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Random Walks with Nonnearest-Neighbor Transitions. II. Analytic One-Dimensional Theory for Exponentially Distributed Steps in Systems with Boundaries

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Exact analytic results for symmetric, nonnearest-neighbor random walks in one-dimensional finite and semiinfinite lattices are presented. Random walks with exponentially distributed step lengths are considered such that variation of a single parameter permits one to cover the whole range of step lengths from nearest-neighbor transitions to steps of aribtrary length. The generating functions for such lattices are derived and used to calculate a number of moment properties (mean first passage times, dispersion in the mean recurrence time). Since explicit expressions for the generating functions for these walks are obtained, additional moment properties can readily be calculated. The results found here for a finite system are compared to results found previously for a system with periodic boundary conditions. Two different semiinfinite systems are also considered.

KEY WORDS: Random walks; finite systems; nonnearest-neighbor transitions; exponentially distributed steps; mean first passage time.

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1. INTRODUCTION

In the first paper of this series[1] (hereafter referred to as I) one-dimensional, nonnearest-neighbor random walks on infinite systems and on systems with periodic boundary conditions were considered. In many physical problems that may be describable by nonnearest-neighbor random walks the system has natural boundaries whose effect on the random walk cannot be ignored. Examples of such systems may be random walks in energy space,[2] exciton diffusion on finite polymers, and electrical conductivity in amorphous semiconductors in the presence of trapping lines or planes.[3]

Exact analytic results for random walks with exponentially distributed step lengths in one-dimensional finite and semiinfinite systems are considered here. Only symmetric random walks are treated, but similar considerations can probably be used to analyze asymmetric walks. Using the modern techniques in this field developed by Montroll and his co-workers,[4-8] the generating functions for several systems are found explicitly and used to evaluate mean first passage times and, in one case, the dispersion in the mean recurrence time, as examples of their applications.

The random walks considered here are treated in terms of a discrete time variable (step number). The passage to continuous-time random walks is straightforward given a distribution of stepping times.[9,10]

Some of the results found in this paper have been given elsewhere for nearest-neighbor random walks.[11]

The following notation will be used:

$p(l, l')$ is the probability that the random walker steps from site l' to site l in one step.

$P_n(l, l')$ is the probability that the random walker starting his walk at site l' is at site l after n steps. These probabilities satisfy the normalization conditions

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

and

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

The generating function $G_{ll'}(z)$ is defined by[4]

$$G_{ll'}(z) \equiv \sum_{n=0}^{\infty} z^n P_n(l, l') \tag{3}$$

The probability $P_n(l, l')$ and the generating function $G_{ll'}(z)$ satisfy the equations

$$P_n(l, l') = \sum_{l''} p(l, l'')P_{n-1}(l'', l') \tag{4a}$$

$$P_0(l, l') = \delta_{ll'} \tag{4b}$$

and

$$G_{ll'}(z) - z \sum_{l''} p(l, l'')G_{l''l'}(z) = \delta_{ll'} \tag{5}$$

where $\delta_{ll'}$ is the Kronecker delta. In addition to Eqs. (4) and (5), $P_n(l, l')$ and $G_{ll'}(z)$ satisfy boundary conditions to be specified later.

In *I* we used the stepping probabilities

$$\begin{aligned} p(l, l') &= \tfrac{1}{2}(e^{a} - 1)e^{-|l-l'|a}, \qquad && |l - l'| > 0 \\ &= 0, && l = l' \end{aligned} \tag{6}$$

to describe a symmetric random walk with exponentially distributed steps on a perfect, infinite, one-dimensional lattice. In this paper Eq. (6) will be used to construct $p(l, l')$ for lattices with boundaries.

In Section 2 generating functions for finite and semiinfinite lattices with nonabsorbing boundaries are derived. In Section 3 generating functions for systems with completely absorbing or trapping boundaries are given. In Section 4 the generating functions are used to obtain several moment properties.

2. GENERATING FUNCTIONS FOR LATTICES WITH FREE END BOUNDARY CONDITIONS

2.1. Finite Lattices

Most random walk calculations in finite systems have been carried out using periodic boundary conditions (PBC)[1,4–8] (Fig. 1a). Since such a ring

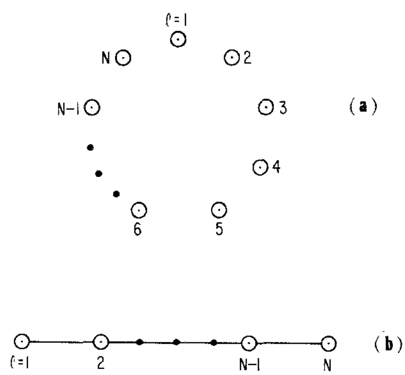

Fig. 1. Finite one-dimensional lattices. (a) System with periodic boundary conditions (no boundaries); (b) system with boundaries.

has no boundary, it is the simplest finite lattice one can consider. In I we treated symmetric and asymmetric walks on a ring with exponentially distributed stepping probabilities, which in the symmetric case are given by

$$
\begin{aligned}
p^{\mathrm{PBC}}(l, l') &= \frac{e^{a} - 1}{2(1 - e^{-Na})} [e^{-|l-l'|a} + e^{-(N-|l-l'|)a}], \qquad l \neq l' \\
&= \frac{(e^{a} - 1)e^{-Na}}{1 - e^{-Na}}, \qquad l = l'
\end{aligned}
\tag{7}
$$

The effect of boundaries can be studied by considering a symmetric random walk on the lattice shown in Fig. 1(b). Corresponding to various physical situations, there are many boundary conditions one can specify for such a system. To clarify the choice made below, it is useful to first consider a symmetric *nearest-neighbor* random walk. On an infinite lattice in the absence of boundaries the stepping probabilities are [cf. Eq. (6) as $a \to \infty$]

$$
\begin{aligned}
p(l, l') &= \tfrac{1}{2} \qquad \text{for} \quad |l - l'| = 1 \\
&= 0 \qquad \text{otherwise}
\end{aligned}
\tag{8}
$$

If a nearest-neighbor random walk takes place in the system of Fig. 1(b), the boundaries do not affect the stepping probabilities unless the walker is at lattice sites 1 or N. That is, for $1 \leqslant l \leqslant N$ and $2 \leqslant l' \leqslant N - 1$, $p^{\mathrm{BB}}(l, l')$ (the superscript indicates the *two* boundaries) is given by Eq. (8). At the boundary sites

$$
p^{\mathrm{BB}}(1, 1) = p^{\mathrm{BB}}(N, N) = K \tag{9a}
$$

and

$$
p^{\mathrm{BB}}(2, 1) = p^{\mathrm{BB}}(N - 1, N) = 1 - K \tag{9b}
$$

with $0 \leqslant K \leqslant 1$, where the choice of K is dictated by the physics of the problem. When $K = 0$ one is dealing with *completely reflecting barriers*. When $K = 1$ the boundary sites are *completely absorbing barriers*, i.e., ones the walker cannot leave. When $0 < K < 1$ it is a matter of semantics whether one calls the boundaries *partially reflecting* or *partially absorbing*. Boundaries defined by $K = \frac{1}{2}$ have been referred to as *free end boundaries*.[11] The choice $K = \frac{1}{2}$ is the only one that preserves the basic symmetry of the walk, i.e., it is the only choice for which $p^{\mathrm{BB}}(l, l') = p^{\mathrm{BB}}(l', l)$ for all l, l' including the boundary sites 1 and N. This symmetry implies that the equilibrium distribution of the system is uniform since Eqs. (1), (2), and (4) then yield $\lim_{n \to \infty} P_n^{\mathrm{BB}}(l, l') = 1/N$ for all l and l'.

The free end boundaries for the *nearest-neighbor* random walk can also be constructed as follows.[11] Consider an infinite lattice without boundaries and the stepping probabilities of Eq. (8). The additional requirement that there be no net flux of probability between sites 0 and 1, and between sites N and $N+1$, can be expressed by the conditions

$$P_n(0, l') = P_n(1, l') \tag{10a}$$

$$P_n(N+1, l') = P_n(N, l') \tag{10b}$$

for all n. For $1 \leqslant l \leqslant N$ and $1 \leqslant l' \leqslant N$, $P_n(l, l')$ in this problem is identical with $P_n^{\rm BB}(l, l')$ obtained in the presence of boundaries with $K = \frac{1}{2}$ in Eqs. (9a) and (9b) and can therefore be used to describe a random walk on a finite lattice. The sites $l \leqslant 0$ and $l \geqslant N+1$ and the probabilities of being at these sites are merely fictitious quantities that enable one to express the boundary conditions in terms of $P_n(l, l')$ instead of $p(l, l')$. This method is equivalent to the method of images in electrostatics.

In a random walk where *steps of any size* can occur there are a large number of ways of defining $p^{\rm BB}(l, l')$ so that the walker remains in the range $1 \leqslant l \leqslant N$. In this case $p^{\rm BB}(l, l')$ will in general differ from the infinite lattice $p(l, l')$ for all l, l' rather than just at the boundary sites. Here, only the generalization of the free end boundary conditions will be considered. Another partially reflecting (or partially absorbing) boundary is treated later for semi-infinite lattices.

To construct $p^{\rm BB}(l, l')$ with free end boundary conditions for a random walk with exponentially distributed steps, consider a fictitious infinite lattice with stepping probabilities given by Eq. (6) and the additional conditions

$$P_n(-l+1, l') = P_n(l, l') \tag{11a}$$

$$P_n(N+l, l') = P_n(N+1-l, l') \tag{11b}$$

for all l, l', and n. Equations (11a) and (11b) are the generalization of the corresponding nearest-neighbor equations (10a) and (10b) to a long-range random walk, and are sufficient conditions for there to be no flux of probability across the boundaries. As shown in Appendix A, Eq. (4a) on the infinite lattice combined with Eqs. (11a) and (11b) for $1 \leqslant l' \leqslant N$ and $1 \leqslant l \leqslant N$ then yields a single equation for $P_n^{\rm BB}(l, l')$ which incorporates the zero flux conditions:

$$P_n^{\rm BB}(l, l') = \sum_{l''=1}^{N} p^{\rm BB}(l, l'') P_{n-1}^{\rm BB}(l'', l') \tag{12}$$

with the initial condition still given by Eq. (4b), and

$$\begin{aligned} p^{\rm BB}(l, l') &= \frac{e^a - 1}{2\sinh Na} \\ &\quad \times \{\cosh[(N - l - l' + 1)a] + \cosh[(N - |l - l'|)a]\}, \quad l \neq l' \\ &= \frac{e^a - 1}{2\sinh Na}\{e^{-Na} + \cosh[(N - 2l + 1)a]\}, \qquad l = l' \end{aligned} \tag{13}$$

Equation (13) then gives stepping probabilities for a nonnearest-neighbor random walk in a finite system with free end boundaries. The probabilities are symmetric in l and l' and hence the equilibrium distribution is uniform. Equation (13) reduces to the corresponding nearest-neighbor case discussed earlier (with $K = \frac{1}{2}$) as $a \to \infty$.

The effect of the boundaries on the stepping probabilities is best seen by comparing Eq. (13) with the corresponding probabilities for a system with periodic boundary conditions, given in Eq. (7). While the latter probabilities depend only on the length $|l - l'|$ of the step, in the presence of boundaries $p^{BB}(l, l')$ depends on both l and l', i.e., the probabilities depend on where the walker is and where he is going. The effect of the boundaries is strongest near the boundaries. As a increases, the difference between $p^{BBC}(l, l')$ and $p^{BB}(l, l')$ shifts more and more toward the boundary sites. As $a \to 0$, both stepping probabilities tend to $1/N$ for all l and l'. Other properties of the two systems will be compared in Section 4.

The generating function for the system with free end boundaries satisfies

$$G_{ll'}^{BB}(z) - z \sum_{l''=1}^{N} p^{BB}(l, l'') G_{l''l'}^{BB}(z) = \delta_{ll'} \tag{14}$$

In terms of the eigenfunctions $f_k(l)$ and the eigenvalues $\lambda(k)$ of the stepping probability matrix $\mathbf{p}^{BB}$ of Eq. (13)

$$G_{ll'}^{BB}(z) = \sum_{k=0}^{N-1} \frac{f_k(l) f_k(l')}{1 - z\lambda(k)} \tag{15}$$

The set of eigenfunctions $f_k(l)$ is just that subset of the eigenfunctions for the infinite lattice that satisfies the boundary conditions (11a) and (11b):

$$\begin{aligned} f_k(l) &= (2/N)^{1/2} \cos[(2l - 1)\pi k/2N] \qquad \text{for} \quad k = 1, 2, \ldots, N - 1 \\ &= (1/N)^{1/2} \qquad\qquad\qquad\qquad\quad\; \text{for} \quad k = 0 \end{aligned} \tag{16}$$

The corresponding eigenvalues are

$$\lambda(k) = \frac{(\exp a) - 1}{2} \left[\frac{1}{\exp(a + i\pi k/N) - 1} + \frac{1}{\exp(a - i\pi k/N) - 1} \right] \tag{17}$$

The sum in Eq. (15) is carried out in Appendix B. The result is

$$\begin{aligned} G_{ll'}^{BB}(z) = \frac{2(e^a \cos\alpha - 1)}{e^a(e^{2a} - 1) \sin\alpha \sin N\alpha} \Big\{ & e^a (\sin\alpha \sin N\alpha) \delta_{ll'} \\ & - (e^{2a} + 1 - 2e^a \cos\alpha) \\ & \times \cos\frac{(2N - l - l' + 1 - |l - l'|)\alpha}{2} \\ & \times \cos\frac{(l + l' - 1 - |l - l'|)\alpha}{2} \Big\} \end{aligned} \tag{18}$$

where

$$\cos \alpha \equiv \frac{1 + e^{2a} + z(e^a - 1)}{e^a[2 + z(e^a - 1)]} \tag{19}$$

Equation (18) reduces to the nearest-neighbor result of Ref. 11 in the limit $a \to \infty$.

2.2. Semiinfinite Lattices

It is of interest for many physical applications to consider nonnearest-neighbor walks on semiinfinite lattices. For some applications, e.g., for random walks in energy space, it may be necessary to deal with asymmetric walks, but we have not found analytic solutions for the generating function equation in such systems.

The generating function $G^{\mathrm{B}}_{ll'}(z)$ for a semiinfinite system with a free end boundary condition at site zero satisfies Eq. (14) with $N \to \infty$ and

$$\begin{aligned} p^{\mathrm{B}}(l, l') &= \lim_{N\to\infty} p^{\mathrm{BB}}(l, l') \\ &= \tfrac{1}{2}(e^a - 1)[e^{-(l+l'-1)a} + e^{-|l-l'|a}], \qquad l \neq l' \\ &= \tfrac{1}{2}(e^a - 1)e^{-(2l-1)a}, \qquad l = l' \end{aligned} \tag{20}$$

The solution is most conveniently obtained by considering Eq. (15) in the limit $N \to \infty$,

$$G^{\mathrm{B}}_{ll'}(z) = \frac{1}{\pi}\int_0^{2\pi} du \frac{\cos[(2l-1)u/2]\cos[(2l'-1)u/2]}{1 - \dfrac{z(e^a - 1)}{2}\left(\dfrac{1}{e^{a+iu} - 1} + \dfrac{1}{e^{a-iu} - 1}\right)} \tag{21}$$

Straightforward contour integration gives

$$\begin{aligned} G^{\mathrm{B}}_{ll'}(z) = {}& \frac{2(x - e^a)(xe^a - 1)}{e^a[2 + z(e^a - 1)](x^2 - 1)}(x^{l+l'-1} + x^{|l-l'|}) \\ &+ \frac{2\delta_{ll'}}{2 + z(e^a - 1)} \end{aligned} \tag{22}$$

where

$$x = \frac{e^{2a} + 1 + z(e^a - 1) - (e^a - 1)\{(1 - z)(e^a + 1)[e^a + 1 + z(e^a - 1)]\}^{1/2}}{e^a[2 + z(e^a - 1)]} \tag{23}$$

A semiinfinite lattice with a different boundary is treated in Appendix C.

3. GENERATING FUNCTIONS FOR LATTICES WITH COMPLETELY ABSORBING BOUNDARIES

Two types of completely absorbing boundaries will be considered here. One type of boundary absorbs the walker only if he steps *on* the boundary, i.e., on a particular lattice site. This occurs, for instance, in the finite lattice of Section 2.1 if site $l = 1$ or site $l = N$ or both are traps (see Fig. 2a). It also occurs in the semiinfinite lattices of Section 2.2 and Appendix C if site $l = 1$ is a trap (Fig. 2b). The second case is one in which a walker is trapped if he steps *on* or *crosses* the absorbing boundary. This situation corresponds to a semiinfinite lattice with traps at all sites $l \geqslant N + 1$ (Fig. 2c). A system with two absorbing boundaries of the second type was treated in I and therefore need not be discussed here. It should be noted that for a nearest-neighbor random walk the two types of boundaries are the same since then a walker cannot cross over a trapping lattice site.

3.1. Finite Lattices

If in the finite system of Section 2.1 lattice site $l = 1$ is a trap and $l = N$ is a free end boundary, then the stepping probability matrix $\mathbf{p}^{TB}$ (the super-

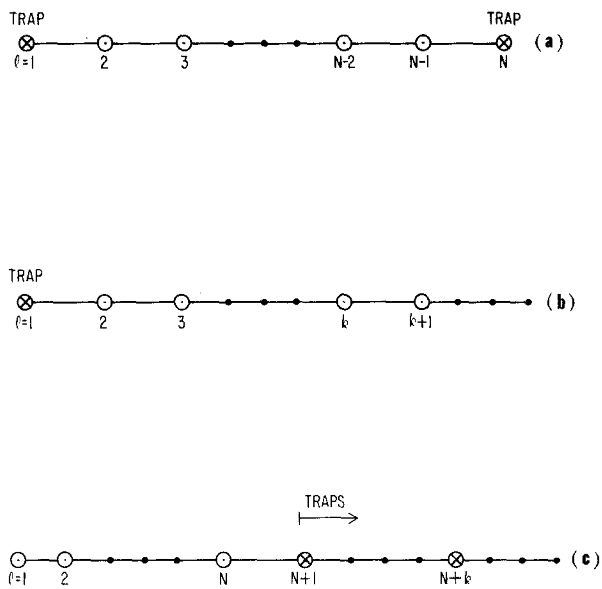

Fig. 2. One-dimensional lattices with absorbing boundaries. (a) Finite system with two trapping boundaries; (b) semiinfinite system with a trapping boundary and an infinite number of nontrapping sites; (c) semiinfinite system with an absorbing boundary and a finite number of nontrapping sites.

script T denotes the trap at the boundary) can be written in terms of $\mathbf{p}^{BB}$ of Eq. (13) as

$$p^{TB}(l, l') = P^{BB}(l, l')(1 - \delta_{l'1}) + \delta_{ll'}\delta_{l'1} \tag{24}$$

Equation (24) expresses the fact that the walker cannot leave site $l = 1$ once he steps on it. The generating function for this system satisfies the equation

$$G_{ll'}^{TB}(z) - z \sum_{l''=1}^{N} p^{BB}(l, l'')G_{l''l'}^{TB}(z) = \delta_{ll'} - z \sum_{l''=1}^{N} \Delta p^{TB}(l, l'')G_{l''l'}^{TB}(z) \tag{25}$$

where, from Eq. (24),

$$\Delta p^{TB}(l, l') = [p^{BB}(l, l') - \delta_{ll'}]\delta_{l'1} \tag{26}$$

Comparison of Eqs. (25) and (14) shows that $G_{ll'}^{BB}(z)$ can be used as a Green function for the solution of Eq. (25):

$$\begin{aligned} G_{ll'}^{TB}(z) &= G_{ll'}^{BB}(z) - z \sum_{j=1}^{N} \sum_{q=1}^{N} G_{lj}^{BB}(z)\, \Delta p^{TB}(j, q)G_{ql'}^{TB}(z) \\ &= G_{l'}^{BB}(z) - z \sum_{j=1}^{N} G_{lj}^{BB}(z)p^{BB}(j, 1)G_{1l'}^{TB}(z) \\ &\quad + zG_{l1}^{BB}(z)G_{1l'}^{TB}(z) \end{aligned} \tag{27}$$

Straightforward manipulations yield

$$G_{ll'}^{TB}(z) = G_{ll'}^{BB}(z) - \frac{G_{l1}^{BB}(z)G_{1l'}^{BB}(z)}{G_{11}^{BB}(z)} + \frac{G_{1l'}^{BB}(z)}{(1 - z)G_{11}^{BB}(z)}\,\delta_{l1} \tag{28}$$

If lattice sites $l = 1$ and $l = N$ are both traps, then there are two absorbing boundaries, and since the walker cannot leave sites 1 or N,

$$p^{TT}(l, l') = p^{BB}(l, l')(1 - \delta_{l'1})(1 - \delta_{l'N}) + \delta_{ll'}(\delta_{l'1} + \delta_{l'N}) \tag{29}$$

Using $G_{ll'}^{BB}(z)$ as a Green function yields

$$\begin{aligned} G_{ll'}^{TT} = G_{ll'}^{BB} &- \frac{G_{l1}^{BB}G_{11}^{BB}G_{1l'}^{BB} - G_{l1}^{BB}G_{1N}^{BB}G_{Nl'}^{BB} + G_{lN}^{BB}G_{NN}^{BB}G_{Nl'}^{BB} - G_{lN}^{BB}G_{N1}^{BB}G_{1l'}^{BB}}{G_{11}^{BB}G_{NN}^{BB} - G_{1N}^{BB}G_{N1}^{BB}} \\ &+ \frac{(G_{11}^{BB}G_{1l'}^{BB} - G_{1N}^{BB}G_{Nl'}^{BB})\delta_{l1} + (G_{NN}^{BB}G_{Nl'}^{BB} - G_{N1}^{BB}G_{1l'}^{BB})\delta_{lN}}{G_{11}^{BB}G_{NN}^{BB} - G_{1N}^{BB}G_{N1}^{BB}} \end{aligned} \tag{30}$$

Equations similar to (28) and (30) are given in Ref. 11 for nearest-neighbor random walks. In that case the lattice with traps at $l = 1$ and $l = N$ is equivalent to a lattice with periodic boundary conditions and a single trap.

3.2. Semiinfinite Lattices

The generating function for the semiinfinite lattice of Section 2.2 with traps at all sites $l \geqslant N + 1$ will be denoted by $G_{ll'}^{\mathrm{BA}}(z)$. Since the walker cannot leave any of the trapping sites, this generating function satisfies

$$\begin{aligned} G_{ll'}^{\mathrm{BA}}(z) &= z \sum_{l''=1}^{N} p^{\mathrm{B}}(l, l'') G_{l''l'}^{\mathrm{BA}}(z) + \delta_{ll'}, & 1 \leqslant l \leqslant N \\ &= z \sum_{l''=1}^{N} p^{\mathrm{B}}(l, l'') G_{l''l'}^{\mathrm{BA}}(z) + z G_{ll'}^{\mathrm{BA}}(z) + \delta_{ll'}, & l > N \end{aligned} \tag{31}$$

with $\mathbf{p}^{\mathrm{B}}$ given by Eq. (20). Equation (31) can be rewritten as

$$G_{ll'}^{\mathrm{BA}}(z) - z \sum_{l''=1}^{\infty} p^{\mathrm{B}}(l, l'') G_{l''l'}^{\mathrm{BA}}(z) = \delta_{ll'} - z \sum_{l''=N+1}^{\infty} \Delta p^{\mathrm{B}}(l, l'') G_{l''l'}^{\mathrm{BA}}(z) \tag{32}$$

where

$$\Delta p^{\mathrm{B}}(l, l'') = p^{\mathrm{B}}(l, l'') - \delta_{ll''}, \qquad l > N \tag{33}$$

The generating function in the absence of the traps at sites $l > N$, $G_{ll'}^{\mathrm{B}}(z)$, can now be used as Green function for the solution of Eq. (32):

$$G_{ll'}^{\mathrm{BA}}(z) = G_{ll'}^{\mathrm{B}}(z) - z \sum_{j=1}^{\infty} \sum_{q=N+1}^{\infty} G_{lj}^{\mathrm{B}}(z)\, \Delta p^{\mathrm{B}}(j, q) G_{ql'}^{\mathrm{BA}}(z) \tag{34}$$

The solution of Eq. (34) for $1 \leqslant l' \leqslant N$ is

$$G_{ll'}^{\mathrm{BA}}(z) = G_{ll'}^{\mathrm{B}}(z) - \frac{f_l^{\mathrm{B}}(z) v_{l'}^{\mathrm{B}}(z)}{1 + h^{\mathrm{B}}(z)} \tag{35}$$

where

$$\begin{aligned} f_l^{\mathrm{B}}(z) &= -(e^{2a} - 1) e^{-(2N-1)a/2} (1 - x) z^2 (x^{N+l} + x^{N-l+1}) \\ &\quad \times \{(1 - z)[2 + z(e^a - 1)](1 + x)(x - e^a)\}^{-1}, \qquad 1 \leqslant l \leqslant N \\ &= -z e^{a/2} \{x(1 + x)(e^a - 1)^2 e^{-la} \\ &\quad + [(1 - x e^a) x^{l+N} + (x - e^a) x^{l-N}](1 - x) e^{-Na}\} \\ &\quad \times [(e^a - 1)(1 - z) x (1 + x)]^{-1}, \qquad l > N \end{aligned} \tag{36}$$

$$\begin{aligned} v_{l'}^{\mathrm{B}}(z) &= [(x - e^a) e^{(2N-1)a/2} + (x e^a - 1) e^{-(2N+1)a/2}](x^{N+l'} + x^{N-l'+1}) \\ &\quad \times \{[2 + z(e^a - 1)](x^2 - 1)\}^{-1}, \qquad 1 \leqslant l' \leqslant N \end{aligned} \tag{37}$$

$$\begin{aligned} h^{\mathrm{B}}(z) &= z e^a (1 - x)\{[(x - e^a) - (1 - x e^a) e^{-2Na}] x^{2N} \\ &\quad + [(1 - x e^a) - (x - e^a) e^{-2Na}]\} \\ &\quad \times [2(1 - z)(e^a - 1)(1 + x)(x - e^a)]^{-1} \end{aligned} \tag{38}$$

4. MOMENT PROPERTIES

4.1. Finite Lattices

The generating functions found in the foregoing sections can be used to calculate various moment properties of the random walk. In this section the mean time (i.e., average number of steps) for a random walker on a finite lattice with free end boundaries to reach site l for the first time is evaluated. The problem of mean first passage time is completely equivalent to that of the mean time for absorption or trapping at site l. The dispersion in the recurrence time of the walker is also given. These results are compared to the corresponding ones for a finite system with periodic boundary conditions.

Let $D_n^{\mathrm{BB}}(l, l')$ be the probability that a walker starting at site l' reaches site l on the nth step for the first time in a finite system with free end boundaries. The generating function

$$E_{ll'}^{\mathrm{BB}}(z) \equiv \sum_{n=1}^{\infty} z^n D_n^{\mathrm{BB}}(l, l') \tag{39}$$

is related to $G_{ll'}^{\mathrm{BB}}$ by[4]

$$E_{ll'}^{\mathrm{BB}}(z) = [G_{ll'}^{\mathrm{BB}}(z) - \delta_{ll'}]/G_{ll}^{\mathrm{BB}}(z) \tag{40}$$

The mean first passage time for arrival at site l is

$$\bar{n}_{ll'}^{\mathrm{BB}} = (\partial/\partial z)E_{ll'}^{\mathrm{BB}}(z)|_{z=1} \tag{41}$$

Using Eqs. (18), (19), and (40) in Eq. (41) with $l \neq l'$ yields

$$\begin{aligned}\bar{n}_{ll'}^{\mathrm{BB}} &= \frac{(e^a - 1)^2}{e^a(e^a + 1)}(l - l')(l + l' - 1) + \frac{2N}{(e^a + 1)}, \qquad l > l' \\ &= \frac{(e^a - 1)^2}{e^a(e^a + 1)}(l' - l)(2N - l - l' + 1) + \frac{2N}{(e^a + 1)}, \qquad l < l'\end{aligned} \tag{42}$$

For $l = l'$ we obtain the mean recurrence time

$$\bar{n}_{ll}^{\mathrm{BB}} = -\frac{\partial}{\partial z}\frac{1}{G_{ll}^{\mathrm{BB}}(z)}\bigg|_{z=1} = N \tag{43}$$

in agreement with a general theorem on recurrence times in Markov chains[4] which is independent of step length. The effect of the boundaries can best be seen by comparing Eq. (42) with the corresponding result in a system with periodic boundary conditions (Fig. 1a), for which[1]

$$\bar{n}_{ll'}^{\mathrm{PBC}} = \frac{(e^a - 1)^2}{e^a(e^a + 1)}|l - l'|(N - |l - l'|) + \frac{2N}{(e^a + 1)}, \qquad l \neq l' \tag{44}$$

$$\bar{n}_{ll}^{\mathrm{PBC}} = N \tag{45}$$

From Eqs. (42) and (44) it follows that the effect of boundaries on mean first passage times is greatest for walks involving short steps with sites l and l' near the boundaries.

Averaging Eq. (42) over starting site l' with $l' \neq l$ yields

$$\begin{aligned}\langle n\rangle_l^{\mathrm{BB}} &\equiv \frac{1}{N-1}\sum_{\substack{l'=1\\ l'\neq l}}^{N} \bar{n}_{ll'}^{\mathrm{BB}} \\ &= \frac{N(e^a-1)^2}{6(N-1)e^a(e^a+1)}[4N^2-6N(2l-1)+3(2l-1)^2-1] \\ &\quad + \frac{2N}{e^a+1} \end{aligned} \tag{46}$$

The corresponding result with periodic boundary conditions is[1]

$$\langle n\rangle_l^{\mathrm{PBC}} = \frac{(e^a-1)^2}{e^a(e^a+1)}\frac{N(N+1)}{6} + \frac{2N}{e^a+1} \tag{47}$$

Hence

$$\begin{aligned}\frac{\langle n\rangle_l^{\mathrm{BB}} - \langle n\rangle_l^{\mathrm{PBC}}}{\langle n\rangle_l^{\mathrm{PBC}}} &= \frac{3(e^a-1)^2(2l-N-1)^2}{(N-1)[(N+1)(e^a-1)^2+12e^a]} \\ &\xrightarrow[a\gg\log N\gg 1]{} \frac{3(2l-N-1)^2}{N^2}\end{aligned} \tag{48}$$

The greatest difference between $\langle n\rangle_l^{\mathrm{BB}}$ and $\langle n\rangle_l^{\mathrm{PBC}}$ again occurs for walks with short steps when $l = 1$ or N. When $a \gg \log N \gg 1$, $\langle n\rangle_N^{\mathrm{BB}}/\langle n\rangle_{NN}^{\mathrm{PBC}} \simeq 4$.

The dispersion in the mean recurrence time of the random walker,

$$d_l^{\mathrm{BB}} \equiv \frac{[\overline{n_{ll}^2}^{\mathrm{BB}} - (\bar{n}_{ll}^{\mathrm{BB}})^2}{(\bar{n}_{ll}^{\mathrm{BB}})^2} \tag{49}$$

with

$$\overline{n_{ll}^2}^{\mathrm{BB}} = -\frac{\partial}{\partial z} z \frac{\partial}{\partial z}\frac{1}{G_{ll}^{\mathrm{BB}}(z)}\bigg|_{z=1} \tag{50}$$

is

$$\begin{aligned} d_l^{\mathrm{BB}} &= \frac{(e^a-1)^2}{3Ne^a(e^a+1)}[4N^2-6N(2l-1)+3(2l-1)^2] \\ &\quad - \frac{e^a-3}{e^a+1} + \frac{2e^{2a}-7e^a-1}{3Ne^a(e^a+1)}\end{aligned} \tag{51}$$

The corresponding result with periodic boundary conditions is[(1),3]

$$d_l^{\mathrm{PBC}} = \frac{N}{3}\frac{(e^a-1)^2}{e^a(e^a+1)} - \frac{e^a-3}{e^a+1} + \frac{2e^{2a}-7e^a-1}{3Ne^a(e^a+1)} \tag{52}$$

[3] Equation (52) corrects two misprints in Eq. (104) of Ref. 1. Also, in Eq. (103) of Ref. 1 there should be a factor $(-z)$ before the second derivative term.

Hence

$$\frac{d_l^{\mathrm{BB}} - d_l^{\mathrm{PBC}}}{d_l^{\mathrm{PBC}}} = \frac{3(e^a - 1)^2(2l - N - 1)^2}{N^2(e^a - 1)^2 - 3Ne^a(e^a - 3) + (2e^{2a} - 7e^a - 1)}$$
$$\xrightarrow[a \gg \log N \gg 1]{} \frac{3(2l - N - 1)^2}{N^2} \tag{53}$$

The greatest difference between d_l^{BB} and d_l^{PBC} thus again occurs for $l = 1$ and $l = N$. For $a \gg \log N \gg 1$, $d_N^{\mathrm{BB}}/d_N^{\mathrm{PBC}} \simeq 4$.

The finite lattice generating functions can be used to evaluate many other moment properties.[4]

4.2. Semiinfinite Lattices

Let $l' \leqslant N$ denote the starting site of the walker. The mean number of steps required for trapping at any site $l \geqslant N + 1$ is found, by reasoning identical to that used in I, to be

$$\begin{aligned}\bar{n}_{l'}^{\mathrm{B}} &= -\frac{\partial}{\partial z}\left[(1 - z)\sum_{l=1}^{N} G_{ll'}^{\mathrm{BA}}(z)\right]_{z=1} \\ &= (N - l')(N + l' - 1)\frac{(e^a - 1)^2}{e^a(e^a + 1)} + 2N\frac{e^a - 1}{e^a + 1} + \frac{2}{e^a + 1}\end{aligned} \tag{54}$$

The mean time to trapping averaged over starting site is

$$\begin{aligned}\langle n\rangle^{\mathrm{B}} &\equiv \frac{1}{N}\sum_{l'=1}^{N} \bar{n}_{l'}^{\mathrm{B}} \\ &= (2N - 1)(N - 1)\frac{(e^a - 1)^2}{3e^a(e^a + 1)} + 2N\frac{e^a - 1}{e^a + 1} + \frac{2}{e^a + 1}\end{aligned} \tag{55}$$

Results with a different partially reflecting boundary are given in Appendix C.

APPENDIX A. DERIVATION OF EQS. (12) AND (13)

To obtain Eqs. (12) and (13), Eq. (4a) for an infinite lattice is first rewritten in three parts,

$$\begin{aligned}\frac{2}{e^a - 1} P_n(l, l') = \sum_{l''=-\infty}^{0} e^{-(l-l'')a} P_{n-1}(l'', l') + \sum_{l''=1}^{N}{}' e^{-|l-l''|a} P_{n-1}(l'', l') \\ + \sum_{l''=N+1}^{\infty} e^{(l-l'')a} P_{n-1}(l'', l')\end{aligned} \tag{A.1}$$

where l, l' are restricted to lie in the interval $(1, N)$ and the prime on the second sum indicates that the term $l'' = l$ is omitted. Consider the first term on the right of Eq. (A.1):

$$\sum_{l''=-\infty}^{0} e^{-(l-l'')a} P_{n-1}(l'', l') = \sum_{l''=1}^{\infty} e^{-(l+l''-1)a} P_{n-1}(-l''+1, l')$$
$$= \sum_{l''=1}^{N} e^{-(l+l''-1)a} P_{n-1}(l'', l')$$
$$+ \sum_{l''=N+1}^{\infty} e^{-(l+l''-1)a} P_{n-1}(l'', l') \tag{A.2}$$

The first equality involves the change of variables $l'' \to -l + 1$; for the second equality use was made of the boundary condition of Eq. (11a). Equation (A.1) can now be rewritten as

$$\frac{2}{e^a - 1} P_n(l, l') = \sum_{l''=1}^{N} [e^{-|l-l''|a} + e^{-(l+l''-1)a} - \delta_{ll''}] P_{n-1}(l'', l')$$
$$+ X_{n-1}(l, l') \tag{A.3}$$

where

$$X_{n-1}(l, l') \equiv \sum_{l''=N+1}^{\infty} [e^{(l-l'')a} + e^{-(l+l''-1)a}] P_{n-1}(l'', l') \tag{A.4}$$

The change of variables $l'' \to l'' + N$ and use of the boundary condition (11b) give

$$X_{n-1}(l, l') = \sum_{l''=1}^{\infty} [e^{(l-l''-N)a} + e^{-(l+l''+N-1)a}] P_{n-1}(N + l'', l')$$
$$= \sum_{l''=1}^{\infty} [e^{(l-l''-N)a} + e^{-(l+l''+N-1)a}] P_{n-1}(N + 1 - l'', l') \tag{A.5}$$

Letting $l'' \to N + 1 - l''$ yields

$$X_{n-1}(l, l') = \sum_{l''=1}^{N} [e^{(l+l''-2N-1)a} + e^{-(l-l''+2N)a}] P_{n-1}(l'', l')$$
$$+ \sum_{l''=-\infty}^{0} [e^{(l+l''-2N-1)a} + e^{-(l-l''+2N)a}] P_{n-1}(l'', l') \tag{A.6}$$

The same steps as those used in Eq. (A.2) can be applied to the second sum in Eq. (A.7) to yield

$$X_{n-1}(l, l') = \sum_{l''=1}^{N} [e^{(l+l''-2N-1)a} + e^{-(l+l''+2N-1)a}$$
$$+ e^{-(l-l''+2N)a} + e^{(l-l''-2N)a}] P_{n-1}(l'', l')$$
$$+ e^{-2Na} X_{n-1}(l, l') \tag{A.7}$$

Solving this equation for $X_{n-1}(l, l')$ and substituting into Eq. (A.3) gives

$$P_n(l, l') = \tfrac{1}{2}(e^a - 1) \sum_{l''=1}^{N} [W_1(l, l'') + W_2(l, l'') - \delta_{ll''}]P_{n-1}(l'', l') \tag{A.8}$$

where

$$\begin{aligned} W_1(l, l'') &= \frac{1}{1 - e^{-2Na}} e^{-(l+l''-1)a} + \frac{e^{-2Na}}{1 - e^{-2Na}} e^{(l+l''-1)a} \\ &= \frac{\cosh[(N - l - l'' + 1)a]}{\sinh Na} \end{aligned} \tag{A.9}$$

and

$$\begin{aligned} W_2(l, l'') &= e^{-|l-l''|a} + \frac{e^{-2Na}}{1 - e^{-2Na}} e^{-(l-l'')a} + \frac{e^{-2Na}}{1 - e^{-2Na}} e^{(l-l'')a} \\ &= \frac{\cosh[(N - |l - l''|)a]}{\sinh Na} \end{aligned} \tag{A.10}$$

Equations (A.8)–(A.10) are equivalent to Eqs. (12) and (13).

APPENDIX B. DERIVATION OF EQ. (18)

The sum indicated in Eq. (15) can be evaluated by a method similar to one of Montroll's[7] and used in Ref. 11 for nearest-neighbor walks. The eigenvalues in Eq. (17) can be rewritten as

$$\lambda(k) = \frac{(e^a - 1)[e^a \cos(\pi k/N) - 1]}{e^{2a} + 1 - 2e^a \cos(\pi k/N)} \tag{B.1}$$

Equation (15) then becomes

$$\begin{aligned} G_{ll'}^{BB} &= \frac{-1}{N(1 - z)} + \frac{2(e^{2a} + 1)}{Ne^a[2 + z(e^a - 1)]} \\ &\quad \times \sum_{k=0}^{N-1} \frac{\cos[(2l - 1)\pi k/2N] \cos[(2l' - 1)\pi k/2N]}{\cos \alpha - \cos(\pi k/N)} \\ &\quad - \frac{4}{N[2 + z(e^a - 1)]} \\ &\quad \times \sum_{k=0}^{N-1} \frac{\cos(\pi k/N) \cos[(2l - 1)\pi k/2N] \cos[(2l' - 1)\pi k/2N]}{\cos \alpha - \cos(\pi k/N)} \end{aligned} \tag{B.2}$$

with $\cos \alpha$ defined in Eq. (19). The denominators occurring in Eq. (B.2) can be separated into partial fractions:

$$\begin{aligned} d &\equiv \frac{1}{\cos \alpha - \cos(\pi k/N)} \\ &= \frac{i}{\sin \alpha} \left\{ \frac{1}{1 - \exp[i(\alpha + \pi k/N)]} - \frac{1}{1 - \exp[-i(\alpha - \pi k/N)]} \right\} \end{aligned} \tag{B.3}$$

Expressing the cosines in the numerators of Eq. (B.2) in terms of exponentials and using Eq. (B.3), one obtains

$$G_{ll'}^{BB} = \frac{e^a \cos\alpha - 1}{2Ne^a(e^{2a} - 1)\sin\alpha}\left\{\frac{2(e^a - 1)^2 \sin\alpha}{1 - \cos\alpha}\right.$$

$$- (e^{2a} + 1)[S(l + l' - 1) + S(l - l')]$$

$$\left. + e^a[S(l + l') + S(l + l' - 2) + S(l - l' + 1) + S(l - l' - 1)]\right\} \tag{B.4}$$

where

$$S(m) \equiv S_1(m) + S_1(-m) \tag{B.5}$$

and

$$S_1(m) = i \sum_{k=0}^{N-1} e^{i\pi km/N}\left\{\frac{1}{\exp[i(\alpha + \pi k/N)] - 1} - \frac{1}{\exp[-i(\alpha - \pi k/N)] - 1}\right\} \tag{B.6}$$

The sum $S_1(m)$ is performed in Ref. 11 by expanding each denominator in Eq. (B.6) in an infinite geometric series, interchanging the order of summation, and performing both sums. The result for $S(m)$ is

$$S(m) = \frac{2 - 2\,\Delta m(1 - \cos\alpha)}{\sin\alpha} + \frac{2N\cos[(N - |m|)\alpha]}{\sin N\alpha} \tag{B.7}$$

where

$$\Delta m \equiv \begin{cases} 0, & m \text{ even} \\ 1, & m \text{ odd} \end{cases} \tag{B.8}$$

Substituting Eq. (B.7) into Eq. (B.4) yields Eq. (18).

APPENDIX C. SEMIINFINITE LATTICE WITH WALL BOUNDARY

Another partially reflecting boundary for a semiinfinite lattice that is easy to consider has the following characteristics. If sites l and l' are away from the boundary ($l, l' > 1$), then the walker steps as on an infinite lattice, i.e., with the probabilities given in Eq. (6). A step which on an infinite lattice would have taken the walker to a site $l \leqslant 1$ now takes him to site $l = 1$ in the presence of the boundary. Finally if the walker is at site $l = 1$, he has probability r of staying there, and exponentially distributed probabilities of returning to sites $l > 1$. Thus the boundary behaves like a "sticky" impenetrable wall, and shall be referred to as the wall boundary. The transition probability matrix $\mathbf{p}^{W}$ for this walk then has elements

$$p^{W}(l, l') = \tfrac{1}{2}(e^{a} - 1)e^{-|l-l'|a}, \qquad l' \geqslant 2, \quad l \geqslant 2, \quad l \neq l'$$

$$p^{W}(1, l') = \tfrac{1}{2}(e^{a} - 1) \sum_{i=1}^{-\infty} e^{-(l'-i)a} = \tfrac{1}{2}e^{2a}e^{-l'a}, \qquad l' \geqslant 2$$

$$p^{W}(l, l) = 0, \quad l \geqslant 2; \qquad p^{W}(1, 1) = r$$
$$p^{W}(l, 1) = (1 - r)(e^{a} - 1)e^{-(l-1)a}, \qquad l \geqslant 2 \tag{C.1}$$

with $0 \leqslant r \leqslant 1$. When $r = 1$, lattice site $l = 1$ becomes a trap. These stepping probabilities lead to a uniform equilibrium distribution only if $r = (e^{a} - 2)/2(e^{a} - 1)$, which in turn requires that $e^{a} \geqslant 2$.

The solution of the equation

$$G_{ll'}^{W}(z) - z \sum_{l''=1}^{\infty} p^{W}(l, l'')G_{l''l'}^{W}(z) = \delta_{ll'} \tag{C.2}$$

is

$$G_{11}^{W}(z) = \frac{e^{a} - x}{z(1 - r)(1 - xe^{a}) - (1 - zr)(x - e^{a})}$$

$$G_{l1}^{W}(z) = \frac{2z(e^{2a} - 1)(e^{a} - 1)(1 - r)}{e^{a}[2 + z(e^{a} - 1)][z(1 - r)(1 - xe^{a}) - (1 - zr)(x - e^{a})]}\, x^{l-1}$$

for $l \geqslant 2$,

$$G_{1l'}^{W}(z) = \frac{z(e^{2a} - 1)}{[2 + z(e^{a} - 1)][z(1 - r)(1 - xe^{a}) - (1 - zr)(x - e^{a})]}\, x^{l'-1}$$

for $l' \geqslant 2$, and

$$G_{ll'}^{W}(z) = Ax^{l+l'-3} + Bx^{|l-l'|} + \frac{2\delta_{ll'}}{[2 + z(e^{a} - 1)]} \tag{C.3}$$

for $l, l' \geqslant 2$; with

$$B = \frac{2(x - e^{a})(1 - xe^{a})}{e^{a}[2 + z(e^{a} - 1)](1 - x^{2})} \tag{C.4}$$

and

$$A = -\frac{2(x - e^{a})(1 - xe^{a})}{e^{a}[2 + z(e^{a} - 1)](1 - x^{2})} \times \frac{z(1 - r)(x - e^{a}) - (1 - zr)(1 - xe^{a})}{z(1 - r)(1 - xe^{c}) - (1 - zr)(x - e^{a})} \tag{C.5}$$

If lattice sites $l \geqslant N + 1$ in this semiinfinite system are traps, then

$$G_{ll'}^{\mathrm{WA}}(z) = G_{ll'}^{\mathrm{W}}(z) - \frac{f_l^{\mathrm{W}}(z) v_{l'}^{\mathrm{W}}(z)}{1 + h^{\mathrm{W}}(z)} \tag{C.6}$$

with

$$\begin{aligned}
f_l^{\mathrm{W}}(z) &= \frac{z(xe^a - 1)x^{N-1}e^{-Na}}{2[z(1-r)(1-xe^a) - (1-zr)(x-e^a)]}, \qquad l = 1 \\
&= \frac{z(e^a - 1)e^{-Na}(Ax^{N+l-2} + Bx^{N-l+1})}{2(e^a - x)}, \qquad 2 \leqslant l \leqslant N \\
&= \frac{z(a^a - 1)e^{-Na}}{2}\left[\frac{Ax^{l+N-2}}{e^a - x} + \frac{Bx^{l-N}}{xe^a - 1}\right] - \frac{z(e^a - 1)e^{-la}}{2(1-z)}, \\
&\qquad l > N
\end{aligned} \tag{C.7}$$

$$\begin{aligned}
v_{l'}^{\mathrm{W}}(z) &= \frac{2(1-r)(e^a - x)e^{Na}x^{N-1}}{z(1-r)(1-xe^a) - (1-zr)(x-e^a)}, \qquad l' = 1 \\
&= \frac{e^{(N+1)a}}{xe^a - 1}(Ax^{N+l'-2} + Bx^{N-l'+1}), \qquad 2 \leqslant l' \leqslant N
\end{aligned} \tag{C.8}$$

$$h^{\mathrm{W}}(z) = \frac{ze^a(e^a - 1)}{2(x - e^a)}\left(\frac{Ax^{2N-1}}{1 - xe^a} + \frac{Bx}{x - e^a}\right) \tag{C.9}$$

In this system an additional absorbing boundary is present at $l = 1$ when $r = 1$. The generating $G_{ll'}^{\mathrm{WA}}(z)$ greatly simplifies in this case.

For $r \neq 1$ the mean number of steps for trapping at any site $l \geqslant N + 1$ and its average over starting site are

$$\begin{aligned}
\bar{n}_{l'}^{\mathrm{W}} &= (N - l')(N + l' - 1)\frac{(e^a - 1)^2}{e^a(e^a + 1)} + 2(N - l')\frac{e^a - 1}{e^a(e^a + 1)} \\
&\quad + 2(l' - 1)\frac{e^a - 1}{e^a + 1} \\
&\quad + \frac{1}{1 - r}\frac{(N - l' + 1)(e^a - 1) + 2}{e^a + 1} + \frac{1 - 2r}{(1 - r)(e^a + 1)}(1 - \delta_{l',1})
\end{aligned} \tag{C.10}$$

$$\begin{aligned}
\langle n \rangle^{\mathrm{W}} &= (2N - 1)(N - 1)\frac{(e^a - 1)^2}{3e^a(e^a + 1)} + (N - 1)\frac{e^a - 1}{e^a} \\
&\quad + \frac{(N + 1)(e^a - 1)}{2(1 - r)(e^a + 1)} + \frac{3 - 2r}{(1 - r)(e^a + 1)} + \frac{2r - 1}{N(1 - r)(e^a + 1)}
\end{aligned} \tag{C.11}$$

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