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Mean first-passage time on loopless aggregates

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We study the mean first-passage time (MFPT) for random walks on the backbone of loopless aggregates. We derive an exact expression for the MFPT on a general aggregate model. The exact MFPT for several deterministic and random disordered structures is calculated. We find that, in general, the exponent $\tau(1)$ describing the asymptotic dependence of the MFPT on the linear size of the system for diffusion is $\tau(1)=1+d_f$, where d_f is the fractal dimension of the aggregate.

I. INTRODUCTION

Diffusion properties on fractals and random aggregates have recently been studied very extensively (see, e.g., the review articles Refs. 1 and 2). An important quantity that characterizes the diffusion is the mean first-passage time (MFPT) of a random walker to reach a given surface. The MFPT for random walks on one-dimensional lattices has received considerable attention in a variety of approaches (see, e.g., Refs. 3 and 4). In the present work we study the MFPT along the backbone of a loopless aggregate. We consider models where along the backbone of the aggregate barriers, traps or dangling ends are distributed. Recently, an approach for solving the first-passage problem for a general network has been considered.[5] This approach has the advantage that it describes all possible characteristics of the dynamics of the network as a function of its components. However, it leads to complicated calculations even for simple structures. In the present work we suggest a simple approach to obtain the MFPT for a certain family of loopless structures.

In Sec. II we obtain a general relation for the MFPT, by reducing an aggregate problem to a one-dimensional problem. We show that the results are consistent with a combinatorial approach.

In Secs. III and IV we apply the relations obtained in Sec. II to various structures. In Sec. III, we examine the one-dimensional hopping model for two different symmetries (barriers and traps). We derive general results for the MFPT in this model, and calculate the MFPT for a deterministic hierarchical hopping model. We show that this model exhibits the same anomalous behavior as the typical MFPT of a random hopping model with a diverging average waiting time.

In Sec. IV we calculate the MFPT for the hierarchical comb and tree models. We discuss the MFPT for self-similar trees. A brief summary is presented in Sec. V.

II. CALCULATION OF THE MFPT

Consider a structure consisting of a backbone to which substructures are connected (see, e.g., Figs. 3 and 5). A walker can travel along the backbone and on the dangling structures. The dynamics is governed by a set of single-step transition probabilities from each site to each of its neighboring sites, subject to the condition that the sum of the transition probabilities from any site is less than or equal to 1. The backbone is a one-dimensional lattice on the interval $[1,L+1]$. We set a reflecting boundary at $x=1$ and wish to calculate the average time for a walker to reach the site $L+1$ for the first time. This is equivalent to placing an absorbing boundary or trap at site $L+1$ and calculating the average time to be trapped. (We have chosen the interval $[1,L+1]$ instead of the more conventional $[0,L]$ for convenience in calculations, but since the length of the system is L in both cases we shall denote mean values by S_L and T_L.) The structures attached to the backbone are finite (otherwise the MFPT is infinite) and are attached to the backbone at a single site, so that no loops are created on the backbone. This will enable us to decimate the dangling structures and associate a waiting time to each site on the backbone.

A. Definition of parameters for a single site

We define $e_i(t)$ to be the probability of a walker that begins at $t=0$ at site i to hop to one of its neighbors for the first time at time t. By assuming no loops on the backbone, and the fact that any structure attached to this site is finite we can ensure that eventually the walker must exit this site. Using $e_i(t)$ we can calculate the mean waiting time at site i, $\tau_i=\sum_0^\infty te_i(t)$. Let us define p_i (and q_i) as the conditional probabilities to leave site i to the right (or left) after waiting at this position. These probabilities are related to the single-step transition probabilities $\tilde{p}_i$ and $\tilde{q}_i$ to the right and left, respectively, by

$$p_i=\frac{\tilde{p}_i}{\tilde{p}_i+\tilde{q}_i}, \quad q_i=\frac{\tilde{q}_i}{\tilde{p}_i+\tilde{q}_i} . \tag{1}$$

The probabilities p_i and q_i obey $p_i+q_i=1$, and from here on they will be referred to as the normalized transition probabilities.

B. MFPT for a site adjacent to the trap

We shall now proceed to calculate a recursive relation for the MFPT of a walker initially placed at site $x=L$, that is adjacent to the absorbing boundary (see Fig. 1).

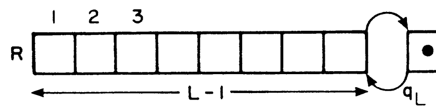

FIG. 1. A walker adjacent to the trap. The walker begins at time $t=0$ at site L. At the right of the segment there is a trap (T) and at the left there is a reflecting boundary (R): $\tilde{q}_1=0$. We wish to calculate the mean time for the walker to be trapped.

Define $Q_L(t)$ as the probability to be trapped at time t for the above initial condition. If we see the structure of length L as composed of a structure of length $L-1$ that is concatenated to a single site, we can write the following relation:

$$Q_L(t)=e_L(t)p_L + q_L \sum_{\tau=1}^{t} e_L(\tau) \sum_{\tau'=1}^{t-\tau} Q_{L-1}(\tau')Q_L(t-\tau-\tau') \; . \quad (2)$$

Relation (2) sums over all possible routes for trapping at time t. Writing the same equation for the generating functions[3–6] $\hat{Q}_L(z)$ and $\hat{e}_L(z)$, we obtain

$$\hat{Q}_L(z)=\frac{\hat{e}_L(z)p_L}{1-q_L\hat{e}_L(z)\hat{Q}_{L-1}(z)} \; . \quad (3)$$

If we define S_L as the MFPT for a walker initially adjacent to the trap, then by differentiation of Eq. (3) with respect to z and setting $z=1$, one obtains a recursive relation for the MFPT:

$$S_L=\frac{q_L}{p_L}S_{L-1}+\frac{1}{p_L}\tau_L \; . \quad (4)$$

Reapplying the recursion relation and using the fact that $S_1=\tau_1$ yields

$$S_L=\tau_1\prod_{n=2}^{L}\left[\frac{q_n}{p_n}\right]+\sum_{i=2}^{L}\frac{\tau_i}{p_i}\prod_{n=i+1}^{L}\left[\frac{q_n}{p_n}\right] \; . \quad (5)$$

Note that Eq. (5) is a generalization of the known expression for the MFPT on a linear chain.[3,4]

C. MFPT for a site at distance L from the trap

We now calculate the MFPT for a walker initially placed at $x=1$ (see Fig. 2). We label $P_L(t)$ as the probability to be trapped at time t, and T_L as the MFPT for this initial condition. In order to be trapped the walker must first reach site $x=L-1$, but from there on one returns to the previous problem of a walker adjacent to the trap. Thus,

$$P_L(t)=\sum_{\tau=1}^{t}P_{L-1}(\tau)Q_L(t-\tau) \; . \quad (6)$$

After transformation to the corresponding generating functions Eq. (6) becomes

$$\hat{P}_L(z)=\hat{P}_{L-1}(z)\hat{Q}_L(z) \; . \quad (7)$$

As before, differentiating and setting $z=1$ gives

$$T_L=T_{L-1}+S_L \; . \quad (8)$$

Applying this recursion relation and taking into account that $T_1=S_1$, it follows that

$$T_L=\sum_{n=1}^{L}S_n \; . \quad (8')$$

Taking the sum in Eq. (8′) only from x to L gives T_L^x, which is the MFPT for a walker placed initially at site x. An interesting observation is that the MFPT from a site adjacent to the trap is the derivative with respect to L of the MFPT from a site at distance L from the trap.

If the normalized transition probabilities along the backbone are constants ($p_n=p, q_n=q$), then one can distinguish between two cases: (a) Diffusion along the backbone ($p=q=\frac{1}{2}$) and (b) bias along the backbone ($p\neq q$). For the case (a) Eq. (5) is reduced to

$$S_L=\tau_1+2\sum_{i=2}^{L}\tau_i, \quad L\geq 2 \; . \quad (9)$$

Using Eqs. (8′) and (9) it follows that

$$T_L=-L\tau_1+2(L+1)\sum_{n=1}^{L}\tau_n-2\sum_{n=1}^{L}n\tau_n \; . \quad (10)$$

For case (b) we obtain in a similar manner

$$T_L=\frac{\tau_1 q}{p-q}\left[\left[\frac{q}{p}\right]^L-1\right]+\frac{1}{p-q}\sum_{n=1}^{L}\tau_n + \frac{1}{p-q}\left[\frac{q}{p}\right]^{L+1}\sum_{n=1}^{L}\tau_n\left[\frac{q}{p}\right]^n \; . \quad (11)$$

When $p<q$ the bias is directed against the trap, the MFPT is dominated by the first term in (11), and the dependence on L is exponential. When $p>q$ expressions (10) and (11) are similar. The first term comes from the fact that site $x=1$ is blocked in one direction and is negligible for large L. The second term is a function of the size of the system and of its components, but is independent on the internal order of the structure. The third represents the dependence on the internal order. In an ordered system where $\tau_n=\tau$, we obtain the well-known results for normal diffusion

$$T_L(v=0)=L^2\tau \; , \quad (12a)$$

$$T_L(v)\approx\frac{L\tau}{v}, \quad L\gg 1 \quad (12b)$$

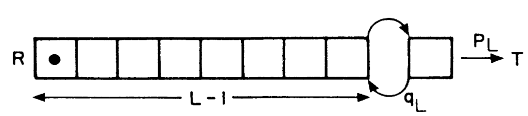

FIG. 2. A walker located a distance L from the trap. The walker begins at time $t=0$ at site 1. At the right of the segment there is a trap (T) and at the left there is a reflecting boundary (R):$\tilde{q}_1=0$. We wish to calculate the mean time for the walker to be trapped.

where $v \equiv p - q$. Before applying the above results [Eqs. (10) and (11)] for particular cases, it should be noted that it is possible to derive these results using a combinatorial method. Since trapping probabilities for FPT problems are in convolution form it is possible to write a set of self-consistent equations for the MFPT's from each site. Solution of this set of equations is equivalent to the following combinatorial approach:

$$T_L = p_L \sum_{n=0}^{\infty} q_L^n [T_{L-1} + \tau_L + n(\tau_L + T_{L-1} + T_{L-2})] . \tag{13}$$

Equation (13) describes the dynamics of exiting a structure of size $L-1$ and returning n times to that structure before being trapped. Calculating the above sum [Eq. (13)] one derives the following equation:

$$T_L - T_{L-1} = \frac{q_L}{p_L}(T_{L-1} - T_{L-2}) + \frac{1}{p_L}\tau_L . \tag{14}$$

Defining $S_L \equiv T_L - T_{L-1}$ we obtain Eq. (4).

III. MFPT FOR ONE-DIMENSIONAL HOPPING MODELS

In this chapter we begin by studying a general one-dimensional hopping model for two different symmetries (barriers and wells which behave as temporary traps). Later, we calculate the MFPT for both models in a particular case where the hopping probabilities are given by a hierarchical model.[17] We also consider the case where the hopping probabilities are random variables with the same distribution as the hierarchical model.

In the one-dimensional hopping lattice model each site is associated with hopping probabilities $\tilde{q}_n$, to the left, and $\tilde{p}_n$, to the right. The probability to remain at the same site is $1 - \tilde{p}_n - \tilde{q}_n$ and the mean waiting time at site i is therefore

$$\tau_n = \frac{1}{\tilde{p}_n + \tilde{q}_n} . \tag{15}$$

The well model is defined by the symmetry condition $\tilde{p}_n = \tilde{q}_n$. Due to the above symmetry, Eq. (5) becomes

$$S_L = \tau_1 + \sum_{n=2}^{L} \frac{\tau_n}{p_n} . \tag{16}$$

Using Eqs. (1) and (15) and the fact that $\tau_1 = 1/\tilde{p}_1$ we obtain

$$S_L = \sum_{n=1}^{L} \frac{1}{\tilde{p}_n} . \tag{17}$$

Note that in contrast to the expressions in the previous chapter, the transition probabilities $\tilde{p}_n$ are the single-step transition probabilities and not the normalized ones. Equation (17) shows some interesting properties of the one-dimensional wells model. A walker adjacent to the trap is able to "see" all the wells, but their internal ordering is of no importance. In a random well model the distribution of the transition probabilities and not their order will define the dynamical behavior. This is similar to the Zwanzig result for the diffusion constant,[8] $D^{-1} = 1/L \sum 1/\tilde{p}_n$. Thus Eq. (17) can be written as $S_L = D^{-1}L$. Using Eqs. (17) and (8) one can calculate T_L,

$$T_L = (L+1) \sum_{n=1}^{L} \frac{1}{\tilde{p}_n} - \sum_{n=1}^{L} \frac{n}{\tilde{p}_n} . \tag{18}$$

The barrier model is defined by the symmetry condition $\tilde{p}_n = \tilde{q}_{n+1}$. Using Eqs. (1), (5), and (15) one obtains

$$S_L = \frac{L}{\tilde{p}_L} . \tag{19}$$

This result is surprising when compared to the well model. A walker adjacent to the trap "sees" an ordered structure composed of L barriers of the same height as the barrier adjacent to the trap. From Eqs. (19) and (8′) follows

$$T_L = \sum_{n=1}^{L} \frac{n}{\tilde{p}_n} . \tag{20}$$

We now consider the MFPT on the hierarchical model introduced by Huberman and Kerszberg.[7] This model has been studied by several authors[9–11] and is shown in Fig. 3. The hopping probabilities are proportional to the inverse of the length of the teeth at each site. The lengths of the teeth l_n are given by the following equations:

$$l_n = R^k, \quad 1 < R < \infty$$
$$n(\mathrm{mod}\,2^{k+1}) = 2^k \quad k \geq 0 . \tag{21}$$

We proceed to calculate the MFPT for the hierachical wells and barriers. In the Appendix we have calculated the sums appearing in Eqs. (18) and (20) as a function of the generation of the structure. The Qth generation of the hierarchical structure is of length $2^{Q+1}-1$, so that the following expressions for the MFPT will be for these lengths only.

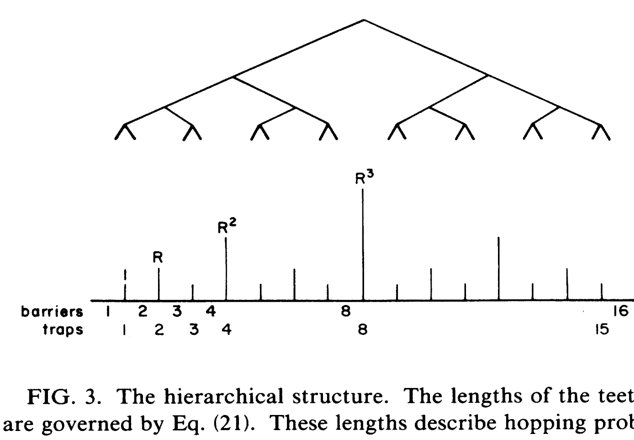

FIG. 3. The hierarchical structure. The lengths of the teeth are governed by Eq. (21). These lengths describe hopping probabilities for the hierarchical barrier and well models or lengths of dangling ends that a walker can walk on them in the hierarchical comb. For the barrier model the sites are defined between the teeth. For the well and comb models sites are defined at the bottom of the teeth.

For the case of hierarchical wells, we use Eqs. (18), (A4), and (A7) to obtain an exact expression for the MFPT,

$$T_L=-L+(L+1)\frac{(L+1)-(L+1)^{\log_2 R}}{2-R} . \quad (22)$$

Two different asymptotic behaviors are seen. For $L\to\infty$ we have

$$T_L\approx\begin{cases}\frac{(L+1)^2}{2-R}\propto L^2, & R\le 2\\ \frac{(L+1)^{1+\log_2 R}}{R-2}\propto L^{1+\log_2 R}, & R>2 .\end{cases} \quad (23)$$

We define the exponent $\tau(1)$ by the relation $T_L\propto L^{\tau(1)}$. The index (1) stands for the first moment of the FPT. Below the critical value $R\le R_c=2$ we have normal diffusive behavior with $\tau(1)=2$. Above the critical value we have anomalous behavior with $\tau(1)=1+\log_2 R$. This transition in the dynamics is similar to that exhibited by the mean-square displacement.[7,9–11] In fact, we find that $\tau(1)$ is equal to the diffusion exponent d_w, both above and below R_c. The diffusion exponent d_w is defined by $\langle x^2\rangle\propto t^{2/d_w}$, where $\langle x^2\rangle$ is the mean-square displacement of the walker after t steps.

For the case of hierarchical barriers one must normalize the hopping probabilities so that $\tilde{p}_n+\tilde{q}_n$ will not exceed unity. We therefore write $\tilde{p}_n=R^{-k}/A$. The constant A will only change the time scale as can easily be seen by examining the master equation governing the dynamics. Using Eqs. (20) and (A7) we derive the MFPT,

$$T_L=A\frac{L+1(L+1)-(L+1)^{\log_2 R}}{2-R} . \quad (24)$$

In Eq. (24) it is seen how the normalization of the hopping probabilities is reflected in the factor that multiplies the MFPT. For large enough systems ($L\gg 1$) the barrier model exhibits the same phase transition exhibited in the well model. That is,

$$\tau(1)=\begin{cases}2, & R\le 2\\ 1+\log_2 R, & R>2 .\end{cases} \quad (25)$$

Until now we have discussed only deterministic models. When the hopping probabilities are random variables, with a probability distribution $\rho(\tilde{p})$, one must take an ensemble average over all the possible configurations. If $\langle 1/\tilde{p}\rangle\equiv D_{av}^{-1}$ converges, the solution is simple. This is exactly case (a) solved by Alexander *et al.*[12] yielding normal diffusion. For this case the ensemble averages over Eqs. (18) and (20) yield the same result,

$$\langle T_L\rangle=\frac{L(L+1)}{2D_{av}} . \quad (26)$$

When the above inverse hopping probability average diverges one finds anomalous diffusion.[12] For this case the divergence of the average waiting time gives rise to an infinite average MFPT. Since the first passage problem deals with a finite system, the typical FPT on such a system will not diverge. One has to take into account a cutoff in the transition probabilities, i.e., a minimum transition rate $\tilde{p}_{min}$, which represents the MFPT for a typical configuration.

Similar to the case of the mean-square displacement on the infinite lattice, here also, the appearance of anomalous behavior is due only to the distribution of the transition probabilities or waiting times, and is not a characteristic of their internal ordering.[9] The transition probability distribution in the hierarchical model is[9] $\phi(\tilde{p})=\tilde{p}^{-\gamma}$ where $\gamma=\ln 2/\ln R$ [the analog for continuous lengths is $\rho(\tilde{p})=(1-\alpha)\tilde{p}^{-\alpha}$ where $\alpha=1-\ln 2/\ln R$]. This distribution coincides with case (*c*) solved by Alexander *et al.* for $R>2$. As previously stated, in order to calculate the typical FPT we must take into account an appropriate cutoff. The cutoff is taken to be the maximum tooth in a Qth generation of the hierarchical model.[11] We therefore find

$$\left\langle\frac{1}{\tilde{p}}\right\rangle=\frac{1}{2}\sum_{n=0}^{Q}R^n(R^n)^{-\log_R 2}=\frac{1-(L+1)^{-1+\log_2 R}}{2-R} . \quad (27)$$

Thus, the average MFPT is

$$\langle T_L\rangle=\frac{L}{2}\frac{(L+1)-(L+1)^{\log_2 R}}{2-R} . \quad (28)$$

If we define $\tau_{typ}(1)$ by $\langle T_L\rangle\propto L^{\tau_{typ}(1)}$ for large L then

$$\tau_{type}(1)=\begin{cases}2, & R\le 2\\ 1+\log_2 R, & R>2 ,\end{cases} \quad (29)$$

which is identical to the exponent $\tau(1)$ for the deterministic model.

IV. MFPT FOR COMBS AND TREES

In this chapter we deal with models that have dangling structures attached to the backbone on which particles can walk. We begin by describing the general method to calculate the MFPT for such models. We then proceed to calculate the MFPT for two examples: the hierarchical comb and the hierarchical tree. The expressions derived are in agreement with previous results for the MFPT asymptotic dependence on the size of the system.[13–15]

Figure 4 shows an arbitrary structure attached to the

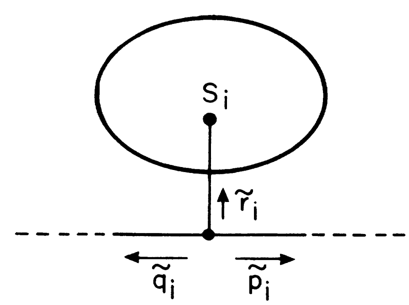

FIG. 4. A dangling structure attached to site i. There is a probability $\tilde{r}_i$ to enter the structure. The mean duration of this sojourn is S_i. The mean waiting time at site i as a function of S_i and $\tilde{r}_i$ is given by Eq. (30).

backbone at site i. Site i has single-step hopping probabilities governing the motion to the right, p_i left, q_i, and up onto the attached structure, $\tilde{r}_i$. (It is possible to define a probability to remain at site i.) We wish to express the mean waiting time at site i, τ_i, as a function of $\tilde{r}_i$ and of the waiting time on the attached structure once it is entered. This is exactly the MFPT of this structure when the walker is adjacent to the trap. Let us depict this value by S_i. We can write, using a combinatorial approach the following expression for τ_i:

$$\tau_i=(1-\tilde{r}_i)\sum_{n=0}^{\infty}\tilde{r}_i^n[1+n(S_i+1)]=1+\frac{\tilde{r}_i}{1-\tilde{r}_i}(S_i+1)\ . \tag{30}$$

The most simple structure to build is a comb structure. In this model a tooth of length l_i is attached to site i of the backbone. In the length l_i we include the site on the backbone, so the structure attached is, in fact, of length l_i-1. Using the fact that for a one-dimensional chain $S_L=2L-1$ and setting $\tilde{r}=\frac{1}{3}$ (all directions are equal), Eq. (30) gives a result convenient for use: $\tau_i=l_i$. The following results are based on the assumption that $\tilde{r}=\frac{1}{3}$, but can easily be generalized for any value of $\tilde{r}$. Moreover, the asymptotic dependence on the linear size of the system is independent on $\tilde{r}$. We now proceed to calculate the MFPT for a deterministic hierarchical comb structure (see Fig. 3), in which the lengths of the teeth are governed by Eq. (21). Since the average waiting time τ_i is exactly the same as in the hierarchical trap model, then for the case of diffusion along the backbone ($\tilde{p}=\tilde{q}=\frac{1}{3}$) the MFPT for the hierarchical comb is exactly the expression derived above for the MFPT of the hierarchical well model:

$$T_L=-L+(L+1)\frac{(L+1)-(L+1)^{\log_2 R}}{2-R}\ . \tag{31}$$

For the case of bias along the backbone ($p\neq q$) we can calculate the MFPT using Eqs. (11), (A4), and (A9),

$$\begin{aligned}T_L=&\frac{q}{p-q}\left[\left[\frac{q}{p}\right]^L-1\right]+\frac{1}{p-q}\frac{(L+1)-(L+1)^{\log_2 R}}{2-R}\\&-\frac{1}{p-q}\left[\frac{q}{p}\right]^{L+1}\left[1-\left[\frac{p}{q}\right]^{L+1}\right]\\&\times\sum_{k=0}^{Q}R^k\left[\frac{p}{q}\right]^{2^k}\left[1-\left[\frac{p}{q}\right]^{2^{k+1}}\right]^{-1}\ .\end{aligned} \tag{32}$$

When $p>q$ and for large systems $L\gg 1$, then according to Eq. (A10) the last term in Eq. (32) converges to a constant and we are able to write

$$T_L\approx\frac{1}{p-q}\frac{(L+1)-(L+1)^{\log_2 R}}{2-R}\ . \tag{33}$$

The asymptotic dependence of T_L on the length of the system, described by $\tau(1)$ is, of course, equivalent to that of the hierarchical well model [Eq. (23)]. This asymptotic result remains valid for the typical FPT on a random comb model with the same length distribution. This can be shown following the same reasoning applied for the random well model. The equivalence of the comb and well models is restricted to the MFPT only. Other moments of the first passage time will be different in value and asymptotic behavior as a function of the size of the system. This is due to the fact that the trapping probabilities $P_L(t)$ are different in the two models. Moreover, $\tau(1)$ for the comb model is different from the diffusion exponent d_w as stated elsewhere.[13,14]

As a last example we consider the hierarchical tree (see Fig. 5). This structure is self-similar in all length scales. A tree of order Q is composed of trees of lower order dangling from the backbone. We consider a tree of coordinate number $z=3$ where all directions are equal, that is, hopping probabilities in all directions are $\frac{1}{3}$. Let us consider the average waiting time at a site that has a tree of order Q attached to it. According to Eq. (30) this value is

$$\tau^{(Q)}=\tfrac{3}{2}+\tfrac{1}{2}S^{(Q)}\ , \tag{34}$$

where $S^{(Q)}$ is the MFPT for the walker initially adjacent to the trap in a tree of order Q. Using Eq. (5) and taking into account the recursive structure of the tree we find

$$\begin{aligned}S^{(Q)}&=2\sum_{n=1}^{L}\tau_n-\tau_1=2S^{(Q-1)}-\tau_1+2(\tfrac{3}{2}+\tfrac{1}{2}S^{(Q-1)})\\&=3S^{(Q-1)}-\tau_1+3\ .\end{aligned} \tag{35}$$

Applying the recursion with the fact that $S^{(0)}=1$ and $\tau_1=1$ we obtain

$$S^{(Q)}=2\times 3^Q-1\ , \tag{36a}$$

$$\tau^{(Q)}=3^Q+1\ . \tag{36b}$$

From here on one can calculate T_L from Eq. (10), using a technique similar to that shown in the Appendix for the hierarchical comb. The result is

$$T_L=-\tfrac{3}{2}L+\tfrac{3}{2}L^{\log_2 6}+2L^{\log_2 3}\ . \tag{37}$$

For large systems ($L\gg 1$) we find the asymptotic dependence on the length is described by $\tau(1)=\log_2 6$.

We can generalize Eq. (37) for an arbitrary fractal tree

FIG. 5. The hierarchical tree. This is a loopless fractal of coordinate number $z=3$. (a) A tree of order $Q=4$ embedded on a square lattice. (b) A tree of order $Q=3$ imbedded on a binary tree.

of coordinate number z (see, e.g., Fig. 6). If all directions on this tree are equal (the hopping transition probability is $(z-2)/z$), then the MFPT obtained is

$$T_L = -\tfrac{3}{2}L + \tfrac{3}{2}L^{1+\log_2 z} + 2L^{\log_2 z} . \quad (38)$$

The fractal dimension of the tree is $d_f = \log_2 z$, so the asymptotic dependence of the MFPT on the length is $\tau(1) = 1 + \log_2 z = 1 + d_f$. This is probably true not only for deterministic fractal trees, but for random ones as well (see, e.g., Ref. 2).

V. SUMMARY

A general method to calculate the MFPT for deterministic loopless structures has been presented. Exact expressions have been derived for several models including combs and trees. For random structures we have calculated the typical FPT by taking the appropriate cutoff. In both cases we can associate the waiting time at a site with a "mass" (this is the real mass in the comb structure or the depth of a well in the well model). The average mass along a segment of length L behaves as $M \sim L^{d_f}$ where d_f is the fractal dimension.[16] The average waiting time per site is, therefore

$$\tau = \frac{M}{L} \sim L^{d_f - 1} . \quad (39)$$

Thus using Eqs. (10) and (11) we can write for diffusion with or without bias along the backbone

$$T_L \propto \begin{cases} L^{1+d_f}, & v = 0 \\ \dfrac{L^{d_f}}{v}, & v \equiv p - q > 0,\ L \gg 1 . \end{cases} \quad (40)$$

This result is consistent with the asymptotic behavior obtained for the MFPT in the preceeding chapters.

Note added. After this work was completed, we learned of complementary results derived by Murthy and Kehr (unpublished) for MFPT on one dimensional hopping models.

ACKNOWLEDGMENTS

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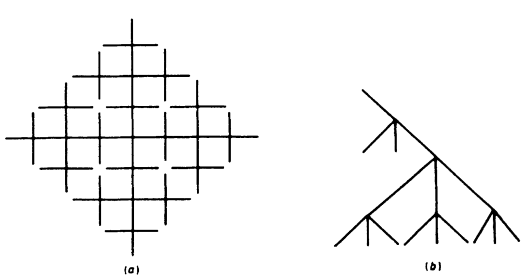

FIG. 6. A fractal of coordinate number $z=4$ embedded (a) on a square lattice (b) on a Cayley tree lattice. Fractals of higher coordination numbers can be embedded only in higher dimensions or on a Cayley tree.

APPENDIX: CALCULATIONS FOR THE HIERARCHICAL STRUCTURE

Here we calculate a few quantities needed for the calculation of the MFPT on hierarchical structures (see Fig. 3). We calculate these values as a function of the generation Q of the hierarchical structure. In the Qth generation the highest tooth is of length R^Q. The number of teeth in structure of order Q is

$$L = 2^{Q+1} - 1 . \quad (A1)$$

The tooth length at site n is given by

$$l_n = R^k , \quad n \bmod 2^{k+1} = 2^k . \quad (A2)$$

We are interested in calculating the value of three expressions that appear in Eqs. (10) and (11):

(a) $\sum_{n=1}^{L} l_n$,

(b) $\sum_{n=1}^{L} n l_n$,

(c) $\sum_{n=1}^{L} l_n a^n$.

Instead of summing over the positions n it is more convenient to sum over teeth of the same size, R^K. Therefore,

$$\sum_{n=1}^{L} \to \sum_{K=0}^{Q} .$$

Since the number of teeth of length R^K is 2^{Q-K}, we write

$$\sum_{n=1}^{L} l_n = \sum_{K=0}^{Q} 2^{Q-K} R^K = 2^Q \sum_{K=0}^{Q} \left[\frac{R}{2} \right]^K = \frac{2^{Q+1} - R^{Q+1}}{2-R} . \quad (A3)$$

We find that value (a) is

$$\sum_{n=1}^{L} l_n = \frac{(L+1) - (L+1)^{\log_2 R}}{2-R} . \quad (A4)$$

In order to calculate the sum (b), we first must calculate the sum of the positions of teeth of length R^K. From Eq. (A2) these positions are

$$2^K + m 2^{K+1} \quad (m = 0, 1, \ldots, 2^{Q-K} - 1) .$$

The sum of the positions is

$$\sum_{m=0}^{2^{Q-K}-1} 2^K + m 2^{K+1} = 2^K 2^{Q-K} + 2^Q (2^{Q-K} - 1) = 2^{2Q-K} . \quad (A5)$$

The sum (b) is therefore

$$\sum_{n=1}^{L} n l_n = \sum_{K=0}^{Q} 2^{2Q-K} R^K = 2^Q \sum_{n=1}^{L} l_n . \quad (A6)$$

Using Eq. (A3) we find

$$\sum_{n=1}^{L} n l_n = \frac{L+1}{2}\,\frac{(L+1)-(L+1)^{\log_2 R}}{2-R} \;. \tag{A7}$$

Before calculating the sum (c), we first sum terms of teeth of length R^K

$$\sum_{m=0}^{2^{Q-K}-1} R^K a^{(2^K+m2^{K+1})} = R^K a^{2^K} \frac{1-a^{2^{Q+1}}}{1-a^{2^{K+1}}} \;. \tag{A8}$$

The sum for the whole structure is therefore

$$\sum_{n=1}^{L} l_n a^n = (1-a^{L+1}) \sum_{K=0}^{Q} \frac{R^K - a^{2^K}}{1-a^{2^{K+1}}} \;. \tag{A9}$$

For large systems ($Q \to \infty$) the sum in Eq. (A9) converges to a constant that does not depend on Q:

$$\sum_{n=1}^{L} l_n a^n \to A(1-a^{L+1}), \quad L \gg 1 \;. \tag{A10}$$

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