Journal of Statistical Physics, Vol. 19, No. 5, 1978

Analytic Results for Asymmetric Random Walk with Exponential Transition Probabilities

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Received March 21, 1978; revised July 13, 1978

We present here exact analytic results for a random walk on a one-dimensional lattice with asymmetric, exponentially distributed jump probabilities. We derive the generating functions of such a walk for a perfect lattice and for a lattice with absorbing boundaries. We obtain solutions for some interesting moment properties, such as mean first passage time, drift velocity, dispersion, and branching ratio for absorption. The symmetric exponential walk is solved as a special case. The scaling of the mean first passage time with the size of the system for the exponentially distributed walk is determined by the symmetry and is independent of the range.

KEY WORDS: Random walks; stochastic processes; exponential models; mean first passage time; branching ratio.

1. INTRODUCTION

The theory of stochastic processes has been successfully applied to a number of physical and chemical problems which can be modeled by master equations or random walks.(1) The wide range of applicability of stochastic models has spurred considerable advances in analytic solutions of the mathematical models,(2) which for the most part are restricted to nearest-neighbor transitions. However, in many problems of experimental interest the long-range transitions cannot be neglected. An example is the case of molecular relaxation,(3) where multiquantum transitions are common and a nearest-neighbor approximation may be insufficient. The realistic description of unimolecular reactions,(4) bimolecular reactions,(5) and chemical lasers(6) requires stochastic models with nonnegligible long-range transition probabilities, which so far have been mostly dealt with by numerical methods.

Supported by the National Science Foundation and the Department of Energy.

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0022-4715/78/1100-0525$05.00/0

In this paper we present an analysis of a random walk on one-dimensional stochastic space with asymmetric exponential transition probabilities characterized by two parameters which control the degree of asymmetry and the range of transitions. Possible applications are molecular processes, electron hopping or exciton migration, and transport phenomena in the presence of gradients in temperature or concentration.

The choice of a random walk, rather than of a master equation, formulation, which is more natural in many problems of interest, was determined by the existing theory of Montroll.[2] The choice is not restrictive, as these two formulations have been shown to be equivalent[7] provided that the time between the steps of a random walk is a Poisson process with the distribution $\psi(t) = (1/\tau_1)e^{-t/\tau_1}$, and the random walk transition matrix M is related to the master equation transition matrix A by $\mathsf{M} = \tau_1\mathsf{A} + \mathsf{1}$. A consequence of this is that, in general, it is impossible to have zero diagonal elements of M, with the exception of the case when all diagonal elements of A are equal and τ_1 is chosen so that $\tau_1 A_{ii} = -1$.

An exponential model has been previously treated in an elegant paper by Lakatos–Lindenberg and Shuler,[8] who considered a symmetric random walk with zero probability of staying at a given site, i.e., zero diagonal elements of M. In the present model the restriction of symmetry is removed; furthermore, a nonzero probability of staying at a site is assumed. However, since in the present model the diagonal elements of the transition matrix in the master equation formulation are all equal, the choice of diagonal elements of M is quite arbitrary if one is interested in the solution of the master equation. Both the analysis in Ref. 8 and the present study are based on Montroll's theory of random walks,[2] which is valid only for translationally invariant transition probabilities.

We consider a one-dimensional stochastic space with two absorbing branches which consist of traps (probability of leaving a trapping site is zero). Thus this model is applicable to situations in which there are two channels available for escape. In addition to definitions needed for subsequent analysis, Section 2 contains a derivation of a general relation between the generating function for the random walk on a perfect lattice (without traps) and that on a lattice with trapping sites. Since the former can be easily evaluated for translationally invariant transition probabilities with Montroll's formulas,[2] this relation enables one to find the latter in a relatively simple manner. Next we derive an expression for the mean first passage time for absorption (MFPT) in terms of the generating function for a lattice with traps. The specific model treated is introduced in detail in Section 3. Since the calculations in this paper are rather lengthy, they have been relegated to appendices and only final results are given in Section 3. Thus after solving for the generating functions, we compute the MFPT, the branching ratio (relative absorption in the two branches), the drift velocity, and the dispersion around the origin. We compare the results with those of the symmetric exponential, as well as nearest-neighbor, models. We show that the asymmetry in the transition probabilities has some interesting and rather unexpected consequences, which do not depend on the range of the jumps. The results are discussed in the last section.

2. THE GENERATING FUNCTIONS

2.1. Introductory Definitions

Consider a perfect lattice and a random walk where the probability of jumping from site l' to l is denoted by $p(l, l')$. Let $P_n(l, l_0)$ be the probability of being at site l after the nth step, with $P_0(l, l_0) = \delta_{l,l_0}$. The normalization conditions are

$$\sum_l p(l, l') = 1 \tag{1}$$

$$\sum_l P_n(l, l_0) = 1 \tag{2}$$

Define now the generating function for the perfect lattice, $G(z, l, l_0)$,

$$G(z, l, l_0) \equiv \sum_{n=0}^{\infty} z^n P_n(l, l_0) \tag{3}$$

We restrict ourselves to problems with translational invariance, i.e.,

$$p(l, l') = p(l - l') \tag{4}$$

where l' is the initial and l the final state in a given jump. With this choice, Eq. (3) can be evaluated with the help of Montroll's theory,[2]

$$G(z, l, l_0) = G(z, l - l_0) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{-i(l-l_0)\phi}}{1 - z\lambda(\phi)}\, d\phi \tag{5}$$

where

$$\lambda(\phi) = \sum_{k=-\infty}^{\infty} p(k) e^{ik\phi}, \qquad k = l - l' \tag{6}$$

so that

$$P_n(l - l_0) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \lambda^n(\phi) e^{-i(l-l_0)\phi}\, d\phi \tag{7}$$

Define $Q_n(l, l_0)$ to be the probability of being at site l after the nth step in the presence of traps, with $Q_0(l, l_0) = \delta_{l,l_0}$. The corresponding generating function is

$$F(z, l, l_0) = \sum_{n=0}^{\infty} z^n Q_n(l, l_0) \tag{8}$$

The calculation of $G(z, l, l_0)$ for translationally invariant systems is relatively easy. A direct evaluation of $F(z, l, l_0)$ presents difficulties. It is useful, therefore, to find a relation between these two generating functions so that one may be evaluated in terms of the other.

2.2. Relationship Between the Generating Functions $G(z, l, l_0)$ and $F(z, l, l_0)$

Let $\mathbf{P}_n(l_0)$ be a vector whose lth element is $\mathbf{P}_n(l, l_0)$ and let $\mathscr{P}$ be a transition matrix for a random walk on a perfect lattice, i.e., $\mathscr{P}_{ll'} = p(l, l')$. The recursion relation for $\mathbf{P}_n(l_0)$ is

$$\mathbf{P}_n(l_0) = \mathscr{P}\mathbf{P}_{n-1}(l_0) = \mathscr{P}^n\mathbf{P}_0(l_0) \tag{9}$$

The generating function for a random walk on a perfect lattice is now written as

$$\mathbf{G}(z, l_0) = \sum_{n=0}^{\infty} z^n\mathbf{P}_n(l_0) = (\mathscr{I} - z\mathscr{P})^{-1}\mathbf{P}_0(l_0) \equiv \mathscr{G}_0\mathbf{P}_0(l_0) \tag{10}$$

From (10) we find

$$z\mathscr{P}\mathscr{G}_0 = \mathscr{G}_0 - \mathscr{I} \tag{11}$$

Now let $\mathscr{P}_N$ be a transition matrix for a random walk on a lattice with traps. Then

$$\mathscr{P}_N = \mathscr{P}(\mathscr{I} - \mathscr{Q}) + \mathscr{Q} \tag{12}$$

where $\mathscr{Q}$ is the projection onto traps, i.e., $\mathscr{Q}_{ll'} = \delta_{l,l'}$ for l trapping and zero for l nontrapping. Let $\mathbf{Q}_n(l_0)$ be a vector whose lth element is $Q_n(l, l_0)$. The recursion relation for $\mathbf{Q}_n(l_0)$ is

$$\mathbf{Q}_n(l_0) = \mathscr{P}_N\mathbf{Q}_{n-1}(l_0) = \mathscr{P}_N{}^n\mathbf{Q}_0(l_0) \tag{13}$$

and the generating function for a random walk on a lattice with traps is

$$\mathbf{F}(z, l_0) = \sum_{n=0}^{\infty} z^n\mathbf{Q}_n(l_0) = (\mathscr{I} - z\mathscr{P}_N)^{-1}\mathbf{Q}_0(l_0) \equiv \mathscr{F}_0\mathbf{Q}_0(l_0) \tag{14}$$

Hence

$$\mathscr{F}_0(\mathscr{I} - z\mathscr{P}_N) = \mathscr{F}_0[\mathscr{I} - z\mathscr{P}(\mathscr{I} - \mathscr{Q}) - z\mathscr{Q}] = \mathscr{I} \tag{15}$$

or since $\mathscr{G}_0^{-1} = \mathscr{I} - z\mathscr{P}$

$$(\mathscr{G}_0^{-1} + z\mathscr{P}\mathscr{Q} - z\mathscr{Q})\mathscr{F}_0 = \mathscr{I} \tag{16}$$

and

$$\mathscr{F}_0 = \mathscr{G}_0 - z\mathscr{G}_0\mathscr{P}\mathscr{Q}\mathscr{F}_0 + z\mathscr{G}_0\mathscr{Q}\mathscr{F}_0 \tag{17}$$

Using (11), we get finally

$$(\mathscr{I} - \mathscr{Q})\mathscr{F}_0 = \mathscr{G}_0 - (1 - z)\mathscr{G}_0\mathscr{Q}\mathscr{F}_0 \tag{18}$$

which allows evaluation of $\mathscr{F}_0$ given $\mathscr{G}_0$.

The generating function used in calculations was defined in (8) and, in terms of $\mathscr{F}_0$, is given by

$$F(z, l, l_0) = \mathbf{Q}_0{}^T(l)\cdot\mathscr{F}_0\mathbf{Q}_0(l_0) \tag{19}$$

From (18)

$$F(z, l, l_0) = G(z, l, l_0) + \sum_{l' \text{ traps}} F(z, l', l_0)[(z - 1)G(z, l, l') + \delta_{l,l'}] \tag{20}$$

Note that this relation is valid whether or not the random walk is translationally invariant.

2.3. Mean First Passage Times

The theory of MFPT as evaluated from solutions of master equations was reviewed by Weiss.[9] In the theory of random walks, the MFPT is given in terms of the average number of steps for absorption. The relation between the two is simply that the master-equation MFPT is the random-walk one times the average time between steps.[7] The relation between the MFPT and the generating functions of the random walk is established with the following argument[8]:

$Q_n(l, l_0)$ was defined as the probability of being at site l after n steps if the motion started at l_0 (nontrapping site), in the presence of traps. The probability of not being trapped by the nth step is

$$\sum_{l \text{ nontrap}} Q_n(l, l_0)$$

The probability of being trapped on or before the nth step is

$$1 - \sum_{l \text{ nontrap}} Q_n(l, l_0)$$

The probability of being trapped on the nth step, η_n, is

$$\begin{aligned}\eta_n &= \Big[1 - \sum_{l \text{ nontrap}} Q_n(l, l_0)\Big] - \Big[1 - \sum_{l \text{ nontrap}} Q_{n-1}(l, l_0)\Big] \\ &= \sum_{l \text{ nontrap}} [Q_{n-1}(l, l_0) - Q_n(l, l_0)]\end{aligned}$$

The average number of steps for trapping is $\langle n\rangle_{\rm tr} = \sum_{n=0}^{\infty} n\eta_n$, or

$$\langle n\rangle_{\rm tr} = \sum_{n=0}^{\infty} n\left\{\sum_{l\,\rm nontrap} [Q_{n-1}(l, l_0) - Q_n(l, l_0)]\right\} \tag{21}$$

But we also have

$$F(z, l, l_0) = \sum_{n=0}^{\infty} z^n Q_n(l, l_0) \Rightarrow \left.\frac{\partial F}{\partial z}\right|_{z=1} = \sum_{n=1}^{\infty} nQ_n(l, l_0) \tag{22}$$

and hence (21) can be written as

$$\langle n\rangle_{\rm tr} = -\frac{\partial}{\partial z}\left[(1 - z) \sum_{l\,\rm nontrap} F(z, l, l_0)\right]_{z=1} \tag{23}$$

On the other hand,

$$\sum_{l} F(z, l, l_0) = \sum_{n=0}^{\infty} z^n \sum_{l} Q_n(l, l_0) = \sum_{n=0}^{\infty} z^n = \frac{1}{1 - z} \tag{24}$$

and

$$\sum_{l\,\rm nontrap} F(z, l, l_0) = \frac{1}{1 - z} - \sum_{l\,\rm trap} F(z, l, l_0)$$

so that

$$\langle n\rangle_{\rm tr} = \frac{\partial}{\partial z}\left[(1 - z) \sum_{l\,\rm trap} F(z, l, l_0)\right]_{z=1} \tag{25}$$

By calculating $G(z, l, l_0)$ and finding $F(z, l, l_0)$ through (20) we are able to calculate the MFPT simply by differentiation. In order to obtain the MFPT in real time we have to multiply (25) by the average time between steps τ_1.[7]

3. THE MODEL

We derive various necessary expressions for a specific model of transition probabilities, first for the perfect 1D lattice (no traps) and then for a lattice segment bounded on each side by trapping sites.

3.1. Random Walk on a Perfect Lattice (No Traps)

Consider a master equation with translationally invariant transition probabilities per unit time given by

$$k_{l\to l'} = \begin{cases} k_0 \exp[-a(l' - l)], & l' > l \\ k_0 \exp[b(l' - l)], & l' < l \end{cases} \tag{26}$$

Note that in the master equation $k_{l \to l}$ is unspecified. Correspondingly, we choose a random walk with the mean time between steps $\tau_1 = c/k_0$ and jump probabilities from l to l':

$$p(l' - l) = \begin{cases} c \exp[-a(l' - l)], & l' - l > 0 \\ c \exp[b(l' - l)], & l' - l < 0 \\ c, & l' - l = 0 \end{cases} \tag{27}$$

where $a \geqslant b > 0$. The normalization constant is

$$c = \frac{(1 - e^{-a})(1 - e^{-b})}{1 - e^{-(a+b)}} = \frac{\epsilon_a \epsilon_b}{\epsilon_a + \epsilon_b - \epsilon_a \epsilon_b} \tag{28}$$

where $\epsilon_a \equiv 1 - e^{-a}$ and $\epsilon_b \equiv 1 - e^{-b}$.

The generating function for this random walk on a perfect lattice is calculated in Appendix A, with the final result

$$G(z, l - l_0) = \begin{cases} x_1^{l - l_0} f(z), & l > l_0 \\ x_2^{l_0 - l} f(z), & l < l_0 \\ 1 + f(z), & l = l_0 \end{cases} \tag{29}$$

where

$$\begin{aligned} x_1 &= e^{-a} g(z) \\ x_2 &= e^{-b} g(z) \\ g(z) &= \tfrac{1}{2}\{(1 + e^{a+b} - e^{a+b}\epsilon_a\epsilon_b z) \\ &\quad - [(1 + e^{a+b} - e^{a+b}\epsilon_a\epsilon_b z)^2 - 4e^{a+b}]^{1/2}\} \\ f(z) &= \frac{[g(z) - 1][e^{a+b} - g(z)]}{g(z)[(1 + e^{a+b} - e^{a+b}\epsilon_a\epsilon_b z)^2 - 4e^{a+b}]^{1/2}} \end{aligned} \tag{30}$$

The pertinent properties of the random walk on the perfect lattice are the drift velocity and the dispersion around the initial point. These properties can be expressed as moments of $P_n(l - l_0)$, where l_0 is the initial site; the moments are given by[2,8]

$$\langle k^m \rangle_n = \sum_{l=-\infty}^{\infty} k^m P_n(k) = \left.\frac{\partial^m}{\partial (i\phi)^m} \lambda^n(\phi)\right|_{\phi=0} \qquad \text{with } k \equiv l - l_0 \tag{31}$$

From Appendix A we have

$$\lambda(\phi) = \frac{(e^a - 1)(e^b - 1)}{(e^{a-i\phi} - 1)(e^{b+i\phi} - 1)} \tag{32}$$

Using (31), we find

$$\langle (l - l_0) \rangle_n = n \frac{e^b - e^a}{(e^a - 1)(e^b - 1)} \tag{33}$$

where here and in the rest of this work we take $a \geqslant b$.

The drift velocity is

$$\langle (l - l_0) \rangle_n / n\tau_1 = k_0(\epsilon_a - \epsilon_b)(\epsilon_a + \epsilon_b - \epsilon_a\epsilon_b) \tag{34}$$

in real time.

The dispersion is

$$\begin{aligned}\langle [(l - l_0) - \langle l - l_0 \rangle_n]^2 \rangle_n &= \langle (l - \langle l \rangle_n)^2 \rangle_n \\ &= n\left\{\frac{(\epsilon_a - \epsilon_b)^2}{\epsilon_a{}^2\epsilon_b{}^2} + \frac{2 - \epsilon_a - \epsilon_b}{\epsilon_a\epsilon_b}\right\}.\end{aligned} \tag{35}$$

Note that in the symmetric case ($\epsilon_a = \epsilon_b$) the dispersion remains proportional to n. We shall find that properties of importance in the random walk on lattices with traps, such as the MFPT and branching ratio, have different behavior for the symmetric and asymmetric walks.

3.2. Random Walk on Lattice with Traps

We consider an infinite 1D lattice such that only $l \in (0, N)$ is a non-trapping site. Equivalently, every $l \notin (0, N)$ is a trapping site, with $p(0) = 1$.

The pertinent time scale in this model is the MFPT for absorption. As the jump probabilities are asymmetric, we are also interested in the relative absorption on the two sets of traps, as a function of the initial conditions.

In Appendix B we find the MFPT as a function of l_0; the result is

$$\begin{aligned}\langle n \rangle_{\rm tr} = 1 &+ \frac{\epsilon_a\epsilon_b}{\epsilon_a - \epsilon_b}\frac{l_0 + (N - l_0)\mu^N - N\mu^{N-l_0}}{1 - \mu^N} \\ &+ \{(\epsilon_b\mu^{N-l_0} - \epsilon_a)[N\mu^N(1 - \mu) - \mu(1 - \mu^N)] \\ &+ (\epsilon_b\mu^N - \epsilon_a\mu^{N-l_0})[1 - \mu^N - N(1 - \mu)]\} \\ &\times \left\{(1 - \mu)(1 - \mu^N)\left(\frac{\epsilon_a}{\epsilon_b} - \frac{\epsilon_b}{\epsilon_a}\mu^N\right)\right\}^{-1}\end{aligned} \tag{36}$$

where $\mu = e^{b-a} \leqslant 1$. If all initial states are equally probable, we can average over l_0 to get

$$\begin{aligned}&\overline{\langle n \rangle}_{\rm tr}(a, b) \\ &\quad = \frac{1}{N - 1}\sum_{l=1}^{N-1} \langle n \rangle_{\rm tr}(a, b, l_0) \\ &\quad = 1 + \frac{1}{2}\frac{N}{N - 1}\frac{N(1 - \mu)(1 + \mu^N) - (1 + \mu)(1 - \mu^N)}{(1 - \mu)(1 - \mu^N)}\frac{\epsilon_a\epsilon_b}{\epsilon_a - \epsilon_b} \\ &\quad + \{[N\epsilon_b\mu(1 - \mu^{N-1}) - (N - 1)\epsilon_a(1 - \mu)][N\mu^N(1 - \mu) - \mu(1 - \mu^N)] \\ &\quad + [(N - 1)\epsilon_b\mu^N(1 - \mu) - N\epsilon_a\mu(1 - \mu^{N-1})][1 - \mu^N - N(1 - \mu)]\} \\ &\quad \times \left\{(N - 1)(1 - \mu)^2(1 - \mu^N)\left(\frac{\epsilon_a}{\epsilon_b} - \frac{\epsilon_b}{\epsilon_a}\mu^N\right)\right\}^{-1}\end{aligned} \tag{37}$$

It is interesting to consider the limit of (37) for large N. We shall see that the scaling of the MFPT is very different for symmetric and asymmetric random walks. Remembering that $\lim_{N\to\infty} \mu^N = 0$, we have

$$\overline{\langle n\rangle}_{\mathrm{tr}}(a, b) = \frac{1}{2}\frac{\epsilon_b(2-\epsilon_a)}{\epsilon_a - \epsilon_b} N + O(1) \tag{38}$$

in the limit of large N. Notice that (38) diverges as we approach the condition for the symmetric walk ($\epsilon_a = \epsilon_b$).

3.3. Branching Ratio

The asymmetry in the jump probabilities is reflected in the form of the branching ratio, which is defined as

$$R(l_0) = \sum_{l=N}^{\infty} Q_\infty(l-l_0) \Big/ \sum_{l=-\infty}^{0} Q_\infty(l-l_0) \tag{39}$$

where $Q_\infty(l-l_0)$ is the stationary distribution, which, in the presence of absorbing states, depends on the initial state.

We calculate the branching ratio in Appendix C, and the result, as a function of l_0, is

$$R(l_0) = \frac{\epsilon_b}{\epsilon_a}\frac{\epsilon_a\mu^{N-l_0} - \epsilon_b\mu^N}{\epsilon_a - \epsilon_b\mu^{N-l_0}} \tag{40}$$

The branching ratio need not be unity even in the symmetric walk since l_0 need not be at the center of the interval $(0, N)$. [The result for R in the symmetric case is (C13).]

It is instructive to study (40) in the limit of large N. As $\mu < 1$, and if l_0 is somewhere in the middle of $(0, N)$, i.e., not too near to N, then $R \to 0$ as $N \to \infty$, unless $\epsilon_a = \epsilon_b$. Thus for a large range of initial conditions, absorption occurs at only one of the two available branches. (All the walkers are trapped on the left, since $a > b$.)

3.4. The Limit of a Symmetric Process

We want to take the limit $a \to b$ such that $a \geqslant b$. Let $a = b + \delta$. Then $\mu = e^{-\delta}$ and $\lim_{\delta\to 0+}$ is equivalent to $\lim_{\mu\to 1-}$. Thus ϵ_b remains unchanged but $\epsilon_a = 1 - \mu(1-\epsilon_b)$ and $\epsilon_a = \epsilon_b$ for $\mu = 1$. By repeated application of L'Hospital's rule we find

$$\lim_{\mu\to 1-} \frac{\epsilon_a\epsilon_b[l_0 + (N-l_0)\mu^N - N\mu^{N-l_0}]}{(\epsilon_a - \epsilon_b)(1-\mu^N)} = \frac{1}{2}\frac{\epsilon_b^2}{1-\epsilon_b} l_0(N-l_0) \tag{41}$$

$$\begin{aligned}\lim_{\mu\to 1-} (\{(\epsilon_b\mu^{N-l_0} - \epsilon_a)&[N\mu^N(1-\mu) - \mu(1-\mu^N)] \\ &+ (\epsilon_b\mu^N - \epsilon_a\mu^{N-l_0})[1 - \mu^N - N(1-\mu)]\} \\ &\times \left\{(1-\mu)(1-\mu^N)\left[\frac{\epsilon_a}{\epsilon_b} - \frac{\epsilon_b}{\epsilon_a}\mu^N\right]\right\}^{-1} \\ &= \tfrac{1}{2}(N-1)\epsilon_b \end{aligned} \tag{42}$$

so that

$$\langle n\rangle_{\text{tr}}(l_0, a) = 1 + \frac{1}{2}(N-1)\epsilon_a + \frac{1}{2}\frac{\epsilon_a^2}{1-\epsilon_a} l_0(N - l_0) \tag{43}$$

where the set of nontrapping sites is (0, N) and l_0 is the initial state. Assuming that all initial states are equally probable, we find

$$\begin{aligned}\overline{\langle n\rangle}_{\text{tr}}(a) &= \sum_{l_0=1}^{N-1} \frac{\langle n\rangle_{\text{tr}}(l_0, a)}{N-1} \\ &= 1 + \frac{1}{2}(N-1)\epsilon_a + \frac{1}{12}\frac{\epsilon_a^2}{1-\epsilon_a} N(2N-1)\end{aligned} \tag{44}$$

Thus, in the limit of large N

$$\overline{\langle n\rangle}_{\text{tr}}(a) \approx \frac{1}{6}\frac{\epsilon_a^2}{1-\epsilon_a} N^2, \qquad N \to \infty \tag{45}$$

Note that in the limit $a \to \infty$, $\langle n\rangle_{\text{tr}}(l_0, a) \propto e^a$ for any N.

It is of interest to compare the MFPT for symmetric and asymmetric walks in the limit of large N (size of the nontrapping subset of the stochastic space). For a given nonzero $\epsilon_a - \epsilon_b$, there exists an N such that total absorption is faster in the asymmetric random walk. On the other hand, for any large but fixed N, there exist values of a and b such that the symmetric walk leads to faster absorption. Thus we see that the limits $N \to \infty$ and $a \to b$ do not commute in this model. In most cases of interest the size of the system is fixed. In this case, if we vary external conditions which control parameters a and b, such that $a \to b$, we see that the MFPT diverges. This behavior, together with the nonanalyticity that is associated with the symmetric limit, bears some resemblance to properties of critical phenomena.

4. CONCLUDING REMARKS

The scaling of the MFPT with the size of the nontrapping subspace N was the subject of a thorough study in the case of nearest neighbor random walks.[8] The general conclusion is that for symmetric walks the scaling depends strongly on the dimensionality of the problem,

$$\langle n\rangle_{\text{tr}} \underset{N\to\infty}{\sim} \begin{cases} N^2, & \text{1D} \\ N \log N, & \text{2D} \\ N, & \text{3D} \end{cases} \tag{46}$$

The MFPT for the asymmetric nearest neighbor random walk scales like N, for large N, i.e.,

$$\langle n\rangle_{\text{tr}} \underset{N\to\infty}{\sim} N, \qquad \text{1D} \tag{47}$$

Thus the first conclusion [from Eqs. (45) and (38)] is that the range of jump probabilities does not change the scaling with N. We also see that the MFPT for 1D asymmetric walks has the same scaling property as the one for the symmetric 3D walk.

APPENDIX A. CALCULATION[3] OF $G(z, l - l_0)$

In order to evaluate G we need to know $\lambda(\phi)$ given by

$$\lambda(\phi) = \sum_{k=-\infty}^{\infty} p(k)e^{ik\phi} = c\,\frac{e^{a+b} - 1}{(e^{a-i\phi} - 1)(e^{b+i\phi} - 1)} \tag{A1}$$

Therefore $G(z, l - l_0) = G(z, m)$ is

$$G(z, m) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi\,\frac{e^{-im\phi}(e^{a-i\phi} - 1)(e^{b+i\phi} - 1)}{(e^{a-i\phi} - 1)(e^{b+i\phi} - 1) - \bar{z}} \tag{A2}$$

where $\bar{z} = c(e^{a+b} - 1)z = e^{a+b}\epsilon_a\epsilon_b z$.

We need to consider three situations: $m > 0$, $m < 0$, and $m = 0$. Using the calculus of residues, we find

$$\begin{aligned} G(z, m) &= x_1{}^m f(z), \qquad m > 0 \\ G(z, m) &= x_2^{|m|} f(z), \qquad m < 0 \end{aligned} \tag{A3}$$

where

$$\begin{aligned} x_1 &\equiv e^{-a}g(z) \\ x_2 &\equiv e^{-b}g(z) \\ g(z) &\equiv \tfrac{1}{2}\{(1 + e^{a+b} - e^{a+b}\epsilon_a\epsilon_b z) \\ &\qquad - [(1 + e^{a+b} - e^{a+b}\epsilon_a\epsilon_b z)^2 - 4e^{a+b}]^{1/2}\} \\ f(z) &\equiv \frac{[g(z) - 1][e^{a+b} - g(z)]}{g(z)[(1 + e^{a+b} - e^{a+b}\epsilon_a\epsilon_b z)^2 - 4e^{a+b}]^{1/2}} \end{aligned} \tag{A4}$$

$$G(z, 0) = 1 + f(z) \tag{A5}$$

APPENDIX B. CALCULATION OF MEAN NUMBER OF STEPS BEFORE TRAPPING

From (25)

$$\langle n \rangle_{\mathrm{tr}} = \frac{\partial}{\partial z}\left\{(1 - z)\sum_{l\,\mathrm{trap}} F(z, l, l_0)\right\}\Bigg|_{z=1} \tag{B1}$$

where, from (20),

$$F(z, l, l_0) = G(z, l, l_0) + \sum_{l'\,\mathrm{trap}} F(z, l', l_0)[(z - 1)G(z, l, l') + \delta_{l,l'}] \tag{B2}$$

[3] The calculations presented here are in a shortened form. Further details may be obtained by writing to the authors.

Equation (B2) can be rewritten as

$$F(z, l - l_0, l_0)G(z, 0) = \frac{G(z, l - l_0)}{1 - z} - \sum_{\substack{l' \text{trap} \\ l' \neq l}} G(z, l - l')F(z, l' - l_0, l_0) \quad \text{(B3)}$$

[From now on we denote $F(z, l' - l_0, l_0)$ by $F(z, \ell' - l_0)$.] Since the trapping sites are in $[-\infty, 0]$ and $[N, \infty]$ we need to consider the following cases:

(i) $-\infty \leqslant l \leqslant -1; l < l_0$. Then, from (B3), (A3)–(A5)

$$\frac{x_2^{l_0 - l}}{1 - z} = F(z, l - l_0)h(z) + \sum_{l'=N}^{\infty} F(z, l' - l_0)x_2^{l'-l} + \sum_{l'=-\infty}^{l-1} F(z, l' - l_0)x_1^{l-l'} + \sum_{l'=l+1}^{\infty} F(z, l' - l_0)x_2^{l'-l} \quad \text{(B4)}$$

(ii) $N + 1 \leqslant l \leqslant \infty; l > l_0$:

$$\frac{x_1^{l-l_0}}{1 - z} = F(z, l - l_0)h(z) + \sum_{l'=-\infty}^{\infty} F(z, l' - l_0)x_1^{l-l'} + \sum_{l'=N}^{l-1} F(z, l' - l_0)x_1^{l-l'} + \sum_{l'=l+1}^{\infty} F(z, l' - l_0)x_2^{l'-l} \quad \text{(B5)}$$

(iii) $l = 0, l < l_0$:

$$\frac{x_2^{l_0}}{1 - z} = F(z, -l_0)h(z) + \sum_{l'=-\infty}^{-1} F(z, l' - l_0)x_1^{-l'} + \sum_{l'=N}^{\infty} F(z, l' - l_0)x_2^{l'} \quad \text{(B6)}$$

(iv) $l = N, l > l_0$:

$$\frac{x_1^{N-l_0}}{1 - z} = F(z, N - l_0)h(z) + x_1^N \sum_{l'=-\infty}^{0} F(z, l' - l_0)x_1^{-l'} + x_2^{-N} \sum_{l'=N+1}^{\infty} F(z, l' - l_0)x_2^{l'} \quad \text{(B7)}$$

The function $h(z)$ is defined as

$$h(z) \equiv \frac{G(z, 0)}{f(z)} = 1 + \frac{1}{f(z)} \quad \text{(B8)}$$

Define

$$A \equiv \sum_{l'=-\infty}^{-1} F(z, l' - l_0)x_1^{-l'} \quad \text{(B9a)}$$

$$B \equiv \sum_{l'=N+1}^{\infty} F(z, l' - l_0)x_2^{l'} \quad \text{(B9b)}$$

Summing (B4) and (B5) over l in the appropriate range, we get, after some algebra

$$\left(h + \frac{x_1}{1-x_1} + \frac{x_2}{1-x_2}\right)\theta_1 = \left(h + \frac{x_1}{1-x_1}\right)F(z, -l_0) - \frac{x_2^{N+1}}{1-x_2}F(z, N-l_0) + \frac{x_2^{l_0+1}}{(1-z)(1-x_2)} + \frac{1}{1-x_1}A - \frac{x_2}{1-x_2}B \tag{B10}$$

$$\left(h + \frac{x_1}{1-x_1} + \frac{x_2}{1-x_2}\right)\theta_2 = \left(h + \frac{x_2}{1-x_2}\right)F(z, N-l_0) - \frac{x_1^{N+1}}{1-x_1}F(z, -l_0) + \frac{x_1^{N-l_0+1}}{(1-z)(1-x_1)} - \frac{x_1^{N+1}}{1-x_1}A + \frac{x_2^{-N}}{1-x_2}B \tag{B11}$$

where

$$\theta_1 \equiv \sum_{l=-\infty}^{0} F(z, l-l_0) \tag{B12a}$$

$$\theta_2 \equiv \sum_{l=N}^{\infty} F(z, l-l_0) \tag{B12b}$$

A and B can be found from (B6) and (B7) in terms of $F(z, -l_0)$ and $F(z, N-l_0)$ as follows:

$$A = \frac{x_1^{N-l_0} - x_2^{l_0-N}}{(1-z)(x_1^N - x_2^{-N})} + \frac{hx_2^{-N} - x_1^N}{x_1^N - x_2^{-N}}F(z, -l_0) + \frac{1-h}{x_1^N - x_2^{-N}}F(z, N-l_0) \tag{B13}$$

$$B = \frac{x_1^N(x_2^{l_0} - x_1^{-l_0})}{(1-z)(x_1^N - x_2^{-N})} + \frac{x_1^N(1-h)}{x_1^N - x_2^{-N}}F(z, -l_0) + \frac{h - x_1^N x_2^N}{x_1^N - x_2^{-N}}F(z, N-l_0) \tag{B14}$$

In order to relate $F(z, -l_0)$ and $F(z, N-l_0)$ to θ_1 and θ_2 we make use of (14), i.e., for l trapping

$$F(z, l-l_0) = z\sum_{l'\,\mathrm{nontrap}} p(l-l')F(z, l'-l_0) + zF(z, l-l_0) \tag{B15}$$

Rearranging and summing over $l \in [-\infty, 0]$ we find

$$(1-z)\sum_{l=-\infty}^{0} F(z, l-l_0) = z\sum_{l'\,\mathrm{nontrap}} F(z, l'-l_0)\sum_{l=-\infty}^{0} p(l-l') = \frac{zc}{1-e^{-b}}\sum_{l'\,\mathrm{nontrap}} F(z, l'-l_0)e^{-bl'} \tag{B16}$$

On the other hand, directly from (B15) and noting that $p(-l') = ce^{-bl'}$ for l' nontrapping,

$$(1 - z)F(z, -l_0) = zc \sum_{l'\,\mathrm{nontrap}} F(z, l' - l_0)e^{-bl'} \tag{B17}$$

so that

$$(1 - z)\theta_1 = (1 - z)F(z, -l_0)/(1 - e^{-b})$$

Finally

$$F(z, -l_0) = \epsilon_b \theta_1 \tag{B18}$$

Similarly

$$F(z, N - l_0) = \epsilon_a \theta_2 \tag{B19}$$

Combining (B10), (B11), (B13), (B14), (B18), and (B19), we find, after some algebra,

$$\Pi\theta_1 = \frac{\phi_1}{1 - z} + \epsilon_b \Lambda_{11}\theta_1 + \epsilon_a \Lambda_{12}\theta_2 \tag{B20}$$

$$\Pi\theta_2 = \frac{\phi_2}{1 - z} + \epsilon_b \Lambda_{21}\theta_1 + \epsilon_a \Lambda_{22}\theta_2 \tag{B21}$$

where

$$\begin{aligned}
\Pi &= (1 - x_1)(1 - x_2)(x_1^{N} - x_2^{-N})\left(h + \frac{x_1}{1 - x_1} + \frac{x_2}{1 - x_2}\right) \\
\phi_1 &= (1 - x_1x_2)(x_1^{N-l_0} - x_2^{l_0-N}) \\
\phi_2 &= (1 - x_1x_2)x_1^{N}x_2^{-N}(x_2^{l_0} - x_1^{-l_0}) \\
\Lambda_{11} &= (h - 1)[x_1^{N}(1 - x_1) + x_1x_2^{-N}(1 - x_2)] \\
\Lambda_{12} &= -(h - 1)(1 - x_1x_2) \\
\Lambda_{21} &= -(h - 1)(1 - x_1x_2)x_1^{N}x_2^{-N} \\
\Lambda_{22} &= (h - 1)[x_1^{N}(1 - x_2) + x_2^{1-N}(1 - x_1)]
\end{aligned} \tag{B22}$$

Therefore, solving (B20) and (B21), we find

$$\theta_1 = \frac{1}{1 - z}\,\frac{\phi_1(\Pi - \epsilon_a\Lambda_{22}) + \phi_2\epsilon_a\Lambda_{12}}{(\Pi - \epsilon_a\Lambda_{22})(\Pi - \epsilon_b\Lambda_{11}) - \epsilon_a\epsilon_b\Lambda_{12}\Lambda_{21}} \tag{B23}$$

$$\theta_2 = \frac{1}{1 - z}\,\frac{\phi_1\epsilon_b\Lambda_{21} + \phi_2(\Pi - \epsilon_b\Lambda_{11})}{(\Pi - \epsilon_a\Lambda_{22})(\Pi - \epsilon_b\Lambda_{11}) - \epsilon_a\epsilon_b\Lambda_{12}\Lambda_{21}} \tag{B24}$$

According to (B1)

$$\langle n\rangle_{\mathrm{tr}} = \frac{\partial}{\partial z}\{(1 - z)(\theta_1 + \theta_2)\}\bigg|_{z=1} \equiv \frac{\partial}{\partial z}\tilde{F}(z)\bigg|_{z=1}$$

where

$$\tilde{F}(z) = \frac{\phi_1(\Pi + \epsilon_b\Lambda_{21} - \epsilon_a\Lambda_{22}) + \phi_2(\Pi + \epsilon_a\Lambda_{12} - \epsilon_b\Lambda_{11})}{(\Pi - \epsilon_b\Lambda_{11})(\Pi - \epsilon_a\Lambda_{22}) - \epsilon_a\epsilon_b\Lambda_{12}\Lambda_{21}} \tag{B25}$$

Finally

$$\begin{aligned}\langle n\rangle_{\text{tr}} = 1 &+ \frac{\epsilon_a\epsilon_b}{\epsilon_a - \epsilon_b}\,\frac{l_0 + (N - l_0)\mu^N - N\mu^{N-l_0}}{1 - \mu^N}\\ &+ \{(\epsilon_b\mu^{N-l_0} - \epsilon_a)[N\mu^N(1 - \mu) - \mu(1 - \mu^N)]\\ &+ (\epsilon_b\mu^N - \epsilon_a\mu^{N-l_0})[1 - \mu^N - N(1 - \mu)]\}\\ &\times \left\{(1 - \mu)(1 - \mu^N)\left(\frac{\epsilon_a}{\epsilon_b} - \frac{\epsilon_b}{\epsilon_a}\mu^N\right)\right\}^{-1}\end{aligned} \tag{B26}$$

where $\mu = e^{b-a} \leqslant 1$, $\epsilon_a = 1 - e^{-a}$, $\epsilon_b = 1 - e^{-b}$.

APPENDIX C. BRANCHING RATIO

We define the branching ratio R as

$$R = \sum_{l=N}^{\infty} Q_\infty(l - l_0)\Big/\sum_{l=-\infty}^{0} Q_\infty(l - l_0) \tag{C1}$$

where $Q_\infty(l - l_0)$ is the stationary distribution, which, in the presence of absorbing states, depends on the initial state. Using the recursion relation (13), we have, for l trapping,

$$Q_n(l - l_0) = c\sum_{l'=1}^{N-1} e^{-a(l-l')}\sum_{k=1}^{n-1} Q_k(l' - l_0), \qquad N \leqslant l \leqslant \infty \tag{C2}$$

$$Q_n(l - l_0) = c\sum_{l'=1}^{N-1} e^{-b(l'-l)}\sum_{k=1}^{n-1} Q_k(l' - l_0), \qquad -\infty \leqslant l \leqslant 0 \tag{C3}$$

Therefore, the stationary distribution is given by

$$Q_\infty(l - l_0) = c\sum_{l'=1}^{N-1} e^{-a(l-l')}F(1, l' - l_0), \qquad N \leqslant l \leqslant \infty \tag{C4}$$

$$Q_\infty(l - l_0) = c\sum_{l'=1}^{N-1} e^{-b(l'-l)}F(1, l' - l_0), \qquad -\infty \leqslant l \leqslant 0 \tag{C5}$$

From (14) we have, after some algebra,

$$\sum_{l=N}^{\infty} Q_\infty(l - l_0) = \frac{e^{-a}}{1 - e^{-a}}\,[F(1, N - 1 - l_0) - \delta_{N-1,l_0}] \tag{C6}$$

$$\sum_{l=-\infty}^{0} Q_\infty(l - l_0) = \frac{e^{-b}}{1 - e^{-b}}\,[F(1, 1 - l_0) - \delta_{1,l_0}] \tag{C7}$$

and

$$R = \mu \frac{\epsilon_b}{\epsilon_a} \frac{F(1, N-1-l_0) - \delta_{N-1,l_0}}{F(1, 1-l_0) - \delta_{1,l_0}} \tag{C8}$$

For l nontrapping we have, from (20),

$$F(1, l-l_0) = G(1, l-l_0) - \lim_{z\to 1-} (1-z)\left\{ \sum_{l'=-\infty}^{0} G(z, l-l')F(z, l'-l_0) + \sum_{l'=N}^{\infty} G(z, l-l')F(z, l'-l_0) \right\}$$

which is found to be

$$F(1, 1-l_0) = \frac{\epsilon_a\epsilon_b(\epsilon_a - \epsilon_b\mu)}{(\epsilon_a - \epsilon_b)(\epsilon_a{}^2 - \epsilon_b{}^2\mu^N)} (\epsilon_a - \epsilon_b\mu^{N-l_0}), \qquad l_0 \neq 1 \tag{C9}$$

and

$$F(1, N-1-l_0) = \frac{\epsilon_a\epsilon_b(\epsilon_a - \epsilon_b\mu)}{(\epsilon_a - \epsilon_b)(\epsilon_a{}^2 - \epsilon_b{}^2\mu^N)} \frac{\epsilon_a\mu^{N-l_0} - \epsilon_b\mu^N}{\mu}, \qquad l_0 \neq N-1 \tag{C10}$$

For $l = 1$, $l_0 = 1$, and for $l = N-1$, $l_0 = N-1$,

$$F(1, 0) = \frac{\epsilon_a\epsilon_b(\epsilon_a - \epsilon_b\mu)}{(\epsilon_a - \epsilon_b)(\epsilon_a{}^2 - \epsilon_b{}^2\mu^N)} (\epsilon_a - \epsilon_b\mu^{N-1}) + 1 \tag{C11}$$

The branching ratio, therefore, is

$$R(l_0) = \frac{\epsilon_b}{\epsilon_a} \frac{\epsilon_a\mu^{N-l_0} - \epsilon_b\mu^N}{\epsilon_a - \epsilon_b\mu^{N-l_0}} \tag{C12}$$

The branching ratio in the symmetric case is found with the L'Hospital rule to be

$$R(l_0, a) = \frac{1 + (l_0 - 1)\epsilon_a}{1 + (N - l_0 - 1)\epsilon_a} \tag{C13}$$

ACKNOWLEDGMENT

We thank one of the referees for a careful review of our paper and for a proof that is more general and elegant than the original one in Section 2.2.

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