Supplementary Material: First passage on disordered intervals

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I. INVERSE ELEMENTS OF A TRIDIAGONAL MATRIX

In this appendix we succinctly reproduce the inverse elements of a general tridiagonal matrix first given in [1]. That is, we will derive the elements of the inverse of the following matrix,

$$\mathbb{B} = \begin{pmatrix} b_1 & c_1 & 0 & 0 & \dots & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & \dots & 0 & 0 \\ 0 & a_3 & b_3 & c_3 & \dots & 0 & 0 \\ \vdots & & & & \ddots & & \\ 0 & 0 & 0 & 0 & \dots & a_N & b_N \end{pmatrix}, \tag{S1}$$

First, we know that the inverse of a general $N \times N$ matrix is given by Cramer's rule as [2],

$$\alpha_{ij} \equiv [\mathbb{B}^{-1}]_{i,j} = \frac{(-1)^{i+j} M_{ji}}{\det(\mathbb{B})}, \tag{S2}$$

where M_{ji} is the minor, i.e., the determinant of the matrix that results from the removal of row j and column i. Our aim is to exploit the triangular nature of the matrix to give analytic expressions for the inverse that can be computed much faster than general matrix inversion (which scales as N^3 for Gauss–Jordan elimination). For brevity we introduce the following determinants,

$$U_i \equiv \begin{vmatrix} b_1 & c_1 & 0 & 0 & \dots & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & \dots & 0 & 0 \\ 0 & a_3 & b_3 & c_3 & \dots & 0 & 0 \\ \vdots & & & & \ddots & & \\ 0 & 0 & 0 & 0 & \dots & a_i & b_i \end{vmatrix}, \qquad L_i \equiv \begin{vmatrix} b_i & c_i & 0 & 0 & \dots & 0 & 0 \\ a_{i+1} & b_{i+1} & c_{i+1} & 0 & \dots & 0 & 0 \\ 0 & a_{i+2} & b_{i+2} & c_{i+2} & \dots & 0 & 0 \\ \vdots & & & & \ddots & & \\ 0 & 0 & 0 & 0 & \dots & a_N & b_N \end{vmatrix}, \tag{S3}$$

with $U_0 = 1$, $U_1 = b_1$ and $L_{N+1} = 1$, $L_N = b_N$. The key step in calculating the α_{ij} is in finding the matrix minors. Let's calculate the minors for a few examples,

$$\begin{aligned} M_{11} &= L_2, \\ M_{22} &= U_1 L_3, \\ M_{33} &= U_2 L_4, \\ M_{12} &= a_2 L_3, \\ M_{13} &= a_2 a_3 L_4, \\ M_{14} &= a_2 a_3 a_4 L_5, \\ M_{N,N} &= U_{N-1}, \\ M_{N,N-1} &= c_{N-1} U_{N-2}, \\ M_{N,N-2} &= c_{N-1} c_{N-2} U_{N-3}. \end{aligned}$$

Here we have made judicious use of Schur's formula [3] for the determinants of block matrices, which states that for the block matrix

$$\mathbb{E} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix}, \tag{S4}$$

with invertible $\mathbf{A}$ and $\mathbf{D}$, we have

$$\det(\mathbb{E}) = \det(\mathbf{A}) \cdot \det(\mathbf{D} - \mathbf{C} \cdot \mathbf{A}^{-1} \cdot \mathbf{B}). \tag{S5}$$

When either $\mathbf{B}$ or $\mathbf{C}$ consist entirely of zeros, the above formula reduces to,

$$\det(\mathbb{E}) = \det(\mathbf{A}) \cdot \det(\mathbf{D}). \tag{S6}$$

We observe that the minors follow the pattern,

$$M_{ji} = \begin{cases} \left(\prod_{k=i}^{j-1} c_k\right) U_{i-1} L_{j+1} & j > i, \\ U_{j-1} L_{j+1} & j = i, \\ \left(\prod_{k=j+1}^{i} a_k\right) U_{j-1} L_{i+1} & j < i, \end{cases} \tag{S7}$$

which is proved by induction in [4]. Substituting M_{ji} into Eq. (S2) then gives our analytic expression for the α_{ij}. Note that $\det(\mathbb{B}) = L_1 = U_N$.

The introduction of orthogonal polynomials comes from the recursive relationship defining the determinants of the sequences $U_0, U_1, \ldots, U_N$ and $L_1, L_2, \ldots, L_{N+1}$. This recurrence is trivially given by Leibniz's rule as,

$$\begin{aligned} &L_{N+1} = 1, \; L_N = b_N, \\ &L_i = b_i L_{i+1} - c_i a_{i+1} L_{i+2}, \\ &U_0 = 1, \; U_1 = b_1, \\ &U_i = b_i U_{i-1} - c_{i-1} a_i U_{i-2}. \end{aligned} \tag{S8}$$

Upon re-labeling $b_i \Rightarrow \beta_i(z)$, $a_i \Rightarrow d_i$, $c_i \Rightarrow b_i$, $N \Rightarrow \bar{N}$, $U_i \Rightarrow q_i(z)$ and $L_i \Rightarrow p_{i-1}(z)$ one then recovers the recursive polynomials defined in Eq. (9) in the main text. Finally, since we only need the terms $\alpha_{i,1}(z)$ and $\alpha_{i,\bar{N}}(z)$, we can use the properties of $U_0 = 1$ and $L_{N+1} = 1$ to arrive at Eqs. (8) in the main text.

II. CONDITIONAL FIRST-PASSAGE PROBABILITY

We are interested in the *conditional* FPT to reach either 0 or N without ever reaching the opposite boundary starting from some initial site i. We focus on the conditional FPT to reach N, and later return to the case of reaching the origin. The probability of reaching N at time t starting from i at $t = 0$ is given by $f_i(t) = P_{i,N}(t)$. Note that $f_i(t)$ has the boundary conditions $f_N(t) = \delta_{t,0}$ and $f_0(t) = 0$. The recurrence relation satisfied by $f_i(t)$ is the same as Eq. (2), but with different boundary conditions. Note that $f_i(t)$ does not strictly correspond to a normalized probability distribution over t since there is a finite probability of being absorbed at the origin and therefore never reaching N. Therefore, we further define,

$$\widetilde{f}_i(t) = \frac{f_i(t)}{\sum_{t=0}^{\infty} f_i(t)} \equiv \frac{f_i(t)}{\phi_i}, \tag{S9}$$

where $\widetilde{f}_i(t)$ is the properly normalized probability density function and we define ϕ_i as the probability for the walk to ultimately reach the boundary at N. This eventual hitting probability is given by

$$\phi_i = \frac{1 + \sum_{k=1}^{i-1} \prod_{i=1}^{k} \frac{d_j}{b_j}}{1 + \sum_{k=1}^{N-1} \prod_{i=1}^{k} \frac{d_j}{b_j}}. \tag{S10}$$

We now define the generating function of $\widetilde{f}_i(t)$ as,

$$\widetilde{F}_i(z) = \sum_{t=0}^{\infty} z^t \widetilde{f}_i(t), \tag{S11}$$

and taking Eq. (2) multiplying by z^t and summing over all t we get the three-term recurrence relation that $\widetilde{F}_i(z)$ satisfies,

$$b_i \phi_{i+1} \widetilde{F}_{i+1}(z) + d_i \phi_{i-1} \widetilde{F}_{i-1}(z) + \beta_i(z) \phi_i \widetilde{F}_i(z) = 0, \qquad i \in 1, 2, \ldots, N-1, \tag{S12}$$

with the boundary conditions now $\widetilde{F}_0(z) = 0$ and $\widetilde{F}_N(z) = 1$ and we have used $\beta_i(z)$ as defined in the main text. For brevity, we henceforth denote $C_i(z) = \phi_i \widetilde{F}_i(z)$. As in the unconditional case, we rewrite Eq. (S12) as a matrix equation,

$$\mathbb{A}(z) \cdot \mathbf{C}(z) = -\mathbf{m}, \tag{S13}$$

with $\mathbf{C}(z) = (C_1(z), C_2(z), \ldots, C_\tau(z))$, $\mathbf{m} = (0, 0, \ldots, 0, b_\tau)$ and $\mathbb{A}(z)$ the $(N-1) \times (N-1)$ matrix defined by Eq. (S1). Since we already have explicit expressions for the elements of the inverse of $\mathbb{A}$, we can readily obtain $\widetilde{F}_i(z) = -b_{\bar{N}} \alpha_{i,\tau}/\phi_i$:

$$\begin{aligned} \widetilde{F}_i(z) &= \frac{-(-1)^{i+\tau} q_{i-1}(z) B_i}{p_0(z)\phi_i}, \qquad i \in \{1, 2, \ldots, \bar{N}-1\}, \\ \widetilde{F}_{\bar{N}}(z) &= \frac{-b_{\bar{N}} q_{-1}(z)}{p_0(z)\phi_{\bar{N}}}. \end{aligned} \tag{S14}$$

By symmetry considerations one can then find the conditional generating functions of the first-passage time to reach $n = 0$ as,

$$\begin{aligned} \widetilde{F}_1(z) &= \frac{-d_1 p_1(z)}{p_0(z)(1-\phi_1)}, \\ \widetilde{F}_i(z) &= \frac{(-1)^i p_i(z) D_i}{p_0(z)(1-\phi_i)}, \qquad i \in \{2, 3, \ldots, \bar{N}\}. \end{aligned} \tag{S15}$$

In the application of the disordered interval in the main text one can use the conditional first-passage time to observe the origin of bimodalities observed for some realizations of disorder. This is possible since the origin of the bimodality seen in Figure 4 (main text) comes from the competition between leaving the opposing ends of the system.

III. ONE REFLECTING AND ONE ABSORBING BOUNDARY

Utilizing methods from the main text we can solve the further problem of having one absorbing and one reflecting boundary on the finite interval. We show the Markovian dynamics of such a process in Fig. 1(b), where we arbitrarily choose the reflecting boundary at $n = 0$ (necessarily having $b_0 > 0$), with the boundary at $n = N$ chosen to be absorbing. For this set of boundary conditions there is no distinction between conditional and unconditional first-passage times since in all cases the process absorbs at the $n = N$ boundary. Only the boundary conditions have changed compared to the calculation in the main text, therefore the recurrence relation remains unchanged, and we restate it from Eq. (3),

$$b_i M_{i+1}(z) + d_i M_{i-1}(z) + \beta_i(z) M_i(z) = 0, \quad i \in \{1, 2, \ldots, N-1\},$$

and we have again denoted $\beta_i(z) = 1 - z^{-1} - b_i - d_i$. As before, if one starts at the boundary at $n = N$ then $\xi_N(0) = \delta_{t,0}$, leading to $M_N(z) = 1$. The other boundary condition is not as trivial, and relates to the connection between the dynamics starting from $n = 0$ and $n = 1$. Intuitively, we know that on the level of the mean first-passage time that $\langle t_1 \rangle - \langle t_0 \rangle = -1/b_0$, since in starting from the state $n = 0$ there is only one possible transition to $n = 1$ with a propensity b_0 occurring with mean time $1/b_0$—presuming that the boundary is completely reflective [5]. However, to find the connection between the generating functions at $n = 0$ and $n = 1$ we first need to find the relationship between $\xi_0(t)$ and $\xi_1(t)$, which are the first-passage time probability distributions to reach $n = N$ at time t given one starts at $n = 0$ and 1 respectively. We find that $\xi_0(t)$ is given by a discrete convolution between the probability to move from $n = 0$ to $n = 1$ and the probability to then move to $n = N$ from $n = 1$,

$$\xi_0(t) = \sum_{t'=1}^{t-1} b_0 (1-b_0)^{t'} \xi_1(t - t' - 1), \tag{S16}$$

where $b_0(1-b_0)^{t'}$ is the geometric probability to move to $n = 1$ at time $t' + 1$, and $\xi_1(t - t' - 1)$ represents the probability to move to $n = N$ in the remaining time $t - t' - 1$. Multiplying this equation by z^t and summing over t

will then give us a relationship between $M_0(z)$ and $M_1(z)$,

$$\begin{aligned} M_0(z) &= b_0 \sum_{t=0}^{\infty} \sum_{t'=1}^{t-1} z^t (1-b_0)^{t'} \xi_1(t-t'-1), \\ &= b_0 \sum_{y=1}^{\infty} \sum_{t=y+1}^{\infty} (1-b_0)^{t-y-1} z^t \xi_1(y), \\ &= b_0 \sum_{y=1}^{\infty} \frac{z}{1+(b_0-1)z} z^y \xi_1(y), \\ &= \frac{b_0 z}{1+(b_0-1)z} M_1(z). \end{aligned}$$

Taking the derivative of this with respect to z gives,

$$M_0'(z) = \frac{b_0 z \left(\left((b_0-1)\, z + 1 \right) M_1'(z) + M_1(z) \right)}{\left((b_0-1)\, z + 1 \right)^2}, \tag{S17}$$

and evaluating at $z=1$ gives us the known boundary condition on the mean-level,

$$\langle t_1 \rangle - \langle t_0 \rangle = -1/b_0. \tag{S18}$$

As was done in the main text, we can now write the matrix formulation of the recurrence relation for $M_i(z)$,

$$\mathbb{C}(z) \cdot \mathbf{M}(z) = -\mathbf{k}, \tag{S19}$$

where $\mathbf{M}$ is as previously defined, $\mathbf{k} = (0, 0, \ldots, 0, b_\tau)$, and $\mathbb{C}(z)$ is identical to $\mathbb{A}(z)$ with the exception of the top-left element which is given by,

$$[\mathbb{C}(z)]_{1,1} = \beta_1(z) + \frac{d_1 b_0 z}{1+(b_0-1)z}. \tag{S20}$$

As previously, one can then find $\mathbf{M}$ by inverting the matrix $\mathbb{C}(z)$, giving,

$$\mathbf{M}(z) = -\mathbb{C}(z)^{-1} \cdot \mathbf{k}. \tag{S21}$$

We now redefine the functions $\beta_i(z)$ to account for the change in the top-left element of $\mathbb{C}(z)$,

$$\beta_i(z) = \begin{cases} 1 - z^{-1} - b_1 - d_1 + \frac{d_1 b_0 z}{1+(b_0-1)z}, & i = 1, \\ 1 - z^{-1} - b_i - d_i, & i \in \{2, 3, \ldots, \tau\}, \end{cases} \tag{S22}$$

in which case the formulae in Eqs. (8) also define the elements of $\mathbb{C}(z)^{-1}$ with the $\beta_i(z)$ as defined in Eq. (S22). Then completing the matrix multiplication in Eq. (S21) we find the generating functions for first-passage on a finite interval with one absorbing and one reflecting boundary,

$$\begin{aligned} M_i(z) &= -\frac{(-1)^{i+\tau} q_{i-1}(z) B_i}{p_0(z)}, \ i \in \{1, 2, \ldots, \tau-1\}, \\ M_\tau(z) &= \frac{-b_\tau q_{\tau-1}(z)}{p_0(z)}. \end{aligned} \tag{S23}$$

IV. SUPPLEMENTARY FIGURES

Figure S1 shows the dependence of the MFPT on starting position for single realizations of the hopping rates, but for varying degrees of disorder. Here $b_i = 1/3 + \mathrm{Uniform}(-a, a)$ and $d_i = 2/3 - b_i$, with a varying between 0 and 1/3. Over this range of a the MFPT varies over three orders of magnitude. The important aspect of these plots is that features of the MFPT versus starting position are qualitatively the same as the degree of disorder is reduced.

Figure S2 shows the counterpart of Fig. (3) in the main text but again with a smaller degree of disorder. We find that the exponent of $-1/2$ that describes the power-law decay of $E_i(f)$ with respect to f is identical to that in the case of stronger disorder shown in Fig. S2.

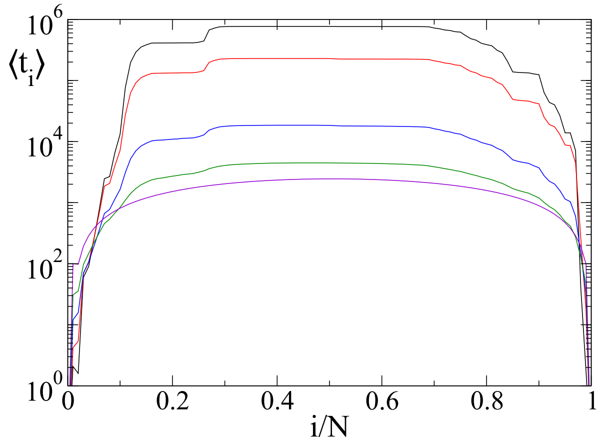

FIG. S1. Similar to Fig. 2(a), but for variable disorder. Here $b_i = 1/3 + \text{Uniform}(-a, a)$ and $d_i = 2/3 - b_i$, with $a = 1/3$ (black), 0.3 (red), 0.2 (blue), 0.1 (green), and 0.0 (magenta).

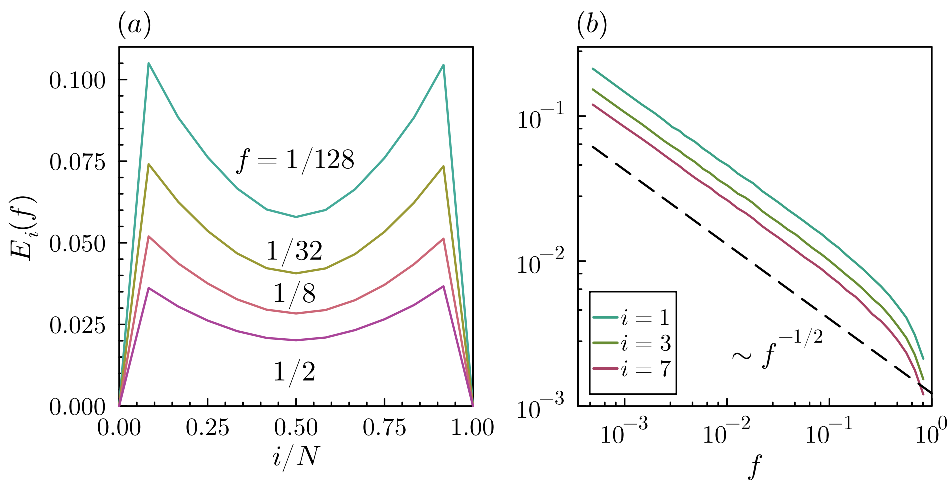

FIG. S2. (a) The average deviation in Eq. (12) when a finite fraction f of all hopping rate realizations are sampled. Interval length $N = 12$. (b) The average deviation as a function of f for various starting positions along the interval. We use a dichotomous distribution with weaker disorder in the hopping rates than that given the main text. Here each b_j takes the values 0.4 or 0.5 equiprobably, while $d_j = 0.9 - b_j$. We find the same power law to describe the deviation as a function of f as in the case of stronger disorder shown in Fig. 2(b).

To show the range of first-passage times for the ensemble described in Figure 3, we show the extreme longest and shortest first-passage times compared to the average MFPT over disorder (Fig. S3). The longest time arises for hopping rates that are biased toward the center of the interval, while the shortest time arises for hopping rate that are biased from the center toward the ends of the interval. The longest and shortest times differ by 2 orders of magnitude, with both these extremal times differing from the disorder average time by an order of magnitude.

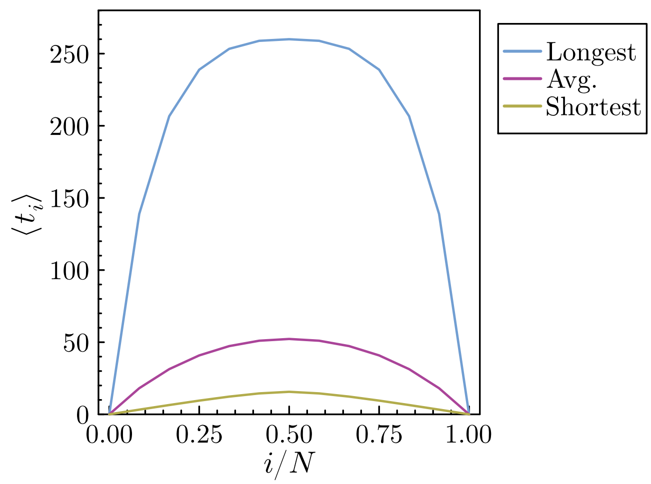

FIG. S3. The longest and the shortest first-passage from the ensemble in Fig. 3. Also shown in the disorder-averaged first-passage time.

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