Letter

First passage on disordered intervals

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We derive unexpected first-passage properties for nearest-neighbor hopping on finite intervals with disordered hopping rates, including (a) a highly variable spatial dependence of the first-passage time, (b) huge disparities in first-passage times for different realizations of hopping rates, (c) significant discrepancies between the first moment and the square root of the second moment of the first-passage time, and (d) bimodal first-passage time distributions. Our approach relies on the backward equation, in conjunction with probability generating functions, to obtain all moments, as well as the distribution of first-passage times. Our approach is simpler than previous approaches based on the forward equation, in which computing the mth moment of the first-passage time requires all preceding moments.

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Introduction. First-passage problems concern the distribution of times for a stochastic process to first reach a defined state [1–7]. Of fundamental importance is the statistics of the time required for a random walk to *first* reach the boundaries of a finite interval. The applications of this type of first-passage problem are vast, including biological processes, such as the Moran model [8,9], migration phenomena [10,11], the behavioral dynamics of ant recruitment [12,13], as well as the dynamics of many types of financial instruments [14,15].

First-passage phenomena are much richer and less well understood when the hopping rates of the random walk are *spatially disordered*. Transport in disordered one-dimensional systems has a host of important applications, such as channel transport across cellular membranes [16], molecular motors walking on microtubules [17], the motion of RNA moving through the ribosome during translation [18], and the search of a transcription factor for a binding site on DNA [19].

While much progress has been made in determining the average first-passage time and its low-order moments [2–4,20–29], understanding the properties of the full *distribution* of first-passage times is incomplete. Here, we solve this fundamental problem by focusing on the generating function for the first-passage probability. The finite interval provides a particularly instructive platform to investigate many basic disorder-controlled physical phenomena, such as the diffusion of a particle in a random potential [26,27,30–35], DNA translocation through a nanopore [36], channel transport [16], and percolation [37,38]. With our formalism, we can readily evaluate first-passage probabilities and their moments for individual realizations of disorder and thereby discover unexpected disorder-controlled phenomena.

The key to our solution lies in first writing the backward equation for the moment generating function of the first-passage probability, and then reformulating the resulting recursion as a linear algebra problem. This approach leads to analytic expressions for the generating function in terms of the elements of the inverse of a tridiagonal matrix [39]. Related methods have previously provided a semianalytic solution to the probability distribution from a one-step master equation in time [40], and to solve the three-term recurrence for the moment generating function [41]. Other pertinent studies derive semianalytic solutions for the first-passage time distribution, again for arbitrary hopping rates [42–44]. These studies start with the Laplace transform of the formal solution to the master equation, and obtain their result in terms of undetermined eigenvalues of the master operator.

However, these past investigations all focused on the forward master equation, whereas we use the backward equation due to its utility in the study of first-passage problems [4,16]. The benefits of our approach are its versatility in elucidating first-passage properties for absorbing boundaries, reflecting boundaries, and conditional waiting times, and its conciseness through the use of linear algebraic results that simplify the generating function. Additionally, our approach does not rely on finding the eigenvalues of the master operator numerically, leading to analytic, as opposed to semianalytic, results.

Formalism. The backward equation is the adjoint of the commonly used master equation for the time evolution of the probability distribution. The backward equation is especially useful in first-passage problems for which the final state is prescribed and the initial state becomes the fundamental dependent variable. Let $P_{i,j}(t)$ be the probability for a random walk to reach a final state j for the *first* time at time t when starting from state i at $t=0$. Here, i denotes a one-dimensional coordinate. The backward equation for this first-passage probability is [2–4,21],

$$\begin{aligned} P_{i,j}(t+\Delta t) = b_i \Delta t P_{i+1,j}(t) + d_i \Delta t P_{i-1,j}(t) \\ + [1-(b_i+d_i)\Delta t] P_{i,j}(t), \end{aligned} \tag{1}$$

where b_i and d_i are arbitrary rates of hopping to the right and left from site i, respectively. This equation states that the probability to first arrive at j starting from i at time $t+\Delta t$

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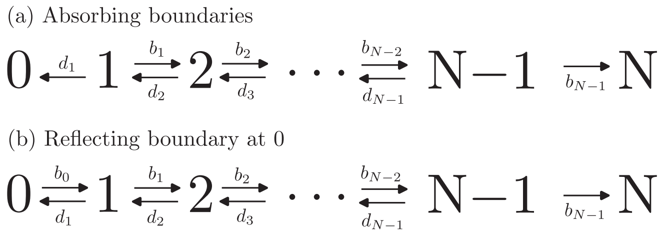

FIG. 1. Hopping rates for the interval with (a) two absorbing boundaries, and (b) one reflecting and one absorbing boundary.

equals the sum of the hopping probabilities in a time Δt from i to either $i-1$, i, or $i+1$ times the first-passage probabilities to j at time t from $i-1$, i, or $i+1$. We set $\Delta t = 1$ so that the hopping probabilities in a time Δt are $b_i\Delta t$ and $d_i\Delta t$, and t now counts the number of hopping events. For $\Delta t = 1$, the hopping rates must satisfy the constraints $0 \leqslant b_i, d_i \leqslant 1$ and $b_i + d_i \leqslant 1$.

We now calculate the generating function of the unconditional first-passage probability for the interval with two absorbing boundaries [Fig. 1(a)]. Define $f_i(t) = P_{i,0} + P_{i,N}$ as the probability density function to first reach either 0 or N at time t when starting from site i. In close analogy with Eq. (1), its governing equation is

$$f_i(t+1) = b_i f_{i+1}(t) + d_i f_{i-1}(t) + [1-(b_i+d_i)]f_i(t). \quad (2)$$

We solve this equation by the generating function technique. Multiplying (2) by z^t, summing over t, and introducing the generating function $F_i(z) = \sum_{t=0}^{\infty} z^t f_i(t)$, gives the following three-term recurrence,

$$b_i F_{i+1}(z) + d_i F_{i-1}(z) + \beta_i(z) F_i(z) = 0, \quad (3)$$

for $1 \leqslant i \leqslant N-1$, where for notational simplicity we introduce $\beta_i(z) \equiv 1 - z^{-1} - b_i - d_i$. This recursion obeys the boundary conditions $F_0(z) = F_N(z) = 1$, since $f_0(t) = f_N(t) = \delta_{t,0}$.

To solve (3), it is helpful to write it as a matrix equation [41]. We first define the column vector $\mathbf{F}(z) = [F_1(z), F_2(z), \ldots, F_{N-1}(z)]$ and using $F_0(z) = F_N(z) = 1$, this recursion becomes

$$\mathbb{A}(z) \cdot \mathbf{F}(z) = -\mathbf{w}, \quad (4)$$

where $\mathbf{w} = (d_1, 0, 0, \ldots, 0, b_{N-1})$ and $\mathbb{A}(z)$ is the tridiagonal matrix of dimension $(N-1) \times (N-1)$,

$$\mathbb{A}(z) = \begin{pmatrix} \beta_1(z) & b_1 & 0 & \ldots & 0 & 0 \\ d_2 & \beta_2(z) & b_2 & \ldots & 0 & 0 \\ \vdots & & & & \ddots & \\ 0 & 0 & 0 & \ldots & d_{N-1} & \beta_{N-1}(z) \end{pmatrix}.$$

The formal solution to Eq. (4) is

$$\mathbf{F}(z) = -\mathbb{A}(z)^{-1} \cdot \mathbf{w}. \quad (5)$$

In what follows we write the ijth elements of $\mathbb{A}(z)^{-1}$ as $\alpha_{i,j}(z)$. Performing the matrix multiplication gives

$$F_i(z) = -[d_1\alpha_{i,1}(z) + b_{\bar N}\alpha_{i,\bar N}(z)], \quad (6)$$

with $\bar N \equiv N-1$. Our task now is to find closed-form expressions for the elements of the inverse $\alpha_{i,j}(z)$. To this end we exploit the tridiagonal form of $\mathbb{A}(z)$, as was done in Ref. [40] for the forward master equation, to give the elements $\alpha_{i,j}(z)$ in terms of computationally simple products of polynomials via Cramer's rule [39]. For later use, we define the following products,

$$B_i \equiv \prod_{k=i}^{\bar N} b_k, \quad D_i \equiv \prod_{k=1}^{i} d_k. \quad (7)$$

To find $F_i(z)$, we only require the elements $\alpha_{i,1}(z)$ and $\alpha_{i,\bar N}(z)$, which are given by

$$\alpha_{i,1} = (-1)^{i+1}\frac{D_i p_i(z)}{d_1 p_0(z)}, \quad \alpha_{i,\bar N} = (-1)^{i+\bar N}\frac{B_i q_{i-1}(z)}{b_{\bar N} p_0(z)}, \quad (8)$$

where we recursively define the polynomials

$$\begin{aligned} p_{\bar N}(z) &= 1, \\ p_{\bar N-1}(z) &= \beta_{\bar N}(z), \\ p_i(z) &= \beta_{i+1}(z)p_{i+1}(z) - b_{i+1}d_{i+2}p_{i+2}(z), \end{aligned} \quad (9a)$$

for $0 \leqslant i \leqslant \bar N - 2$, and

$$\begin{aligned} q_0(z) &= 1, \\ q_1(z) &= \beta_1(z), \\ q_i(z) &= \beta_i(z)q_{i-1}(z) - d_i b_{i-1} q_{i-2}(z), \end{aligned} \quad (9b)$$

for $2 \leqslant i \leqslant N$. Although this calculation seems complicated, it is much faster than matrix inversion via Cramer's rule, since it avoids calculating the multiple zeros encountered in the evaluation of the minors of $\mathbb{A}(z)$ [45]. More details are given in Sec. I of the Supplemental Material (SM) [46].

We can now write the generating functions for the first-passage probability for each starting position i as

$$\begin{aligned} F_1(z) &= \frac{1}{p_0(z)}[(-1)^{\bar N}B_1 - d_1 p_1(z)], \\ F_{\bar N}(z) &= \frac{1}{p_0(z)}[(-1)^{\bar N}D_{\bar N} - b_{\bar N}q_{\bar N-1}(z)], \\ F_i(z) &= \frac{(-1)^i}{p_0(z)}[p_i(z)D_i + (-1)^{\bar N-1}q_{i-1}(z)B_i], \end{aligned} \quad (10)$$

where the last equality holds for $2 \leqslant i \leqslant \bar N - 1$. Note that $p_{\bar N-i}$ and q_i are polynomials of order i in z^{-1}, and each $F_i(z)$ is a rational function that is made up of polynomials in z. In practice, for an interval of length N and given a set of $\{b_i, d_i\}$, we find the polynomials p_i and q_i via Eq. (9), after which we can use Eqs. (10) to compute the generating function and its series expansion. Practically, for the expansion about $z = 1$ we series expand $\beta_i(z)$, $p_i(z)$, and $q_i(z)$ up to the order of the moment of interest before utilizing Eq. (10). We cannot conduct a similar series expansion about $z = 0$ [due to the singularity in $\beta_i(z)$] and hence use the full generating function expressions in Eq. (10) to calculate the probability distribution.

Our formalism can be readily extended to the *conditional* first-passage probability, namely, the probability to first reach a specified boundary without touching the other boundary (Sec. II of the SM [46]). We can also treat the case of a reflecting boundary. Here, the dynamics at the reflecting end of the interval must be treated as a special case in which some

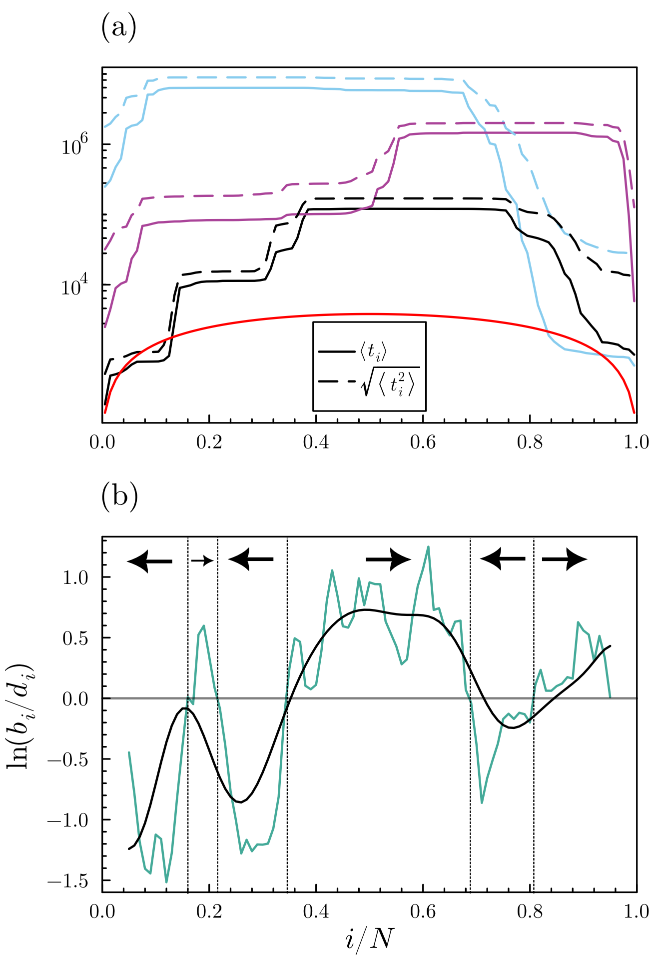

FIG. 2. (a) Mean first-passage times on a disordered interval of length $N = 100$ for three realizations of the hopping rates as a function of starting position i (solid). The dashed curves show the square root of the second moment of the first-passage time for these same realizations. The red solid curve shows the mean first-passage time of the homogeneous interval with $b_i = d_i = 1/3$ for all i. (b) The local bias $\ln(b_i/d_i)$ [smoothed over a 10-point range (green) and by a Bezier curve (black)] for the realization in black in (a). The arrows show the direction of the local average bias.

of the elements of $\mathbb{A}(z)$ are altered, although the functional forms in Eqs. (10) remain the same. Details of this calculation are shown in Sec. III of the SM [46].

Application to the disordered interval. A salient feature of first passage in the interval is the huge disparity in the mean first-passage time (MFPT) between different realizations of the hopping rates $\{b_j, d_j\}$. We use Eq. (10) to derive the exact MFPT that represents an average over all random-walk trajectories. We choose each b_j from a uniform distribution on $[0, 2/3]$, so that each $d_j = 2/3 - b_j$. Since $b_j + d_j = 2/3$, there is a $1/3$ probability for the walk to remain at the same site in a single event. This choice eliminates the annoying and obfuscating even-odd oscillations that arise for the nearest-neighbor random walk with $b_j + d_j = 1$.

Figure 2(a) illustrates this disparity in the MFPT between several representative realizations of the $\{b_j, d_j\}$ (up to three orders of magnitude for an interval of length 100). Even larger realization-specific variations occur for higher moments of the FPT [dashed lines of Fig. 2(a)]. Moreover, the first moment and the square root of the second moment for a *single* realization of hopping rates can differ by more than an order of magnitude (especially near the ends of the interval). This fact demonstrates that the statistics of the first-passage time are not captured by the MFPT. Finally, the dependence of the MFPT on starting position has no resemblance to the parabolic profile that arises in the absence of disorder [4]. This is also true for cases of weaker disorder (see Fig. S1 [46]). Instead, the MFPT is nearly independent of the starting location in certain subintervals and changes rapidly within intervening boundary layers. This behavior stems from the existence of local potential wells that are induced by the disordered hopping rates.

For the realization shown in black in the figure, there is a negative bias over most of the first ≈40% of the interval [Fig. 2(b)] so that the MFPT for starting points in this range is small. A small region of positive bias at $i/N \approx 0.2$ is responsible for a steplike increase in the FPT at this point. The bias suddenly becomes positive for $i/N \gtrsim 0.4$ which causes the rapid increase in the MFPT over this range of i/N. The effective potential well for $0.4 \lesssim i/N \lesssim 0.8$, keeps the MFPT roughly constant in this range. In general, wherever the local bias leads to an effective potential well, the MFPT (and higher moments) is nearly independent of starting location within this well and then suddenly jumps when the local bias changes sign.

It is revealing to determine the convergence of the MFPT to its true value upon averaging over progressively larger numbers of realizations of the hopping rates. Here, we use the dichotomous distribution in which each b_j takes the values 0.3 or 0.6 equiprobably, while $d_j = 0.9 - b_j$. With this choice, there is a countably finite number of hopping-rate realizations so that we can average over all random walk trajectories *and* over all realizations of the hopping-rate disorder for a given (albeit short) interval length.

For a given realization of hopping rates indexed by α, we define the MFPT starting from site i as $\langle t_i^{(\alpha)} \rangle$. The true average MFPT, averaged over all $\mathcal{M} = 2^{N-1}$ realizations of the hopping rates, is then

$$\overline{\langle t_i \rangle} \equiv \frac{1}{\mathcal{M}} \sum_{\alpha=1}^{\mathcal{M}} \langle t_i^{(\alpha)} \rangle. \tag{11a}$$

How close is the MFPT over a subset of realizations of the hopping rates to the average over *all* realizations of the hopping rates? To address this basic question, we define the partial average in which we select a random fraction $f = M/\mathcal{M}$ of all hopping-rate realizations and compute the exact MFPT for this subset, again for random walks that start at site i:

$$\overline{\langle t_i \rangle}_f \equiv \frac{1}{M} \sum_{\alpha=1}^{M} \langle t_i^{(\alpha)} \rangle. \tag{11b}$$

An appropriate deviation measure is the relative difference between the true average and the partial average as a function of f, which we define as $E_i(f)$:

$$E_i(f) \equiv \frac{\overline{\langle t_i \rangle} - \overline{\langle t_i \rangle}_f}{\overline{\langle t_i \rangle}}. \tag{12}$$

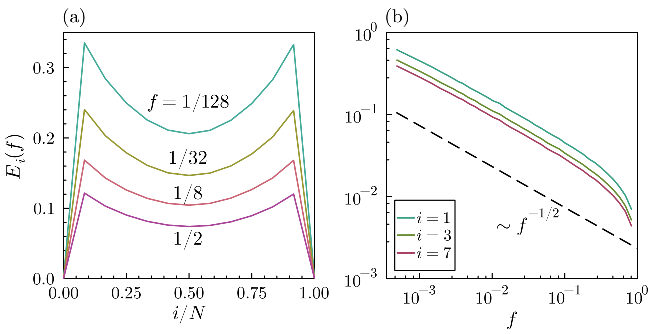

FIG. 3. (a) The average deviation in Eq. (12) when a finite fraction f of all hopping-rate realizations is sampled for an interval length $N = 12$. (b) The average deviation as a function of f for various starting positions along the interval.

Figure 3(a) shows this deviation $E_i(f)$ vs i for various ensemble fractions f. Using 50% of all possible realizations leads to a deviation of roughly 10%, while using 1% of all realizations gives a deviation of roughly 25%. Since any simulation can realistically only sample an infinitesimal fraction of all realizations, simulations of first-passage properties in disordered systems will be pointless because of their poor accuracy. Again, the deviations for the higher-order moments are much larger than that of the mean (not shown). We additionally show the dependence of $E_i(f)$ on f across three orders of magnitude. Surprisingly, this is well fit by a power law with exponent $-1/2$, a result which holds even when a less disordered dichotomous distribution is used (see Fig. S2 in the SM [46]).

Another unexpected feature that emerges from our exact approach is that *bimodal* first-passage distributions arise for certain realizations of the hopping rates. Related "echo" phenomena have been observed previously in systems where disparate paths with very different timescales contribute to the first-passage probability [4,47,48]. We show one such example in Fig. 4(a) with b_i chosen uniformly in the range $(0, 1/3)$ and $d_i = 1/3 - b_i$, with the walk starting at $i = 2$ on an interval of length 10. Also shown in this figure are the local biases at each site i, $\ln(b_i/d_i)$. The essential feature of this bias profile is that it is negative at $i = 1$, almost neutral at $i = 2$, and generally positive for $i > 2$. Thus a particle starting at $i = 2$ exits via the left edge with appreciable probability and does so quickly because of the strong negative bias at $i = 1$. However, if the particle initially hops to the right, it then experiences a rightward bias, which leads to the second later-time peak in the first-passage probability. To verify this crude picture, we construct a synthetic interval of length 20 in which the segment [0,5] has a bias to the left and the segment [5,20] has a bias to the right, with both biases of magnitude $|v| = 0.3$ [Fig. 4(b)]. When the random walk starts at $i \leqslant 5$, it is likely to remain in the region $i \leqslant 5$ and exit the interval on the left side, corresponding to the early-time peak in Fig. 4(b). However, if the random walker traverses to the region $i > 5$, it is likely to remain on this side of the interval, ultimately leading to the second, longer-time peak in Fig. 4(b).

Summary. We analytically derived the generating function of the first-passage probability and all its moments on intervals with arbitrary nearest-neighbor hopping rates. It is in only

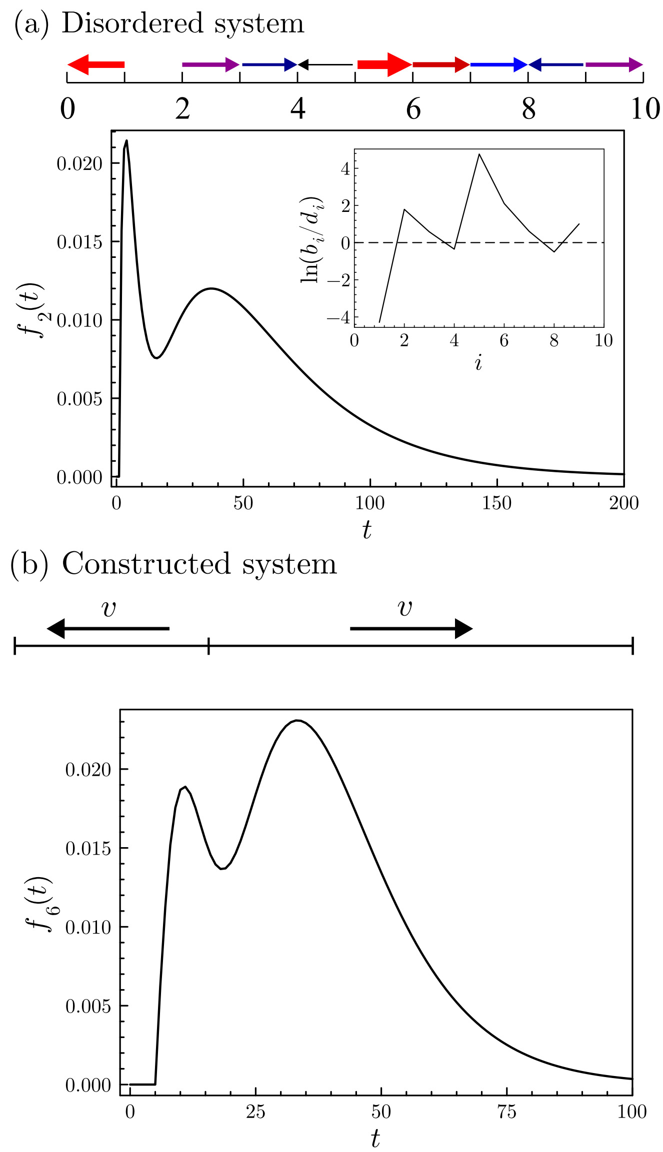

FIG. 4. (a) The first-passage probability $f_2(t)$ on the interval [0,10]. The schematic shows the local bias $\ln(b_i/d_i)$ at each site. The inset shows the explicit values of $\ln(b_i/d_i)$. (b) The first-passage probability $f_6(t)$ for an interval of length $N = 20$ in which the synthetically generated bias changes sign at $i = 5$ with $|v| = |b_i - d_i| = 0.3$.

one dimension, where disorder can lead to anomalous scaling laws, for which our techniques can reveal the full probability distribution of first-passage times and all its moments. Our exact approach reveals and elucidates unexpected anomalies in first-passage properties, such as the steplike spatial dependence of the first-passage time for individual hopping-rate realizations, the huge disparities in the first-passage time in different realizations of hopping rates, and the similarly huge disparities between the first moment and the square root of the second moment of the FPT. We additionally found that bimodal first-passage distributions can arise in certain realizations that possess a general outward bias in the hopping rates from an interior point. Here, a random walk that starts near this interior point may exit via the "downstream" side of the interval and do so quickly. Conversely, the walk may also exit via the "upstream" side, but with a much longer exit time. When the exit probabilities via the downstream and upstream sides are comparable, two well-resolved peaks in the first-passage probability arise. This bimodality is unexpected for a system without any reflecting boundaries.

We also quantified the slow convergence of the first-passage time, averaged over a finite fraction of all hopping-rate realizations, to the true average over all such realizations. This slow convergence has profound implications for computational studies of first passage. Since realistic simulations can only sample a tiny fraction of all hopping-rate realizations, numerical results for first-passage properties from such simulations are doomed to be wildly inaccurate. It is only through analytical methods, such as those presented here, that one can obtain accurate results for first-passage properties.

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