Analytic method for calculating properties of random walks on networks

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Unlike the case of regular networks, such as lattices, no method of general applicability exists for dealing with random walks on complex networks. We propose a method, which is based on the identification of certain types of walks on a one-dimensional segment as basic. Generating functions for complex networks or for complex types of walks can all be constructed from the generating functions corresponding to these basic walks. We also define basic walks corresponding to a network. The properties of walks in a network composed of "black boxes," each containing a network by itself, can be expressed in terms of the basic walks defined for the single black box. This result can be compared to the way the Kirchhoff rules allow one to calculate properties of a network of "elements" in terms of the impedances of each of the elements. In the present case the combination rules are more complex than in the electrical case. Our method is demonstrated by calculating mean first-passage times on several structures: a segment, a segment with a single dangling bond, a segment with many dangling bonds, and a looplike structure. The results are analyzed and related to the question of applicability of the Einstein relation between conductance and diffusion.

I. INTRODUCTION

The importance of the random-walk problem in many areas of science and technology and as a mathematical problem in its own right is well known. Some excellent textbooks[1] and reviews[2] provide details of the enormous advances this field has experienced since its inception at the beginning of the century.

Many important problems related to random walks are still open; others are only partially understood—and new questions have arisen only lately. For example, the problems of self-avoiding random walks or random walks on random lattices (with or without traps) or on fractals are still subjects of many investigations. The recent interest in these and related problems is partially due to their relevance to the theories of percolation[3–9] or flow through porous media.[10] In many problems the long-time properties or the diffusion limit is of interest. In some, one may be interested in transients.

Most methods that were applied to random walks of complex nature (*not* on regular lattices, for example) are approximate. Typical methods would be of the mean-field type, effective-medium theory, renormalization group (RG), and numerical simulations. Interesting results were obtained in the case of anomalous diffusion (i.e., $D \sim$ power of the length scale) using scaling and RG methods and assuming the Einstein relation to hold in this case.[4–8] For example, one may calculate the diffusion laws on finite scales and relate them to anomalous wave-vector and frequency dependence of ac conductivities or ac dielectric functions.[4–8]

While we see no point in presenting a survey of the enormous literature in the field of random walks, we wish to single out the problems associated with percolation,[9] because in this case it is the *geometry* which is the source of anomalous behavior. So far, mainly scaling arguments and numerical simulations were employed in this field.[3–6] However, a microscopic understanding is still lacking.

In this paper we present a method of calculating properties of discrete random walks on networks, which—we hope—is a first step towards the development of a microscopic approach to random-walk problems on branched (and other complex) networks, as well as to the related diffusion problems.

The problems we deal with can, in principle, be solved using a master equation approach.[11] However, even for relatively simple structures, this approach requires an enormous amount of labor. In more complex cases (some of which are solved in this paper), the application of this method becomes impractical. In contrast, the method presented here remains fairly simple even for quite complicated structures.

In this paper we demonstrate our method by calculating the mean first-passage times for several systems. The basic idea is to divide complex networks into simpler units whose contribution to the mean first-passage time is calculated. One can then proceed by further iterating the simplified network. When the system is geometrically self-similar, the procedure resembles the renormalization-group process. Among the results we obtain, we find worthwhile mentioning the fact that the effect of many "short" dangling bonds may be equivalent or different from that of one or a few "long" dangling bonds (depending on the "limits" considered), in contrast to a simple argument based on a naive interpretation of the Einstein relation. We also study the two channel in parallel structure ("loop") and compare the result to a one-channel structure. In this paper we present only relatively simple cases,

since our *main aim* here is demonstrating our method. Applications will be presented in future publications.

The structure of the paper is as follows. Section II contains a definition of the problem and an outline of our method. In Sec. III we apply our method to the random-walk problem on a straight segment. Except for the obvious role of this section—to demonstrate that our method actually works—it is being used to define and calculate some basic quantities, which are then employed in all subsequent sections. Section IV deals with the problem of a random walk on a segment with a single dangling bond. In Sec. V we treat the loop configuration. The problem of many dangling bonds is treated in Sec. VI. Section VII provides a summary of the results obtained in this paper as well as some remarks on possible generalizations and future work.

II. DEFINITIONS AND OUTLINE OF THE METHOD

Mathematically, the problem we deal with is that of a random walk on a finite collection of points. A random walker starts at a given point. At each "step" the walker has a given probability to move to any point in the collection, including its present point. Thus, if we label the points by $i=1,2,\ldots,N$, we are given a set of probabilities p_{ij} to move, at each step, from point i to point j. The numbers p_{ij} must, of course, satisfy

$$\sum_{j=1}^{N} p_{ij}=1 , \tag{2.1}$$

$$p_{ij}\geq 0 \quad \text{for all } 1\leq i,j\leq N , \tag{2.2}$$

and are otherwise unrestricted, in principle. A realization or a path of an n-step walk is the (ordered) set of points a walker has "actually" visited: $i_1,i_2,\ldots,i_n$. The numbers i_k belong to the set $\{1,2,\ldots,N\}$. Repetition (say $i_k=i_l$, $l\neq k$) is allowed, in principle, and n can be any natural number. Given that the walker starts at i_1, the probability of the above realization is $\prod_{r=1}^{n-1} p_{i_r,i_{r+1}}$. A *walk* is a set of paths satisfying some restrictions. For example, we may wish to consider a walk from a given point A to a given point B in n steps. The probability of a given walk is the sum of probabilities of *all* distinct paths (i.e., differ from each other in at least one step) that satisfy the restrictions of the walk. We define a walk from A to B as "for the first time," a walk in which the walker starts at point A and reaches point B for the first time, namely point B was not reached in any path before the walk ended at B.

Consider now a walk from A to B, in n steps, in which a third point C was visited on the way. Define $P_{AC}(n_1)$ as the probability of a walk to start at A and reach point C for the first time in n_1 steps and $\tilde{P}_{CB}(n_2)$ as the probability to start at C and reach B in n_2 steps. Note the restriction on the walk from A to C (first time) and the absence of this restriction when moving from C to B. The role of the restriction is to avoid "overcounting" of paths. The probability $P_{AB}(n)$ to move from A to B "through" C in n steps is

$$\tilde{P}^{C}_{AB}(n)=\sum_{n_1=0}^{n}\sum_{n_1=0}^{n} P_{AC}(n_1)\tilde{P}_{CB}(n_2)\delta_{n_1+n_2,n} , \tag{2.3}$$

where δ is Kronecker's symbol. (Note that if $A=C$, the $n_1=0$ term contributes.)

Let $P_W(n)$ be the probability for a given walk to be performed in n steps. Here W represents the relevant parameters of the walk (such as AC in the above example). It is common to define the *corresponding generating* function[1,2] $G_W(\phi)$ as[12]

$$G_W(\phi)\equiv\sum_{n=0}^{\infty} e^{i\phi n}P_W(n) , \tag{2.4}$$

where $0\leq\phi\leq 2\pi$. In what follows we may write G for $G(\phi)$, the ϕ dependence being understood. We shall also call $G(\phi)$ the ϕ probability of this walk, for reasons to become clear later.

It follows from (2.3) and (2.4) that

$$\tilde{G}^{C}_{AB}(\phi)=G_{AC}(\phi)\tilde{G}_{CB}(\phi) , \tag{2.5}$$

where the notation is obvious. The advantage of using ϕ probabilities is that, as we see from Eq. (2.5), ϕ probabilities of parts of walks (such as AC and CB) multiply. The restriction embodied in the Kronecker δ in Eq. (2.3) does not appear at the level of ϕ probabilities. Equation (2.3) can be generalized for a walk from a point A_0 to a point A_N that goes through the points $A_1,A_2,\ldots,A_{N-1}$ in that precise order. Using obvious notation

$$\tilde{P}_{A_0,A_1,\ldots,A_N}(n)=\sum_{n_1=0}^{N}\sum_{n_2=0}^{N}\cdots\sum_{n_N=0}^{N} P_{A_0,A_1}(n_1)P_{A_1,A_2}(n_2)\cdots\tilde{P}_{A_{N-1},A_N}(n_N)\delta_{n_1+n_2+\cdots+n_N,n} . \tag{2.6}$$

For reasons similar to those described above the probabilities, $P_{A_i,A_{i+1}}$ $(0\leq i\leq N-2)$ refer to reaching A_{i+1} for the first time and $\tilde{P}_{A_{N-1},N}$ is not restricted this way. Going over to ϕ probabilities,

$$\tilde{G}_{A_0,A_1,\ldots,A_N}(\phi)=G_{A_1A_1}(\phi)G_{A_1A_2}(\phi)\cdots\tilde{G}_{A_{N-1},A_N}(\phi) . \tag{2.7}$$

Thus, the ϕ probabilities for subpaths (property restricted) multiply.

Another kind of walk we wish to define is a *branched walk*. It is a walk whose paths can be divided into distinct subsets we call branches. For example, a walker may be required to go, in n steps, from a point A to a point B through a point C *or* D, but not through both. The probability of doing so is (using obvious notation)

$$\tilde{P}_{AB}^{C;D}(n)=\sum_{n_1=0}^{n}\sum_{n_2=0}^{n}\tilde{P}_{AC}^{(-D)}(n_1)P_{CB}^{(-D)}(n_2)\delta_{n_1+n_2,n}$$
$$+\sum_{n_1=0}^{n}\sum_{n_2=0}^{n}\tilde{P}_{AD}^{(-C)}(n_1)P_{DB}^{(-C)}(n_2)\delta_{n_1+n_2,n}\ ,$$

where the restrictions applying to the various P's are obvious. In the ϕ-probability language

$$\tilde{G}_{AB}^{C;D}(\phi)=\tilde{G}_{AC}^{(-D)}(\phi)G_{CB}^{(-D)}(\phi)+\tilde{G}_{AD}^{(-C)}(\phi)G_{DB}^{(-C)}(\phi)\ . \tag{2.8}$$

This result, too, can be generalized to the case of many branches and many subpaths. We write symbolically

$$G_{AB}(\phi)=\sum_{\alpha}\sum_{r}G_{\alpha_1}^{\alpha}(\phi)G_{\alpha_2}^{\alpha}(\phi)\cdots G_{\alpha_r}^{\alpha}(\phi)\ , \tag{2.9}$$

where α symbolizes the different branches, r denotes the number of subpaths (each branch may be divided into sets of subpaths of different r's), and α_i labels the subpaths. Equation (2.9) means that ϕ probabilities add and multiply precisely as regular probabilities do (hence their name), except that one does not have to worry about the number of steps. As is well known,[1,2] the knowledge of a ϕ probability $G(\phi)$ is equivalent to the knowledge of all the corresponding probabilities $P(n)$, since the inversion is trivial (in principle).

So far we have dealt with a general set of points. It is convenient for ease of labeling (and for obvious physical reasons) to arrange the points on simple geometric structures such as segments (Fig. 1), segments with dangling bonds (Figs. 2 and 3), loops (Fig. 4), lattices, etc. We work in discrete time. (Hopping time distributions will be considered in future publications.) Finally, for the sake of definiteness of the calculations that follow (and for simplicity), we define the probability distributions to be used in this work as follows: (a) Each point has at most four nearest neighbors, (b) when a point has fewer than four nearest neighbors we consider it to have "fictitious" bonds to itself (see Fig. 5) so that its total number of bonds is four, and (c) a walker at a given point has a probability of $\frac{1}{4}$ to use any of these four bonds (to itself and to its nearest neighbors) (see Fig. 5).

We reiterate that our specific choice of probabilities does not limit the generality of our results (as the reader can verify).[13] Our method can be applied to *any* choice of probabilities (e.g., the expression for X [see Eq. (2.10)], where the number of nearest neighbors is not four, is changed, but it plays the same role in the expressions for the more complex networks).

One consequence of introducing the fictitious bonds is that the probability to stay at an "end point" like A in Fig. 2, for one step, is $\frac{3}{4}$, whereas the similar probability

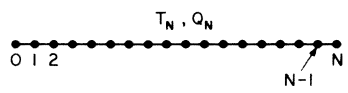

FIG. 1. Straight segment configuration.

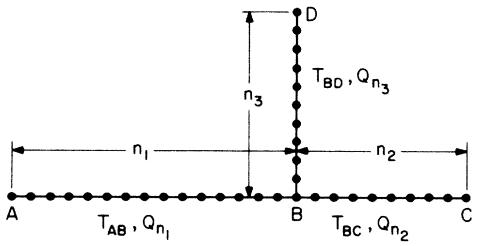

FIG. 2. A segment with a single dangling bond.

at point B in Fig. 2 is $\frac{1}{4}$. At a middle point on a segment (such as point 2 in Fig. 1) this probability is $\frac{1}{2}$. The corresponding ϕ probabilities [i.e., of staying at a given point for *one step* (this is a well-defined walk)] are $\frac{3}{4}e^{i\phi}$, $\frac{1}{4}e^{i\phi}$, and $\frac{1}{2}e^{i\phi}$, respectively.

In order to demonstrate our method we present in this section a calculation of the ϕ probabilities in two simple cases. The first is the ϕ probability for a walker to stay at its initial point (not necessarily for one step, i.e., sum all n), which is assumed to have r fictitious bonds (or $4-r$ nearest neighbors). The probability per step to stay at the initial point is $r/4$ and the corresponding ϕ probability is $e^{i\phi}(r/4)$. Thus, the ϕ probability to stay at a given initial point with $4-r$ nearest neighbors, $X_{r/4}(\phi)$, is

$$X_{r/4}(\phi)=\sum_{n=0}^{\infty}[e^{i\phi}(r/4)]^n$$

or

$$X_{r/4}(\phi)=\frac{1}{1-(r/4)e^{i\phi}}\ . \tag{2.10}$$

The next example is representative of the kind of techniques we wish to develop. Assume a random walker wishes to start at point A, and get to point C after having visited a third point B at least once (see Fig. 6). Define the following quantities: T_{AB}, the ϕ probability to start at A and get to B for the first time, without having reached C or returned to A in the process; T_{BC}, the ϕ probability to start at B and get to C for the first time without having reached A or returned to B in the process; and Q_{BB}, the ϕ probability to start at B, leave B (i.e., not making any move through a fictitious bond of B), and return to B for the first time without touching either A or C in the process. X_B is defined as the ϕ probability to stay at B. Note that no information on the nature of the different paths is given. As far as the ϕ probability to get from A to C via B (which we define as G_{AC}^{B}) is concerned, only these three quantities are of interest. We call T_{AB} and T_{BC} the prop-

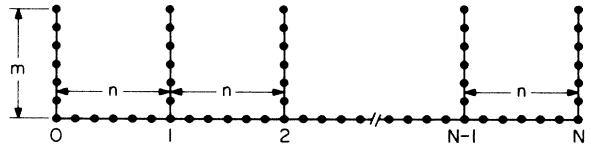

FIG. 3. A segment with many dangling bonds.

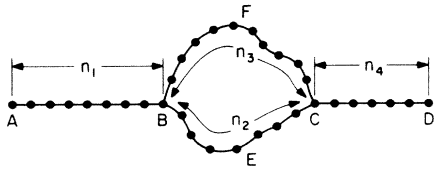

FIG. 4. Loop configuration.

agators from A to B and from B to C, respectively. Q_{BB} is called the B vertex.

There are many types of routes that contribute to G^B_{AC}. For example, $A\to B\to C$ or $A\to B\to B\to A\to B\to C$, where the notation is obvious. To take all of these into account we proceed in several steps. First, we calculate the ϕ probability to get from B to B (not necessarily for the first time) without touching A or C. The ϕ probability to do so, R_B, is

$$R_B = X_B + X_B Q_B X_B + X_B Q_B X_B Q_B X_B + \cdots . \quad (2.11)$$

The first term in (2.11) represents the possibility of just staying at B (including also "zero step," i.e., not staying there). This probability is represented by the term "1" in X_B). The second term represents the possibility that the walker stays at B for some time, then takes a path out of B (that does not touch A or C), which ultimately leads back to B and then stays at B for some time (which can be zero, as mentioned before). The other terms are "repetitions" of the paths represented by the second term. Obviously the different terms in (2.11) represent distinct paths, whose ϕ probabilities should be added. The "renormalized" B vertex is, from (2.11),

$$R_B = \frac{X_B}{1 - X_B Q_B} . \quad (2.12)$$

Similarly we can define R_A.

Next we take into account the fact that a walker can go from B to A and return. Assuming $T_{BA} = T_{AB}$ (with obvious notation), we calculate S_{AB}, the probability to get from A to B (not necessarily the first time) without touching C, and eventually remaining at B. It is

$$S_{AB} = R_A T_{AB} R_B + R_A T_{AB} R_B T_{AB} R_A T_{AB} R_B + R_A T_{AB} R_B T_{AB} R_A T_{AB} R_B T_{AB} R_A T_{AB} R_B + \cdots . \quad (2.13)$$

The first term represents the paths that start at A, return to A an unspecified number of times (without touching B or C), then reach B without returning to A on the way, and finally move from B to B without touching A or C for an unspecified number of steps. The next terms involve getting from A to B, moving from B to B as before, then returning to A and moving back to B (represented by T^2_{AB}), and so on. Summing up (2.13) we obtain

$$S_{AB} = \frac{R_A T_{AB} R_B}{1 - T^2_{AB} R_A R_B} . \quad (2.14)$$

The final path is to C. Thus we finally obtain

$$G^B_{AC} = \frac{T_{AB} R_A R_B T_{BC}}{1 - T^2_{AB} R_A R_B} . \quad (2.15)$$

Equation (2.15) is the result in this case. It has been obtained by successive renormalizations, each renormalization taking into account a set of subpaths whose ϕ probabilities can be summed up as a geometric series. These renormalizations are constructed so as to take into account the different branches of paths. In Secs. III–VI we shall treat specific examples and calculate explicitly the propagators and vertices themselves.

To conclude this section, we define mean first-passage times in terms of the ϕ probabilities (as is standardly done in the literature). Let $P_{AB}(n)$ be the probability to reach B for the first time in n steps, after having started at A. The mean first-passage time $\langle t \rangle$ from A to B defined as

$$\langle t \rangle = \frac{\sum_{n=0}^{\infty} n P_{AB}(n)}{\sum_{n=0}^{\infty} P_{AB}(n)} . \quad (2.16)$$

Let G_{AB} be the ϕ-probability corresponding to P_{AB}. Then

$$\langle t \rangle = \left. \frac{\frac{d}{di\phi} G_{AB}(\phi)}{G_{AB}(\phi)} \right|_{\phi=0} . \quad (2.17)$$

It is easy to see that for structures for which A and B are connected, $G_{AB}(\phi)\,|_{\phi=0} = 1$; hence

$$\langle t \rangle = \frac{d}{di\phi} G_{AB}(\phi)\,|_{\phi=0} . \quad (2.18)$$

Now that the essentials of our method have been presented we turn to several specific examples.

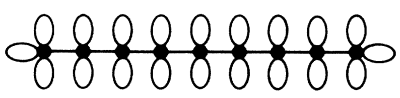

FIG. 5. "Fictitious" bonds.

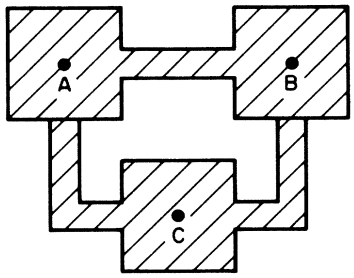

FIG. 6. Black boxes containing points A, B, and C (see Sec. II).

III. RANDOM WALK ON A SEGMENT

In this section we present a detailed calculation of the generating function of the random walk on a segment (see Fig. 1). This problem can be obviously solved using standard master equation methods; the aim of the calculations in this section is to further present details of our method and, of course, show how it works on a simple test case.

We wish to calculate the probability $P_N(n)$ of a walker starting at one end of a segment to reach the other end for the first time in n steps. We shall do so by calculating the appropriate generating function, which will subsequently be used to calculate the corresponding mean first-passage time.

The points on the segment (of length N) are denoted by $0,1,\ldots,N$. The problem is to calculate the generating function G_N corresponding to P_N. To this end we define, as in Sec. II, the following quantities (the φ dependence of these quantities is suppressed).

(i) T_N, the φ probability to leave 0 on the first step and reach N for the first time, without having returned to 0 in the process.

(ii) Q_N, the φ probability to leave 0 and return to it for the first time without having reached N in the process.

Note that

$$Q_1(\varphi)=0 \tag{3.1}$$

(i.e., such a walk does not exist for $N=1$).

The generating function G_N can be expressed in terms of T_N, Q_N, and $X_{3/4}$ [see (2.10)]. A walker at point 0 can stay there for a number of steps (with φ probability $X_{3/4}$), move out of 0 and return to 0 without having touched N (with φ probability Q_N), then stay at 0 and repeat the process a number of times. Eventually it will start out at 0 and reach N without returning to 0 again (with φ probability T_N). Thus, the processes that lead the walker back to 0 have the φ probability

$$X_{3/4}+X_{3/4}Q_NX_{3/4}+X_{3/4}Q_NX_{3/4}Q_NX_{3/4}+\cdots = \frac{X_{3/4}}{1-Q_NX_{3/4}} .$$

The last process is starting at 0 and reaching N without returning to 0 any longer. Its φ probability is T_N. Hence

$$G_N=\frac{X_{3/4}T_N}{1-X_{3/4}Q_N} . \tag{3.2}$$

It remains now to calculate T_N and Q_N. This is done by finding and solving recursion relations for these quantities.

The walker that wishes to walk from 0 to 0 under the conditions specified in the definition of Q_N has to start by moving from 0 to 1. This process has a φ probability of $\frac{1}{4}e^{i\varphi}$. At 1 it may stay as long as it pleases [with φ probability $X_{1/2}$; see Eq. (2.10)]. It may subsequently leave 1 for the part of the segment between 2 and N and return to 1 (with φ probability Q_{N-1}). Then it may stay at 1 for some time (again with φ probability $X_{1/2}$) and repeat the process that leads it back to 1 without touching N or returning to 0. The φ probability describing these processes is

$$\tfrac{1}{4}e^{i\varphi}(X_{1/2}+X_{1/2}Q_{N-1}X_{1/2} +X_{1/2}Q_{N-1}X_{1/2}Q_{N-1}X_{1/2}+\cdots) = \tfrac{1}{4}e^{i\varphi}\frac{X_{1/2}}{1-Q_{N-1}X_{1/2}} . \tag{3.3}$$

Note that each term in the geometric series in Eq. (3.3) represents a certain number of repetitions of the process $1\rightarrow$segment $(2,N)\rightarrow 1$. Finally, the walker returns to 0 with φ probability $\frac{1}{4}e^{i\varphi}$. Hence

$$Q_N=(\tfrac{1}{4}e^{i\varphi})^2\frac{X_{1/2}}{1-X_{1/2}Q_{N-1}} , \tag{3.4}$$

which is a recursion relation for Q_N. Before we turn to a solution of (3.4) we derive a second recursion relation for Q_N. To do that we consider two distinct types of paths that contribute to Q_N: those paths that contain the point $N-1$ and those that do not. The contribution of the paths that do not reach the point $N-1$ is precisely Q_{N-1}. The φ probability of leaving 0 and reaching $N-1$ (without returning to 0 in the process) for the first time is T_{N-1}. Upon reaching point $N-1$ the walker may choose to stay there (with φ probability $X_{1/2}$), then move into the segment between point 1 and point $N-1$ and return to point $N-1$ (with φ probability Q_{N-1}). The process can then be repeated. This set of paths has a total φ probability

$$T_{N-1}(X_{1/2}+X_{1/2}Q_{N-1}X_{1/2} +X_{1/2}Q_{N-1}X_{1/2}Q_{N-1}X_{1/2}+\cdots) = T_{N-1}\frac{X_{1/2}}{1-X_{1/2}Q_{N-1}} . \tag{3.5}$$

The fact that the different terms in the geometric series are repetitions of a type of process should by now be clear. Finally, the walker returns to point 0 (remember that it should not get to N if it wishes to contribute to Q_N) with φ probability T_{N-1}. The total contribution of the paths that contain the point $N-1$ is thus

$$T_{N-1}^2\frac{X_{1/2}}{1-X_{1/2}Q_{N-1}} .$$

Adding the φ probabilities of the two types of paths we obtain

$$Q_N=Q_{N-1}+\frac{T_{N-1}^2X_{1/2}}{1-X_{1/2}Q_{N-1}} , \tag{3.6}$$

from which we obtain a formula for T_N,

$$T_N=\left[\frac{(Q_{N+1}-Q_N)(1-X_{1/2}Q_N)}{X_{1/2}}\right]^{1/2} . \tag{3.7}$$

The sign of T_N will be dealt with later. Thus, upon solving Eq. (3.4) and using (3.7) we obtain all we need to calculate G_N.

We start by solving the recursion relation for Q_N. Define

$$S_N \equiv X_{1/2} Q_N \tag{3.8}$$

and

$$a = (\tfrac{1}{4} e^{i\varphi} X_{1/2})^2 . \tag{3.9}$$

It follows from Eq. (3.4) that

$$S_{N+1} = a \frac{1}{1-S_N} . \tag{3.10}$$

Define

$$S_N \equiv \frac{A_N}{B_N} . \tag{3.11}$$

Substituting (3.11) into (3.10) we obtain

$$A_{N+1} = c_N a B_N \tag{3.12}$$

and

$$B_{N+1} = c_N (B_N - A_N) , \tag{3.13}$$

where $c_N \neq 0$ is an arbitrary constant. Define $B_N \equiv (\prod_{n=0}^{N-1} C_n) \tilde{B}_N$ and $A_N = (\prod_{n=0}^{N-1} C_n) \tilde{A}_N$. Obviously, $S_N = \tilde{A}_N / \tilde{B}_N$. It follows from Eqs. (3.12) and (3.13) that

$$\tilde{A}_{N+1} = a \tilde{B}_N , \tag{3.14a}$$

$$\tilde{B}_{N+1} = \tilde{B}_N - \tilde{A}_N . \tag{3.14b}$$

Hence,

$$\tilde{B}_{N+1} + a \tilde{B}_{N-1} - \tilde{B}_N = 0 . \tag{3.14c}$$

Equation (3.14c) has two independent solutions of the form $\lambda_{1,2}^N$ where $\lambda_{1,2}$ solve the quadratic equation $\lambda^2 - \lambda + a = 0$, i.e.,

$$\lambda_{1,2} = \frac{1 \pm \sqrt{1-4a}}{2} . \tag{3.15}$$

Note that

$$\lambda_1 \lambda_2 = a \tag{3.16}$$

and

$$\lambda_1 + \lambda_2 = 1 . \tag{3.17}$$

Thus, the general solution of (3.10) is

$$S_N = \frac{a(H_1 \lambda_1^{N-1} + H_2 \lambda_2^{N-1})}{H_1 \lambda_1^N + H_2 \lambda_2^N} , \tag{3.18}$$

where the numerator in (3.18) is $\tilde{A}_n$ and the denominator is the general solution of Eq. (3.14c). H_1 and H_2 are so far arbitrary constants. Using now (3.8) and (3.9)

$$Q_N = (\tfrac{1}{16} e^{2i\varphi} X_{1/2}) \frac{\lambda_1^{N-1} + (H_2/H_1)\lambda_2^{N-1}}{\lambda_1^N + (H_2/H_1)\lambda_2^N} . \tag{3.19}$$

Using now (3.1), we finally obtain

$$Q_N = (\tfrac{1}{16} e^{2i\varphi} X_{1/2}) \frac{\lambda_1^{N-1} - \lambda_2^{N-1}}{\lambda_1^N - \lambda_2^N} . \tag{3.20}$$

Equations (2.10), (3.2), (3.7), (3.15), and (3.20) thus constitute a closed solution of $G_N(\varphi)$.

Finally, we turn to obtaining numbers with this calculation. We wish to obtain the mean first-passage time (MFT) from point 0 to point N. Using (2.17),

$$\langle t \rangle = \left. \frac{\frac{d}{di\varphi} G_N(\varphi)}{G_N(\varphi)} \right|_{\varphi=0} , \tag{3.21}$$

which means we have to know $G_N(\varphi)$ only to first order in $i\varphi$. To do so, we expand Q_N, T_N, $X_{1/2}$, $X_{3/4}$, $\lambda_{1,2}$, and a to first power in $i\varphi$. It turns out to be convenient to define $i\varphi \equiv \epsilon^2$ and expand all quantities in powers of ϵ. It follows from (2.10) that to order ϵ^3

$$X_{1/2} = 2 + 2\epsilon^2 \tag{3.22}$$

and

$$X_{3/4} = 4 + 12\epsilon^2 , \tag{3.23}$$

and, using Eqs. (3.9) and (3.22),

$$a = \tfrac{1}{4} + \epsilon^2 + O(\epsilon^4) . \tag{3.24}$$

Substituting (3.24) into (3.15)

$$\lambda_{1,2} = \tfrac{1}{2} \pm i\epsilon + O(\epsilon^3) . \tag{3.25}$$

Note that it suffices to calculate $\lambda_{1,2}$ to first order in ϵ because in Eq. (3.20) both numerator and denominator vanish in the limit $\epsilon \to 0$. The first-order terms then cancel, and only a term of $O(\epsilon^2)$ survives. Using (3.22) and (3.25) in (3.20) we obtain

$$Q_N = \frac{N-1}{4N} + \frac{(4N+1)(N-1)}{12N} \epsilon^2 + O(\epsilon^4) . \tag{3.26}$$

It follows now from (3.26), (3.22), and (3.7) that

$$T_N = \frac{1}{4N} + \frac{2N^2+1}{12N} \epsilon^2 + O(\epsilon^4) . \tag{3.27}$$

Now, from (3.2), (3.23), (3.26), and (3.27) we obtain

$$G_N = 1 + 2(N^2+N)\epsilon^2 + O(\epsilon^4) . \tag{3.28}$$

Note that $G_N(\varphi=0) = 1$ as it should. Finally, using (3.21) and (3.28) it follows that

$$\langle t \rangle = 2N^2 + 2N , \tag{3.29}$$

which is the dependence of the MFT on the length of the segment. Note that for large N we obtain $N^2 \sim \frac{1}{2} \langle t \rangle$. If we wish to define a diffusion constant this way, we obtain

$$\tilde{D} \equiv \frac{N^2}{2\langle t \rangle} \to \frac{1}{4} . \tag{3.30}$$

We also wish to note that in a *finite system* the regular definition of a diffusion constant, i.e., (distance)^2/time, in the long-time limit is useless since the distance is bounded. The above result suggests a possible meaningful definition in this case.

The functions $T_N(\varphi)$ and $Q_N(\varphi)$, which we have defined and calculated in this section, as well as $X_{1/4}(\varphi)$, are important building blocks of many other generating functions, as the examples in Secs. IV–VI will show. We

went into great detail in this section in order to demonstrate our method in as clear a fashion as we can. The key idea in the derivation is that of dressing the "bare" propagator $T_N(\varphi)$ by processes Q and X. One then uses recursion relations to obtain the full generating function.

IV. A SEGMENT WITH A SINGLE DANGLING BOND

The configuration that is the subject of this section is depicted in Fig. 2. We wish to calculate the φ probability for a walker starting at point A to reach point C for the first time. Using this φ probability we shall calculate the corresponding mean first-passage time. The power of our method now shows up—the desired generating functions depend solely on quantities that were already defined and calculated in Secs. I–III: the T, Q, and X functions. Using these entities it is now a matter of a few lines to calculate the generating function G in this case (the master equation approach becomes rather messy here).

As seen in Fig. 2, the problem involves three segments AB, BC, and BD of lengths n_1, n_2, and n_3, respectively. The corresponding basic functions are T_{n_1},Q_{n_1}; T_{n_2},Q_{n_2}; and T_{n_3},Q_{n_3} (as defined in Sec. III).

We start by defining V_A, the renormalized A vertex, as the φ probability to start at A and return to A without reaching B in the process. The argument goes as in Sec. III, resulting in

$$V_A = X_{3/4} + X_{3/4}Q_{n_1}X_{3/4} + X_{3/4}Q_{n_1}X_{3/4}Q_{n_1} + \cdots$$

or

$$V_A = \frac{X_{3/4}}{1 - X_{3/4}Q_{n_1}} . \tag{4.1}$$

The partially renormalized B vertex Q_B is defined as the φ probability to start at B and return to B without having reached A, C, or D in the process. Noting that the φ probability to stay at B is $X_{1/4}$ and that the walker can perform excursions into AB, CB, or DB after having stayed at B (each such excursion being represented by Q_{n_1}, Q_{n_2}, or Q_{n_3}, respectively), we obtain

$$\begin{aligned} Q_B = {} & X_{1/4} + X_{1/4}(Q_{n_1} + Q_{n_2} + Q_{n_3})X_{1/4} \\ & + X_{1/4}(Q_{n_1} + Q_{n_2} + Q_{n_3})X_{1/4}(Q_{n_1} + Q_{n_2} \\ & + Q_{n_3})X_{1/4} + \cdots \end{aligned}$$

or

$$Q_B = \frac{X_{1/4}}{1 - X_{1/4}(Q_{n_1} + Q_{n_2} + Q_{n_3})} . \tag{4.2}$$

Another path that leads from B to B is going to A or to D and returning to B for the first time (recall that in the processes represented by Q_{n_1} or Q_{n_3} the end points A or D, respectively, were not touched because of the definition of the Q's), a process whose φ probability we define as S_B.

The φ probability of going from B to A and back to B involves $T_{n_1}^2$ and is renormalized by repeated Q_{n_1} excursions from A to A. This leads to a total φ probability to go from B to A and back to B for the first time,

$$T_{n_1}^2 \frac{X_{3/4}}{1 - Q_{n_1}X_{3/4}} ,$$

and a similar contribution from the excursion to D. Thus

$$S_B = \frac{T_{n_1}^2 X_{3/4}}{1 - Q_{n_1}X_{3/4}} + \frac{T_{n_3}^2 X_{3/4}}{1 - Q_{n_3}X_{3/4}} . \tag{4.3}$$

The walker starting at B can make any number of excursions without touching A or D (including the possibility of staying at B all the time or only for zero steps) which are represented by Q_B. Then it can perform an excursion in which A or D are reached, rest at B, and so on. Defining R_B, the renormalized B vertex, as the φ probability to go from B to B without reaching C, we obtain

$$R_B = \frac{Q_B}{1 - Q_B S_B} . \tag{4.4}$$

Now, to reach C, the walker starts at A, performs motions represented by V_A, then moves to B (with φ probability T_{n_1}), performs motions whose φ probability is R_B, and finally reaches C with φ probability T_{n_2}. Consequently,

$$G = V_A T_{n_1} R_B T_{n_2} . \tag{4.5}$$

Equation (4.5) expresses the desired generating function in terms of known quantities and is, therefore, a closed analytic solution for G. To calculate the corresponding MFT we have to calculate the quantities in (4.5) to first order in $i\varphi$ or second order in ϵ.

As a consistency check we find it useful to evaluate G at $\varphi = 0$. This is a relatively easy calculation that should yield $G = 1$. Indeed, we obtain in this limit

$$T_n = \frac{1}{4n} , \tag{4.6a}$$

$$Q_n = \frac{n-1}{4n} , \tag{4.6b}$$

$$X_{3/4} = 4 , \tag{4.6c}$$

$$X_{1/4} = \tfrac{4}{3} , \tag{4.6d}$$

$$V_A = 4n_1 , \tag{4.6e}$$

$$Q_B = \frac{4}{\frac{1}{n_1} + \frac{1}{n_2} + \frac{1}{n_3}} , \tag{4.6f}$$

$$S_B = \frac{1}{4n_1} + \frac{1}{4n_3} , \tag{4.6g}$$

$$R_B = 4n_2 , \tag{4.6h}$$

and

$$G(\varphi = 0) = 1 . \tag{4.6i}$$

This is an easy check that is recommended in all calculations of MFT's. As far as the calculation of $\langle t \rangle$ goes, it is useful to employ the following trivial identity. If

$$G = \prod_{i=1}^{m} A_i , \tag{4.7}$$

where A_i are any ϵ^2-dependent functions, then

$$\frac{1}{G}\frac{\partial G}{\partial \epsilon^2}=\sum_{i=1}^{m}\frac{1}{A_i}\frac{\partial A_i}{\partial \epsilon^2} . \tag{4.8}$$

In our specific case

$$\frac{1}{G}\frac{\partial G}{\partial \epsilon^2}=\frac{1}{V_A}\frac{\partial V_A}{\partial \epsilon^2}+\frac{1}{T_{n_1}}\frac{\partial T_{n_1}}{\partial \epsilon^2}+\frac{1}{R_B}\frac{\partial R_B}{\partial \epsilon^2}+\frac{1}{T_{n_2}}\frac{\partial T_{n_2}}{\partial \epsilon^2} . \tag{4.9}$$

Note the appearance of quantities such as $(1/T)(\partial T/\partial \epsilon^2)$, whose value can be calculated and tabulated once and for all. The aim is to reduce the expression in specific cases to a sum of such "universal" expressions. For example, $(1/V_A)(\partial V_A/\partial \epsilon^2)$ can be further reduced, using Eq. (4.1),

$$\frac{1}{V_A}\frac{\partial V_A}{\partial \epsilon^2}+\frac{1}{X_{3/4}}\frac{\partial X_{3/4}}{\partial \epsilon^2}+\frac{1}{1-X_{3/4}Q_{n_1}}\frac{\partial}{\partial \epsilon^2}(X_{3/4}Q_{n_1}) , \tag{4.10}$$

or

$$\frac{1}{V_A}\frac{\partial V_A}{\partial \epsilon^2}=\frac{1}{X_{3/4}}\frac{\partial X_{3/4}}{\partial \epsilon^2}+\frac{X_{3/4}Q_{n_1}}{1-X_{3/4}Q_{n_1}}\frac{1}{Q_{n_1}}\frac{\partial Q_{n_1}}{\partial \epsilon^2}+\frac{X_{3/4}Q_{n_1}}{1-X_{3/4}Q_{n_1}}\frac{1}{X_{3/4}}\frac{\partial X_{3/4}}{\partial \epsilon^2} . \tag{4.11}$$

In the limit $\epsilon^2\to 0$ we obtain

$$\langle t\rangle=\frac{1}{G}\frac{\partial G}{\partial \epsilon^2}=2(n_1+n_2)^2+2(n_1+n_2)+4n_2n_3 . \tag{4.12}$$

Note that when $n_3=0$ we recover the result of the straight segment, Eq. (3.29). Another interesting aspect of this result is the asymmetry between n_1 and n_2. This effect follows from the fact that it matters whether the random walker goes from A to B or from B to A, because in one of these cases it meets the dangling bond earlier than in the other. The linear dependence on n_3 is also worth mentioning. It means that the time spent in the dangling bond is proportional to its length, which indicates a uniform probability distribution in the dangling bond. Whether this effect is general remains to be seen. The effective diffusion constant in this case is sensitive to the limits considered. For example, when $n_1\to\infty$, n_2,n_3 remaining fixed we obtain $D=\frac{1}{4}$, as in the case of the simple segment. In the limits $n_1,n_2,n_3\to\infty$ but $n_3/n_1^4\to$const and $n_2/n_1\to$const, we obtain an anomalous diffusion constant that behaves like $t^{-3/5}$.

We conclude this section by mentioning again the power of the "dressing" technique we have presented. In Sec. V we turn to a slightly more complex case.

V. A LOOP CONFIGURATION

We turn now to our third example. It is slightly more complicated than the previous ones, but we can still calculate the appropriate generating function with the aid of our basic functions. The geometry of the loop configuration is depicted in Fig. 4. The structure is composed of four segments AB, BEC, BFC, and CD, of lengths n_1, n_2, n_3, and n_4, respectively. The corresponding basic functions are T_{n_1},Q_{n_1}; T_{n_2},Q_{n_2}; T_{n_3},Q_{n_3}; and T_{n_4},Q_{n_4}. We shall also need $X_{3/4}$ (for the vertices A and D) and $X_{1/4}$ (for the vertices B and C). As in the preceding, we wish to calculate the generating function G for starting at A and reaching D for the first time and deduce the MFT, which is denoted by $\langle t\rangle$ as before. The calculation proceeds by a series of renormalizations as before.

First, we renormalize the A vertex. This renormalization includes the possibility that the walker starting at A may stay there (with φ probability $X_{3/4}$) or make an excursion into the segment AB without touching B (the corresponding φ probability is Q_{n_1}). The contribution of these processes is the φ probability Q_A for the walker to start at A and return to A without having reached B. Considerations similar to these appearing in previous sections lead to

$$Q_A=\frac{X_{3/4}}{1-X_{3/4}Q_{n_1}} . \tag{5.1}$$

The first renormalization of the B vertex, Q_B, will include the following possibilities: the walker stays at B (corresponding to $X_{1/4}$) and/or wanders into BA, BEC, or BFC without reaching A or C (the corresponding φ probabilities are Q_{n_1}, Q_{n_2}, and Q_{n_3}). The resulting formula for Q_B is

$$Q_B=\frac{X_{1/4}}{1-X_{1/4}(Q_{n_1}+Q_{n_2}+Q_{n_3})} . \tag{5.2}$$

Similarly we renormalize the C vertex by including excursion from C into the segments CD, CEB, and CFB. The resulting renormalized vertex Q_C is

$$Q_C=\frac{X_{1/4}}{1-X_{1/4}(Q_{n_2}+Q_{n_3}+Q_{n_4})} . \tag{5.3}$$

Next we define a further renormalization of the B vertex, which includes all possible excursions leading from B back to B. The walker may go to A (with φ probability T_{n_1}), perform motions described by Q_A, and then return to B (again with φ probability T_{n_1}). This process thus has a φ probability $T_{n_1}^2Q_A$. Alternatively, the walker may choose to go to C via BEC and eventually return through BEC, a process whose φ probability is $T_{n_3}Q_C$. It may wish to perform a similar walk through BFC, contributing $T_{n_3}^2Q_C$ to the φ probability. Finally, it may use segment BEC to reach C and return through BFC or go the other way around. This possibility has a φ probability of $2T_{n_2}T_{n_3}Q_C$. All together, the φ probability of leaving B and reaching A or C *before* returning to B is

$$S_B\equiv T_{n_1}^2Q_A+(T_{n_2}+T_{n_3})^2Q_C . \tag{5.4}$$

Now the walker starting at B may perform a Q_B-type walk. (Q_B includes the possibility that this walk lasts for zero steps, i.e., it is not performed. This possibility is represented in Q_B by the $n=0$ term of the sum defining $X_{1/4}$, which is 1. This 1 then multiplies whatever walks

are subsequently performed. This is why we consider Q_B as the first possibility, since S_B does not contain a zero-step term.) Then it can perform an S_B-type walk, then a Q_B-type walk, and so on. It follows that the fully renormalized B vertex, which we denote by R_B, and which contains all walks from B to B which do not reach D, is

$$R_B=\frac{Q_B}{1-Q_BS_B} . \tag{5.5}$$

Now G is the product of (a) the renormalized A vertex Q_A, (b) a term T_{n_1} representing the motion from A to B, (c) the fully renormalized B vertex (whose significance was explained before), (d) a term $(T_{n_2}+T_{n_3})$ representing the transition from B to C (via BEC or BFC), (e) a term Q_C representing the renormalized C vertex, and (f) a term T_{n_4} representing the transition from C to D. Thus, we finally obtain

$$G=Q_AT_{n_1}R_B(T_{n_2}+T_{n_3})Q_CT_{n_4} . \tag{5.6}$$

At this point we wish to mention that if we had tried to solve this problem by the master equation approach, we would have had to perform an extremely tedious calculation. The method we presented makes the derivation of the result (5.6) a rather straightforward task (which, after gaining a little experience, becomes almost trivial). A useful diagram showing the possible distinct paths for the loop case is shown in Fig. 7. The "ends" appearing in the diagram contain points that the walker has previously encountered. At such a point x the walker is assumed to "go back" to a point x^* represented by the same symbol x as the end point. This point x^* is the first time the point x is encountered by the walker. For example, once one reaches a B end point, go to B^* and continue "walking" until point D is reached. We found that diagrams such as Fig. 7 are useful in deciding which paths should be included in each renormalization of the vertices. The calculation of $\langle t\rangle$ is now a matter of straightforward algebra (although somewhat tedious). The result is

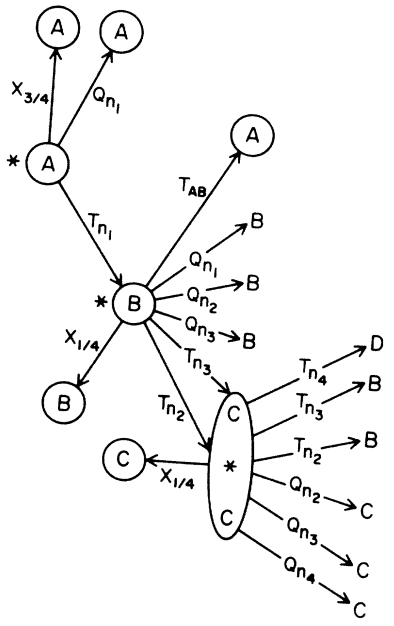

FIG. 7. Branching of paths in the loop case. Each arrow is labeled by the appropriate φ probability.

$$\begin{aligned}\langle t\rangle=&\frac{4n_1^2+6n_1-1}{3}\left[1+\left[n_4+\frac{1}{\Sigma_{2,3}}\right]\frac{1}{n_1}\right]+\frac{4n_{1,2,3}-\Sigma_{1,2,3}-6}{3\Sigma_{1,2,3}}\left[1+\left[n_4+\frac{1}{\Sigma_{2,3}}\right]\frac{1}{n_1}+\left[n_4+\frac{1}{\Sigma_{2,3}}\right]\frac{\Sigma_{2,3}^2}{\Sigma_{2,3,4}}\right]\\&+\frac{4n_{2,3,4}-\Sigma_{2,3,4}-6}{3\Sigma_{2,3,4}}\left[1+\left[n_4+\frac{1}{\Sigma_{2,3}}\right]\frac{\Sigma_{2,3}^2}{\Sigma_{2,3,4}}\right]+\frac{2n_1^2+1}{3}\left[1+2\left[n_4+\frac{1}{\Sigma_{2,3}}\right]\frac{1}{n_1}\right]\\&+\frac{2n_2^2+1}{3}\left[\frac{1}{n_2\Sigma_{2,3}}+2\left[n_4+\frac{1}{\Sigma_{2,3}}\right]\frac{1}{n_2}\frac{\Sigma_{2,3}}{\Sigma_{2,3,4}}\right]+\frac{2n_3^2+1}{3}\left[\frac{1}{n_3\Sigma_{2,3}}+2\left[n_4+\frac{1}{\Sigma_{2,3}}\right]\frac{1}{n_3}\frac{\Sigma_{2,3}}{\Sigma_{2,3,4}}\right]+\frac{2n_4^2+1}{3} ,\end{aligned} \tag{5.7}$$

where $n_{ij}=n_i+n_j$, $n_{i,j,k}=n_i+n_j+n_k$, $\Sigma_{ij}=1/n_i+1/n_j$, and $\Sigma_{ijk}=1/n_i+1/n_j+1/n_k$. We found no way to simplify Eq. (5.7) in the general case. In simple limiting cases, though, one obtains more transparent results. For instance, when $n_1=n_2=n_4=n$ we obtain

$$\langle t\rangle=20n^2 . \tag{5.8}$$

The MFT corresponding to a straight segment of length $3n$ (which is what we obtain by completely disconnecting one of the two segments of which the loop is "composed") is $18n^2+6n$. Thus in the large-n limit, the "addition" in parallel of a segment of length n to another segment of length n does not change $\langle t\rangle$ very much. Choosing $n_1=n_2=n_4\equiv n$ and $n_3=n+n\delta$, δ satisfying $|\delta|\ll 1$ (strictly speaking, $n\delta$ should be an integer), we obtain

$$\langle t\rangle=20n^2+7n^2\delta+O(\delta^2) , \tag{5.9}$$

which shows the direction in which small changes in the lengths of one of the two segments of which the loop is composed change the MFT. It increases when the seg-

ment is made slightly longer and becomes smaller in the opposite case. It is, of course, interesting to check other limits of $\langle t \rangle$, but since we are mainly interested in presenting our method, we shall not dwell on this point here. We turn now to our last example.

VI. A SEGMENT WITH MANY DANGLING BONDS

The system that we treat in this section is depicted in Fig. 3. The segment is of length Nn. Each subsegment has a length n and has two dangling bonds—one at each end. Thus there are $N+1$ dangling bonds, each of length m. We wish to calculate $\langle t \rangle$, the MFT for getting from point 0 to point N, and the corresponding generating function. To this end we define the following functions.

(i) $Q_N(\varphi)$, the φ probability to leave 0 and return for the first time to 0, without reaching N on the way (but it is allowed to reach end points of the dangling bonds).

(ii) $T_N(\varphi)$, the φ probability to leave 0 and reach N for the first time, without having returned to 0 on the way.

(iii) $r_m(\varphi)$, the φ probability to leave 0, move into the first dangling bond (the one connected to 0), and return for the first time to 0 (it is allowed to touch the end point of the first dangling bond).

(iv) $t_n(\varphi), t_m(\varphi), q_n(\varphi), q_m(\varphi)$, the T and Q functions of simple segments of lengths n and m, respectively. [Note the change of notation—t's and q's here are the same as T's and Q's in Secs. II–V. The T's and Q's are reserved for the whole segment, as defined in (i) and (ii).]

(v) $X_{1/4}, X_{1/2}, X_{3/4}$, as previously defined.

We now turn to the renormalization of the vertices. First we calculate r_m. It is obvious that a walker that leaves 0 for the first dangling bond can *either* return to 0 without having touched the end point of the dangling bond (with φ probability q_m) *or* reach this end point for the first time (with φ probability t_m), stay there (with φ probability $X_{3/4}$), then move into the dangling segment and return to the end point, without having touched 0 (with φ probability q_m). Then it may repeat this process, and eventually return to 0 (with φ probability t_m). Consequently,

$$r_m = q_m + t_m^2 \frac{X_{3/4}}{1 - X_{3/4} q_m} . \tag{6.1}$$

To solve for T_N and Q_N, we derive recursion relations, in N, for these quantities. The first relation is

$$Q_N = q_n + r_m + t_m^2 \frac{X_{1/4}}{1 - X_{1/4}(Q_{N-1} + q_n)} . \tag{6.2}$$

The first two terms in (6.2) represent the fact that the walker can *either* start out at 0, move into the segment (0,1) without touching 1 and return to 0, *or* move into the first dangling bond and return to 0. Alternatively, it may choose to move to 1 (with φ probability t_n). It can then stay at 1 (with φ probability $X_{1/4}$). It may leave 1 and return to 1 for the first time without having touched 0 or N (with φ probability $Q_{N-1}+q_n$). After having stayed at 1, left it, and returned to it as many times as it pleased, with φ probability

$$\frac{X_{1/4}}{1 - X_{1/4}(Q_{N-1} + q_n)} ,$$

the walker eventually returns to 0 (with φ probability t_n). All together, the motion from 0 to 1, the excursion from 1 to 1 without touching 0 or N, and the return to 0 produce the third term in (6.2).

The second recursion relation that we derive is

$$Q_N = Q_{N-1} + T_{N-1}^2 \frac{X_{1/4}}{1 - X_{1/4}(Q_{N-1} + q_n)} . \tag{6.3}$$

The first term in (6.3) represents all paths leading from 0 to 0 without reaching the point $N-1$. The second term represents all paths in which the walker reaches point $N-1$ (with φ probability T_{N-1}) and eventually returns to 0 (again with φ probability T_{N-1}). In the meantime it can stay at $N-1$, move to the right into the segment $(N-1,N)$ without touching N, and return to $N-1$ for the first time (with φ probability q_n). It may choose to move upwards or to the left of $N-1$, without touching 0, and return to $N-1$ for the first time (with φ probability Q_{N-1}). Thus an excursion leaving $N-1$ and returning to $N-1$ for the first time without having touched 0 or N has a φ probability of $Q_{N-1}+q_n$, and the totality of such excursions, including resting periods at $N-1$, has a φ probability of

$$\frac{X_{1/4}}{1 - X_{1/4}(Q_N + q_n)} ,$$

which yields the second term in (6.3).

The only unknowns in Eq. (6.2) are the Q_N's. To find them we solve the recursion relation (6.2) in much the same way as we solved Eq. (3.4). Define

$$S_N \equiv Q_N - q_n - r_m . \tag{6.4}$$

Note that

$$S_1 = 0 . \tag{6.5}$$

The recursion relation for S_N reads

$$S_{N+1} = \frac{a}{b - S_N} , \tag{6.6}$$

where

$$a = t_n^2 \tag{6.7a}$$

and

$$b = \frac{1}{X_{1/4}} - (2q_n + r_m) . \tag{6.7b}$$

Define

$$S_N = \frac{A_N}{B_N} ; \tag{6.8}$$

then, from (6.6),

$$A_{N+1} = a B_N , \tag{6.9a}$$

$$B_{N+1} = a B_N - A_N , \tag{6.9b}$$

up to a multiplicative constant taken to be 1 (see Sec. III).

It follows as in Sec. III that

$$S_N = a\frac{\lambda_1^{N-1}-\lambda_2^{N-1}}{\lambda_1^N-\lambda_2^N} , \tag{6.10}$$

where

$$\lambda_{1,2}=\frac{b\pm\sqrt{b^2-4a}}{2} , \tag{6.11}$$

and Eq. (6.5) was used. Now using (6.4) we can find Q_N. The algebra is somewhat tedious, but straightforward, and we obtain

$$Q_N=\frac{1}{2}-\frac{1}{4Nn}+\epsilon^2\left[m+\frac{4n^2-1}{12n}+(N-1)\left[\frac{n+m}{3}+\frac{1-2nm}{12Nn}\right]\right]+O(\epsilon^4) , \tag{6.12}$$

where $\epsilon^2\equiv i\varphi$ as in previous sections. T_N is subsequently found from Eq. (6.3). In the limit $\epsilon^2\to 0$ its value is

$$T_N=\frac{1}{4nN} . \tag{6.13}$$

To calculate the MFT we need the corresponding generating function G_N. Considerations that should be obvious by now lead to

$$G_N=\frac{X_{1/2}}{1-X_{1/2}Q_N}T_N , \tag{6.14}$$

which lead to the following MFT:

$$\langle t\rangle = 2N^2n(n+m)+2Nn(m+1) . \tag{6.15}$$

Note that for fixed n and m the leading dependence on N is quadratic. When $m=0$ we regain the formula for a straight segment of length Nn, as we should. The dependence of $\langle t\rangle$ on m is linear, as in the case of a single dangling bond (meaning, perhaps, that the probability distribution along the dangling segments is uniform).

In the limit of large N, $\langle t\rangle$ is invariant under the transformations

$$N\to N/k , \tag{6.16a}$$

$$m\to km , \tag{6.16b}$$

$$n\to kn , \tag{6.16c}$$

which means that a dilution of the "density" of dangling bonds by a factor k, keeping the total length of the segment $(0,N)$ fixed (i.e., Nn is fixed) and also keeping Nm, the total length of the dangling bonds [its exact value is actually $(N+1)m$] fixed, does not change $\langle t\rangle$. This result would imply that a naive Einstein relation approach (see Sec. VII) could work here. Note also that by making the following replacements,

$$n\to\frac{Nn}{2} , \tag{6.17a}$$

$$N\to 2 , \tag{6.17b}$$

$$m\to\frac{(N+1)m}{3} , \tag{6.17c}$$

which keep Nn and $(N+1)m$ fixed (i.e., replace the original segment by a segment with three dangling bonds), we obtain that $\langle t\rangle$ remains unchanged.

In summary, we have shown in this section how our method enables one to perform the calculation of the generating function corresponding to a rather nontrivial case. To leading order in N it seems that diluting the dangling bonds, while keeping their total length fixed, leaves the MFT unchanged. Thus the effective diffusion constant $\tilde{D}=N^2n^2/2\langle t\rangle$ also remains unchanged. In other limits (m very large) this statement may not hold. The conclusion is that such geometrical transformations should be approached with care.

VII. SUMMARY AND CONCLUSIONS

We have presented a method for calculating properties of discrete random walks on a discrete network. The method involves the definition of "basic walks" on a segment, whose probabilities are denoted by T, Q, and X. Once the probabilities of these basic walks have been calculated, the probability of any walk on a network can be calculated, in principle. In practice, the algebra may be tedious, yet much simpler than that involved in a straightforward solution of master equations. It should be obvious from our calculations that given a black box (which contains a network) to which only two points A and B are "connected," all the properties of a random walk which involves entering the black box and leaving it (except for the properties that are directly related to events inside the box) can be calculated from T_{AB}, T_{BA}, Q_{AA}, and Q_{BB} (the notation, we hope, is obvious). The result can be obviously generalized to a black box with a larger number of "exists." The meaning of this result is that when dealing, e.g., with networks, one may replace parts of a network by their "effective" properties (T's and Q's) in an exact way. Such an approach can be useful when dealing with self-similar objects. For example, using this approach one can calculate properties of a walk on networks, which contain (infinite) sets of nested loops, fractals (at least some), etc. More details will be presented in future publications, where application to physical systems will also be presented. Some of our results can be generalized to continuous (in time and/or space) random walks. Efforts in this direction are being pursued by the authors.

It is interesting to note that exact iterative processes have been used in the literature (sometimes known as multiple-scattering techniques) to solve certain aspects of random-walk problems (cf. Eq. 1 in Ref. 14) such as hopping conductivity or motion (decay) of excitations (Refs. 14–18). In the present paper we have mainly concentrat-

ed on mean-first-passage-time problems. The problems of transport using our method will be dealt with in subsequent publications. We shall only reiterate that one of the novel elements in our approach is the identification of some basic random walks, which differ with respect to other approaches. This fact is shown to be useful in calculating a large variety of physical quantities.

Our final remark concerns the relation between the effective diffusion constant $\tilde{D}$ defined for MFT calculations, and the real diffusion constant D, which appears in the Einstein relation. Strictly speaking, the two quantities are different. We expect, though, that $\tilde{D}$ and D will have the same asymptotic dependence on the geometry for homogeneous systems (e.g., a long segment). For more complicated systems the situation is, however, different. Let us consider the example of a segment with a dangling bond [cf. Eq. (4.12) and Fig. 2]. A naive interpretation of the Einstein relation $D \sim \sigma/\tilde{n}$, σ being the electrical dc conductivity and $\tilde{n}$ being the volume fraction of the metallic cluster within a box of linear size (n_1+n_2), yields (we choose $n_1 \gg n_2$)

$$D \sim 1 \quad \text{for } n_3 < n_1 \ , \tag{7.1a}$$

$$D \sim \frac{n_3}{n_1} \quad \text{for } n_3 > n_1 \ . \tag{7.1b}$$

By contrast, from Eq. (4.15) we obtain (for $n_3 \gg n_1$, $n_1^2 \ll n_2 n_3$)

$$\tilde{D} = \frac{(n_1+n_2)^2}{2 \cdot 4 \cdot n_2 \cdot n_3} \sim \frac{n_1^2}{n_2 n_3} \ . \tag{7.2}$$

The difference between Eqs. (7.1b) and (7.2) results from the fact that in the calculation of $D = n^2/2\langle t \rangle$, the average of t includes paths that contribute extremely large "trapping times" in the dangling bond. In general, when $\langle t \rangle$ has a very long tail, one should expect that $D \neq \tilde{D}$ (which is related to the fact that $\langle 1/t \rangle \neq 1/\langle t \rangle$). Thus, the results presented in this paper indicate that one has to be extremely cautious when calculating the finite time diffusion constant in an inhomogeneous system.

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