

Anomalous diffusion on a random comblike structure

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We have recently studied a random walk on a comblike structure as an analog of diffusion on a fractal structure. In our earlier work, the comb was assumed to have a deterministic structure, the comb having teeth of infinite length. In the present paper we study diffusion on a one-dimensional random comb, the length of whose teeth are random variables with an asymptotic stable law distribution $\phi(L) \sim L^{-(1+\gamma)}$ where $0 < \gamma \leq 1$. Two mean-field methods are used for the analysis, one based on the continuous-time random walk, and the second a self-consistent scaling theory. Both lead to the same conclusions. We find that the diffusion exponent characterizing the mean-square displacement along the backbone of the comb is $d_w = 4/(1+\gamma)$ for $\gamma < 1$ and $d_w = 2$ for $\gamma \geq 1$. The probability of being at the origin at time t is $P_0(t) \sim t^{-d_s/2}$ for large t with $d_s = (3-\gamma)/2$ for $\gamma < 1$ and $d_s = 1$ for $\gamma > 1$. When a field is applied along the backbone of the comb the diffusion exponent is $d_w = 2/(1+\gamma)$ for $\gamma < 1$ and $d_w = 1$ for $\gamma \geq 1$. The theoretical results are confirmed using the exact enumeration method.

I. INTRODUCTION

Anomalous diffusion is a common feature of diffusion on fractal structures.¹⁻⁴ One knows in general that the anomalous diffusion is due to the diffusion particles being stuck in bottlenecks and dead ends of the fractal. A general theory relating the exponents of various statistical properties of the diffusion process to properties of the fractal structure is yet to be formulated.

Recently we have analyzed a random walk on a comblike structure,⁵ which allows exact calculation of statistical properties, and which exhibits the phenomenon of anomalous diffusion. That model included an infinite line in the x direction, each site of which is intersected by an infinite line perpendicular to it as shown in Fig. 1. We showed that the properties of a random walk on the x axis of such a structure includes that of anomalous diffusion. This

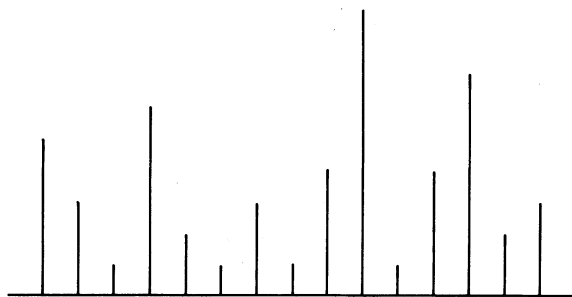


FIG. 1. Illustration of a random comblike structure. The backbone is the x axis and the teeth of the comb, characterized by the length distribution in Eq. (1), consist of the vertical lines.

property of the comb model can be regarded as the analog of anomalous diffusion along the backbone of a fractal. The anomalous properties clearly result from excursions taken by the random walker in the y direction along so-called dead ends. These excursions are analogs of excursions of diffusing particles into the dead ends of fractal structures. In our original comb model the length of the dead ends were all infinite. A more realistic analog of diffusion on fractals is one in which the dead ends are all finite but have a distribution of lengths. In particular, we will consider a lattice comb in which the length of each tooth is described by a probability distribution having the property

$$\phi(L) \sim L^{-(1+\gamma)}, \quad L \gg 1 \quad (1)$$

with $0 < \gamma \leq 1$. This distribution will be shown to lead to anomalous diffusion, the characteristic exponents of which depend on the value of γ . When the average tooth length is finite, $\gamma > 1$, one finds that the random walker moves as a simple diffusing particle, i.e., $\langle x^2 \rangle \approx t$. Two techniques will be used to calculate the diffusion exponents. The first is a mean-field-type argument that makes use of a formalism involving the continuous-time random walk (CTRW) and the second is a self-consistent scaling theory, which is also implicitly a mean-field approximation. The results of both analyses are in agreement, and are confirmed by numerical simulations. Our results for the characteristic exponents also apply to diffusion on deterministic geometrical hierarchical structures (see Fig. 2).

II. THE CTRW ANALYSIS

The CTRW analysis is a mean-field approach in which the random walker moves along the backbone of the

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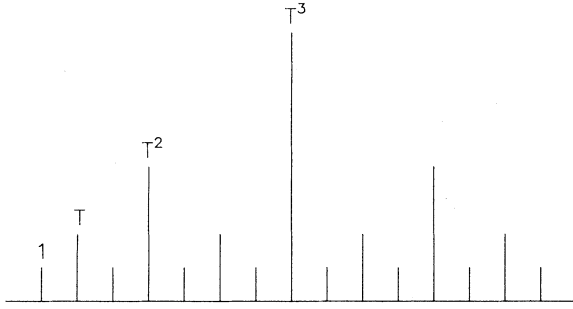


FIG. 2. A deterministic hierarchical structure of the kind discussed in the text. The scale of the teeth is determined by a parameter $T > 1$, so that teeth of a size $1, T, T^2, T^3, \dots$ can appear in the structure.

comb, without memory. That is to say, when the random walker returns to a site already visited, he can see a dead end with a value of L different from that seen the first time. The formalism for calculating the behavior of $\langle x^2(n) \rangle$ (for a random walker in discrete time) is very close to that presented in Ref. 5, which the reader should consult for further details. It was shown there that $\langle x^2(n) \rangle$ can be expressed as

$$\langle x^2(n) \rangle = \sigma^2 \langle j(n) \rangle, \quad (2)$$

where σ^2 is the variance of displacement of a single step of the random walk ($\sigma^2 = 1$ for a symmetric nearest-neighbor walk), the average is taken over all possible lengths, and $\langle j(n) \rangle$ is the expected number of steps that are taken along the backbone out of a total of n steps. The generating function of $\langle j(n) \rangle$ with respect to n will be denoted by $J(z)$, i.e.,

$$J(z) \equiv \sum_{n=0}^{\infty} \langle j(n) \rangle z^n. \quad (3)$$

Let ψ_n be the probability that the interval between two successive sojourns at a site of the backbone is equal to n , and let $\langle \psi(z) \rangle$ be the corresponding generating function. An argument analogous to that given in Ref. 5 can be used to show that $J(z)$ has the form

$$J(z) = \langle \psi(z) \rangle / \{ (1-z)[1 - \langle \psi(z) \rangle] \}. \quad (4)$$

Our strategy for calculating the asymptotic n dependence of $\langle x^2(n) \rangle$ will be to use a Tauberian theorem⁶ to infer the n dependence from the analytic behavior of $J(z)$ in the neighborhood of $z = 1$. It is shown in the Appendix that the asymptotic behavior of $\langle \psi_n \rangle$ is

$$\langle \psi_n \rangle \sim n^{-(3+\gamma)/2}, \quad (5)$$

which allows us to infer that as $z \rightarrow 1$ $\langle \psi(z) \rangle$ has the behavior

$$\langle \psi(z) \rangle \sim 1 - k(1-z)^{(1+\gamma)/2}, \quad (6)$$

where k is a constant that plays no further role in the analysis, and it is assumed that $\gamma \leq 1$. When $\gamma > 1$, the first moment corresponding to $\langle \psi_n \rangle$ is finite so that $\langle \psi(z) \rangle \sim 1 - k(1-z)$ as $z \rightarrow 1$. The case $\gamma = 1$ has to be

handled separately since it introduces a logarithmic term which has no effect on the exponent. When Eq. (6) is substituted into Eq. (4), one finds that

$$J(z) \sim (1-z)^{-(3+\gamma)/2}, \quad \gamma \leq 1 \\ \sim (1-z)^{-2}, \quad \gamma > 1 \quad (7)$$

as $z \rightarrow 1$. This allows us to infer that $\langle x^2(n) \rangle$ has the asymptotic form

$$\langle x^2(n) \rangle \sim n^{(1+\gamma)/2}, \quad \gamma \leq 1 \\ \sim n^2, \quad \gamma > 1. \quad (8)$$

If the diffusion exponent d_w is defined by the relation $\langle x^2(n) \rangle \sim n^{2/d_w}$, it follows that for the present model

$$d_w = 4/(1+\gamma), \quad 0 < \gamma < 1 \\ = 2, \quad \gamma \geq 1. \quad (9)$$

III. SELF-CONSISTENT SCALING ANALYSIS

The analysis of Sec. II has the characteristics of a mean-field theory in that the space-dependent structure of the comblike teeth are replaced by a waiting-time distribution independent of the x coordinate. Thus, the detailed structure of the comb is taken into account in an approximate rather than an exact way. An alternative mean-field approach is available to obtain the same results. The effect of the dangling ends is to provide random delays at each value of x . These delays are characterized by an average waiting time $\tau(L)$, where, in the absence of a field,⁷

$$\tau(L) \sim L, \quad L \gg 1. \quad (10)$$

The transition rate $w(L)$ at which random walkers return to the backbone from a comblike tooth of length L is therefore of the order of L^{-1} . Since the distribution of lengths has the asymptotic property shown in Eq. (1), it follows that the distribution of the waiting times is $p(w)$, where

$$p(w) = \phi(L) / (dw/dL) \sim w^{-(1+\gamma)}. \quad (11)$$

We next calculate the value of the diffusion exponent d_w , starting from some results for $\langle x^2(t) \rangle$ for diffusion in a one-dimensional random medium first given by Machta⁸ and Zwanzig,⁹ and more recently for higher-dimensional systems by Kundu and Philips.¹⁰ The result relates the square displacement $x^2(t)$ to the number of distinct sites visited, N , and the transition rates $\{w_i\}$ where w_i is the transition rate at site i . They find that

$$t/x^2 = (1/N) \sum_{i=1}^N (1/w_i) \quad (12)$$

in the limit of large t and N . At any finite time t or finite displacement x there is always a minimum transition rate that we denote by w_{\min} , and whose dependence on n will be found later. This quantity allows us to rewrite Eq. (12) as

$$t/x^2 \sim \int_{w_{\min}}^1 [p(w)/w] dw \sim w_{\min}^{(\gamma-1)}, \quad \gamma < 1. \quad (13)$$

The quantity w_{\min} is a measure of the smallest transition rate the random walker sees during a displacement x . Note that fluctuations in w_{\min} are neglected which implies that any argument based on Eq. (13) is a form of mean-field argument. The rate w_{\min} can be estimated as the inverse of the maximum span L_{\max} made by the walker in the y direction.¹¹ There are two characteristic lengths in the y direction. One is the maximum tooth length sampled in the same time as the random walk along the backbone has traveled a distance x . This scales as $x^{1/\gamma}$.¹¹ The second is the span of a random walk diffusing in the y direction on the assumption of a semi-infinite tooth. Since $x^{d_w} \sim t$, it follows that since the span in the y direction can be shown to go like $y^2 \sim t$, one finds

$$y \sim x^{d_w/2}. \quad (14)$$

The maximum span L_{\max} will therefore be the minimum of these two lengths, i.e.,

$$L_{\max} \sim \min(x^{d_w/2}, x^{1/\gamma}) \quad (15)$$

As will be seen, $x^{d_w/2}$ is smaller than $x^{1/\gamma}$ when $\gamma < 1$. Substituting Eq. (15) into Eq. (13), we obtain

$$t/x^2 \sim x^{-d_w(\gamma-1)/2}, \quad (16)$$

from which one finds a self-consistent equation for d_w ,

$$d_w = 2 - d_w(\gamma - 1)/2 \quad (17)$$

or

$$\begin{aligned} d_w &= 2 \quad \text{for } \gamma \geq 1 \\ &= 4/(1 + \gamma) \quad \text{for } 0 < \gamma < 1. \end{aligned} \quad (18)$$

This result is indeed consistent with the assumption that $d_w/2 < 1/\gamma$ when $\gamma < 1$.

It is evident that the result in this last equation agrees with the solution obtained from the CTRW argument that is found in Eq. (9). The reason is that the very long dead ends have a negligible effect since Eqs. (14) and (15) imply that a random walker rarely visits tips of these dead ends. Thus large fluctuation in the size of the dead ends are not relevant and a mean-field approach such as that of the CTRW is valid. Equation (18) was tested numerically by performing random walks on random combs with several values of γ . Numerical results for $\langle x^2 \rangle$ as a function of t were obtained using the exact enumeration method,¹² as shown in Fig. 3. For the values of $\gamma = 1, \frac{2}{3}, \frac{1}{2}, \frac{2}{5}, \frac{1}{3},$ and $\frac{1}{10}$ we found from the slopes of Fig. 3, $d_w = 2.08 \pm 0.1$ ($d_{w,\text{theor}} = 2$), 2.38 ± 0.5 (2.4), 2.69 ± 0.5 (2.67), 2.82 ± 0.5 (2.86), 3.24 ± 0.10 (3.33), and 3.60 ± 0.10 (3.63), in excellent agreement with the predicted values of Eqs. (9) and (18) for the values of n used in the simulation. We believe that these are true asymptotic results but this would be impossible to prove from simulations alone.

A similar approach can be applied to calculate the long-time autocorrelation function $P_0(t) \sim t^{-d_s/2}$ which is the probability that a random walker initially at the origin is also found at time t at the origin. It was shown by Alexander and Orbach¹ that

$$d_s/2 = d_f/d_w, \quad (19)$$

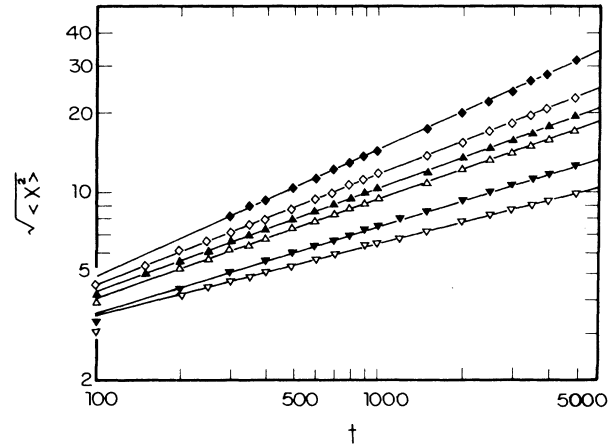


FIG. 3. Plot of the mean-squared displacement along the backbone $\langle x^2 \rangle^{1/2}$ as a function of t for several values of γ : $\gamma = 1$ (\blacklozenge), $\gamma = \frac{2}{3}$ (\diamond), $\gamma = \frac{1}{2}$ (\blacktriangle), $\gamma = \frac{2}{5}$ (\triangle), $\gamma = \frac{1}{3}$ (\blacktriangledown), $\gamma = \frac{1}{10}$ (∇). In the calculations, combs of sizes $-400 \leq x \leq 400$ were studied and averages were made over 100 configurations each.

where d_f is the fractional dimension. In our case, since the random walker does not visit the entire structure, d_f should represent the fractal dimension of the volume, M , visited by the walker. This can be approximated as

$$M \sim \sum_{L'=1}^x L' \sim x \int_0^{L_{\max}} L' p(L') dL' \sim x L_{\max}^{1-\gamma}, \quad (20)$$

where L_{\max} is found from Eq. (15). This leads to

$$M \sim x^{d_f} \equiv x^{1+d_w(1-\gamma)/2}, \quad (21)$$

from which it follows that

$$d_f = 1 + d_w(1 - \gamma)/2. \quad (22)$$

This relation can also be derived by using the resistivity coefficient, ξ , defined by $R \sim L^\xi$ in the Einstein relation,¹ $d_w = d_f + \xi$. On using this relation with the value $\xi = 1$ in Eq. (17) we find the result shown in Eq. (22). Furthermore, the combination of Eqs. (18), (19), and (22) allows us to express d_s as

$$\begin{aligned} d_s/2 &= (3 - \gamma)/4, \quad \gamma < 1 \\ &= \frac{1}{2}, \quad \gamma \geq 1. \end{aligned} \quad (23)$$

There are two limiting cases in which contact can be made with earlier results. When $\gamma \geq 1$, the first moment of the length distribution in Eq. (1) is finite and the mean sojourn time on a tooth is also finite. For the transition value $\gamma = 1$ one finds $d_w = 2$ and $d_s = \frac{1}{2}$ which is the same as for a one-dimensional random walk when the variance of step length is finite. The case $\gamma = 0$ corresponds to a comb in which the teeth are all infinite, for which it has been shown that $d_w = 4$ and $d_s = \frac{3}{4}$.⁵

The result shown in Eqs. (18) and (23) are also valid for diffusion on deterministic hierarchical combs,¹³⁻¹⁶ exemplified by that shown in Fig. 2. The relation between γ and the magnification factor T is^{14,16}

$$\gamma = (\ln 2) / (\ln T) . \quad (24)$$

On substituting this result into Eqs. (18) and (23) we find that the resulting exponents d_w and d_s for these structures are

$$\begin{aligned} d_w &= 2, \quad T \leq 2 \\ &= 4(\ln T) / (\ln 2T), \quad T > 2 \\ d_s &= \frac{1}{2}, \quad T \leq 2 \\ &= [\ln(T^3/2)] / (4 \ln T), \quad T > 2 . \end{aligned} \quad (25)$$

Whereas recent studies have used hierarchical structures as a model for a series of energy barriers, in the present work they are used as a model of the geometric structure of the system. It is interesting to compare the results shown in Eq. (25) with those obtained in models of diffusion in the presence of hierarchical energy barriers (cf., for example, Refs. 13 and 14). The exponent d_w found here is smaller than that found for the energy barriers in the cited references. This is because it is impossible to pass through an infinitely high barrier, while in the present model all the nearest-neighbor sites to a given one can be reached in a single step.

IV. EFFECTS OF A UNIFORM FIELD

The problem of diffusion on a random comb performed in a uniform field can be studied using the same techniques as discussed in Sec. III. The problem of a uniform field in the y direction only has been analyzed earlier where it was shown that $\langle x^2 \rangle$ is asymptotically proportional to $(\ln t)^{2\gamma}$, the coefficient being a function of the field.¹¹ It is known that in isotropic diffusion on a translationally invariant lattice the average displacement is equal to zero, but the presence of a field induces a mean drift so that $\langle x \rangle$ is asymptotically proportional to t . This result is obviously modified in diffusion on a comb structure where diffusion along a tooth is not influenced by the field. When the length of each tooth is long compared to that of a single step, one expects the majority of the time to be spent in motion along the teeth. This leads to a modification of the time dependence of the mean-squared displacement along the backbone.

The self-consistent argument given earlier can be used to suggest the form of the results expected in the case of the uniform field in the x direction. The time to make a displacement equal to x , for large x , can be approximated by

$$t \sim \sum_{i=1}^x (1/w_i) , \quad (26)$$

in which w_i is the transition rate at site i . This will be approximated by

$$t \sim x \int_{w_{\min}}^1 [p(w)/w] dw \sim x w_{\min}^{-\gamma} . \quad (27)$$

We find from Eq. (14) that

$$w_{\min} \sim 1/L_{\max} \sim x^{-d_w/2} \quad (28)$$

so that

$$t \sim x^{1+d_w(1-\gamma)/2} . \quad (29)$$

This implies that the self-consistency condition is

$$d_w = 1 + d_w(1-\gamma)/2 \quad (30)$$

with the result that

$$\begin{aligned} d_w &= 1 \quad \text{for } \gamma \geq 1 \\ &= 2/(1+\gamma) \quad \text{for } 0 < \gamma < 1 . \end{aligned} \quad (31)$$

The limits $\gamma = 0$ ($d_w = 2$) and $\gamma = 1$ ($d_w = 1$) correspond to the limits of long and short (i.e., with a finite mean length) dead ends.

V. DISCUSSION AND SUMMARY

We have found the exponents that characterize anomalous diffusion on comb structures when there is an inverse power law distribution of the length of the dead end. Because, on average, the random walker may not traverse the entire dead end on a given sojourn, the CTRW approach leads to a value for the diffusion exponent which is consistent with both the self-consistent scaling approach and numerical data. This behavior can be contrasted with that of diffusion on a loopless fractal in which, due to the property of self-similarity, the random walk tends to visit all accessible sites.¹⁶ This can be explained in terms of the expression for the exponent d_s which can be written in terms of d_l , the fractal dimension of a tree in the space of chemical distances. The exponent d_s is found to be¹⁷

$$d_s = 2d_l / (1 + d_l) , \quad (32)$$

which is always less than 2. The critical fractal dimension is $d_s = 2$, below which the number of distinct sites visited scales as the mass of the cluster.⁴

It is interesting to see how the present approach can be used to obtain results for different fractal models. As an example, let us consider diffusion on the incipient percolation cluster generated on a Cayley tree. This can be put into correspondence with diffusion along a one-dimensional backbone, with the excursions along dead ends modeled in terms of excursions along the teeth of the comb. The distribution of cluster sizes, s , along the backbone has been shown to be¹⁸

$$\rho(s) \sim s^{-3/2} . \quad (33)$$

It is physically reasonable to assume that the transition rates $\{w_i\}$ scale as the inverse of cluster size, so that the distribution of these transition rates for small w is

$$p(w) \sim \rho(s) ds/dw \sim w^{-1/2} . \quad (34)$$

Hence, the parameter γ is equal to $\frac{1}{2}$. In this case $w_{\min} \sim s_{\max}^{-1} \sim x^{-1/\gamma}$ so that if we substitute this result into Eq. (13) we have

$$d_w = (1 + \gamma) / \gamma = 3 , \quad (35)$$

as has been found earlier; see, for example (Ref. 19). It is interesting to apply a similar approach to the case of field acting only along the backbone but not along the dead ends of such a structure. This case is suggested by the

problem of modeling the dispersion of a tracer particle in flow through porous media.²⁰ The flow through a structure with a main channel with dead ends reacts to a field along the channel but the flow in the dead ends is modeled in terms of an ordinary diffusion process. If we use similar arguments to those leading to Eq. (31), in the case of flow on a percolation cluster of a Cayley tree we find for the diffusion of the tracer

$$d_w = 3/(1+2\gamma) = \frac{3}{2}, \quad (\text{A36})$$

changing the diffusion exponent from $d_w = 1$ to $d_w = \frac{3}{2}$.

APPENDIX: CALCULATION OF THE ASYMPTOTIC FORM OF $\langle \psi_n \rangle$

Consider a nearest-neighbor random walk on a discrete line $(0, L)$ in which the point $y=0$ is absorbing and $y=L$ is reflecting. We determine the asymptotic form for the probability that the time between two successive steps on the backbone is equal to n , in the limit of large n . In this calculation the first step is to find the probability that the random walker takes at lead n steps before being trapped, given that the starting point is at $y=1$. Call this quantity T_n . The probability that trapping occurs exactly at step n is

$$U_n = T_{n-1} - T_n. \quad (\text{A37})$$

However, for the problem whose solution is required, a return to $y=0$ does not guarantee an immediate step along the backbone, since there is a finite probability that the random walker can over back from $y=0$ to $y=1$. Hence, our final step is to take this into account.

Let $p_n(y)$ be the probability that the random walker is at y at step n given an initial position $y=1$. These probabilities satisfy

$$p_{n+1}(y) = \frac{1}{2}[p_n(y+1) + p_n(y-1)], \quad (\text{A38})$$

subject to the initial and boundary conditions

$$\begin{aligned} p_0(y) &= \delta_{y,1}, \quad p_{n+1}(0) = 0, \\ p_{n+1}(L) &= \frac{1}{2}[p_n(L) + p_n(L-1)]. \end{aligned} \quad (\text{A39})$$

The boundary condition on the second line of this equation implies that a random walker at the reflecting end either remains there with probability $\frac{1}{2}$ or moves to $L-1$ with probability $\frac{1}{2}$. For the model in Eqs. (A2) and (A3) standard methods of solution suffice to show that

$$p_n(y) = \frac{2}{L+1} \sum_{j=0}^{L-1} \cos^n \lambda_j \sin \lambda_j \sin(\lambda_j y), \quad (\text{A40})$$

$$\lambda_j = \pi(2j+1)/(2L+1),$$

from which one finds T_n to be

$$\begin{aligned} T_n &= \sum_{y=1}^L p_n(y) = \frac{8}{2L+1} \sum_{j=0}^{L-1} \cos^n \lambda_j \cos(\lambda_j/2) \sin(\lambda_j/2) \\ &\quad \times \sin[\lambda_j(L+1)/2]. \end{aligned} \quad (\text{A41})$$

Since the large- n behavior of T_n comes from sojourns on the longest teeth, we may pass to the continuum limit in Eq. (A5). If we fix j and let $L \rightarrow \infty$, then $\lambda_j \sim \pi j/L$ which allows us to make the following estimates:

$$\begin{aligned} \cos^n \lambda_j &\sim \exp[-n\pi^2 j^2/(2L^2)], \quad \cos(\lambda_j/2) \sim 1, \\ \sin(\lambda_j L/2) \sin[\lambda_j(L+1)/2] &\sim \sin^2(\pi j/2). \end{aligned} \quad (\text{A42})$$

These limiting values imply that

$$T_n \sim (4/L) \sum_{s=0}^{\infty} \exp[-n\pi^2(2s+1)^2/(2L^2)], \quad (\text{A43})$$

valid for L fixed. We will now distinguish between two cases according to whether $\gamma < 1$ or $\gamma > 1$; the case $\gamma = 1$ is special but not interesting and will not be analyzed here. When $\gamma < 1$, the average of T_n with respect to the stable law distribution in Eq. (1) is

$$\begin{aligned} \langle T_n \rangle &\sim 4 \sum_{s=0}^{\infty} \int_0^{\infty} \frac{1}{L^{2+\gamma}} \exp\left[-\frac{\pi^2 n(2s+1)^2}{2L^2}\right] dL \\ &\sim K n^{-(1+\gamma)/2}, \end{aligned} \quad (\text{A44})$$

where K is a constant. It is evident that in this case the mean first passage time to return to the backbone is infinite. In contrast, when $\gamma > 1$, the mean time to return to the backbone is finite.

As a final step we can calculate the asymptotic behavior of the probability $\langle \psi_n \rangle$ defined earlier. When the random walker is at $y=0$, it either moves along the backbone with probability $\frac{1}{2}$ or back along a dead end with probability $\frac{1}{2}$. Hence, the expected number of visits to the backbone before a step is made along it is

$$\sum_{n=1}^{\infty} n \left(\frac{1}{2}\right)^n = 2, \quad (\text{A45})$$

so that

$$\langle \psi_n \rangle \sim n^{-(3+\gamma)/2}, \quad (\text{A46})$$

which is the result used in Eq. (5).

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