Global first-passage times of fractal lattices

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The global first passage time density of a network is the probability that a random walker released at a random site arrives at an absorbing trap at time T. We find simple expressions for the mean global first passage time $\langle T \rangle$ for five fractals: the d-dimensional Sierpinski gasket, T fractal, hierarchical percolation model, Mandelbrot-Given curve, and a deterministic tree. We also find an exact expression for the second moment $\langle T^2 \rangle$ and show that the variance of the first passage time, $\mathrm{Var}(T)$, scales with the number of nodes within the fractal N such that $\mathrm{Var}(T) \sim N^{4/\bar{d}}$, where $\bar{d}$ is the spectral dimension.

I. INTRODUCTION

The study of diffusion on statistically self-similar disordered media (e.g., percolation clusters and diffusion limited aggregates) is simplified by modeling their structure by deterministic fractals [1]. Although scaling theory has been central in studying diffusive processes on a variety of deterministic fractals [2], it has been noted that scaling laws do not provide a complete picture of dynamic phenomena on fractals [3], and exact relationships are useful.

Lately there has been interest in calculating the mean time $\langle T \rangle$ taken for a walker released from a randomly chosen node on a fractal to arrive at a trap. We call the underlying probability density of T the global first passage time (GFPT). It is found by a simple average of the node-to-trap first passage times over the entire fractal. The mean of the GFPT was first obtained for the Sierpinski gasket lattice by Kozak and Balakrishnan [4,5], and an analogous study has been recently performed for the T fractal [6]. The mean $\langle T \rangle$ has been associated [6] with important questions such as the exploration of a random walker on a fractal lattice [7], providing further motivation for the study of global first passage times.

In general, deterministic fractals have played a key role in explaining diffusion in disordered materials because their properties can be exactly studied. In this paper we use a renormalization method to derive an exact expression for the full moment generating function of the GFPT. The method is exact, and can be applied to any finitely ramified deterministic fractal, making the exploration of higher moments of the GFPT possible. There is interest in higher moments of random walk quantities [8,9] as such results give further insight into the nature of transport on fractals. Knowledge of these moments is also useful to investigate the variance of the bimolecular reaction $A + B \rightarrow A$ [10].

The paper is organized as follows. In Sec. II we formulate the problem of continuum diffusion on networks of pipes as an algebraic system of equations involving Laplace transforms of the fluxes and concentrations at each node. We show how the equations are solved on a d-dimensional Sierpinski gasket lattice using a renormalization procedure. In Sec. III, we derive the general formula for the Laplace transform of the GFPT density for a trap at an arbitrary node on the gasket. We demonstrate our method for the apex of the nth iteration of the d-dimensional gasket. Our results, for the

mean of the GFPT, agree with prior work [4,5], and are extended to show that, for any given trap, there is an exact analytic expression for the moment generating function of the GFPT.

In Sec. IV, we demonstrate that the method can be used to calculate the GFPT moment generating function for at least one node on any structure provided that a renormalization procedure exists. A general formula is provided for the GFPT moment generating function for a finitely ramified deterministic fractal with two end nodes. As examples we consider the Mandelbrot-Given curve, deterministic tree, hierarchical percolation model, and the T tree [6]. The calculation of higher moments is demonstrated for the T tree in Sec. V.

II. CONTINUUM DIFFUSION ON NETWORKS

We begin by solving the diffusion equation

$$D\frac{\partial^2}{\partial x^2}C(x,t) = \frac{\partial}{\partial t}C(x,t) \tag{1}$$

on a bar of length L with the nonhomogeneous boundary conditions

$$C(0,t) = P_1(t), \quad C(L,t) = P_2(t),$$

and initial condition $C(x,0)=0$. Taking Laplace transforms of Eq. (1) and solving using the boundary and initial conditions we find

$$c(x,s) = p_2(s)\frac{\sinh\left(x\sqrt{\frac{s}{D}}\right)}{\sinh\left(L\sqrt{\frac{s}{D}}\right)} + p_1(s)\frac{\sinh\left[(L-x)\sqrt{\frac{s}{D}}\right]}{\sinh\left(L\sqrt{\frac{s}{D}}\right)}, \tag{2}$$

where we denote Laplace transformed functions by lower case letters;

$$c(x,s) = \mathcal{L}[C(x,t)] \equiv \int_0^\infty C(x,t)e^{-st}dt.$$

The flux entering the bar at the point $x=0$ is $F_1 = -D\frac{\partial}{\partial x}C(x,t)\big|_{x=0}$ and the flux entering the bar at $x=L$ is $F_2 = D\frac{\partial}{\partial x}C(x,t)\big|_{x=L}$. For networks it is useful to express these
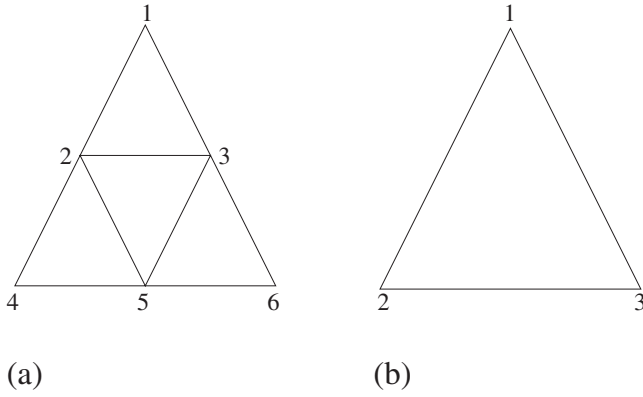
FIG. 1. (a) First iteration of the Sierpinski Gasket lattice. (b) Zeroth iteration of the Sierpinski gasket lattice. The labeling used in the above (a) and (b) implies that the left corner of the nth iteration of the 2D Sierpinski gasket lattice is denoted by $3(3^n+1)/2-2^n$, the right corner by $3(3^n+1)/2$ and the apex by 1.

fluxes in terms of the concentrations p_i at either end. This gives rise to the equations

$$g\begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} 1 & -\operatorname{sech}\left(\sqrt{\frac{s}{D}}L\right) \\ -\operatorname{sech}\left(\sqrt{\frac{s}{D}}L\right) & 1 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \end{bmatrix}, \quad (3)$$

where $g = \tanh(\sqrt{\frac{s}{D}}L)/\sqrt{sD}$. We call the above a flux-concentration matrix. For simplicity we set D and L to be unity.

Using these relations, diffusion on an arbitrary network can be formulated as a system of algebraic equations. To link two or more bars at a node we set the concentrations to be equal. As an example the system for the first iteration of the Sierpinski gasket lattice shown in Fig. 1(a) is

$$g\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix} = \begin{bmatrix} 2a_0 & -b_0 & -b_0 & 0 & 0 & 0 \\ -b_0 & 4a_0 & -b_0 & -b_0 & -b_0 & 0 \\ -b_0 & -b_0 & 4a_0 & 0 & -b_0 & -b_0 \\ 0 & -b_0 & 0 & 2a_0 & -b_0 & 0 \\ 0 & -b_0 & -b_0 & -b_0 & 4a_0 & -b_0 \\ 0 & 0 & -b_0 & 0 & -b_0 & 2a_0 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \\ p_5 \\ p_6 \end{bmatrix}. \quad (4)$$

Here $a_0 = 1$ and $b_0 = \operatorname{sech}(\sqrt{s})$.

A. Initial and boundary conditions

The f_i in Eq. (4) are understood to represent the total flux entering node i. For mass conservation $f_i = 0$, but if we take an instantaneous unit source at node i, then the flux entering the node is $F_i = \delta(t)$, where $\delta(t)$ is the Dirac δ function. This means that $f_i = \mathcal{L}(F_i) = \mathcal{L}[\delta(t)] = 1$. The matrix has a similar form to a simple finite difference scheme for modeling diffusion and probability on a lattice. Prior studies [11–13] have also formulated the problem of diffusion on networks in

terms of the Laplace transform of the concentration and flux at a node. Here, linear algebra is used to extend these ideas.

It is useful to illustrate the formulation of two different but closely related problems. If we take $\mathbf{f}^T = (0,0,0,0,0,1)$ the solution $\mathbf{p}^T = (p_1,p_2,p_3,p_4,p_5,p_6)$ provides the Laplace transforms of the concentrations at the nodes if an instantaneous source is released at node 6, and mass is conserved at every node (including node 6). Next consider taking $\mathbf{f}^T = (1,0,0,0,0,f_6')$ and $\mathbf{p}^T = (p_1',p_2',p_3',p_4',p_5',0)$ and solving the six equations for p_i' $(i=1,\ldots,5)$ and f_6'. In this case the equations correspond to an instantaneous source at node 1, a homogenous Dirichlet condition (i.e., a trap) at node 6, and mass conservation at nodes $i=1,\ldots,5$. The quantity f_6' is just the flux entering at the "trap." It can be shown [14] that this flux can be calculated from p_1 and p_6 derived in the former problem, the result being $f_6' = -p_1/p_6$. Note the negative sign arises from our convention for defining the flux. The result (a convolution in time) can also be derived using a continuum random walker argument. We use a generalization of this result in Sec. III.

B. First passage times and concentrations

In order to analyze the flux-concentration matrix for higher order generations of the Sierpinski gasket we apply a renormalization method. We first show how the 6×6 system (4) can be reduced to a 3×3 system associated with the 0th order Sierpinski gasket [see Fig. 1(b)]

$$g\begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} = \begin{bmatrix} 2a_0 & -b_0 & -b_0 \\ -b_0 & 2a_0 & -b_0 \\ -b_0 & -b_0 & 2a_0 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}. \quad (5)$$

To do this we consider the three equations associated with nodes 2, 3, and 5 in Eq. (4)

$$\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} -b_0 & 4a_0 & -b_0 & -b_0 & -b_0 & 0 \\ -b_0 & -b_0 & 4a_0 & 0 & -b_0 & -b_0 \\ 0 & -b_0 & -b_0 & -b_0 & 4a_0 & -b_0 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \\ p_5 \\ p_6, \end{bmatrix},$$

where we have set $f_2 = 0$, $f_3 = 0$, and $f_5 = 0$. Solving this under determined system gives

$$\begin{bmatrix} p_2 \\ p_3 \\ p_5 \end{bmatrix} = \frac{1}{(4\rho_0+1)(2\rho_0-1)} \begin{bmatrix} \dfrac{2}{\rho_0} & \dfrac{2}{\rho_0} & 1 \\ \dfrac{2}{\rho_0} & 1 & \dfrac{2}{\rho_0} \\ 1 & \dfrac{2}{\rho_0} & \dfrac{2}{\rho_0} \end{bmatrix} \begin{bmatrix} p_1 \\ p_4 \\ p_6 \end{bmatrix}, \quad (6)$$

where $\rho_0 = \frac{a_0}{b_0}$. Eliminating p_2, p_3, and p_5 from Eq. (4) by using Eq. (6) gives

$$g\begin{bmatrix} f_1 \\ f_4 \\ f_6 \end{bmatrix} = \begin{bmatrix} 2a_1 & -b_1 & -b_1 \\ -b_1 & 2a_1 & -b_1 \\ -b_1 & -b_1 & 2a_1 \end{bmatrix} \begin{bmatrix} p_1 \\ p_4 \\ p_6 \end{bmatrix},$$

with

$$b_1 = \frac{a_1 b_0^2}{a_0(4a_0 - 3b_0)} = \frac{b_0^2(2a_0 + b_0)}{(2a_0 - b_0)(4a_0 + b_0)}.$$

Note that this flux-concentration matrix is of the same form as a flux-concentration matrix (5) of the triangle in Fig. 1(b). Continuing, we find that the system of equations for the nth iteration of the Sierpinski gasket has the form (5) with a_0 and b_0 replaced by

$$a_n = \rho_n b_n = \rho_n \frac{b_{n-1}(2\rho_{n-1} + 1)}{(4\rho_{n-1} + 1)(2\rho_{n-1} - 1)}. \quad (7)$$

Here ρ_n is the renormalization of the inverse FPT equation on a 2D Sierpinski gasket, which satisfies

$$\rho_n = \rho_{n-1}(4\rho_{n-1} - 3).$$

A detailed discussion of the equation can be found in Refs. [15–17].

The recurrence relationship for the d-dimensional Sierpinski gasket lattice is

$$a_n = \rho_n b_n = \rho_n \frac{(d\rho_{n-1} + 1)b_{n-1}}{[d\rho_{n-1} - (d-1)][2d\rho_{n-1} + (3-d)]}, \quad (8)$$

where

$$\rho_n(d) = 2d\rho_{n-1}^2 - 3(d-1)\rho_{n-1} + (d-2) \quad (9)$$

is the renormalization of the inverse FPT equation in d dimensions. Equation (9) has been derived in Refs. [18,19], however, the above recurrence relationships (7) and (8) are new, and allow the concentration to be calculated everywhere within the nth iteration of the d-dimensional Sierpinski gasket lattice given that an instantaneous unit source is released at a corner of the structure.

Before proceeding, a comment needs to be made about Eq. (6). The relation between the concentrations calculated in Eq. (6) holds for any iteration. By this it is understood that if p_2, p_3, p_5 can be expressed in terms of p_1, p_4, p_6 through Eq. (6) using ρ_0 for the first iteration of the Sierpinski gasket, then p_4, p_6, p_{13} can be expressed in terms of p_1, p_{11}, p_{15} through Eq. (6) using ρ_1 on the second iteration of the 2D Sierpinski gasket. In our notation (Fig. 1), node 13 is the mid base node equidistant to the nodes 11 and 15, with the other nodes having a similar labeling to Fig. 1. The fact that the concentrations at the nodes can be expressed through Eq. (6) will be used when we derive a similar relation that holds for the concentrations at the nodes of other fractal structures in Sec. IV.

III. FIRST PASSAGE TIME

Let $F_{kj}(t)$ be the first passage time for a random walker released at node j to reach node k. The GFPT is given by
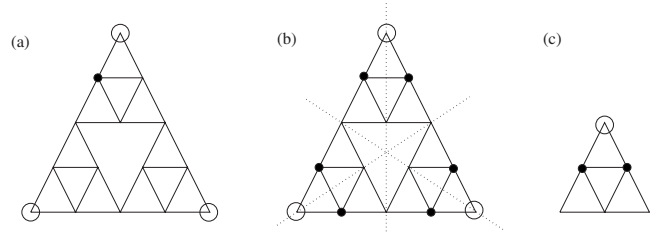

FIG. 2. Illustration of the method of images argument used to prove the result $\alpha_{k,n} = p_{1k,n-1}$. The filled circles denote sources and the open circles are the concentrations of interest.

$$F_k(t) = \frac{1}{N} \sum_{j=1, j \neq k}^{N+1} F_{kj}(t),$$

where $N+1$ is the total number of nodes and N the number of starting nodes on the fractal. Let $p_{kj,n}$ be the concentration at a node k given that an instantaneous unit source is released at a node j, and there is no loss of mass at all nodes (the first problem discussed in Sec. II A). The additional subscript n denotes the iteration of the fractal. As in Sec. II A we consider a complementary problem where a trap is placed at node k and a unit source is released at node j. The flux "entering" at k due to the source at j is

$$f_{kj,n} = -\frac{p_{jk,n}}{p_{kk,n}}.$$

The Laplace transform of the GFPT for node k is

$$f_{k,n} = \frac{1}{N}\left(-1 + \sum_{j=1}^{N+1} |f_{jk,n}|\right) = \frac{1}{N}\left(-1 + \frac{\sum_{j=1}^{N+1} p_{jk,n}}{p_{kk,n}}\right). \quad (10)$$

The mean of the GFPT is

$$\langle T_{k,n} \rangle = \int_0^\infty tF_k(t)dt = \left. -\frac{df_{k,n}(s)}{ds} \right|_{s=0}.$$

The form of $f_{k,n}$ (10) is simplified for the Sierpinski gasket through the use of conservation of probability. We integrate Eq. (2) for every pipe of the gasket and sum to find

$$\frac{d(\alpha_{k,n} + 2\beta_{k,n})[\cosh(\sqrt{s}) - 1]}{\sqrt{s}\sinh(\sqrt{s})} = \frac{1}{s}. \quad (11)$$

Here $\alpha_{k,n}$ is the sum of concentrations at the corner nodes and the apex for the closed Sierpinski gasket and $\beta_{k,n}$ is the sum of the concentrations at the other $(d+1)[(d+1)^n - 1]/2$ nodes. Note that Eq. (11) is true because there are d pipes stemming from the corner nodes and there are $2d$ pipes stemming from each interior node.

Using the method of images we show that $\alpha_{k,n} = p_{1k,n-1}$. Here we have identified the apex of the nth iteration of the d-dimensional Sierpinski gasket by the label 1. We consider the release of a walker at point $k=2$ of the second iteration of the 2D gasket [see Fig. 2(a)] to show the result, but the extension to arbitrary k and higher dimensions is clear. We first place an additional five sources at the image points of

$k=2$ in the three lines of symmetry of the gasket [Fig. 2(b)]. If we denote the sum of concentrations at the corner and apex nodes by $\alpha'_{2,2}$, then it can easily be seen (through symmetry) that $\alpha_{2,2}=\alpha'_{2,2}/6$. Now, by symmetry, there will be no flux between the three 1st iteration gaskets used to construct the second iteration, and each problem [see Fig. 2(c)] can be treated alone. It is clear that the concentration at the apex of the reduced problem is $2p_{12,1}$. Therefore, $\alpha'_{2,2}=3(2p_{12,1})$ and finally $\alpha_{2,2}=p_{12,1}$. For a source at a point which lies on a line of symmetry (such as a corner), only two copies of the source need to be considered. In the above argument k is limited to values which appear in the $(n-1)$th iteration. All other points in the nth iteration have an image point corresponding to an acceptable k value.

Using Eq. (11) reduces the GFPT (10) to

$$f_{k,n}=\frac{1}{2N}\left(\frac{p_{kk,n}^{-1}\sinh(\sqrt{s})}{d\sqrt{s}[\cosh(\sqrt{s})-1]}+\frac{\alpha_{k,n}}{p_{kk,n}}-2\right), \quad (12)$$

where $N(d)=[(d+1)^{n+1}+d-1]/2$ is the number of starting nodes. Setting $\alpha_{k,n}=p_{1k,n-1}$ in Eq. (12) gives

$$f_{k,n}=\frac{1}{2N}\left(\frac{p_{kk,n}^{-1}\sinh(\sqrt{s})}{d\sqrt{s}[\cosh(\sqrt{s})-1]}+\frac{p_{1k,n-1}}{p_{kk,n}}-2\right). \quad (13)$$

As an example, consider a trap at the apex which requires evaluation of $p_{11,n}$, which is provided in Eq. (A3) of Appendix A. After simplification the moment generating function of the GFPT for a trap at the apex is

$$f_{1,n}=\frac{1}{2N}\left(\frac{d\rho_n+1}{d\rho_n-(d-1)}-2+\prod_{j=0}^{n}\frac{d\rho_j+1}{d\rho_j-(d-1)}\right). \quad (14)$$

Note that the diffusion equations and first passage times considered above correspond to a continuous-space/continuous-time random walker. We have chosen to formulate the problem in this way because it makes the working significantly simpler. For example, Eq. (10) applies to all networks, while it must be modified to account for local coordination numbers in the discrete formulation. From $f_{k,n}(s)$ we can find results for discrete-time or discrete-space walkers using the simple transformation discussed below.

Let $F_{kj}^{*}(m)$ denote the probability that a walker released at j arrives at k on the mth step for the first time, so the GFPT is given by

$$F_{k}^{*}(m)=\frac{1}{N}\sum_{j=1,j\neq k}^{N+1}F_{jk}^{*}(m).$$

Here, and below, we denote quantities associated with a discrete walker by an asterisk. The moment generating function of $F_{kj}^{*}(m)$ is defined as

$$f_{kj}^{*}(\lambda)=\sum_{m=0}^{\infty}F_{kj}^{*}(m)e^{m\lambda}.$$

$f_{kj}^{*}(\lambda)$ is the counter part of $f_{kj}(s)$ descibed above (the iteration for the fractal is irrelevant here). The two quantities are related by

$$f_{kj}^{*}(\lambda)=f_{kj}\{[\text{arsech}(e^{\lambda})]^2\}.$$

For example, on a single bar $T_{12}^{*}(m)=\delta_{m1}$, so $f_{12}^{*}(\lambda)=e^{\lambda}$ and for a continuum walker $f_{12}(s)=1/\rho_0(s)=\text{sech}(\sqrt{s})$. A derivation of the transformation is given in Appendix B.

Thus, the moment generating function of the GFPT for a discrete walker is given by

$$f_{k}^{*}(\lambda)=f_{k}\{[\text{arsech}(e^{\lambda})]^2\}, \quad (15)$$

so we can write

$$\langle T_{k}^{*}\rangle=\sum_{m=0}^{\infty}mF_{k}^{*}(m)=\left.\frac{df_{k}^{*}(\lambda)}{d\lambda}\right|_{\lambda=0}.$$

Since the location of the trap is generally clear, we simply write the mean as $\langle T^*\rangle$. To explicitly calculate $F_{k}^{*}(m)$, we form the probability generating function $f_{k}^{*}[\ln(z)]$ and note that $F_{k}^{*}(m)$ is the coefficient of the mth term of the Taylor series expansion of $f_{k}^{*}[\ln(z)]$ about $z=0$.

For the remainder of the paper, we first calculate $f_{k}(s)$, and then use Eq. (15) to determine $f_{k}^{*}(\lambda)$. For the Sierpinski gasket example, a Taylor series exansions of the moment generating function $f_{k}^{*}(\lambda)$ [Eq. (14) with Eq. (15)] determines the moments of the GFPT:

$$f_{1,n}^{*}(\lambda)=1+\frac{\{(d+1)^n[(d+3)^{n+1}-1]+(d+2)(d+3)^n\}d^2}{[(d+1)^{n+1}+d-1](d+2)}\lambda$$
$$+O(\lambda^2). \quad (16)$$

The coefficient of λ is the mean GFPT which matches the results found in Refs. [4,5]. The first and higher moments of the GFPT for alternative nodes can be calculated using our method. For example, the GFPT for a trap at the midbase of the 2D Sierpinski gasket is

$$f_{k,n}(s)=\frac{1}{2N}\left(\frac{(2\rho_n-1)}{\rho_n}\prod_{j=0}^{n}\frac{2\rho_j+1}{2\rho_j-1}-2+\frac{4\rho_{n-1}-1}{\rho_n}\right),$$

where $k=3(3^{n-1}+1)/2-2^{n-1}$ for $n\geq 1$, using the labeling in Fig. 1. For a discrete walker, we find

$$\langle T^*\rangle=\frac{2(15^n)-3^n+11(5^{n-1})}{3^{n+1}+1}.$$

IV. METHOD FOR OTHER RENORMALIZABLE STRUCTURES

For completeness it is useful to determine whether $f_{k,n}^{*}(\lambda)$ for any finitely ramified deterministic structure can be found. In the next section we are able to obtain at least one exact analytic expression. $f_{k,n}^{*}(\lambda)$ for other structures can also be calculated depending on the coordination number of the nodes in the network. For the Sierpinski gasket a simple expression for $f_{k,n}^{*}(\lambda)$ can be found for more than one node. This is due partly to the structure of the Sierpinski gasket, where every node is connected to $2d$ other nodes with the exception of the corners. In that case, conservation of prob-
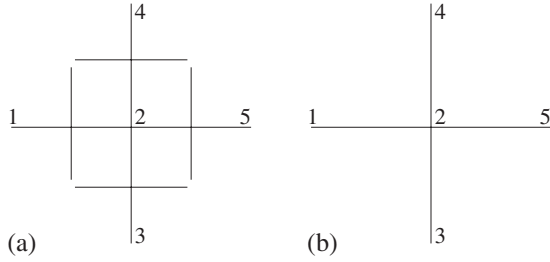
FIG. 3. Deterministic tree (a) $n=1$ (b) $n=0$. The labeling of the nodes 1 to 5 remain the same regardless of the iteration.

ability simplified the solution but such a formula might not exist for other structures. However, for all finitely ramified deterministic fractals there is always a renormalization scheme which allows us to calculate $f^*_{k,n}(\lambda)$ for the case of an end node.

In the next section, we will always calculate $f_{k,n}(s)$ for node 1. The trick in determining Eq. (10) is to express the concentrations at the interior nodes in terms of the concentrations at the exterior (end) nodes. This is relevant when calculating Eq. (10) in terms of the concentrations throughout the fractal, which can then be explicitly written as a function of the renormalization of the inverse FPT equation. $f^*_{k,n}(\lambda)$ can then be found from Eq. (15). As examples we calculate $f^*_{k,n}(\lambda)$ for four different fractals.

A. Deterministic tree

For the deterministic tree (Fig. 3) we calculate $f_{k,n}(s)$ for the end node 1. We can relate the concentrations at the nodes 2 to 4, for the iteration $n=0$, to the concentrations at nodes 1 and 5 in the following way:

$$\begin{bmatrix} p_{21,0} \\ p_{31,0} \\ p_{41,0} \end{bmatrix} = \frac{1}{2(2\rho_0^2-1)} \begin{bmatrix} \rho_0 & \rho_0 \\ 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} p_{11,0} \\ p_{51,0} \end{bmatrix}. \qquad (17)$$

Here $\rho_{n+1}=4\rho_n^2-3$ is the renormalization of the inverse FPT equation. We can deduce from Eq. (17) that

$$\sum_{i=2}^{4} p_{i1,0} = \frac{\rho_0+2}{2(2\rho_0^2-1)} \qquad (18)$$

and also that

$$\sum_{i=1}^{5} \kappa_i p_{i1,0} = \frac{2\rho_0(1+\rho_0)}{2\rho_0^2-1}, \qquad (19)$$

where κ_i is the coordination number associated with the ith node. These equations are essential, as they can be used repeatedly on any iteration of the deterministic tree to express the concentrations at the interior nodes in terms of the concentrations at the nodes 1 and 5. This will now be demonstrated for iteration 1, shown in Fig. 3, which we label consistently with iteration 0 (we are not concerned with the labeling of the new nodes). We denote θ_{2j} to be the sum of the concentrations at the nodes between node 2 (i.e., the center node) and node j on iteration 1. Using Eq. (18)

$$\theta_{21} = \frac{\rho_0+2}{2(2\rho_0^2-1)}(p_{11,1}+p_{21,1}).$$

Repeating this process for all unlabeled nodes and summing leads to

$$\theta_{21} + \theta_{23} + \theta_{24} + \theta_{25} = \frac{\rho_0+2}{2(2\rho_0^2-1)} \sum_{i=1}^{5} \kappa_i p_{i1,1}.$$

The final step is recalling (Sec. II) that if the sum of concentrations on the LHS of Eq. (19) gives the RHS of Eq. (19) with ρ_0 for iteration 0, then one can automatically assume that the LHS of Eq. (19) gives the RHS of Eq. (19) with ρ_0 being replaced by ρ_1 for iteration 1. In doing so, one finds the sum of the concentrations at all non-labeled nodes on the fractal at iteration 1 is

$$\theta_{21} + \theta_{23} + \theta_{24} + \theta_{25} = \frac{(\rho_0+2)(1+\rho_1)\rho_1}{(2\rho_0^2-1)(2\rho_1^2-1)}.$$

Furthermore, one can show that all concentrations at any node at any iteration can be expressed in terms of the concentrations at nodes 1 and 5 with the sum of concentrations at every node being

$$\sum_{j=1}^{N} p_{j1,n} = (p_{11,n}+p_{51,n})$$

$$\times \left[1 + \sum_{m=0}^{n} \left(\frac{(\rho_m+2)}{(4\rho_m^2-2)} \prod_{i=m+1}^{n} 2\frac{\rho_i(\rho_i+1)}{2\rho_i^2-1} \right) \right].$$

We know that there are exactly $N=4^{n+1}$ starting nodes, so $f_{1,n}(s)$ can be calculated from Eq. (10)

$$f_{1,n}(s) = \frac{1}{N} \left[\frac{1}{\rho_{n+1}} + \left(1 + \frac{1}{\rho_{n+1}} \right) \right.$$

$$\left. \times \sum_{m=0}^{n} \left(\frac{(\rho_m+2)}{(4\rho_m^2-2)} \prod_{i=m+1}^{n} 2\frac{\rho_i(\rho_i+1)}{2\rho_i^2-1} \right) \right].$$

Substituting for λ (15) and taking Taylor series expansions gives

$$f^*_{1,n}(\lambda) = 1 + \left(3(2^{n-1}) + \frac{6}{7}8^{1+n} - \frac{17}{28} \right)\lambda + O(\lambda^2).$$

More generally, one can construct a formula for any finitely ramified deterministic fractal, provided that it has two end nodes each having a coordination number of 1. In this case, one can find the following quantities:

$$y_1(\rho_0) = \frac{1}{p_{11,0}+p_{\nu1,0}} \sum_{\alpha} p_{\alpha1,0}, \qquad (20)$$

where α is an interior node and

$$y_2(\rho_0) = \frac{1}{p_{11,0}+p_{\nu1,0}} \sum_{j=1}^{N} \kappa_j p_{j1,0}. \qquad (21)$$

For consistency we always let 1 and ν represent the two end nodes of the nth iteration of the specific fractal. One can then

TABLE I. The first and second derivates of $\rho_n^*(\lambda)$, evaluated at $\lambda=0$, for the d-dimensional Sierpinski gasket, the Mandelbrot-Given curve (MG), the T tree, the deterministic tree (D), and the hierarchical percolation model (HP).

Lattice	$(\rho_n^*)'$	$(\rho_n^*)''$
Sierpinski	$-(d+3)^n$	$[4d(d+3)^n+d+6+d^2]/$ $[(d+3)^{1-n}(2+d)]$
MG curve	-22^n	$22^{n-1}[359+103(22^n)]/21$
T tree	-6^n	$6^n(4+6^n)/5$
D tree	-8^n	$8^n(6+8^n)/7$
HP model	-10^n	$10^{n-1}[7+3(10^n)]$

show that the GFPT density for a random walker to arrive at node 1 can be expressed as

$$f_{1,n}(s) = \frac{1}{N}\left[\frac{p_{\nu 1,n}}{p_{11,n}} + \left(1 + \frac{p_{\nu 1,n}}{p_{11,n}}\right)\sum_{m=0}^{n}\left(y_1(\rho_m)\prod_{i=m+1}^{n}y_2(\rho_i)\right)\right],$$

which becomes, using the fact that $p_{\nu 1,n}/p_{11,n}=\rho_{n+1}^{-1}$,

$$f_{1,n}(s) = \frac{1}{N}\left[\rho_{n+1}^{-1} + (1 + \rho_{n+1}^{-1})\sum_{m=0}^{n}\left(y_1(\rho_m)\prod_{i=m+1}^{n}y_2(\rho_i)\right)\right]. \tag{22}$$

Here ρ_n is the renormalization of the inverse FPT equation of the nth iteration of a finitely ramified deterministic fractal with two end nodes 1 and ν. To calculate $\langle T^*\rangle$ for discrete walkers we use $\rho_n^*(\lambda)|_{\lambda=0}=1$, and the first derivative of $\rho_n^*(\lambda)$ given in Table I. The method will be demonstrated on three simple examples.

B. T tree

Consider the T tree shown in Fig. 4. The decimation procedure assumes that flux leaves only through the end nodes 1 and 4 for every iteration n. The concentrations at nodes 2 and 3 for the iteration $n=0$ can be expressed in terms of the concentrations at nodes 1 and 4 in the following way:

$$\begin{bmatrix} p_{21,0} \\ p_{31,0} \end{bmatrix} = \frac{1}{3\rho_0^2 - 1}\begin{bmatrix} \rho_0 & \rho_0 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} p_{11,0} \\ p_{41,0} \end{bmatrix}.$$
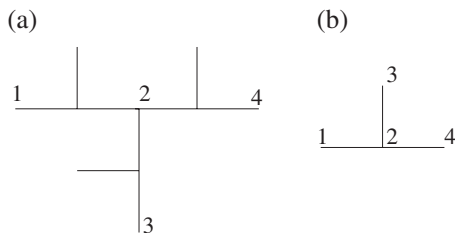
Hence, the quantities defined in Eqs. (20) and (21) are

(a)

(b)

FIG. 4. The T tree (a) $n=1$, (b) $n=0$. The labeling of the nodes remains the same for all iterations.

$$y_2(\rho_0) = 3\rho_0 y_1(\rho_0) = 3\frac{\rho_0(1 + \rho_0)}{3\rho_0^2 - 1}.$$

We use the renormalization of the inverse FPT equation $\rho_{n+1}=3\rho_n^2-2$ and $N=3^{n+1}$ in Eq. (22), to find

$$f_{1,n}(s) = \frac{1}{N}\left[\rho_{n+1}^{-1} + (1 + \rho_{n+1}^{-1})\right.$$

$$\left.\times \sum_{m=0}^{n}\left(\frac{(1 + \rho_m)}{3\rho_m^2 - 1}\prod_{i=m+1}^{n}3\frac{(1 + \rho_i)\rho_i}{3\rho_i^2 - 1}\right)\right]. \tag{23}$$

Substituting for λ (15) in Eq. (23) and taking Taylor series expansions gives

$$f_{1,n}^*(\lambda) = 1 + \left(\frac{2^{n+2}}{3} + \frac{4}{5}6^{n+1} - \frac{7}{15}\right)\lambda + O(\lambda^2).$$

The mean coincides with $\langle T^*\rangle$ for a trap at the center (node 2) of the T tree of iteration $n-1$ (replace n by $n-1$ in the above formula), which agrees with Ref. [6]. For the next two examples we just state N, the renormalization of the inverse FPT equation, and the two essential quantities $y_1(\rho_0), y_2(\rho_0)$.

C. Mandelbrot-Given curve

The Mandelbrot-Given curve is shown in Fig. 5. We find that $N=[6(8^{n+1})+1]/7$, $\rho_{n+1}=-21\rho_n+13/2\rho_n^{-1}-1/2\rho_n^{-3}+16\rho_n^3$,

$$y_1(\rho_0) = \frac{2\rho_0^2 + 2\rho_0 - 1}{8\rho_0^3 - 6\rho_0^2 - 2\rho_0 + 1}$$

and

$$y_2(\rho_0) = \frac{2\rho_0(4\rho_0^2 + \rho_0 - 1)}{8\rho_0^3 - 6\rho_0^2 - 2\rho_0 + 1}.$$

Substituting these expressions into Eq. (22), we find in the usual way that

$$f_{1,n}^*(\lambda) = 1 + 4/7\frac{1518(176^n) - 39(8^n) + 187(22^n)}{1 + 48(8^n)}\lambda + O(\lambda^2).$$

The coefficient of λ is the mean GFPT for a random walker to reach node 1 of the nth iteration of the Mandelbrot-Given curve.

D. Hierarchical percolation model

The hierarchical percolation model shown in Fig. 6 has the properties $N=[2(4^{n+1})+1]/3$, $\rho_{n+1}=\rho_n(9\rho_n^2-7)/2$ and
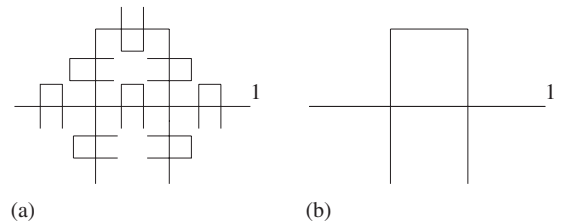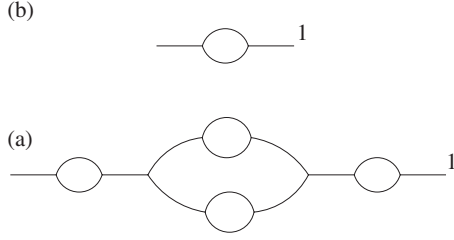

(a)

(b)

FIG. 5. Mandelbrot-Given curve (a) $n=1$, (b) $n=0$.

FIG. 6. Hierarchicial percolation model (a) $n=1$, (b) $n=0$.

$$y_2(\rho_0) = (3\rho_0 + 1)y_1(\rho_0) = \frac{(3\rho_0 + 1)}{3\rho_0 - 2}.$$

Using these results in Eq. (22), transforming to λ, and taking Taylor series expansions gives

$$f_{1,n}^*(\lambda) = 1 + 2\frac{10^{n+1} + 30(40^n) - 4^n}{1 + 2(4^{n+1})}\lambda + O(\lambda^2).$$

Here, as in all other examples, the coefficient of λ is the mean of the GFPT for node 1.

V. SCALING OF HIGHER ORDER MOMENTS

To find higher moments of the GFPT, it is necessary to calculate higher derivatives of $\rho_n^*(\lambda)$. We have given the relevant results in Table I. As an example, we calculate the second moment of the GFPT on a T tree. From the coefficient of λ^2 in the Taylor expansion of $f_n^*(\lambda)$ [Eq. (23) with Eq. (15)] we find that the second moment is given by

$$\langle (T^*)^2 \rangle = \frac{72}{5}12^n - \frac{16}{15}2^n + \frac{8928}{175}36^n - \frac{208}{25}6^n + \frac{53}{175}.$$

$$(24)$$

It is interesting to examine how the first and second moments, expressed as a function of the number of nodes $N_T = N + 1$, scale with the spectral dimension $\bar{d}$ [20]. Usually, $\bar{d}$ is determined through the analysis of the concentration at the origin $C_0(t)$, which is known to scale as

$$C_0(t) \sim t^{-\bar{d}/2}.$$

In Ref. [4,5], the mean GFPT expressed in terms of the total number of nodes N_T on the Sierpinski gasket was related to the spectral dimension $\bar{d} = 2 \ln(d+1)/\ln(d+3)$. This was done by rearranging the formula for the number of nodes on a d-dimensional gasket, $N_T = N + 1 = (d+1)[(d+1)^n + 1]/2$, to set $(d+1)^n = N_T^{\frac{2}{d+1}} - 1$ and $(d+3)^n = (N_T^{\frac{2}{d+1}} - 1)^{2/d}$. Substituting these values into Eq. (16) and taking the limit for large N_T gives $\langle T^* \rangle \sim N_T^{2/\bar{d}}$.

We perform a similar analysis for the second moment of the GFPT given in Eq. (24). There are $N_T = 3^{n+1} + 1$ nodes available on the nth iteration of the T fractal. By replacing 3^n by $(N_T - 1)/3$ and 2^n by $[(N_T - 1)/3]^{2/\bar{d}-1}$ in the expression for the second moment of the GFPT (24) we find
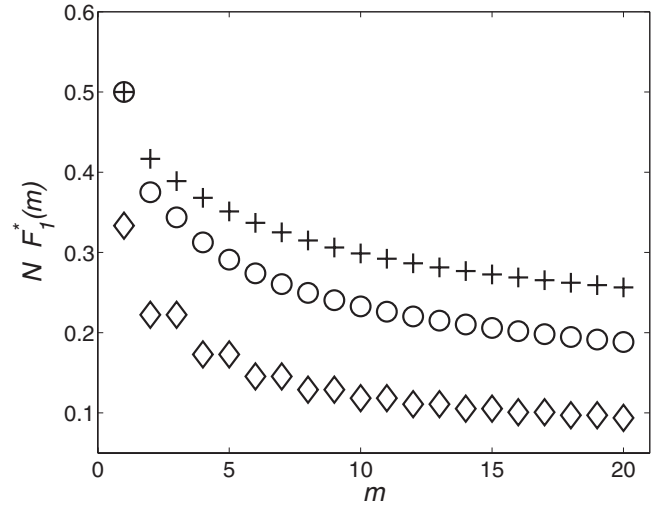

FIG. 7. The normalized probability for a random walker to arrive at a trap at node 1 on the mth jump for the 10th iteration of the Sierpinski gasket ($d=2$) ($\bigcirc$), Sierpinski gasket ($d=3$) ($+$), and the hierarchical percolation model ($\diamondsuit$). The values are calculated from the Taylor series of the GFPT generating function $f_1^*[\ln(z)]$. A symbolic algebra package was used.

$$\langle (T^*)^2 \rangle = 6/5(N_T - 1)^{4/\bar{d}-1} - \frac{8}{15}(N_T - 1)^{2/\bar{d}-1} + \frac{248}{175}(N_T - 1)^{4/\bar{d}}$$

$$- \frac{104}{75}(N_T - 1)^{2/\bar{d}} + \frac{53}{175}.$$

$$(25)$$

Asymptotically we find that $\langle (T^*)^2 \rangle \sim N_T^{4/\bar{d}}$. Since we have an exact expression for the mean and second moment we can show that the variance scales as

$$\mathrm{Var}(T^*) \sim N_T^{4/\bar{d}}.$$

$$(26)$$

All other structures considered above yield the same asymptotic behavior.

VI. CONCLUSION

We have used the properties of the renormalization of the first passage time equation to find the first passage time moment generating function for a variety of fractals. From this, we were able to derive simple expressions for the first and second moments of the global first passage time.

Our results can be applied to a diffusion controlled reaction experiment of the form $A + B \rightarrow B$. Here A is a particle which performs a random walk on the structure until it is absorbed by a single immobile particle B. If there are an infinite number of A particles then the reaction rate at node k is the deterministic function $F_k^*(m)$. This reaction rate, at node $k=1$, for the gasket in two and three dimensions, and the hierarchical percolation model, is shown for small time in Fig. 7. The first and second moment we have calculated are the moments of the reaction rate. An alternate experiment would involve a single walker, in which case the expected time of completion is $\langle T \rangle$ with the outcome being extremly variable, the variance being given by $\mathrm{Var}(T^*) \sim N_T^{4/\bar{d}}$.

Since the variance of the first passage time scales as Eq. (26), we relate the variance to the mean by calculating the reduced moment $R(N_T) = \text{Var}(T^*)^{1/2}/\langle T^* \rangle$. This type of approach has been used in the study of the variance of the range of an n-step random walk [8,21]. As in Ref. [21] we expect that $\lim_{N_T \to \infty} R(N_T)$ exists and remains finite, for every fractal structure with a spectral dimension of $\bar{d} < 2$. Using Eq. (14), we find the reduced second moment for the Sierpinski gasket to be

$$\lim_{N_T \to \infty} R(N_T) = \left(1 + \frac{8}{(d+3)(d+4)d} \right)^{1/2},$$

which decreases monotonically with d.

ACKNOWLEDGMENTS

APPENDIX A: CORNER CONCENTRATIONS

Here we show how the concentration at the apex and the corners of the nth iteration of the d-dimensional Sierpinski gasket can be calculated if a walker is released at the apex. We define $p_{c(i)1,n}$ to be the concentration at the $i = 1 \cdots d$ corners of the gasket. Recall that the concentration at the apex is given by $p_{11,n}$. The flux-concentration matrix has the simple (circulant) form

$$\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} da_n & -b_n & \dots & -b_n \\ -b_n & da_n & -b_n & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ -b_n & \dots & -b_n & da_n \end{pmatrix} \begin{pmatrix} p_{11,n} \\ p_{c(1)1,n} \\ \vdots \\ p_{c(d)1,n} \end{pmatrix}.$$

This is the natural extension of Eq. (5), with a_n and b_n defined in Eq. (8). The solution of the equations are

$$p_{c(i)1,n} = \frac{b_n}{d(a_n - b_n)(da_n + b_n)} = \frac{1}{db_n(\rho_n - 1)(d\rho_n + 1)}$$

(A1)

for $i = 1, \dots, d$ and

$$p_{11,n} = \frac{[da_n - (d-1)b_n]}{d(a_n - b_n)(da_n + b_n)} = \frac{[d\rho_n - (d-1)]}{db_n(\rho_n - 1)(d\rho_n + 1)}.$$

(A2)

If we use the renormalization of first passage time equation $\rho_n(d) = 2d\rho_{n-1}^2 - 3(d-1)\rho_{n-1} + (d-2)$ [see Eq. (9)] on the term $(\rho_n - 1)$ in $p_{11,n}$ (A2), we find that

$$p_{11,n} = \frac{[d\rho_n - (d-1)]}{db_n(2d\rho_{n-1} - d + 3)(\rho_{n-1} - 1)(d\rho_n + 1)}.$$

Using

$$b_n = \frac{(d\rho_{n-1} + 1)b_{n-1}}{[d\rho_{n-1} - (d-1)][2d\rho_{n-1} + (3-d)]},$$

we obtain

$$p_{11,n} = \frac{[d\rho_{n-1} - (d-1)]}{db_{n-1}(\rho_{n-1} - 1)(d\rho_{n-1} + 1)} \frac{[d\rho_n - (d-1)]}{(d\rho_n + 1)}.$$

Note the similarities with Eq. (A2). If we repeat the above procedure we get the result

$$p_{11,n} = \frac{\sinh(\sqrt{s})}{d\sqrt{s}[\cosh(\sqrt{s}) - 1]} \prod_{j=0}^{n} \frac{d\rho_j - (d-1)}{d\rho_j + 1}.$$

(A3)

The concentration at the corner points, defined in Eq. (A1), can be found using the same procedure used above. The result can be expressed as $p_{c(i)1,n} = p_{11,n}/[d\rho_n - (d-1)]$. From the two preceeding results it can be shown that $p_{11,n} + dp_{c(i)1,n} = p_{11,n-1}$ which agrees with the more general result given in Sec. III.

APPENDIX B: CONTINUUM TO DISCRETE TRANSFORMATIONS

The results we derive for a continuous space/continuous time random walker can be applied to a discrete walker by simple transformations. For a discrete walker the probability flux and probabilities at ends 1 and 2 of a bar are related by

$$F_1^*(m) = \frac{P_1^*(m)}{\kappa_1} - \frac{P_2^*(m-1)}{\kappa_2},$$

$$F_2^*(m) = \frac{P_2^*(m)}{\kappa_2} - \frac{P_1^*(m-1)}{\kappa_1},$$

where $m \geq 0$ and κ_i is the coordination number of the ith node. These equations are quite formal and are easier to understand when they are combined for a network.

Multiplying both equations by z^n and summing from $n = 0, \dots, \infty$ leads to

$$\begin{bmatrix} \hat{f}_1 \\ \hat{f}_2 \end{bmatrix} = \begin{bmatrix} 1/\kappa_1 & -z/\kappa_2 \\ -z/\kappa_1 & 1/\kappa_2 \end{bmatrix} \begin{bmatrix} \hat{p}_1 \\ \hat{p}_2 \end{bmatrix},$$

(B1)

where $\hat{p}_i(z) = \sum_{m=0}^{\infty} P^*(m)z^m$ is the probability generating function of $P^*(m)$. We have used the fact that $\sum_{i=0}^{\infty} P_i^*(m-1)z^m = P_i^*(-1) + z\sum_{i=0}^{\infty} P_i^*(m)z^m$ and define $P_i^*(-1) = 0$. Equation (B1) is the direct analog of Eq. (3).

The transformations we need to derive are most easily shown by example. Using Eq. (B1) for the first iteration of the 2D Sierpinski gasket gives

$$
\begin{bmatrix} \hat{f}_1 \\ \hat{f}_2 \\ \hat{f}_3 \\ \hat{f}_4 \\ \hat{f}_5 \\ \hat{f}_6 \end{bmatrix} = \begin{bmatrix} a_0 & -\dfrac{b_0}{4} & -\dfrac{b_0}{4} & 0 & 0 & 0 \\[2mm] -\dfrac{b_0}{2} & a_0 & -\dfrac{b_0}{4} & -\dfrac{b_0}{2} & -\dfrac{b_0}{4} & 0 \\[2mm] -\dfrac{b_0}{2} & -\dfrac{b_0}{4} & a_0 & 0 & -\dfrac{b_0}{4} & -\dfrac{b_0}{2} \\[2mm] 0 & -\dfrac{b_0}{4} & 0 & a_0 & -\dfrac{b_0}{4} & 0 \\[2mm] 0 & -\dfrac{b_0}{4} & -\dfrac{b_0}{4} & -\dfrac{b_0}{2} & a_0 & -\dfrac{b_0}{2} \\[2mm] 0 & 0 & -\dfrac{b_0}{4} & 0 & -\dfrac{b_0}{4} & a_0 \end{bmatrix} \begin{bmatrix} \hat{p}_1 \\ \hat{p}_2 \\ \hat{p}_3 \\ \hat{p}_4 \\ \hat{p}_5 \\ \hat{p}_6 \end{bmatrix},
$$

$$(B2)$$

where $a_0=1$ and $b_0=z$. We release a walker at site 1 at $t=0$ and place a trap at site 6 with probability conservation at other nodes. This means $\hat{\mathbf{p}}^T=(\hat{p}_1,\hat{p}_2,\hat{p}_3,\hat{p}_4,\hat{p}_5,0)$ and $\hat{\mathbf{f}}^T=(1,0,0,0,0,\hat{f}_6)$, where $-\hat{f}_6$ is the probability generating function of the first passage time. The matrix equation given above can also be directly derived from the equations governing the probability of a discrete walker on the gasket [i.e., $P_1^*(m+1)=P_2^*(m)/4+P_3^*(m)/4$ for node 1, etc.]. The initial and boundary conditions are represented in our flux vector.

If we write the matrix equation (B2) as $\hat{\mathbf{f}}=A\hat{\mathbf{p}}$ and multiply by $g=\tanh(\sqrt{s})/\sqrt{s}$, we obtain

$$g\hat{\mathbf{f}} = gA\hat{\mathbf{p}}. \qquad (B3)$$

Rescaling $\hat{\mathbf{p}}$ as

$$
\hat{\mathbf{p}}^T = \left(\frac{2\hat{p}_1'}{g}, \frac{4\hat{p}_2'}{g}, \frac{4\hat{p}_3'}{g}, \frac{2\hat{p}_4'}{g}, \frac{4\hat{p}_5'}{g}, 0 \right)
$$

transforms the matrix equation (B3) to $g\hat{\mathbf{f}}=A'\hat{\mathbf{p}}$. Because of our rescaling of $\hat{\mathbf{p}}$, the matrix A' is now identical to the flux-concentration matrix defined in Eq. (4) if z is replaced by $\mathrm{sech}(\sqrt{s})$. Comparing the variables in both problems shows how first passage time and probability generating functions for discrete walkers are related to their continuum counterparts.

More generally, for the quantities considered in this paper, the above example establishes the following transformations;

$$
p_{ij}(s) = \frac{1}{\kappa_i} \left. \frac{\tanh(\sqrt{s})}{\sqrt{s}} \hat{p}_{ij}(z) \right|_{z=\mathrm{sech}(\sqrt{s})},
$$

and $f_{ij}(s)=\hat{f}_{ij}[\mathrm{sech}(\sqrt{s})]$. Recall $\hat{f}$ is the probability generating function of the first passage time. In order to relate $\hat{f}$ to the moment generating function f^*, we make the further substitution $f^*(\lambda)=\hat{f}(e^\lambda)$. Thus the quantities in the main text are given by

$$
f_{kj}^*(\lambda) = \hat{f}_{kj}(e^\lambda) = f_{kj}[\mathrm{arcsech}(e^\lambda)^2]
$$

which is the transformation used throughout the paper.

We have not seen these transformations before, but they are analogous to the Montroll-Weiss transformations [Ref. [9], p. 254, Eq. (5.51)]. which relate the properties of a continuous time discrete space random walker to those of a discrete time discrete space random walker.

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