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Reflection Principles for Biased Random Walks and Application to Escape Time Distributions

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We present a reflection principle for an arbitrary *biased* continuous time random walk (comprising both Markovian and non-Markovian processes) in the presence of a *reflecting* barrier on semi-infinite and finite chains. For biased walks in the presence of a reflecting barrier this principle (which cannot be derived from combinatorics) is completely different from its familiar form in the presence of an absorbing barrier. The result enables us to obtain closed-form solutions for the Laplace transform of the conditional probability for biased walks on finite chains for all three combinations of absorbing and reflecting barriers at the two ends. An important application of these solutions is the calculation of various first-passage-time and escape-time distributions. We obtain exact results for the characteristic functions of various kinds of escape time distributions for biased random walks on finite chains. For processes governed by a long-tailed event-time distribution we show that the mean time of escape from bounded regions diverges even in the presence of a bias—suggesting, in a sense, the absence of true long-range diffusion in such "frozen" processes.

KEY WORDS: Continuous time random walk; biased random walk; reflection principle; escape time distribution.

1. INTRODUCTION

A classic and elegant way of solving random walk problems on finite or semi-infinite domains bounded by barriers is by means of the reflection principle, also known as the method of images in boundary value problems.[1-3] In this method, the solution to the more difficult problem of a random walk in the presence of barriers is expressed as a superposition of solutions in the absence of the barriers. In random walk theory, the proof

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of the reflection principle involves combinatorics. The most familiar and widely used form[2] of the principle pertains to the case of *symmetric* or unbiased random walks on a semi-infinite chain with a reflecting or absorbing barrier at one end. The method is extended easily to symmetric random walks on finite chains with such barriers at both ends; the result is an infinite sum over solutions corresponding to the infinite chain, since the image set due to repeated reflections at the two barriers is an infinite one. For unsymmetric or *biased* random walks, the reflection principle in the case of an absorbing barrier is known.[2] However, there is no analogous result in the case of a reflecting barrier. A direct superposition of infinite-chain solutions as in the previous cases is incorrect. In fact, a simple reflection principle does not exist in this case, basically because of the complexity in enumerating paths in a biased random walk with repeated reflections at a point.

In this paper, we present a form of reflection principle for a discrete biased random walk in the presence of a reflecting barrier. Our solution expresses the Laplace transform (with respect to time) of the conditional probability for a random walk on the set of positive integers $\{1, 2,...\}$ (0 being a perfectly reflecting barrier) as a linear combination of the transforms of solutions to the random walk problem on an infinite chain (the set of integers, $\mathbb{Z}$), with a frequency-dependent coefficient. Reexpressed in terms of the original functions of time, this relation involves an integration over a memory kernel of the solution on $\mathbb{Z}$, even in the case of a Markovian random walk. This is a consequence of the complexity in path enumeration mentioned earlier, and incidentally helps explain why a simple reflection principle cannot obtain when a reflecting barrier and bias are *both* present. Our results are derived for a general random walk governed by a renewal process with an arbitrary waiting time distribution—a "continuous time random walk," or CTRW. They are therefore valid for a wide class of random walks, ranging from the simple Markovian one to walks that are highly correlated in time, including those "frozen" processes for which the mean residence time at a site is infinite. (These are of interest in the problem of transport in amorphous media.)

In Section 2, we present the new reflection principle for a biased CTRW on the semi-infinite chain $\{1, 2,...\}$, 0 being a reflecting barrier. (Its form in the continuum limit of Markovian diffusion with uniform drift on the half-line $[0, \infty)$ is also given.) Used in conjunction with the already known reflection principle for an absorbing barrier, this result enables one to arrive at compact exact solutions for the Laplace transform of the conditional probability for random walks on finite chains with all three combinations of absorbing and reflecting barriers at the two ends. We list these in Section 3, and comment upon the structure of the different expressions.

Finally, in Section 4, we use our results to obtain various kinds of escape time distributions for biased CTRW's on finite chains, including the one corresponding to an arbitrary starting point for the walk. (In the particular case of a symmetric walk from the center of the chain, this distribution has been found in an earlier work.[4]) We show also that the mean escape time diverges for any CTRW governed by an interval density that has no moments, even if the walk is biased.

2. THE REFLECTION PRINCIPLE

2.1. Boundary Conditions and Known Results

For the sake of clarity, we write down first the reflection principle for unbiased and biased random walks in the already known cases.[1-3] Let $P(m, t \mid m_0)$ be the conditional probability of finding the random walker at the point (site) m at time t, given that the walker started from m_0 at $t=0$ on an infinite chain. Let $P_0(m, t \mid m_0)$ [respectively, $P_{\bar{0}}(m, t \mid m_0)$] represent the corresponding solution for a random walk on the set $\{1, 2,...\}$ in the presence of a reflecting (absorbing) barrier at 0—the bar over the subscript in $P_{\bar{0}}$ serving to remind us of the termination of the walk once the barrier is reached. Consider a biased nearest-neighbor random walk in which the *a priori* probability of a jump to the right is p and that to the left is $q=1-p$. For an absorbing barrier at 0, the boundary condition on the conditional probability is

$$P_{\bar{0}}(0, t \mid m_0)=0 \tag{2.1a}$$

for both biased $(p \neq q)$ and unbiased $(p=q=1/2)$ walks. This condition represents absorption as it ensures that the random walker and the image walker "annihilate" each other on coming together at the boundary, thus terminating the walk. In the physical context of diffusion, this is equivalent to a vanishing concentration of the diffusing species at the boundary. For a reflecting barrier at 0, the boundary condition is

$$P_0(0, t \mid m_0)=P_0(1, t \mid m_0) \qquad \text{when} \quad p=q=\tfrac{1}{2} \tag{2.1b}$$

i.e., for an unbiased walk; and

$$pP_0(0, t \mid m_0)=qP_0(1, t \mid m_0) \qquad \text{when} \quad p \neq q \tag{2.1c}$$

i.e., for a biased walk. These conditions imply that the barrier is a perfect reflector. With reference to diffusion, these conditions ensure that the current (rather than the concentration itself) vanishes at the boundary; see also Eq. (2.16) below.

The reflection principle[2] yields the following relationships between $P(m, t \mid m_0)$ and $P_{\bar{0}}(m, t \mid m_0)$ [respectively, $P_0(m, t \mid m_0)$]:

With an *absorbing* barrier at 0,

$$P_{\bar{0}}(m, t \mid m_0) = P(m, t \mid m_0) - P(m, t \mid -m_0) \qquad (\text{unbiased, } p = q = \tfrac{1}{2}) \tag{2.2a}$$

and

$$P_{\bar{0}}(m, t \mid m_0) = P(m, t \mid m_0) - (q/p)^{m_0} P(m, t \mid -m_0) \qquad (\text{biased, } p \neq q) \tag{2.2b}$$

With a *reflecting* barrier at 0,

$$P_0(m, t \mid m_0) = P(m, t \mid m_0) + P(m, t \mid -m_0 + 1) \qquad (\text{unbiased, } p = q = \tfrac{1}{2}) \tag{2.2c}$$

There is no simple analog of Eq. (2.2b) for a reflecting barrier. It is evident that the relations in Eqs. (2.2) are valid as they stand for the corresponding Laplace transforms. Using certain symmetry properties of the infinite chain solution $P(m, t \mid m_0)$ (see below), it may be verified that the solutions in Eqs. (2.2) satisfy Eqs. (2.1a) and (2.1b).

2.2. Continuous Time Random Walk on $\mathbb{Z}$

For a random walk by nearest-neighbor jumps on the infinite chain $\mathbb{Z}$, we have

$$P(m, t \mid m_0) = P(m - m_0, t \mid 0) = \sum_{n = |m - m_0|}^{\infty} W(n, t)\, p_n(m - m_0) \tag{2.3}$$

where $W(n, t)$ is the normalized probability for exactly n jumps to occur in the time interval t, and $p_n(m - m_0)$ is the probability of reaching the point m from m_0 in n steps. This is of course given by

$$p_n(r) = \binom{n}{\frac{n - r}{2}} p^{(n+r)/2} q^{(n-r)/2} \tag{2.4}$$

when $(n - |r|)/2$ is a nonnegative integer, and is zero in all other cases. Let $W(n, t)$ be generated by an ordinary renewal process[2,5] which is specified by a normalized event-time density $\psi(t)$. It can be shown in a straightforward manner[4,6] that the Laplace transform of $W(n, t)$ is given by

$$\tilde{W}(n, u) = u^{-1}(1 - \tilde{\psi})[\tilde{\psi}(u)]^n \tag{2.5}$$

Inserting (2.4) and (2.5) in (2.3) and carrying out the summation yields the following result for the Laplace transform of the conditional probability:

$$\tilde{P}(m, u \mid m_0) = (p/q)^{(m-m_0)/2}\, u^{-1}(1-4pq\tilde{\psi}^2)^{-1/2} \times (1-\tilde{\psi})\left[\frac{1-(1-4pq\tilde{\psi}^2)^{1/2}}{2(pq)^{1/2}\,\tilde{\psi}}\right]^{|m-m_0|} \tag{2.6}$$

Equation (2.6) is a special case of a general solution obtained earlier in another context[7] for an arbitrary biased CTRW with a first event-time distribution $\psi_0(t)$ that is distinct from $\psi(t)$. In the present work $\psi_0(t)$ has been taken to be the same as the interval density $\psi(t)$, keeping in mind the main physical applications of CTRW's, namely, transport in amorphous media.[8] If need be, our results may be modified easily to cover the case when $\psi_0(t)$ is distinct from $\psi(t)$.

In what follows, it is convenient to introduce the variable

$$\xi(u) = \operatorname{arcsech}[2(pq)^{1/2}\,\tilde{\psi}] \tag{2.7}$$

and to define also

$$\alpha = \tfrac{1}{2}\ln(p/q) \tag{2.8}$$

Then

$$\tilde{P}(m, u \mid m_0) = u^{-1}(1-\tilde{\psi})\coth\xi\,\exp[(m-m_0)\alpha - |m-m_0|\,\xi] \tag{2.9}$$

2.3. The Reflection Principle for Biased Walks

As mentioned in the Introduction, a direct enumeration of paths in the presence of a reflecting barrier is not feasible when the walk is biased, because of the nature of the boundary condition (2.1c). Therefore a generalization of Eq. (2.2c) to cover the case $p \neq q$ is not possible by combinatorial methods. Thus, even for a Markovian walk—the original "random walk"—for which $P(m, t \mid m_0)$ is essentially a modified Bessel function, we cannot wirte down a simple answer for $P_0(m, t \mid m_0)$ when $p \neq q$, although we can do so for $P_{\bar{0}}(m, t \mid m_0)$.

We present below a reflection principle that expresses $\tilde{P}_0(m, u \mid m_0)$ for an arbitrary, biased CTRW in terms of the corresponding infinite chain function $\tilde{P}(m, u \mid m_0)$, by actually using an explicit solution for $\tilde{P}_0$ found in an entirely different context: In the study of hopping conductivity in a bond-percolation model in a constant external field,[9] an exact solution was obtained for the conditional probability $\tilde{P}_{0,N}(m, u \mid m_0)$ of a biased random walk on the set $\{1, 2,..., (N-1)\}$, with reflecting barriers at 0 and N. The reflection principle is essentially deduced *post facto* by an inspection of the form of this solution (in the limit $N \to \infty$) vis-à-vis that of $\tilde{P}(m, u \mid m_0)$. In Section 3, we use the principle so obtained to find easy solutions to related problems.

Consider a biased CTRW on the set $\{1, 2,..., (N-1)\}$ with perfectly reflecting barriers at 0 and N. Although the random walk is not Markovian except in the single instance of the exponential density $\psi(t) = 2W\exp(-2Wt)$, $P(m, t \mid m_0)$ still obeys a master equation with a memory kernel.[10,11] The algebraic equations obtained from this for the set of transforms $\tilde{P}_{0,N}(m, u \mid m_0)$, where $1 \leqslant m,\ m_0 \leqslant N-1$ can be written in matrix form and solved exactly.[9] After a great deal of algebra, we obtain the result

$$\begin{aligned}\tilde{P}_{0,N}(m, u \mid m_0)&\\ &= e^{\alpha(m-m_0-1)}[\sinh(N-m_>)\xi - e^{\alpha}\sinh(N-m_>-1)\xi]\\ &\quad\times[e^{\alpha}\sinh m_<\xi - \sinh(m_<-1)\xi][u\sinh\xi\,\sinh(N-1)\xi]^{-1} \qquad (2.10)\end{aligned}$$

where $m_> = \max(m, m_0)$ and $m_< = \min(m, m_0)$. Letting $N \to \infty$ in Eq. (2.10), we obtain the following solution to the random walk problem on the semi-infinite chain $\{1, 2,...\}$ with a reflecting barrier at the site 0:

$$\tilde{P}_0(m, u \mid m_0) = \frac{e^{\alpha(m-m_0)-m_>\xi}(e^{\xi-\alpha}-1)[e^{\alpha}\sinh m_<\xi - \sinh(m_<-1)\xi]}{u\sinh\xi} \qquad (2.11)$$

An inspection of Eq. (2.11) and a comparison with Eq. (2.9) reveals that this solution may be rewritten in the form

$$\tilde{P}_0(m, u \mid m_0) = \tilde{P}(m, u \mid m_0) + e^{-2m_0\alpha}K(\xi, \alpha)\,\tilde{P}(m, u \mid -m_0+1) \qquad (2.12)$$

where

$$K(\xi, \alpha) = e^{\alpha}\sinh\tfrac{1}{2}(\xi-\alpha)/\sinh\tfrac{1}{2}(\xi+\alpha) \qquad (2.13)$$

This is the desired "reflection principle." Comparing it with that of Eq. (2.2b), we observe the similarity of form—note that $\exp(-2m_0\alpha) = (q/p)^{m_0}$—as well as the presence of the extra factor $K(\xi, \alpha)$. This factor reduces to unity when there is no bias ($p = q$), i.e., when $\alpha = 0$.

The superposition expressed by Eq. (2.12) is valid for the Laplace transform of the conditional probability. In terms of the original time variable, therefore, the relationship involves a convolution over a memory kernel. Although the transform K of this kernel appears to be quite simple, it is not possible to invert it to find the kernel in closed form even for the standard Markovian random walk. This also corroborates our earlier statement that it does not appear to be feasible to arrive at the reflection principle for $P_0(m, t \mid m_0)$ by combinatorial methods when a bias is present.

2.4. The Continuum Case

It is instructive to look at the form of the reflection principle deduced above in the continuum limit of (Markovian) biased diffusion on the half-line $[0, \infty)$ with a reflecting boundary at 0. We first set the interval density $\psi(t) = 2W \exp(-2Wt)$, where $2W$ is the constant jump rate out of a site, and introduce the lattice spacing a wherever appropriate. Letting $W \to \infty$, $a \to 0$, and $p \to q$ such that the static diffusion constant $D = \lim Wa^2$ and the drift velocity $c = \lim 2Wa(p-q)$ are finite, leads to the continuum limit; α and ξ then approach zero like $(p-q)$ and $a(c^2 + 4uD)^{1/2}/2D$, respectively. We then find from (2.12) and (2.13) that the transform of the conditional probability density, $\tilde{P}_0(x, u \mid x_0)$ $(0 \leqslant x, x_0 < \infty)$, is expressible in terms of the transform $\tilde{P}(x, u \mid x_0)$ for diffusion on the infinite line according to

$$\tilde{P}_0(x, u \mid x_0) = \tilde{P}(x, u \mid x_0) + \left[\frac{(c^2 + 4uD)^{1/2} - c}{(c^2 + 4uD)^{1/2} + c}\right] \times e^{-x_0 c/D} \tilde{P}(x, u \mid -x_0) \tag{2.14}$$

This "reflection principle" may be verified directly by starting with the Smoluchowski equation for diffusion with a constant drift, namely,

$$(\partial/\partial t + c\, \partial/\partial x - D\, \partial^2/\partial x^2)\, f(x, t) = 0 \tag{2.15}$$

subject to the initial condition $f(x, 0) = \delta(x - x_0)$. The solution in $(-\infty, \infty)$ with natural boundary conditions corresponds to $P(x, t \mid x_0)$, and is the usual Gaussian peaked at the point $(x_0 + ct)$. The solution[12] obeying the boundary condition

$$(D\, \partial/\partial x - c)\, f(x, t)\, |_{x=0} = 0 \tag{2.16}$$

corresponds to $P_0(x, t \mid x_0)$. Taking the Laplace transforms of $P_0(x, t \mid x_0)$ and $P(x, t \mid x_0)$, one may verify that they are related as in Eq. (2.14). The memory kernel corresponding to the inverse transform of the u-dependent coefficient in (2.14) is not a simple one. However, it is evident that the behavior of this kernel is characterized by the time scale expected on physical grounds, $4D/c^2$.

3. SOLUTIONS FOR BIASED CTRW's ON FINITE CHAINS

The relation found in (2.12) completes the set listed in Eqs. (2.2). These may now be used to advantage to get closed expressions for $\tilde{P}_{\bar{0},\bar{N}}(m, u \mid m_0)$ and $\tilde{P}_{0,\bar{N}}(m, u \mid m_0)$, without again going through the lengthy algebra involved in arriving at the solution (2.10) for $\tilde{P}_{0,N}(m, u \mid m_0)$.

3.1. Random Walk Between Two Absorbing Boundaries

Consider a biased CTRW on the set $\{0, 1,..., N\}$ with absorbing ends at 0 and N. Equation (2.2b) is the appropriate reflection principle in this case. As the interval is finite, the image set of barrier points is infinite[2,3] because of repeated reflections at the two end points. Using Eq. (2.2b) for each point in the image set, we find that $\tilde{P}_{\bar{0},\bar{N}}$ can be expressed in terms of the infinite chain solution according to

$$\tilde{P}_{\bar{0},\bar{N}}(m, u \mid m_0) = \sum_{n=-\infty}^{\infty} \{\exp(-2nN\alpha)\, \tilde{P}(m, u \mid m_0 - 2nN) \\ - \exp[-2\alpha(m_0 - nN)]\, \tilde{P}(m, u \mid 2nN - m_0)\} \quad (3.1)$$

[As the coefficients of $\tilde{P}$ in the above equation are independent of u, the Laplace transform may be inverted directly to yield a series solution for $P_{\bar{0},\bar{N}}(m, t \mid m_0)$ if required.] Substituting for $\tilde{P}$ from Eq. (2.9) and carrying out the summation in (3.1), we obtain

$$\tilde{P}_{\bar{0},\bar{N}}(m, u \mid m_0) = \frac{2(1-\tilde{\psi})\exp \alpha(m - m_0)\sinh(m_< \xi)\sinh(N - m_>)\xi}{u \tanh \xi \sinh N\xi} \quad (3.2)$$

From the structure of $\tilde{P}_{\bar{0},\bar{N}}$ in (3.2), it is obvious that the boundary conditions at 0 and N [Eq. (2.1a)] are satisfied. The solution in (3.2) is often sufficient in many applications, and it is not necessary to find $P_{\bar{0},\bar{N}}(m, t \mid m_0)$ explicitly. One such application is discussed in Section 4.

3.2. Random Walk Between an Absorber and Reflector

Consider now a biased CTRW on the set $\{1, 2,..., (N-1)\}$ with a reflecting boundary at 0 and an absorbing one at N. For this set of boundary conditions, the appropriate use of both Eq. (2.2b) and Eq. (2.12) is necessary. The number of images of the interval is again infinite. However, the image of the walker at m_0 due to reflection at 0 (the reflecting end) is at

$(-m_0+1)$ rather than $-m_0$, whereas the image of the walker at m_0 due to reflection at N (the absorbing end) is at $(2N-m_0)$. Taking account of this difference and using Eqs. (2.2b) and (2.12) repeatedly, we find that $\tilde{P}_{0,\bar{N}}(m, u \mid m_0)$ can be expressed in the form

$$\begin{aligned}
&\tilde{P}_{0,\bar{N}}(m, u \mid m_0) \\
&\quad = \sum_{n=0}^{\infty} (-1)^n \exp(-2\alpha nN)\, K^n[\tilde{P}(m, u \mid m_0 - n(2N-1)) \\
&\qquad + K \exp(-2\alpha m_0)\, \tilde{P}(m, u \mid -2nN - m_0 + n + 1)] \\
&\qquad + \sum_{n=1}^{\infty} (-1)^n \exp(2\alpha nN)\, K^{n-1}\{\exp[-2\alpha(n + m_0 - 1)] \\
&\qquad \times \tilde{P}(m, u \mid 2nN - m_0 - (n-1)) + \exp(-2\alpha n)\, K\tilde{P}(m, u \mid 2nN + m_0 - n)\}
\end{aligned} \tag{3.3}$$

where K has been defined in Eq. (2.13). Once again the summations in Eq. (3.3) can be carried out explicitly after using Eq. (2.9) for $\tilde{P}$. The final result for $\tilde{P}_{0,\bar{N}}$ is

$$\begin{aligned}
\tilde{P}_{0,\bar{N}}(m, u \mid m_0) &= 2(\cosh\xi - \cosh\alpha)[e^{\alpha(m-m_0)} \sinh(N - m_>)\xi] \\
&\quad \times \frac{e^{\alpha} \sinh m_< \xi - \sinh(m_< - 1)\xi}{u \sinh\xi[e^{\alpha} \sinh N\xi - \sinh(N-1)\xi]}
\end{aligned} \tag{3.4}$$

It is easy to verify that the required boundary conditions at 0 and N [Eqs. (2.1c) and (2.1a), respectively] are satisfied by Eq. (3.4). As a further check, letting $N \to \infty$ in Eq. (3.4) we recover the solution given earlier in Eq. (2.11) for a random walk on a semi-infinite chain with a reflector at 0. We have thus obtained expressions for the Laplace transforms of the probability distributions for biased CTRW's on finite chains with all three possible combinations of boundary conditions. The similarity of structure exhibited by these solutions is evident on comparing Eqs. (2.10), (3.2), and (3.4).

3.3. Distribution of First Passage Time for a Biased CTRW on a Finite Chain

The results we have obtained in the foregoing enable us to derive quite easily an expression for the distribution of the first passage time for a biased CTRW on a bounded set of points.

Consider a biased CTRW on the set $\{1, 2,...\}$ with a *reflecting* boundary at 0, so that the random walk is bounded from below, without any "leakage." It is required to find the probability $Q(m, t \mid m_0)\, dt$ that the random walker, starting at the point m_0 at time 0, reaches the point m ($>m_0$) for the first time in the interval $(t, t+dt)$. The characteristic function corresponding to the distribution of the time of first passage is the transform $\tilde{Q}(m, u \mid m_0)$ evaluated at $u = i\omega$. In an earlier paper[13] we have calculated this quantity for a biased Markovian random walk with the help of a renewal principle[14,15] that is specific to a Markov process. For general (non-Markovian) CTRW's, other methods[3,4] must be used to obtain $\tilde{Q}$. The most direct way is to observe that if the final point m is regarded as an absorbing boundary, $Q(m, t \mid m_0)$ may be found from the rate of change of the probability of the survival of the walker without absorption according to

$$Q(m, t \mid m_0) = -\frac{d}{dt} \sum_{m'=1}^{m-1} P_{0,\bar{m}}(m', t \mid m_0) \qquad (1 \leqslant m_0 < m) \tag{3.5}$$

In the preceding section [see Eq. (3.4)], we have computed $\tilde{P}_{0,\bar{m}}(m', u \mid m_0)$. Using this result in the transform of Eq. (3.5), we find

$$\begin{aligned}\tilde{Q}(m, u \mid m_0) &= 1 - u \sum_{m'=1}^{m-1} \tilde{P}_{0,\bar{m}}(m', u \mid m_0)\\ &= \frac{e^{(m-m_0)\alpha}[e^{\alpha} \sinh m_0 \xi - \sinh(m_0 - 1)\xi]}{[e^{\alpha} \sinh m\xi - \sinh(m-1)\xi]} \qquad (m > m_0)\end{aligned} \tag{3.6}$$

This is the characteristic function sought. The moments of the time of first passage from m_0 to m are obtained easily from (3.6). In particular, the mean first passage time is given by

$$\begin{aligned}\langle t_{m_0 \to m} \rangle &= -(\partial \tilde{Q}/\partial u)_{u=0}\\ &= \frac{\tau}{(p-q)} \left\{ (m - m_0) + \frac{p}{p-q} [(q/p)^m - (q/p)^{m_0}] \right\}\end{aligned} \tag{3.7}$$

in the case of all CTRW's for which the interval density $\psi(t)$ has a finite first moment

$$\tau = \int_0^{\infty} t\psi(t)\, dt = -[d\tilde{\psi}(u)/du]_{u=0} \tag{3.8}$$

(τ is the mean residence time at a site.)

Equations (3.6) and (3.7) are generalizations of the results derived in Ref. 13 for Markovian walks.

4. ESCAPE TIME DISTRIBUTIONS FOR A BIASED CTRW

The distribution of the time of escape of the random walker from a given region and the corresponding mean exit time find application in a variety of physical problems.[3,4,16-18] With the help of the solution obtained for $P_{\bar{0},\bar{N}}$, it is possible to derive expressions for escape time distributions of various kinds for an arbitrary, biased CTRW on the set $\{1, 2,..., (N-1)\}$. Let $Q_e(t; m_0)\,dt$ be the probability of the escape of the walker from either end (0 or N) in the time interval $(t, t+dt)$, for a walk starting from m_0 $(1 \leqslant m_0 \leqslant N-1)$ at $t=0$. As before, analytic continuation of the transform $\tilde{Q}_e(u; m_0)$ to $u = i\omega$ yields the characteristic function of the escape time distribution. Once again, the escape rate $Q_e(t; m_0)$ is just the survival rate with a change of sign, i.e.,

$$Q_e(t; m_0) = -\frac{d}{dt} \sum_{m=1}^{N-1} P_{\bar{0},\bar{N}}(m, t \mid m_0) \tag{4.1}$$

or

$$\tilde{Q}_e(u; m_0) = 1 - \sum_{m=1}^{N-1} u\tilde{P}_{\bar{0},\bar{N}}(m, u \mid m_0) \tag{4.2}$$

Using Eq. (3.2) for $\tilde{P}_{\bar{0},\bar{N}}$, we get after simplification

$$\tilde{Q}_e(u; m_0) = \frac{\sinh(N-m_0)\xi + e^{N\alpha} \sinh m_0 \xi}{e^{m_0\alpha} \sinh N\xi} \tag{4.3}$$

While this expression has been derived for $1 \leqslant m_0 \leqslant N-1$, it is valid also for $m_0 = 0$ or N: for, setting $m_0 = 0$ or N in it yields $\tilde{Q}_e(u; 0) = \tilde{Q}_e(u; N) = 1$, which implies that $Q_e(t; 0) = Q_e(t; N) = \delta(t)$, as expected.

If the origin of the random walk is unspecified, and is thus any one of the sites with equal probability, the relevant escape time distribution may be defined naturally as

$$Q_e(t) = \frac{1}{N+1} \sum_{m_0=0}^{N} Q_e(t; m_0) \tag{4.4}$$

Our result for $\tilde{Q}_e(u; m_0)$ then yields the very symmetrical expression

$$\tilde{Q}_e(u) = \frac{1}{N+1}\left[1 + \frac{\sinh \xi(\cosh N\xi - \cosh N\alpha)}{\sinh N\xi(\cosh \xi - \cosh \alpha)}\right] \tag{4.5}$$

The corresponding mean exit (or escape) time from the region $(0, N)$, starting with equal probability from any initial point, is given by

$$\langle t_e \rangle = \int_0^\infty tQ_e(t)\,dt = -[d\tilde{Q}_e(u)/du]_{u=0} \tag{4.6}$$

For all CTRW's for which τ (the mean residence time at a site) is finite, Eqs. (4.5) and (4.6) yield

$$\langle t_e \rangle = \frac{N\tau}{2(N+1)(p-q)} \left[\frac{N(p^N+q^N)}{(p^N-q^N)} - \frac{1}{(p-q)} \right] \tag{4.7}$$

In the absence of bias, the results for $\tilde{Q}_e$ and $\langle t_e \rangle$ reduce further to the following simple forms:

$$\tilde{Q}_e(u) = \frac{1}{N+1} \left[1 + \frac{\tanh(N\xi_0/2)}{\tanh(\xi_0/2)} \right] \tag{4.8}$$

where $\xi_0 = \operatorname{arcsech} \tilde{\psi}(u)$, and

$$\langle t_e \rangle = \tfrac{1}{6}N(N-1)\tau \tag{4.9}$$

A case of special interest is that of escape from either end starting from an origin exactly midway between the end points. For convenience, consider a biased CTRW on the set $\{-N, ..., 0, ..., +N\}$, starting from the point 0. The transform of the escape time distribution (in an obvious notation) is then found to be simply

$$\tilde{Q}_e(\pm N, u \mid 0) = (\cosh N\alpha)/(\cosh N\xi) \tag{4.10}$$

The corresponding mean time of escape from the region $(-N, N)$ starting from the origin (the mean "exit" time) is[4] found to be

$$\langle t_e(\pm N) \rangle = \frac{N\tau}{(p-q)} \left(\frac{p^N - q^N}{p^N + q^N} \right) \tag{4.11}$$

for CTRW's for which τ is finite. Once again, in the limit of zero bias, Eqs. (4.10) and (4.11) reduce, respectively, to

$$\tilde{Q}_e(\pm N, u \mid 0) = \operatorname{sech} N\xi_0 \tag{4.12}$$

and

$$\langle t_e(\pm N) \rangle = N^2\tau \tag{4.13}$$

These results show that the mean escape time from a bounded region is finite only for those walks for which the first moment τ of the interval density $\psi(t)$ is finite. When the latter has a long tail, its moments may diverge.[14] It turns out to be necessary to invoke such distributions to explain anomalous charge transport in amorphous solids.[19-22] A physically interesting, explicit realization of this type of interval density corresponds to a temporally fractal (self-similar) clustering of epoch times at which jumps occur: $\psi(t)$ may then be represented[23] as an infinite superposition of exponentials in which the jump rate $\lambda\beta^k$ occurs with a probability proportional to γ^k, where $0<\beta<\gamma<1$ and λ^{-1} is a positive constant with the dimensions of time. It can be shown that the Laplace transform of such a density has a small-u behavior given by

$$\tilde{\psi}(u) \underset{u \to 0}{=} 1 + u^H K(u) + O(u) \tag{4.14}$$

where $K(u)$ is a logarithmic correction to the power law behavior. The leading power H is the fractal dimension characterizing the CTRW, and is given by

$$H = \ln \gamma / \ln \beta \tag{4.15}$$

so that $0 < H < 1$. Using the asymptotic form (4.14) in Eq. (4.5), the small-u behavior of $\tilde{Q}_e(u)$ is also found to be

$$\tilde{Q}_e(u) \underset{u \to 0}{=} 1 + (\text{const})\, u^H K(u) + O(u) \tag{4.16}$$

It is then evident from (4.6) that $\langle t_e \rangle$ diverges for such CTRW's, even if they are biased walks. Writing $\langle t_e \rangle = \lim_{T \to \infty} \langle t_e \rangle_T$ where

$$\langle t_e \rangle_T = \int_0^T t Q_e(t)\, dt \tag{4.17}$$

we find in fact that the divergence has the power law behavior T^{1-H} as the time of observation, T, goes to infinity. In this sense, therefore, such a random walk does not correspond to a true long-range diffusive process.

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