1-2\lambda)T_y^{(N)}]\\&=2[2\times4^Nu+(1-2\lambda)(2R)^NT_y].\end{aligned} \qquad (6)$$

This exhibits a dynamical transition at $R=2$. When $R<2$, the first term dominates asymptotically, leading to one-dimensional diffusive behaviour, while for $R>2$, the second term dominates, leading to anomalous diffusion. The corresponding scaling exponent, τ_1, defined by $\langle t\rangle\sim L^{\tau_1}$, where L is the length of the system, equals 2 when $R<2$, and equals $\ln 2R/\ln 2$ when $R>2$.

Alternatively, generating function methods can be used to solve (4) directly. Introducing $g(z)=\Sigma_{N=0}^{\infty}T_x^{(N)}z^N$ one finds from (4) that

$$g(z)=\frac{1}{1-4z}+\frac{8z}{(1-2Rz)(1-4z)}. \qquad (7)$$

For $R<2$, the smallest singularity of $g(z)$ is a simple pole at $z=\frac{1}{4}$, and this leads to $\langle t\rangle_N\sim4^N$. Conversely, for $R>2$ the smallest singularity of $g(z)$ is a simple pole at $z=1/2R$, leading to $\langle t\rangle_N\sim(2R)^N$. At $R=2$, however, the confluence of the two

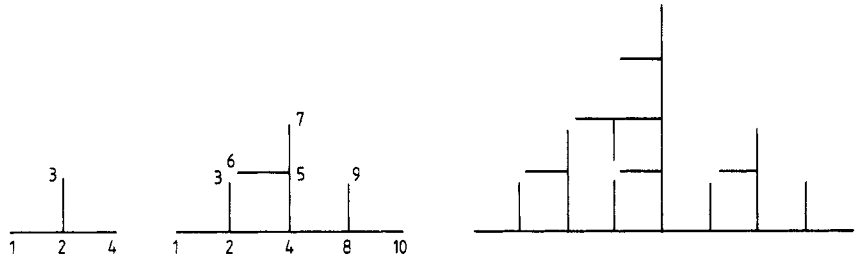

Figure 2. The first three iterations of the hierarchical tree.

singularities leads to a second-order pole at $z=\frac{1}{4}$. Using this, together with the solution to (4*b*), we find $\langle t\rangle_N = 2\times 4^N(4N+3)$. Since $L=2^N$, this leads to $\langle t\rangle_N \sim 8L^2 \ln L/\ln 2$. Thus there is a logarithmic correction to the mean first-passage time in the marginal case $R=2$.

For the hierarchical tree (cf figure 2), $T_x = T_y$, so that from (4*a*), $T'_x = 6T_x$. This immediately gives $\tau_1 = \ln 6/\ln 2$. We will rederive these results, as well as information about higher moments of the first-passage time, from an analysis of the master equations, in the next section.

3. Diffusion on the hierarchical tree

The first-passage probability for the hierarchical tree with an absorbing point at one end can be calculated by successive decimation of the discrete-time master equations. Let $P_i(n)$ be the probability for a random walker to be at site i on the nth step. Then for a zeroth-order tree, with site 4 being an absorber, the master equations are

$$P_1(n+1)=\tfrac{1}{3}P_2(n) \qquad P_2(n+1)=P_1(n)+P_3(n)$$
$$P_3(n+1)=\tfrac{1}{3}P_2(n) \qquad P_4(n+1)=\tfrac{1}{3}P_2(n). \tag{8}$$

For a random walk initially at site 1, the corresponding master equations for the generating functions, $P_i(z)=\Sigma_{n=0}^{\infty} P_i(n)z^n$, are

$$P_1(z)=aP_2(z)+1 \qquad P_2(z)=3aP_1(z)+3aP_3(z)$$
$$P_3(z)=aP_2(z) \qquad P_4(z)=aP_2(z) \tag{9}$$

with $a=\frac{1}{3}z$. Due to the absorbing boundary condition, $P_4(z)$ also coincides with the generating function for the first-passage probability and solving for this quantity yields

$$P_4(z)=3a^2/(1-6a^2). \tag{10}$$

To compute the first-passage probability for the Nth-order tree, we first eliminate the occupation probabilities of the Nth-order sites from the master equations. This yields renormalised equations which are identical in form to the bare master equations for an $(N-1)$th-order tree, except that $a\to a' = a^2/(1-6a^2)$, and the initial condition factor of unity in the equation for $P_1^{(N-1)}(z)$ is replaced by $(1-3a^2)/(1-6a^2)$. This procedure is illustrated in appendix 2 for the first-order tree. Iterating this procedure, the generating function of the first-passage probability on an Nth-order tree is

$$P_4^{(N)}(z)=3(a^{(N)})^2/[1-6(a^{(N)})^2] \tag{11a}$$

where

$$a^{(N)} = (a^{(N-1)})^2/[1-6(a^{(N-1)})^2] \tag{11b}$$

and $a^{(0)} = \frac{1}{3}z$. Notice that a single-parameter renormalisation involving only a is sufficient to compute the first-passage probability exactly.

The kth moment of the first-passage time on an Nth-order tree is formally obtained from

$$\langle t^k \rangle_N = \left(z \frac{\partial}{\partial z} \right)^k P_4^{(N)}(z) \bigg|_{z=1} \tag{12}$$

or equivalently by computing the series expansion of $P_4^{(N)}(z)$ in powers $\varepsilon = 1-z$. Writing this power series as

$$P_4(z) = 1 + \sigma_1 \varepsilon + \sigma_2 \varepsilon^2 + \ldots \tag{13}$$

where we temporarily drop the superscript referring to the iteration order, and applying (12), we identify $\sigma_1 = -\langle t \rangle$, $\sigma_2 = \frac{1}{2}(\langle t^2 \rangle - \langle t \rangle)$, etc. The scaling properties of these moments can be conveniently obtained from the transformation of the power-series expansion for $a^{(N)}$ upon iterating the tree. Thus writing

$$\begin{aligned} a^{(N)} &= \tfrac{1}{3} P_4^{(N-1)} \\ &= \tfrac{1}{3}(1 + \sigma_1^{(N-1)} \varepsilon + \sigma_2^{(N-1)} \varepsilon^2) \end{aligned} \tag{14}$$

we then find from (11b)

$$P_3^{(N-1)} = 1 + 6\sigma_1^{(N-1)} \varepsilon + \varepsilon^2 [6\sigma_2^{(N-1)} + 27(\sigma_1^{(N-1)})^2]. \tag{15}$$

We therefore infer $\sigma_1^{(N)} = 6\sigma_1^{(N-1)}$ and $\sigma_2^{(N)} = 6\sigma_2^{(N-1)} + 27(\sigma_1^{(N-1)})^2$. The former immediately yields $\langle t \rangle_N = 6^N$. Since $\langle t \rangle_N$ increases by a factor of 6 at each iteration, while the length of the tree increases by a factor of 2, we obtain $\tau_1 = \ln 6/\ln 2$, as already found in § 2. The recursion relation involving the second moment can be solved by the diagonalisation procedure of the previous section. Introducing $u_N \equiv \langle t^2 \rangle_N + \lambda \langle t \rangle_N^2$, and choosing $\lambda = -\frac{9}{5}$, gives $u_N = 6u_{N-1}$. With the initial condition $u_0 = -\frac{4}{5}$, we find $\langle t^2 \rangle_N = \frac{9}{5}(6^{2N}) - \frac{4}{5}(6^N)$. Thus we conclude that $\langle t^2 \rangle_N \sim (\langle t \rangle_N)^2$, i.e. the second moment scales as the square of the first moment. This calculation can be extended to the higher moments, leading to the general conclusion $\langle t^q \rangle_N \sim (\langle t \rangle_N)^q$. Thus in the hierarchical tree a single timescale suffices to describe all the moments of the first-passage time. We expect that this will continue to hold for any exact self-similar structure.

The survival probability at the nth step, $S(n)$, is the probability that the random walk has not yet reached the output site. It is related to the first-passage probability via $S(n) = 1 - \Sigma_{n'=1}^{n} P_4(n')$. For any finite graph, $S(n)$ decays exponentially in n at long times, and we investigate the relation between the characteristic time of this exponential decay and the moments of the first-passage time. Now if $S(n)$ decays as μ^n, then so does $P_4(n)$. Consequently, the corresponding generating function, $P_4(z)$, will have a simple pole at $z_c = \mu^{-1}$. As the order of the tree becomes large the survival probability decays more slowly, so that z_c approaches unity from above. Thus to locate the pole in $P_4^{(N)}(z)$, we make the ansatz $z_c \simeq 1 + \varepsilon$, and substituting in (11b) gives $a^{(N)} \simeq \frac{1}{3}(1 + 6^N \varepsilon)$. Using this in (11$a$), we find that $P_4^{(N)}(z)$ has a simple pole when $\varepsilon \equiv \varepsilon^{(N)} = \frac{1}{4}(\frac{1}{6})^N$. Thus the characteristic time in the exponential decay of $S(n)$ increases as 6^N as the tree is iterated, and this scaling is identical to that of the moments of the first-passage time. Thus ail dynamical properties of diffusion on the hierarchical tree are described by a single exponent.

4. Diffusion on the hierarchical comb

For the comb, a decimation approach similar to that given for the hierarchical tree gives a formal solution for the first-passage probability. Our calculation proceeds in two stages. First we account for a side branch in terms of a 'waiting-time polynomial', and thereby solve for the first-passage probability of a system with a single side branch. Next we solve for the first-passage probability for the full hierarchical comb.

4.1. First-passage probability for a single side branch

For concreteness, consider a linear chain n of length 2 and a side branch of height R (figure 3). A random walker starts at site 1 and is absorbed at site 3. The equations for the occupation probabilities of the sites on the side branch can be eliminated successively, as discussed in appendix 3. This leads to the master equations

$$\begin{aligned} w_0(z)P_1(z) &= \tfrac{1}{3}zP_2(z)+1 \\ w_R(z)P_2(z) &= zP_1(z) \\ P_3(z) &= \tfrac{1}{3}zP_2(z) \end{aligned} \tag{16}$$

with solution for the first-passage probability

$$P_3(z) = z^2/(3w_0(z)w_R(z)-z^2). \tag{17}$$

Here we introduce $w_0(z)=1$ for later convenience, and $w_R(z)$ is the waiting-time polynomial that accounts for the modification of $P_2(z)$ by sojourns of a random walk on a side branch of length R. This polynomial has the form $w_R(z)=1-\frac{2}{3}f_R(z)$, where f_R is the finite continued fraction

$$f_R = \frac{\frac{1}{4}z^2}{1-f_{R-1}} \tag{18}$$

with the initial condition $f_1=\frac{1}{2}z^2$.

To compute f_R in closed form, we employ the method outlined by Goldhirsch and Gefen [19]. Writing

$$f_R \equiv \frac{g_R}{h_R} = \frac{\frac{1}{4}z^2}{1-g_{R-1}/h_{R-1}} \tag{19}$$

we see that g_R and h_R obey the recursion relations

$$g_R = \tfrac{1}{4}z^2 h_{R-1}c_R \qquad h_R = (h_{R-1}-g_{R-1})c_R \tag{20}$$

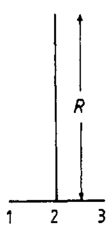

Figure 3. A chain of three sites to which a side branch of length R is attached.

with c_R an arbitrary constant. This constant can be eliminated by introducing $g_R = c_1 c_2 \ldots c_R \tilde{g}_R$ and $h_R = c_1 c_2 \ldots c_R \tilde{h}_R$. Then $\tilde{g}_R$ and $\tilde{h}_R$ obey

$$\tilde{g}_R = \tfrac{1}{4} z^2 \tilde{h}_{R-1} \qquad \tilde{h}_R = \tilde{h}_{R-1} - \tilde{g}_{R-1}. \tag{21}$$

Since we are interested in f_R, which is the ratio of g_R to h_R (or $\tilde{g}_R$ to $\tilde{h}_R$), we may henceforth omit the tildes in (21). We therefore have $h_R = h_{R-1} - \frac{1}{4}z^2 h_{R-2}$, and the solution is a linear combination of α_+ and α_-, where $\alpha_\pm = \frac{1}{2}(1 \pm \sqrt{1-z^2})$. Since $z > 1$, $\alpha_\pm$ can be written as $a \exp(\pm i\phi)$, with $\phi = \tan^{-1}(\sqrt{z^2-1})$ and $i = \sqrt{-1}$. Using the initial condition, $f_1 = 2a^2$, we finally obtain

$$\begin{aligned} f_R &= \frac{z^2}{4}\left(\frac{\alpha_+^{R-1} + \alpha_-^{R-1}}{\alpha_+^R + \alpha_-^R}\right) \\ &= \frac{z}{2}\left(\frac{\cos[(R-1)\phi]}{\cos R\phi}\right). \end{aligned} \tag{22}$$

This result, together with (17) provides a solution for the first-passage probability on a chain of length 2 with a side branch of length R. Note also that when $R = \infty$, the recursion relation (18) reduces to the algebraic relation $f_\infty = \frac{1}{4}z^2/(1-f_\infty)$, which has the solution

$$f_\infty = \tfrac{1}{2} z^2 (1 - \sqrt{1-z^2}). \tag{23}$$

We will discuss the physical consequences of these results for the asymptotic behaviour of the survival probability in § 6.

4.2. *First-passage probability for the hierarchical comb*

We now exploit the solution of a single side branch to solve for the first-passage probability on an arbitrary Nth-order comb. The master equations for this structure are

$$\begin{aligned} &w_0(z)P_1(z) = \tfrac{1}{3}zP_2(z) + 1 && w_1(z)P_2(z) = zP_1(z) + \tfrac{1}{3}zP_3 \\ &w_2(z)P_3(z) = \tfrac{1}{3}zP_2(z) + \tfrac{1}{3}zP_4 && w_1(z)P_4(z) = \tfrac{1}{3}zP_3(z) + \tfrac{1}{3}zP_5 \\ &w_3(z)P_5(z) = \tfrac{1}{3}zP_4(z) + \tfrac{1}{3}zP_6 && \text{etc} \end{aligned} \tag{24}$$

where we now define $w_N(z) = 1 - \frac{2}{3} f_{R^{N-1}}$ for $N \geq 1$, with f_R the continued fraction given in (18). By decimating out the even-index sites (those with the shortest side branch attached), the master equations are transformed to those of an $(N-1)$th-order comb, but with the following rescaled waiting-time polynomials

$$w'_0(z) = \frac{3}{z}\left(w_1(z)w_0(z) - \frac{z^2}{3}\right) \tag{25a}$$

$$w'_N(z) = \frac{3}{z}\left(w_1(z)w_{N+1}(z) - \frac{2z^2}{9}\right) \qquad N \geq 1 \tag{25b}$$

and the initial condition factor of unity in the equation for $P_1(z)$ is replaced by $3w_1/z$. Successively applying this decimation to the shortest branches at each stage ultimately leads to a renormalised zeroth-order structure, which is easily solved. We therefore find the general solution for the first-passage probability on an Nth-order structure

$$P^{(N)}(z) = z^2/(3w_0^{(N)}(z)w_1^{(N)}(z) - z^2) \tag{26}$$

where the superscript in $w_0^{(N)}$ and $w_1^{(N)}$ indicates N applications of the renormalisation transformation (25). In principle, the moments of the transit time can be found by a direct expansion of the first-passage probability in powers of $\varepsilon = 1 - z$. This is a tedious task, however, and we therefore turn to an alternative approach which is based on the anisotropic scaling structure of the comb.

5. Scaling for the first-passage time moments and the survival probability

To compute the moments of the first-passage time on the comb, we exploit the fact that the comb iterates anisotropically in the x and y directions, leading to an anisotropic rescaling of the hopping probabilities. Accordingly, we generalise from one hopping rate, a, to hopping rates $a-f$, as defined in figure 4. This is the minimal set of rates needed to close a direct renormalisation from an Nth-order to an $(N-1)$th-order comb. With these rates, the master equations for the first-order comb are

$$P_1(z) = aP_2(z) + b \qquad P_2(z) = 3cP_1(z) + dP_4(z)$$
$$P_3(z) = fP_2(z) \qquad P_4(z) = eP_2(z) \tag{27}$$

with the solution for the first-passage probability

$$P_3(z) = 3bcf/(1 - 3ac - de). \tag{28}$$

For concreteness, we investigate the renormalisation of an $R = 3$ first-order comb (cf appendix 4), and later generalise to arbitrary R. By decimating the first-order sites, one obtains master equations of the zeroth-order comb, but with the renormalised hopping rates

$$a' = ac/A \tag{29a}$$
$$c' = c^2(1 - \tfrac{9}{4}e^2)/B_3 \tag{29b}$$
$$d' = \tfrac{9}{4}e^2 d(1 - de)/B_3 \tag{29c}$$
$$e' = \tfrac{9}{4}e^3/(1 - \tfrac{27}{4}e^2) \tag{29d}$$
$$g' = cg/A \tag{29e}$$

where $A = (1 - de - 3ac)$, $B_3 = (1 - de)(1 - \tfrac{9}{4}e^2 - \tfrac{1}{2}de) - 2c^2(1 - \tfrac{9}{4}e^2)$ and where b and f naturally appear together as the product $g = bf$.

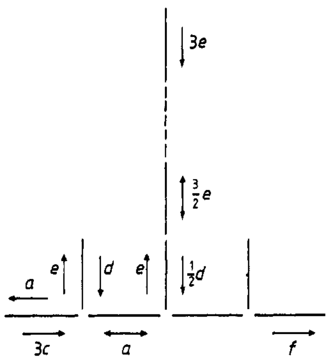

Figure 4. A first-order hierarchial comb showing the general set of hopping rates needed to close the renormalisation of the comb.

To compute the moments of the first-passage time for this generalised structure, we first expand each of the hopping rates in powers of $\varepsilon = 1-z$, e.g.

$$a = a_0(1 + a_1\varepsilon + a_2\varepsilon^2) + O(\varepsilon^3) \tag{30}$$

and similarly for c, d, e, and g. By evaluating (29) at $z=1$, the leading term in a, e, and g equals $\frac{1}{3}$, while the leading term in c and d depends on the order of the comb. Accordingly the power series expansion for $P_3(z)$ is

$$\begin{aligned} P_3(z) = 1 + \varepsilon[2c_1 + g_1 + a_1 + (d_0/3c_0)(e_1 + d_1)] \\ + \varepsilon^2(2c_2 + g_2 + a_2 + 2g_1c_1 + 2c_1a_1 + c_1^2 + g_1a_1 \\ + (d_0/3c_0)(e_2 + d_2 + e_1d_1 - c_1e_1 - c_1d_1 - g_1e_1 - g_1d_1)] + O(\varepsilon^3). \end{aligned} \tag{31a}$$

Retaining only the asymptotically dominant contributions under rescaling leads to

$$P_3(z) \sim 1 + m_1\varepsilon + m_2\varepsilon + O(\varepsilon^3) \tag{31b}$$

where $m_1 \sim O((d_0/c_0)e_1)$ and $m_2 \sim O((d_0/c_0)e_2)$. For $R=3$, a straightforward calculation shows that these dominant contributions rescale as

$$d_0'/c_0' = 2d_0/3c_0 \qquad e_1' = 9e_1 \qquad e_2' \sim 81e_2 \tag{32a}$$

leading to the scaling laws $\langle t\rangle_{N+1} = 6\langle t\rangle_N$ and $\langle t^2\rangle_{N+1} \sim 54\langle t^2\rangle_N$.

For general R, a similar calculation shows that the asymptotically dominant contributions rescale as

$$d_0'/c_0' = 2d_0/Rc_0 \qquad e_1' = R^2e_1 \qquad e_2' \sim R^4e_2. \tag{32b}$$

From the manner in which these terms appear in the power series for $P_3(z)$, we can interpret the quantity d_0/c_0 as the probability for a random walk to enter a side branch at a junction with the backbone, and e_q as the qth moment of the residence time on the side branch. Since e is the hopping rate in the y direction, it is physically clear that $e_q' = R^{2q}e_q$, although we cannot provide a proof of this fact within the present context. These rescaling factors conspire to yield an overall contribution of R^{2q-1} for the rescaling factor of the qth moment of the first-passage time. Correspondingly, the scaling exponent, defined by $\langle t^q\rangle \sim L^{\tau_q}$, is $\tau_q = \ln 2R^{(2q-1)}/\ln 2$.

Thus we have found multifractal behaviour, as $\tau_q \neq q\tau_1$, with τ_q becoming strictly proportional to q only in the limit $q \to \infty$. However, this multifractality is of a trivial character which arises from the anisotropy of the comb. Our prediction for τ_q is in good agreement with the simulations of Havlin and Matan [9]. For $R=3$, their data for τ_q is almost linear for large q, as we would expect (see figure 3 of their paper). Furthermore, their numerical data for τ_q for $q=1$, 4 and 5 are 2.585 ± 0.02, 11.70 ± 0.04 and 14.80 ± 0.04, respectively, compared to our corresponding theoretical values (to four significant figures) of 2.585, 12.09 and 15.26. The agreement is excellent for $q=1$, and somewhat less good for $q=4$ and $q=5$. We attribute the discrepancies to the presence of lower-order correction terms to the first-passage moments. These will be seen in numerical simulations on a finite structure, while our calculation for the exponents involves only the asymptotically dominant term.

We can also use the above rescaling properties to determine the behaviour of the characteristic time in the asymptotic decay of the survival probability. From (31) and (32), we have, for $z = 1-\varepsilon$,

$$P_3'(z) \sim 1 + (2/R)[m_1(R^2\varepsilon) + m_2(R^2\varepsilon)^2 + O((R^2\varepsilon)^3)]. \tag{33}$$

That is, the generating function for the first-passage probability rescales as

$$P_3'(\varepsilon)-1=(2/R)(P_3(R^2\varepsilon)-1). \tag{34}$$

From the inversion integral for the generating function, this implies that the first-passage probability as a function of the number of steps, n, rescales as

$$P_3'(n)\sim(2/R^3)P_3(n/R^2). \tag{35}$$

Consequently, the characteristic time, t^*, rescales as $t^{*'}=R^2t^*$, so that the corresponding scaling exponent τ^*, equals $\ln R^2/\ln 2$. This yields $\tau^*=3.17$ for $R=3$, and $\tau^*=4$ for $R=4$, compared with the respective numerical data [9, 18] of $\tau^*=3.06\pm0.06$ and 3.94. The discrepancy between the theoretical and numerical values is significant for $R=3$ and we will discuss the source of the discrepancy by a more complete calculation of the survival probability in the next section.

6. Asymptotic behaviour of the survival probability

As first discussed for the hierarchical tree, we need to locate the smallest singularity of the first-passage probability to determine the scaling behaviour of t^*. Consider first a linear chain of length 2 with a side branch of length R. From (17), the condition that locates the singularity in the first-passage probability on this structure is

$$f_R(z_c)=\tfrac{1}{2}(3-z_c^2) \tag{36}$$

and a solution can be found graphically (figure 5). Note that when $z=1$, $f_R=\frac{1}{2}$ for all R. However, for $z\gtrsim 1$, f_R is a rapidly increasing function which diverges at

$$z_\infty=[1+\tan^2(\phi/2R)]^{1/2}\simeq 1+\pi^2/8R^2.$$

Since the right-hand side of (36) equals unity at $z=1$, and is a relatively slowly decreasing function of z, we know that $1<z_c<z_\infty$. Furthermore, since $z_\infty\to 1$ as $O(R^{-2})$, and because the slope of f_R at $z=1$ is proportional to R, it follows that the leading behaviours of z_c-1 and $z_\infty-1$ coincide. To obtain the next-order approximation for z_c, we write $z_c\sim 1+(\pi^2/8R^2)(1-\tau)$, with $\tau\ll 1$. Substituting this into (36) yields

$$z_c\simeq 1+\pi^2/8R^2-\pi^2/4R^3+O(1/R^4) \tag{37}$$

and higher-order terms are, in principle, calculable. This result shows that $t^*\sim(z_c-1)^{-1}$ increases as R^2, as expected. The comparison between this approximation and the exact value of z_c is shown in table 1.

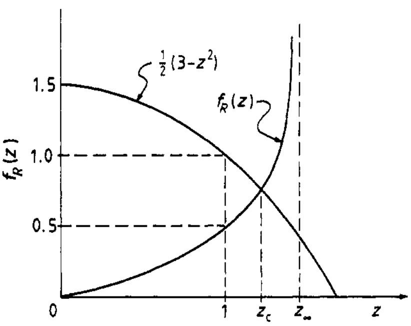

Figure 5. Illustration of the graphical solution to (36). The divergence of $f_R(z)$ at z_∞ is indicated, as well as the location of the root of (36).

It is also worth noting that for an infinite-length side branch, the waiting-time polynomial has a square root singularity at $z=1$. This implies that the first-passage time is divergent, while the survival probability decays with time as $t^{-1/2}$.

Table 1. Comparison between the 'exact' value of z_c given by the numerical solution to (36), and the approximate values of z_c obtained by keeping the first two or the first three terms in (37). To see the differences between these quantities more clearly, we tabulate the values of $(z_c-1)8R^2/\pi^2$ rather than z_c.

	$(z_c-1)8R^2/\pi^2$		
R	Two term	Three term	Exact
2	1	0.00	0.408 63
3	1	0.33	0.551 56
4	1	0.50	0.639 32
5	1	0.60	0.697 60
10	1	0.80	0.830 37
20	1	0.90	0.908 62
50	1	0.96	0.961 51
100	1	0.98	0.980 39

For the first-passage probability on the Nth-order comb, a first approximation to z_c is obtained by locating the divergence of the most singular contribution to $w_1^{(N)}(z)$. For a side branch of length R^N

$$z_\infty^{(N)}=[1+\tan^2(\phi/2R^N)]^{1/2}\simeq 1+\pi^2/8R^{2N}.$$

Thus for an Nth-order comb, we write $z_c^{(N)}\simeq 1+(\pi^2/8R^{2N})(1-\tau)$, and we attempt to find the correction term τ.

Writing the waiting-time polynomial for a side branch of length R^N as $w_{N+1}=1-\frac{2}{3}f_{R^N}\equiv 1-\frac{2}{3}g_N$, then at $z=z_c^{(N)}$ a simple calculation yields

$$g_N=\tfrac{1}{2}[1+2/(R^N\tau)] \tag{38a}$$

$$g_k=\tfrac{1}{2}(1+\mathrm{O}(R^{-2N+k})) \qquad k<N. \tag{38b}$$

Thus to order R^{-N}, we replace g_k by its value at $z=1$, namely $g_k=\frac{1}{2}$ for $k<N$.

In the spirit of this approximation, we evaluate $w_0^{(N)}$ at $z=1$, and keep only the dominant contribution to $w_1^{(N)}$ in the condition $3w_0^{(N)}(z)w_1^{(N)}(z)=z^2$ that locates the singularity of the first-passage probability. Thus in (25*b*) we write $w'_N(z)\simeq 2w_{N+1}(z)-\frac{2}{3}$, and iterating this linearised relation yields, after some algebra,

$$w_1^{(N)}(z)=2^N w_N(z)+\tfrac{2}{3}(1-2^N). \tag{39}$$

Substituting this into (26) and using the approximation (38) for g_N gives, finally, $\tau\simeq 2(2/R)^N$. Thus the singularity in the first-passage probability for an Nth-order comb is located at

$$z_c^{(N)} = 1 + \frac{\pi^2}{8R^{2N}}\left[1 - 2\left(\frac{2}{R}\right)^N\right] \tag{40}$$

and this leads to the characteristic decay time,

$$t_N^* \simeq \frac{8R^{2N}}{\pi^2}\left[1 + 2\left(\frac{2}{R}\right)^N\right]. \tag{41}$$

Notice that the correction term in the decay time depends on the order of iteration, N. This means that numerical estimates of t_N^* should exhibit curvature when plotted on a double logarithmic scale. Thus the value of the associated exponent τ^* determined from such data may not agree with the asymptotic formula $\tau^* = \ln R^2/\ln 2$ which arises when all correction terms are ignored. Furthermore for $R = 3$ and $N = 1$, the correction term leads to $z_c < 1$, and higher-order terms in R^{-1} play a relatively large role. While the correction is straightforward to obtain in principle, it is tedious computationally. A comparison between the values of t_N^* obtained from the numerical solution to (26) and the estimate given by (41) is shown in figure 6.

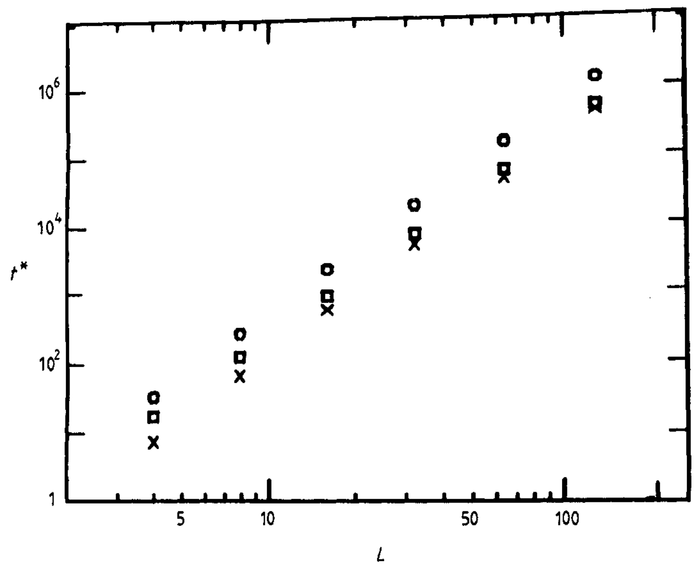

Figure 6. Comparison of the exact value (○) of t^* obtained from the solution to equation (39) with the approximate values obtained from equation (41) by retaining only the first two terms (×) or all three terms (□) of equation (41).

7. Summary

We have calculated the first-passage probability, the moments of the first-passage time and the survival probability for random walks on hierarchical structures. In the case of exact self-similarity, e.g. the hierarchical tree, a single timescale suffices to characterise all the dynamical behaviour of random walks. The moments of the first-passage time to go from an input point to an absorbing sink are characterised by a unique timescale, i.e. $\langle t^q\rangle \sim \langle t\rangle^q$, where $\langle t\rangle \sim L^\tau$, with $\tau = \ln 6/\ln 2$. Similarly, the probability that the random walk does not hit the sink decays asymptotically as $\exp(-t/t^*)$, with a characteristic decay time, t^*, that also scales as $\langle t\rangle$.

For the hierarchical comb, there is a dynamical transition between normal and anomalous diffusion at $R=2$, where R is the rescaling factor of the teeth of the comb upon rescalings of the backbone by a factor of 2. In the anomalous regime ($R>2$), the qth moment of the first-passage time scales as $\langle t^q\rangle \sim L^{\tau_q}$, with $\tau_q = 1+(2q-1)\ln R/\ln 2$. This behaviour is very similar to the scaling behaviour of the moments of the transit-time distribution for the hydrodynamic dispersion problem on percolation clusters [20].

For the survival probability on the comb, the characteristic time t^* scales as L^{τ^*}, with $\tau^* = \ln R^2/\ln 2$. This is different from the exponent, τ_1, of the first-passage time, but is related to the exponents characterising the higher moments by $\tau^* = \lim_{q\to\infty} \tau_q/q$. Thus both the survival probability and the higher moments of the transit time are governed by the walks which traverse the longest side branch of the comb. However, for values of $R \geqslant 2$ there are appreciable corrections to the scaling behaviour of t^*, and these are needed in order to understand numerical simulation results.

It is worth noting the dichotomy between the moments of the first-passage probability, and the moments of the displacement distribution. The former pertain to the temporal behaviour at a fixed observation point while the latter pertain to the spatial distribution at a fixed observation time. The second moment of the displacement, $\langle r^2\rangle$, may be characterised by the fractal dimension of the walk, d_w, via the scaling law $\langle r^2\rangle \sim t^{2/d_w}$. If diffusion were characterised by a unique timescale, then τ_1 would coincide with d_w. This generally appears to be the case for exact self-similar structures. However, for the hierarchical comb, Havlin *et al* [7] have obtained $d_w = 4\ln R/\ln 2R$, which is very different from the value $\tau_1 = \ln 2R/\ln 2$. A plausible explanation for this discrepancy is that moments of the first-passage time at a fixed observation point are strongly influenced by the 'slowest' particles, while moments of the displacement distribution at fixed time are strongly influenced by the 'fastest' particles. Cases where $\tau_1 \neq d_w$ deserve more attention in order to clarify the essential differences between the fixed time and fixed observation point ensembles.

After this work was completed, we learned of complementary results derived by Weiss *et al* [18] for random walks on deterministic structures. We thank these authors for sending a copy of their work prior to publication.

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Appendix 1. Mean first-passage time on the hierarchical comb

The equations governing the first-passage times for a random walk starting at a given site of the first-order comb are (cf figure 1(*b*))

$$
\begin{aligned}
t_1 &= T_x + t_2 \\
t_2 &= \tfrac{1}{3}(T_x + t_1) + \tfrac{1}{3}(T_y + t_6) + \tfrac{1}{3}(T_x + t_3) \\
t_3 &= \tfrac{1}{3}(T_x + t_2) + \tfrac{1}{3}(T_y + t_7) + \tfrac{1}{3}(T_x + t_4) \\
t_4 &= \tfrac{1}{3}(T_x + t_3) + \tfrac{1}{3}(T_y + t_{R+7}) + \tfrac{1}{3}T_x \\
t_6 &= T_y + t_2 \\
t_7 &= \tfrac{1}{3}(T_y + t_8) + \tfrac{1}{2}(T_y + t_3) \\
t_k &= \tfrac{1}{2}(t_{k-1} + t_{k+1}) + T_y \qquad \text{for } k = 8, \ldots, R+5 \\
t_{R+6} &= T_y + t_{R+5} \\
t_{R+7} &= T_y + t_4 .
\end{aligned}
\tag{A1}
$$

By eliminating the equations associated with all sites except 1, 3, 5 and $R+6$, the first-order sites are decimated out, and one obtains (3) for the average first-passage time.

Appendix 2. First-passage probability on the hierarchical tree

For the first-order hierarchical tree (figure 2), the master equations for the generating function are

$$
\begin{aligned}
P_1(z) &= aP_2(z) + 1 \\
P_2(z) &= 3aP_1(z) + 3aP_3(z) + aP_4(z) \\
P_3(z) &= aP_2(z) \\
P_4(z) &= aP_2(z) + aP_5(z) + aP_8(z) \\
P_5(z) &= aP_4(z) + 3aP_6(z) + 3aP_7(z) \\
P_6(z) &= P_7(z) = aP_5(z) \\
P_8(z) &= aP_4(z) + 3aP_9(z) \\
P_9(z) &= P_{10}(z) = aP_8(z).
\end{aligned}
\tag{A2}
$$

By decimating out the first-order sites in the tree, namely 2, 3, 5, 6, 8 and 9, and identifying sites 1, 4, 7 and 10, with 1′, 2′, 3′ and 4′, respectively, we obtain the rescaled master equations

$$
\begin{aligned}
P_{1'} &= a'P_{2'} + c \qquad & P_{2'} &= 3a'P_{1'} + 3a'P_{3'} \\
P_{3'} &= a'P_{2'} \qquad & P_{4'} &= (a'/c)P_{2'}
\end{aligned}
\tag{A3}
$$

with $a' = a^2/(1-6a^2)$ and $c = (1-3a^2)/(1-6a^2)$. These are of the same form as the master equations for the zeroth-order structure, except that the hopping rate has been renormalised, and a new parameter, c, has been introduced. The solution to these renormalised master equations yields the first-passage probability, $P_{4'} = 3a'^2/(1-6a'^2)$, in the form given in (10).

Appendix 3. Master equations for a single side branch

For a side branch of length R attached to a linear chain at site i, the master equations for the sites on the side branch are (cf figure 7)

$$\begin{aligned}
P_i(z) &= aP_{i-1}(z) + aP_{i+1}(z) + aP_1(z) \\
P_1(z) &= \tfrac{2}{3}aP_i(z) + aP_2(z) \\
P_2(z) &= aP_1(z) + aP_3(z) \\
&\vdots \\
P_{R-1}(z) &= aP_{R-2}(z) + 2aP_R(z) \\
P_R(z) &= aP_{R-1}(z)
\end{aligned} \tag{A4}$$

with $a = z/2$, while the master equations for the sites $\{j\}$ on the linear chain have the form

$$P_j(z) = aP_{j-1}(z) + aP_{j+1}(z). \tag{A5}$$

Here $a = z/2$. In (A4), we first eliminate the variable $P_R(z)$. The master equation for $P_{R-1}(z)$ then becomes

$$(1 - 2a^2)P_{R-1}(z) = aP_{R-2}(z). \tag{A6}$$

Next the variable P_{R-1} is eliminated, and this yields the master equation for $P_{R-2}(z)$,

$$\left(1 - \frac{a^2}{1 - 2a^2}\right) P_{R-2}(z) = aP_{R-3}(z). \tag{A7}$$

Continuing this process until the occupation probabilities associated with all the sites on the side branch are eliminated leads to the effective master equation for the junction site,

$$w_R(z)P_i(z) = aP_{i-1}(z) + aP_{i+1}(z) \tag{A8}$$

where $w_R(z)$ is the waiting-time polynomial defined in (18).

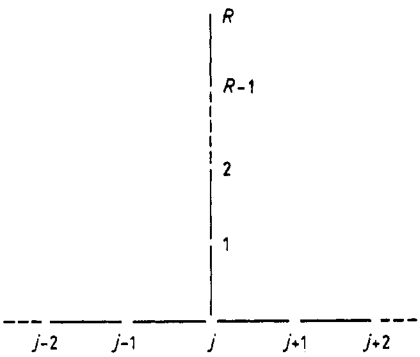

Figure 7. A linear chain with an attached side branch of length *R*.

Appendix 4. Generalised master equations for the first-order comb

For the first-order $R=3$ hierarchical comb, the master equations for the generating function are (using the notation of (27) for the coefficients and that of figure 1(*b*) for the site labels)

$$
\begin{aligned}
P_1 &= aP_2 + b \\
P_2 &= 3cP_1 + aP_3 + dP_6 \\
P_3 &= aP_2 + aP_4 + \tfrac{1}{2}dP_7 \\
P_4 &= aP_3 + dP_{10} \\
P_5 &= fP_4 \\
P_6 &= eP_2 \\
P_7 &= eP_3 + \tfrac{3}{2}eP_8 \\
P_8 &= \tfrac{3}{2}eP_7 + 3eP_9 \\
P_9 &= \tfrac{3}{2}eP_8 \\
P_{10} &= eP_4.
\end{aligned}
\qquad \text{(A9)}
$$

As in the case of the hierarchical tree, we first decimate out the first-order sites (2, 4, 6, 7, 8 and 10) and sites 1, 3, 5 and 9 are identified with 1′, 2′, 3′ and 4′, respectively. This leads to master equations of the same form as those in (27) for the zeroth-order comb, but with renormalised coefficients given in (29).

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