Validity of the mean-field approximation for diffusion on a random comb

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We consider unbiased diffusion on a random comb structure (an infinitely long backbone with loopless branches of arbitrary length emanating from it). If $\langle t(\pm j|0)\rangle_w = T_0$ is the mean time (averaged over all random walks) for first passage from an arbitrary origin 0 on the backbone to either of the sites $+j$ or $-j$ on it in a given realization of the structure, the exact diffusion constant for the problem is defined as $K = \lim_{j\to\infty} j^2 \langle 1/T_0\rangle_c$, where $\langle\ \rangle_c$ stands for the configuration average over the realizations of the random comb. The diffusion constant in the mean-field approximation is given by $K_{\mathrm{MF}} = \lim_{j\to\infty} j^2/\langle T_0\rangle_c$. We compute T_0 exactly for an arbitrary realization of the comb and then show rigorously that, owing to the suppression of the relative fluctuations in T_0 in the "thermodynamic limit" $j\to\infty$, we have $K_{\mathrm{MF}} = K$ whenever the moments of certain random variables $\Gamma(L,\alpha,\beta)$ are finite; here the site-dependent random variables L, α, and β are, respectively, the branch length, stay probability at the tip of a branch, and the backbone-to-branch jump probability. Finally, we discuss different situations in which K will not be equal to K_{MF}, although the transport remains diffusive, as opposed to those in which anomalous diffusion occurs. [S1063-651X(96)04508-4]

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I. INTRODUCTION

The important problem of transport in disordered media has received a great deal of attention for a number of years now [1]. In particular, random walks on comblike structures—regular, hierarchical, and random—have been studied in detail in recent times. These structures provide tractable models for investigating transport in more complex systems, such as percolation clusters, finitely ramified fractals, porous media, etc. A comb consists of an infinitely long backbone of sites to which teeth (loopless branches) are attached. Transport along the backbone is the object of interest. If all the branches are of the same (finite) length we have a regular comb. In this case motion along the backbone is purely diffusive (the mean square displacement diverges linearly with time); the presence of the branches simply provides for a delay and leads to a smaller value of the diffusion constant. However, if the branches all are of infinite length, the diffusion is anomalous [2], in that the mean square displacement diverges as $t^{1/2}$, although the distribution of the position of the random walker is asymptotically Gaussian. If the branches have hierarchical lengths, one can have regular as well as anomalous diffusion depending on the values of the parameters that describe the structure ([3–10] and the references cited therein).

Random combs constitute another class of structures on which a wide variety of diffusive and subdiffusive processes occur. Here, branches of random lengths (with a given distribution) are attached to random sites on the backbone. Both unbiased diffusion and field-induced drift have been studied [11–16] on random combs. A comprehensive treatment of the problem has been given recently [17], delineating the precise conditions on the branch length distribution under which different kinds of behavior ensue. Analytical treatments of the problem have essentially used a "mean-field" approach—in the present context, this means a premature configuration averaging over the realizations of the random comb. As a result, a random walk on the random comb is reduced to a random walk on a regular linear lattice with a certain common effective waiting-time distribution at each site. In view of the extensive applicability of the random comb model, it is important to examine carefully whether this approximation is justified. It is the purpose of this paper to establish explicitly the validity of the mean-field approximation when the motion on the comb is diffusive: in other words, when normal diffusion occurs on the random comb, we show that the diffusion constant in the mean-field approximation is equal to the true diffusion constant.

The rest of the paper is organized as follows. In the next section we define the diffusion constant K in terms of the mean first passage time T_0 to reach boundary sites $\pm j$ from an origin 0 on the backbone, in the limit $j\to\infty$ (the "thermodynamic limit" in the present context). An exact expression for T_0 is derived for an arbitrary realization of the random comb. In Sec. III we use this to compute first the mean-field value K_{MF} of the diffusion constant. The fluctuations in T_0 are then analyzed to show that their contribution to K vanishes in the thermodynamic limit, leading to the equality of K_{MF} and K. The precise conditions under which this takes place are identified. In Sec. IV we discuss situations in which the mean-field approximation does not hold good even at the level of the diffusion constant.

II. THE DIFFUSION CONSTANT ON A RANDOM COMB

A. Definition of the diffusion constant

The diffusion constant on a statistically homogeneous structure such as the random comb under consideration can be defined in either of two equivalent ways [18,19]. From the asymptotic ($n\to\infty$) behavior of the variance of the displacement $j(n)$ in time n, we have

$$K = \lim_{n\to\infty} n^{-1} \langle\langle j^2(n)\rangle_w\rangle_c, \tag{1}$$

where $\langle\ \rangle_w$ denotes the average over random walks on a given realization of the random comb, and $\langle\ \rangle_c$ denotes the subsequent configuration average over these realizations. The alternative definition of K involves the asymptotic ($j\to\infty$) behavior of the mean first passage time (MFPT) to start from some origin and reach either one of the two exit points at $+j$ and $-j$:

$$K=\lim_{j\to\infty} j^2\langle\langle t(\pm j|0)\rangle_w^{-1}\rangle_c . \tag{2}$$

We shall use this definition, as it is relatively easier to calculate the MFPT concerned. We use the abbreviation T_0 for the MFPT $\langle t(\pm j|0)\rangle_w$ on a given realization of the structure. Strictly speaking, the thermodynamic limit in Eqs. (1) and (2) should precede the configuration averaging. As long as the expressions concerned converge uniformly, the interchange of the order of operation is permissible. We shall assume that this is the case and defer a discussion of the exceptional cases to Sec. IV.

B. Calculation of the MFPT

The derivation of a formula for T_0 proceeds in several steps. Consider first a chain $(-j,\ldots,0,\ldots,j)$ of $(2j+1)$ sites, such that the jump probability from any site to either of its neighbors is $+1/2$, the only exception being a particular site r. At this site, the random walker stays on at the end of a time step with a probability γ_r, or jumps to site $(r\pm1)$ with a probability $(1-\gamma_r)/2$. Writing T_l for the MFPT $\langle t(\pm j|l)\rangle_w$ to start from site l and reach either of the exit points at $+j$ and $-j$, we have the set of linear equations:

$$T_l=1+\tfrac{1}{2}(T_{l-1}+T_{l+1}),\quad -(j-2)\leqslant l\leqslant(j+2),\quad l\neq r, \tag{3}$$

$$T_{\pm(j-1)}=1+\tfrac{1}{2}T_{\pm(j-2)}, \tag{4}$$

$$T_r=(1-\gamma_r)^{-1}+\tfrac{1}{2}(T_{r-1}+T_{r+1}). \tag{5}$$

Solving for T_0, we find

$$T_0=\langle t(\pm j|0)\rangle_w=j^2+(j-|r|)\left(\frac{\gamma_r}{1-\gamma_r}\right). \tag{6}$$

Next, consider the same chain, but with an arbitrary *set* $\{r\}$ of sites at which the random walker has stay probabilities $\{\gamma_r\}$. As a direct consequence of the Markov property of the walk, and *at the level of the MFPT*, the contribution (to T_0) of different sites is verified in a straightforward manner to be simply *additive*. We thus arrive at the crucial result

$$T_0=j^2+\sum_r (j-|r|)\left(\frac{\gamma_r}{1-\gamma_r}\right). \tag{7}$$

When every $\gamma_r=0$, this reduces to the well-known result $T_0=j^2$ for a simple unbiased random walk on a linear chain.

Now suppose there is a branch of L_r sites at the backbone site r, with transition probabilities as indicated in Fig. 1. For the sake of generality, we have introduced a backbone-to-branch jump probability β_r as well as a stay probability α_r at the end of the branch. This enables one to encompass at one stroke a variety of possible physical situations and boundary

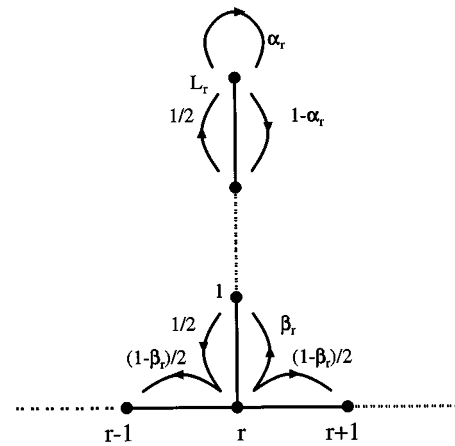

FIG. 1. Branch of L_r sites at backbone site r. Jump probabilities out of different sites are indicated.

conditions. Once again, at the level of the MFPT, the presence of the branch at r is *entirely equivalent* to a branchless site with a certain *specific* stay probability γ_r: if $\langle t(r\pm1|r)\rangle_w$ is the MFPT to escape from r to the neighboring sites $r\pm1$ in the presence of the branch at r, this equivalence is expressed by

$$\gamma_r=1-\langle t(r\pm1|r)\rangle_w^{-1}. \tag{8}$$

[Some reflection shows that $\langle t(r\pm1|r)\rangle_w$ is identically equal to $(1-\gamma_r)^{-1}$]. Now, a straight-forward calculation similar to the one leading to Eq. (6) yields

$$\langle t(r\pm1|r)\rangle_w=\frac{1}{1-\beta_r}\left[2\beta_r(L_r-1)+1+\frac{\beta_r}{1-\alpha_r}\right]. \tag{9}$$

Using this in Eq. (8), we get, say,

$$\frac{\gamma_r}{1-\gamma_r}=\left(\frac{\beta_r}{1-\beta_r}\right)\left[2L_r+\frac{\alpha_r}{1-\alpha_r}\right]\equiv\Gamma_r . \tag{10}$$

Substitution in Eq. (7) gives, finally, the compact formula

$$T_0=\langle t(\pm j|0)\rangle_w=j^2+\sum_r (j-|r|)\Gamma_r\delta_r , \tag{11}$$

where Γ_r has been defined in Eq. (10); further, $\delta_r=1$ if there is a branch $(L_r\geqslant1)$ at the site r, and $\delta_r=0$ otherwise $(L_r=0)$. On the random comb we may regard $\{L_r,\beta_r,\alpha_r\}$ as a set of independent random variables that are identically distributed at each site r of the backbone. The difficulty, of course, is the fact that it is the *reciprocal* of T_0 that must be configuration averaged in Eq. (2) for K.

Various special cases are read off easily from Eq. (11). In particular, a *myopic* random walk corresponds to $\beta_r=1/3$ and $\alpha=0$, leading to

$$T_0=j^2+\sum_r \delta_r L_r(j-|r|). \tag{12}$$

III. EQUALITY OF THE MEAN-FIELD AND EXACT VALUES OF K

The mean-field (MF) approximation to the diffusion constant K corresponds to neglecting the fluctuations in T_0 from one realization of the comb to another, and thus to replacing $\langle T_0^{-1}\rangle_c$ by $\langle T_0\rangle_c^{-1}$ in the thermodynamic limit $j\to\infty$ involved in the computation of K using Eq. (2). Since $\sum_{r=-(j-1)}^{j-1}(j-|r|)=j^2$, we have

$$\langle T_0\rangle_c=j^2\left[1+\left\langle\frac{\beta}{1-\beta}\left(2L+\frac{\alpha}{1-\alpha}\right)\right\rangle_c\right]=j^2(1+\langle\Gamma\rangle_c), \tag{13}$$

where we have dropped the site label r on the quantities α, β, L, and Γ for brevity. Thus

$$K_{\mathrm{MF}}=\lim_{j\to\infty}\frac{j^2}{\langle T_0\rangle_c}=(1+\langle\Gamma\rangle_c)^{-1}$$
$$=\left[1+\left\langle\frac{\beta}{1-\beta}\left(2L+\frac{\alpha}{1-\alpha}\right)\right\rangle_c\right]^{-1}. \tag{14}$$

If, further, β and α are constants that do not vary randomly from site to site, Eq. (14) reduces to

$$K_{\mathrm{MF}}=\left[1+\frac{\beta}{1-\beta}\left(2\langle L\rangle_c+\frac{\alpha}{1-\alpha}\right)\right]^{-1}, \tag{15}$$

where $\langle L\rangle_c$ is the average length of a branch. In particular, for a myopic walk $(\beta=1/3,\alpha=0)$ we have the simple expression

$$K_{\mathrm{MF}}=(\langle L\rangle_c+1)^{-1}, \tag{16}$$

while a reflecting boundary condition at the branch tips $(\alpha=1/2)$ gives $K_{\mathrm{MF}}=(\langle L\rangle_c+3/2)^{-1}$, etc.

We now show that the mean-field result, Eq. (14), is in fact the *exact* value of K as defined in Eq. (2). Defining $\delta T_0=T_0-\langle T_0\rangle_c$ and assuming that all the moments of δT_0 exist, we have from Eqs. (2) and (14)

$$K=K_{\mathrm{MF}}+\lim_{j\to\infty}\sum_{n=2}^{\infty}(-1)^n j^2\langle T_0\rangle_c^{-n-1}\langle(\delta T_0)^n\rangle_c$$
$$=K_{\mathrm{MF}}+\sum_{n=2}^{\infty}(-1)^n(1+\langle\Gamma\rangle_c)^{-n-1}$$
$$\times\lim_{j\to\infty}j^{-2n}\langle(\delta T_0)^n\rangle_c. \tag{17}$$

We have used $\langle\delta T_0\rangle=0$ and the fact that $\langle T_0\rangle$ scales as j^2. What is needed, therefore, is the leading behavior (as $j\to\infty$) of $\langle(\delta T_0)^n\rangle_c$ for $n\geqslant 2$. Recalling that $\delta T_0=T_0-\langle T_0\rangle_c$, we have

$$j^{-2n}\langle(\delta T_0)^n\rangle_c=\sum_{l=0}^{n}\binom{n}{l}(-1)^l(1+\langle\Gamma\rangle_c)^{n-l}j^{-2l}\langle T_0^l\rangle_c. \tag{18}$$

The correction to K_{MF}, if any, is therefore controlled by the leading [or $O(j^{2l})$] term in $\langle T_0^l\rangle_c$. From Eq. (11) we have

$$j^{-2l}\langle T_0^l\rangle_c=\sum_{k=0}^{l}\binom{l}{k}j^{-2k}\left\langle\left[\sum_r(j-|r|)\delta_r\Gamma_r\right]^k\right\rangle_c. \tag{19}$$

We therefore require the leading [or $O(j^{2k})$] term in

$$\sum_{r_1}\cdots\sum_{r_k}(j-|r_1|)\cdots(j-|r_k|)\langle\Gamma_{r_1}\cdots\Gamma_{r_k}\rangle_c. \tag{20}$$

An inspection of the summand shows that this leading behavior can only arise from that term in the multiple sum in which all the indices r_i are distinct and no two of them are equal. The $O(j^{2k})$ term therefore comes only from the restricted sum

$$\sum_{r_1}{}'\cdots\sum_{r_k}{}'\langle\Gamma_{r_1}\rangle_c\cdots\langle\Gamma_{r_k}\rangle_c(j-|r_1|)\cdots(j-|r_k|)$$
$$=\langle\Gamma\rangle_c^k\sum_{r_1}{}'\cdots\sum_{r_k}{}'(j-|r_1|)\cdots(j-|r_k|); \tag{21}$$

the primes denote the restriction $r_i\neq r_j$. As a consequence, only the first moment $\langle\Gamma\rangle_c$ of the random variable Γ_r appears in the quantities of interest in the present context. But the leading, or $O(j^{2k})$, term in Eq. (21) is precisely the same as that of the *unrestricted* sum

$$\langle\Gamma\rangle_c^k\sum_{r_1}{}'\cdots\sum_{r_k}{}'(j-|r_1|)\cdots(j-|r_k|), \tag{22}$$

which is trivially evaluated to yield $j^{2k}\langle\Gamma\rangle_c^k$. Using this in Eq. (19), we have

$$\langle T_0^l\rangle_c=j^{2l}(1+\langle\Gamma\rangle_c)^l+\text{lower orders in } j. \tag{23}$$

Insertion in Eq. (18) shows at once that the coefficient of j^{2n} in $\langle(\delta T_0)^n\rangle_c$ vanishes, so that (in view of the limit $j\to\infty$)

$$K=K_{\mathrm{MF}}. \tag{24}$$

While the explicit derivation we have given above helps us understand the precise conditions under which the result of Eq. (24) is obtained, a shorter formal proof is also possible, along the lines of the central limit theorem. The linear dependence of T_0 on the set of random variables $\{\Gamma_r\}$ in Eq. (11) implies at once that the corresponding characteristic functions

$$G(\theta)=\langle\exp\{i\theta T_0\}\rangle_c \tag{25}$$

and

$$g(\theta)=\langle\exp\{i\theta\Gamma\}\rangle_c \tag{26}$$

are related by

$$G(\theta)=\exp\{ij^2\theta\}\prod_{r=-(j-1)}^{(j-1)} g[(j-|r|)\theta]$$
$$=\exp\{ij^2\theta\}g(j\theta)\prod_{r=1}^{j-1} g^2(r\theta). \tag{27}$$

If all the moments of the random variable Γ exist, we have the cumulant expansion

$$\ln g(\theta)=\sum_{n=1}^{\infty}\frac{(i\theta)^n k_n}{n!} \tag{28}$$

and similarly, for the random variable T_0,

$$\ln G(\theta)=\sum_{n=1}^{\infty}\frac{(i\theta)^n \chi_n}{n!}. \tag{29}$$

Equation (27) then yields, on equating the coefficients of θ on both sides,

$$\chi_1=\langle T_0\rangle_c=j^2(1+k_1)=j^2(1+\langle\Gamma\rangle_c), \tag{30}$$

which is just Eq. (13); further,

$$\chi_2=\langle(\delta T_0)^2\rangle_c=\frac{1}{3}k_2(2j^3+j), \tag{31}$$

where $k_2=\langle\Gamma^2\rangle_c-\langle\Gamma\rangle_c^2$ In general, χ_n is related to k_n by

$$\chi_n=k_n\left[j^n+2\sum_{r=1}^{j-1} r^n\right],\quad n\geqslant 2. \tag{32}$$

The leading large-j behavior of $\Sigma_{r=1}^{j-1}r^n$ is $j^{n+1}/(n+1)$. This implies at once that, for very large values of j,

$$\frac{\chi_n^{1/n}}{\chi_1}\to\left(\frac{2k_n}{n+1}\right)^{1/n}(1+\langle\Gamma\rangle_c)^{-1}j^{1/n-1}. \tag{33}$$

This shows precisely how the fluctuations of T_0 about its mean value $\langle T_0\rangle_c$ are suppressed in the limit $j\to\infty$: that is, the *distribution* of T_0 converges to a degenerate distribution with a single point of increase at $\langle T_0\rangle_c$, validating Eq. (24). The precise factors responsible for this result are as follows: (i) the additivity property of the contributions to the MFPT, T_0, from different branches; (ii) the linear dependence of T_0 upon the random site variables $\{\Gamma_r\}$; and (iii) the linear dependence of the coefficients of Γ_r upon the distance $(j-|r|)$ or, equivalently, the distance $|r|$, in the expression for T_0 [see Eq. (11)].

IV. EXCEPTIONS TO THE MEAN-FIELD RESULT

We have seen that the diffusion constant for an unbiased random walk on a random comb is given by the mean-field approximation when all the moments of the site variable Γ exist—essentially when all the moments of the branch length distribution are finite. It is clear from the definition of K in Eq. (2) that, as long as $\langle\Gamma\rangle_c$ (essentially the mean branch length $\langle L\rangle_c$) is finite, the diffusion is normal; i.e., the MFPT $\langle T_0\rangle_c$ scales as j^2 asymptotically; or, equivalently, the mean square displacement of the random walk has a leading asymptotic behavior proportional to the time n. If the higher moments of Γ_r (or L_r) diverge, the diffusion constant is renormalized by the fluctuations in $\{L_r\}$ to a value other than the mean field one. On the other hand, if $\langle\Gamma\rangle_c$ (or $\langle L\rangle_c$) *itself* diverges, the diffusion is anomalous; i.e., the random walk along the backbone of the comb is subdiffusive, with the mean square displacement diverging typically as $t^\nu, \nu\leqslant 1$. The central quantity of interest is then the exponent ν. This is a separate problem that is addressed elsewhere ([14,17], and references therein). We are concerned here with the situation in which K can differ from $K_{\rm MF}$ owing to the nonexistence of the second and higher moments of the branch-length distribution.

In this context, it is worth remembering that K may differ from $K_{\rm MF}$ even if all the moments of L exist, if the branches at different sites are sufficiently *correlated* instead of being independently distributed. As an extreme instance, suppose all the branches are *identical*, i.e., the random variables $\Gamma_{-(j-1)}=\Gamma_{-j}=\cdots\Gamma_0=\Gamma_1=\cdots\Gamma_{j-1}$ in each realization. Now, the expression we have derived for T_0, Eq. (11), is valid for any given set of variables $\{\Gamma_r\}$. Therefore

$$K=\lim_{j\to\infty}\left\langle\frac{j^2}{j^2+\Gamma\Sigma_r(j-|r|)}\right\rangle_c=\langle(1+\Gamma)^{-1}\rangle, \tag{34}$$

in contrast to the mean-field answer

$$K_{\rm MF}=(1+\langle\Gamma\rangle)^{-1}. \tag{35}$$

Even if the variables $\{\Gamma_r\}$ are uncorrelated to each other (and this is the random comb problem in which we are interested at present), when Γ_r does not have finite moments of all orders, the preceding demonstration that $K=K_{\rm MF}$ does not go through. It is precisely here that the question of uniform convergence in j, mentioned at the end of Sec. II, comes up. A simple example illustrates the kind of situation that can arise. Consider the case when there is no branch at any site except the origin, and consider a myopic random walk on such a structure. From Eq. (12), we have $T_0=j^2+Lj$, so that $j^2/T_0=[1+(L/j)]^{-1}$ on this structure. It is obvious that the behavior of this quantity depends on the manner in which the limits are taken: if $L,j\to\infty$ such that L/j is finite, we have a finite diffusion constant (as defined here) on the backbone. If L and j are allowed to become unbounded independently, the limiting value of $[1+(L/j)]^{-1}$ is 1 or 0, depending on whether $j\to\infty$ or $L\to\infty$ first. It is therefore clear that various kinds of subdiffusive behavior (on the backbone) can be obtained by letting the length L of the sole branch tend to infinity such as some power of j greater than unity. These are the situations considered in greater detail by Goldhirsch and Gefen [20,21]. All these possibilities show that the physical problem of interest must be specified carefully in each case. As already stated, we have been concerned in this paper with a random comb in which all the sites on the backbone are *statistically equivalent*, the random variables $\{L_r,\beta_r,\alpha_r\}$ being *independently and identically distributed* at each site r. If, therefore, one takes the view that the thermodynamic limit $j\to\infty$ is unrelated to the manner in which the branch lengths $\{L_r\}$ may become unbounded in some realization of the random comb, then the averaging over the distribution of the latter must be done independently, preceding the $j\rightarrow\infty$ limit. The (exact) relation between the characteristic functions G and g [see Eq. (27)] must be used to compute $\langle j^2/T_0\rangle_c$, and the $j\rightarrow\infty$ limit must be taken subsequently. [We note that $\langle 1/T_0\rangle_c = -i\lim_{s\rightarrow 0}\widetilde{G}(s)$, where $\widetilde{G}(s)$ is the Laplace transform of $G(\theta)$]. The divergence of the second and higher moments of $\{L_r\}$ will be reflected, of course, in the nonanalyticity of $\ln G(\theta)$ at $\theta=0$; the expansion of Eq. (29) breaks down, and the second term in the small-θ behavior of $\ln G(\theta)$ will typically be $O(\theta^{\gamma})$ where $0<\gamma<1$, signaling the departure of the true K from the mean-field value K_{MF}.

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