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Random Walks on Lattices. IV. Continuous-Time Walks and Influence of Absorbing Boundaries

Elliott W. Montroll[1] and Harvey Scher[2]

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The general study of random walks on a lattice is developed further with emphasis on continuous-time walks with an asymmetric bias. Continuous time walks are characterized by random pauses between jumps, with a common pausing time distribution $\psi(t)$. An analytic solution in the form of an inverse Laplace transform for $\tilde{P}(l, t)$, the probability of a walker being at l at time t if it started at l_0 at $t = 0$, is obtained in the presence of completely absorbing boundaries. Numerical results for $\tilde{P}(l, t)$ are presented for characteristically different $\psi(t)$, including one which leads to a non-Gaussian behavior for $\tilde{P}(l, t)$ even for large t. Asymptotic results are obtained for the number of surviving walkers and the mean $\langle l \rangle$ showing the effect of the absorption at the boundary.

KEY WORDS: Random walks; transport theory; stochastic processes; boundary value problems; continuous-time walks.

1. INTRODUCTION

This paper is a continuation of the development of the theory of random walks on lattices, the earlier stages of which are given in Ref. 1–6. It is

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[1] Institute for Fundamental Studies, Department of Physics and Astronomy, University of Rochester, Rochester, New York.

[2] Xerox Rochester Research Center, Xerox Square, Rochester, New York.

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primarily concerned with random walks on lattices with an extensive number of traps, permanent and temporary. The investigation of this type of system was motivated by experiments on transient photoconductivity of amorphous semiconductors.[7,8] In such materials some localized states correspond to deep traps or hopping sites for electrons (holes) which, after being trapped for some time, finally escape from the trap only to be retrapped at another localized state or hop to another site. The time a carrier spends in a trapped state may be considerably longer than the time of flight from one site to the next. In the conductivity experiments the electric field which gives rise to the current creates a bias in the direction in which the carrier jumps after it escapes from the trap. Finally, those electrons (holes) which reach the edge of the sample are captured forever by positive (negative) charges. Hence the edge of the crystal acts as an absorbing barrier or a trap so deep that escape never occurs. The detailed application to the problems mentioned above will be developed elsewhere.

In this section we review very briefly the ideas in the previous papers of the series which are relevant for the problem at hand. Section 2 is a general discussion of the effect of temporary traps, and Section 3 contains an exposition of the rate of disappearance of walkers into the absorbing barrier and the dynamics of a pulse of walkers which have been injected into the sample and which undergo a biased walk.

The starting point of our general theory is that of walks on a network such that at regular time intevals (a) the walker must jump to a new point and (b) the transition probability for a jump from l' to l, $p(l, l')$, is the same anytime a walker is at l'. Then if $P_n(l)$ is the probability that a walker is at network point l after n steps,

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

with

$$\sum_{l} p(l, l') = 1 \tag{2}$$

The generating function for the walks is defined as

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

If the initial distribution function of location of walkers is $P_0(l)$, then by multiplying Eq. (1) by z^{n+1} and summing over n, one obtains[3]

$$P(l, z) - z \sum p(l, l')P(l', z) = P_0(l) \tag{4}$$

The $P(l, z)$ can be expressed in terms of the Green's function $G(l, z)$ which satisfies

$$G(l, z) - z \sum p(l, l')G(l', z) = \delta_{l,0} \tag{5}$$

for

$$P(l, z) = \sum_{l'} G(l - l', z)P_0(l') \tag{6}$$

Now suppose that steps do not occur at regular time intervals, but that there exists a probability density function $\psi(t)$ such that after a walker arrives at any network point the probability that he will make his next step between time t and $t + \delta t$ is $\psi(t)\,\delta t$. Let $\tilde{P}(l, t)$ be the probability of a walker being at l at time t. Then it can be shown[4] that the Laplace transform of $\tilde{P}(l, t)$,

$$\tilde{P}^*(l, u) = \int_0^\infty e^{-ut}\,\tilde{P}(l, t)\,dt \tag{7}$$

has the form

$$\tilde{P}^*(l, u) = Q^*(l, u)\,[1 - \psi^*(u)]/u \tag{8}$$

where $\psi^*(u)$ is the Laplace transform of $\psi(t)$,

$$\psi^*(u) = \int_0^\infty e^{-ut}\,\psi(t)\,dt \tag{9}$$

and $Q^*(l, u)$ is directly related to the generating function (3) with

$$Q^*(l, u) \equiv P[l, \psi^*(u)] \tag{10}$$

with z in (3) set equal to $\psi^*(u)$.

Once $\tilde{P}^*(l, u)$ is known its inverse Laplace transform can be found to yield $\tilde{P}(l, t)$ just as one can obtain $P_n(l)$ from the generating function (3) by finding the coefficient of z^n. These results are only valid when all network points have the same $\psi(t)$; i.e., when the distribution of pausing times is independent of the network point. The theory can be extended to situations in which there are several classes of network points, each class having its own $\psi(t)$. This will be discussed elsewhere.

A network in the form of a periodic lattice has a simple Green's function $G(l, z)$ and the theory has a relatively simple form. Let us suppose that all lattice points are equivalent, as is the case in a square lattice or a simple cubic lattice. In this case

$$p(l, l') \equiv p(l - l') \tag{11}$$

depends only on the vector distance $l - l'$. In a k-dimensional lattice with periodic boundary conditions and with N_1 lattice points in the first direction, N_2 in the second, etc.,

$$G(l, z) = (N_1^{-1}N_2^{-1}\cdots) \sum_{s_1=1}^{N_1} \sum_{s_2=1}^{N_2} \cdots \frac{\exp 2\pi i(s_1 l_1 N_1^{-1} + s_2 l_2 N_2^{-1} + \cdots)}{1 - z\lambda(k_1, k_2, k_3, \ldots)} \tag{12}$$

where $\lambda(k)$ is the structure function defined by [2,3]

$$\lambda(k_1, k_2, \ldots) = \sum_l p(l) \exp - ik \cdot l \qquad \text{with} \quad k_j \equiv 2\pi s_j/N_j \tag{13}$$

Note that

$$\sum_l p(l) = 1 \tag{14}$$

and

$$\bar{l}_j = \sum l_j p(l) = i(\partial\lambda/\partial k_j)_{k=0} \tag{15}$$

is the mean displacement in the jth direction on each step, while

$$\overline{l_j^2} = \sum_l l_j^2 p(l) = -(\partial^2\lambda/\partial k_j^2)_{k=0} \tag{16}$$

is the second moment of the displacement and the dispersion is

$$\overline{(l_j - \bar{l}_j)^2} = \overline{l_j^2} - \bar{l}_j^2 \tag{17}$$

An explicit lattice model which we will use frequently in the remainder of this paper is

$$\begin{aligned} &p(0, 1, 0) = p(0, -1, 0) = p(0, 0, 1) = p(0, 0, -1) = q \\ &p(1, 0, 0) = 2\eta p; \qquad p(-1, 0, 0) = 2(1 - \eta)p \end{aligned} \tag{18}$$

with all other $p(l_1, l_2, l_3)$ vanishing. This corresponds to nearest-neighbor hopping on a simple cubic lattice with a bias for hops in the $+x$ direction over those in the $-x$ direction. From Eq. (14)

$$4q + 2p = 1 \tag{19}$$

The appropriate form for the structure function $\lambda(k)$ is

$$\lambda(k_1, k_2, k_3) = 2q(C_2 + C_3) + 2pC_1 - 2(2\eta - 1)piS_1 \tag{20}$$

with

$$C_j \equiv \cos k_j \qquad \text{and} \qquad S_j = \sin k_j \qquad \text{with} \qquad k_j \equiv 2\pi s_j/N_j \tag{21}$$

s_j being an integer in the range 1, 2,..., N_j . As $k \to 0$

$$\lambda(k_1, k_2, k_3) \sim 1 - 2pi(2\eta - 1)k_1 - qk_2^2 - qk_3^2 - pk_1^2 + \cdots \quad (22)$$

An alternative traditional way of discussing continuous-time random walks on lattices is through a master equation[6] which is obtained by letting the time interval between jumps as described through Eq. (1) become smaller and smaller. If we let $t = n\tau$ and consider $p(l, l'; \tau)$ to be a function of τ, then

$$P_{t+\tau}(l) - P_t(l) = \sum_{l'} [p(l, l'; \tau) - \delta_{l,l'}] P_t(l') \quad (23)$$

so that as $\tau \to 0$

$$dP_t(l)/dt = \sum_{l'} P_t(l')A(l, l') \quad (24)$$

where

$$A(l, l') = \lim_{\tau\to 0}[p(l, l'; \tau) - \delta_{l,l'}]/\tau \quad (25)$$

Then the discussion of the lattice walk problem is based on solving the differential equation.

In order to be a bit more explicit about the limit process (25), let us consider several forms of the probability density function $\psi(t)$ for steps away from a lattice point. First we choose

$$\psi(t) = \lambda e^{-\lambda t} \quad (26)$$

Then the probability that a step to a new lattice point is made in time τ is

$$\int_0^\tau \psi(t)\, dt = 1 - e^{-\lambda\tau} = \lambda\tau + O(\tau^2) \quad (27)$$

while the probability that the walker remains at his lattice point for a time τ is

$$e^{-\lambda\tau} = 1 - \lambda\tau + O(\tau^2) \quad (28)$$

Hence

$$A(l, l) = \lim_{\tau\to 0} \tau^{-1}[1 - \lambda\tau + O(\tau^2) - 1] = -\lambda \quad (29)$$

If $l \neq l'$,

$$p(l, l'; \tau) = p(l, l')\{\lambda\tau + O(\tau^2)\} \quad (30)$$

where $p(l, l')$ is the probability that if a step is made from l', the walker ends at l. Then, if $l \neq l'$,

$$A(l, l') = \lambda p(l, l') \quad (31)$$

Hence (24) has the form

$$dP_t(l)/dt = -\lambda P_t(l) + \lambda \sum_{l \neq l'} p(l, l')P_t(l') \tag{32}$$

It has been shown by Bedeaux *et al.*[9] that when $\psi(t)$ has the exponential form (26), the solution of (32) is exactly the same as that obtained from taking the Laplace inverse of (7) when $\tilde{P}^*(l, u)$ is found from the generating function $P[l, \psi^*(u)]$. For other forms of $\psi(t)$ this is not necessarily true. For example, if $\psi(t)$ is not given by (26), but if all positive integral moments

$$\mu_n \equiv \int_0^\infty t^n \psi(t)\, dt, \qquad n = 0, 1, 2, 3,... \tag{33}$$

exist, and if the limit (25) exists, then for all times long compared with

$$\gamma \equiv \sup(\mu_n/n!)^{1/n} \tag{34}$$

the solution of the master equation (24) is essentially the same as the inverse Laplace transform of $P^*(l, u)$ as defined by (8) and (10).

There are some elementary forms of $\psi(t)$ for which the limit (24) does not exist. Consider

$$\psi(t) = \lambda(\pi\lambda t)^{-1/2}\, e^{-\lambda t} \tag{35}$$

Then for small τ

$$\int_0^\tau \psi(t)\, dt = 2\tau^{1/2} - \tfrac{2}{3}\lambda\tau^{3/2} + \cdots$$

so that

$$\begin{aligned} A(l, l) &= \lim_{\tau\to 0}[(1 - 2\tau^{1/2} - \tfrac{2}{3}\lambda\tau^{3/2} + \cdots) - 1]/\tau \\ &= \lim_{\tau\to 0}(-2\tau^{-1/2}) \to \infty \end{aligned}$$

and our required limit does not exist. In cases such as

$$\psi(t) = (2a/\pi)\,(a^2 + t^2)^{-1} \tag{36}$$

the moments μ_n do not exist, so that from the theorem derived in Ref. 9 there might not be any time regime in which the solution of (24) would approximate the solution to our problem as obtained from lattice generating functions. It was indeed for these cases in which a master equation might not be valid that our generating function technique was developed. Since there is some evidence that in transient photoconductivity experiments $\psi(t)$ may have a long tail such that moments do not exist, we base our analysis of the next sections on the generating function technique.

2. RANDOM WALKS WITH A BIAS IN ONE DIRECTION

The general formula for the probability of a random walker going from the origin to a point l in time t is obtained by calculating the Laplace inverse of Eq. (7). If a walker is originally at the origin of a periodic lattice, the generating function $P(l, z)$ is exactly $G(l, z)$ of Eq. (12). Hence using the standard inversion formula, we find

$$\tilde{P}(l, t) = (1/2\pi i) \int_{c-i\infty}^{c+i\infty} (du/u)e^{ut}[1 - \psi^*(u)]G(l, \psi^*(u)) \tag{37}$$

To proceed further we need an explicit form for $\psi^*(u)$.

We consider several classes of pausing time distribution functions. The first is

$$\psi(t) = \alpha(\alpha t)^{\alpha\bar{t}-1}e^{-\alpha t}/\Gamma(\alpha\bar{t}) \tag{38a}$$

where it is easily seen that

$$\bar{t} = \int_0^\infty t\psi(t)\, dt \tag{38b}$$

Equation (38a) reduces to the exponential distribution when $\alpha\bar{t} = 1$. Since all moments of (38a) exist, the asymptotic form for $\tilde{P}(l, t)$ for large t could be found from a transport equation such as (24). The Laplace transform of $\psi(t)$ is

$$\psi^*(u) = [1 + (u/\alpha)]^{-\alpha\bar{t}} \tag{38c}$$

which is to be inserted into (37) if $\tilde{P}(l, t)$ is to be calculated.

Since the most interesting applications of (37) will be for cases in which higher moments of $\psi(t)$ do not exist and therefore for which the transport equation (24) is not appropriate, we note two examples of such a distribution. The first is

$$\begin{aligned} \psi_1(t) &= a(\pi t)^{-1/2} - a^2[\exp(ta^2)]\ \mathrm{Erfc}(at^{1/2}) \\ &\sim (\pi^{1/2}at^{3/2})^{-1} \qquad \text{as} \quad t \to \infty \end{aligned} \tag{39a}$$

The Laplace transform of $\psi_1(t)$ is

$$\psi_1^*(u) = [1 + (u^{1/2}/a)]^{-1} \sim 1 - (u^{1/2}/a) + \cdots \tag{39b}$$

The second is

$$\begin{aligned} \psi_2(t) &= 4a^2[\exp(ta^2)]i^2\ \mathrm{Erfc}(at^{1/2}) \\ &\sim (\pi^{1/2}at^{3/2})^{-1} \qquad \text{as} \quad t \to \infty \end{aligned} \tag{40a}$$

with

$$\psi_2^*(u) = [1 + (u^{1/2}/a)]^{-2} \sim 1 - (2u^{1/2}/a) + \cdots \tag{40b}$$

The quantity i^2 Erfc z is the second repeated integral of the complementary error function of which the nth is defined by

$$i^n \operatorname{Erfc} z = (2/\pi^{1/2}n!) \int_z^\infty (t-z)^n (\exp -t^2)\, dt \tag{41}$$

Both forms (39a) and (40a) diminish as $t^{-3/2}$ for large t rather than exponentially. Forms (39) and (40) differ qualitatively for small t since (39a) diverges as $t^{-1/2}$ as $t \to 0$, while (40a) approaches a constant value in that limit. Since the Laplace transforms of the functions (41) are elementary, they are useful examples.[10]

An alternative form for $P(l, t)$ which can be used instead of (37) is the finite Fourier representation:

$$\tilde{P}(l, t) = (1/N_1N_2N_3) \sum_{s_1=1}^{N_1} \sum_{s_2=1}^{N_2} \sum_{s_3=1}^{N_3} \gamma(k_1, k_2, k_3; t) \exp(il \cdot k) \tag{42}$$

where

$$k_j \equiv 2\pi s_j/N_j \tag{43}$$

In the limit as N_1, N_2, and $N_3 \to \infty$, $\tilde{P}(l, t)$ becomes

$$\tilde{P}(l, t) = (2\pi)^{-3} \iiint_{-\pi}^{\pi} \gamma(k, t) \exp(il \cdot k)\, d^3k \tag{42a}$$

If (48) is substituted into (37) and the result compared with (42), it is clear that

$$\gamma(k, t) = (1/2\pi i) \int_{c-i\infty}^{c+i\infty} (du/u) e^{ut} [1 - \psi^*(u)][1 - \lambda(k)\psi^*(u)]^{-1} \tag{44a}$$

where $\lambda(k)$ is the structure function defined by (13).

The Fourier component $\gamma(0, 0, 0, t)$ is clearly equal to one, since $\lambda(0) = 1$ and, with $(\mathscr{L}^{-1}[f(u)]$ the inverse Laplace transform of the function f,

$$\mathscr{L}^{-1}[1/u] = 1 = \gamma(0, t) \tag{44b}$$

Various moments of $\tilde{P}(l, t)$ are easily obtained from $\gamma(k, t)$. Since

$$\gamma(k, t) = \sum_l \tilde{P}(l, t) \exp - il \cdot k \tag{45}$$

we have

$$i[\partial\gamma(k, t)/\partial k_j]_{k=0} = \langle l_j \rangle \tag{46}$$

$$-[\partial^2\gamma(k, t)/\partial k_j\, \partial k_{j'}]_{k=0} = \langle l_j l_{j'} \rangle, \quad \text{etc.} \tag{47}$$

We now consider the case in which at each step there is a bias for a step to the right in preference to one to the left. Equal weight is given to steps in to steps in the $\pm y$, and $\pm z$ directions. As in Eqs. (11) and (13), we define $p(l) \equiv p(l_1, l_2, l_3)$ to be the probability of a displacement vector l each time a step is taken. In the case of interest

$$p(l_1, l_2, l_3) = p(l_1, -l_2, l_3) = p(l_1, l_2, -l_3) = p(l_1, -l_2, -l_3) \tag{48}$$

Hence

$$\sum_{l_2} l_2 p(l_1, l_2, l_3) = \sum_{l_3} l_3 p(l_1, l_2, l_3) = 0 \tag{49}$$

We also define μ_1, μ_2, and μ_2':

$$\langle l_1^2 \rangle = \mu_2, \qquad \langle l_2^2 \rangle = \langle l_3^2 \rangle = \mu_2' \tag{50a}$$

$$\langle l_1 \rangle = \sum_{l} l_1 p(l_1, l_2, l_3) = \mu_1 \tag{50b}$$

then, if $\langle l_i l_j \rangle = 0$ for $i \neq j$,

$$\lambda(k) = 1 - i\mu_1 k_1 - \tfrac{1}{2}\mu_2 k_1^2 - \tfrac{1}{2}\mu_2'(k_2^2 + k_3^2) + \cdots \qquad \text{as} \quad k \to 0 \tag{51}$$

We now consider the explicit calculation of the characteristic function $\gamma(k, t)$.

We can use (44a) and (44b) to rewrite $\gamma(k, t)$ as

$$\gamma(k, t) = 1 - \frac{1 - \lambda(k)}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{du}{u} \frac{e^{ut}}{[\psi^*(u)]^{-1} - \lambda(k)} \tag{52}$$

In general one will not be able to carry out the integration in closed form. However, we have chosen our examples of $\psi(t)$, Eqs. (38a), (39a), and (40a), so that the integration can be performed.

Let

$$I\{h(s)\} \equiv \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{e^{s\tau}\, ds}{s\{h(s) - \lambda(k)\}} \tag{53}$$

Then, if we use the form (38c) for $\psi^*(u)$ and define

$$\tau \equiv \alpha t, \qquad \bar{\tau} \equiv \alpha \bar{t}, \qquad s = u/\alpha \tag{54a}$$

we have

$$h(s) = (1 + s)^{\bar{\tau}} \tag{54b}$$

and

$$I\{(1 + s)^{\bar{\tau}}\} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{e^{s\tau}\, ds}{s\{(1 + s)^{\bar{\tau}} - \lambda(k)\}} \tag{55}$$

From Laplace transform tables one finds elementary forms when $\bar{\tau} = \frac{1}{2}$, 1, 2, as well as for certain other values of $\bar{\tau}$. The respective values for $\gamma(k, t)$ are

$$\bar{\tau} = 2: \qquad \gamma(k, t) = e^{-\tau}\{\cosh[\tau(\lambda(k))^{1/2}] + [\lambda(k)]^{-1/2} \sinh [\tau(\lambda(k))^{1/2}]\} \tag{56}$$

$$\bar{\tau} = 1: \qquad \gamma(k, t) = \exp - \tau\{1 - \lambda(k)\} \tag{57}$$

$$\bar{\tau} = \tfrac{1}{2}: \qquad \gamma(k, t) = [1 + \lambda(k)]^{-1} (1 - \operatorname{erf} \tau^{1/2} + \lambda(k) \times \exp\{-[1 - \lambda^2(k)]\tau\} \operatorname{Erfc}[-\lambda(k)\tau^{1/2}]) \tag{58}$$

With the choice (39a) of $\psi(t)$ and the transform (39b) one finds after letting

$$s \equiv u/a^2, \qquad \tau = ta^2 \tag{59a}$$

$$h(s) = 1 + s^{1/2} \tag{59b}$$

that

$$\gamma(k, t) = \exp\{[1 - \lambda(k)]^2\tau\} \operatorname{Erfc}\{[1 - \lambda(k)]\tau^{1/2}\} \tag{60}$$

Similarly with the choice (40a) of $\psi(t)$,

$$\begin{aligned}\gamma(k, t) = {} & \tfrac{1}{2}\lambda^{-1/2}(k)[1 + \lambda^{1/2}(k)] \exp\{\tau[1 - \lambda^{1/2}(k)]^2\} \\ & \times \operatorname{Erfc}\{[1 - \lambda^{1/2}(k)]\tau^{1/2}\} \\ & -\tfrac{1}{2}\lambda^{-1/2}(k)[1 - \lambda^{1/2}(k)] \exp\{\tau[1 + \lambda^{1/2}(k)]^2\} \\ & \times \operatorname{Erfc}\{[1 + \lambda^{1/2}(k)]\tau^{1/2}\}\end{aligned} \tag{61}$$

One form for $\psi(t)$ and $\lambda(k)$ for which an explicit closed expression can be derived for $\tilde{P}(l, t)$ is that with $\bar{\tau} = 1$ in Eq. (38a), so that

$$\psi(t) = \alpha e^{-\alpha t} \qquad \text{and} \qquad \psi^*(u) = [1 + (u/\alpha)] \tag{62}$$

and with the choice (20) for $\lambda(k)$. Then, from (57) and (42a)

$$\tilde{P}(l, t) = (2\pi)^{-3} \iiint_{-\pi}^{\pi} \exp\{ik \cdot l - \tau[1 - \lambda(k)]\}\, d^3k \tag{63}$$

When the form for $\lambda(k)$ is substituted into this expression the three k integrals separate and can be evaluated individually using the following Bessel function formula:

$$\left\{\frac{a + ib}{(a^2 + b^2)^{1/2}}\right\}^l I_l([a^2 + b^2]^{1/2}) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{ikl}\, e^{a \cos k + b \sin k}\, dk \tag{64}$$

In the k_2 and k_3 integrals of (63) $b = 0$ and $a = 2q\tau$, while in the k_1 integral $a = 2p\tau$ and $b = -2p(2\eta - 1)i\tau$. Hence

$$\tilde{P}(l, t) = [(1 - \eta)/\eta]^{l_1/2} e^{-\alpha t} I_{l_2}(2q\alpha t) \times I_{l_3}(2q\alpha t) I_{l_1}(4p\alpha t[\eta(1 - \eta)]^{1/2}) \tag{65}$$

The one-dimensional analog of this result was discussed by Montroll[11] many years ago. When τ is very large the main contribution to the integral (63) comes from small values of k and (63) is approximated by

$$\tilde{P}(l, t) \sim (2\pi)^{-3} \iiint_{-\pi}^{\pi} \exp\{i[k \cdot l + 2\tau p(1 - 2\eta)k_1]\} \times \exp\{-\tau[qk_3^2 + qk_2^2 + pk_1^2 + O(k^3)]\} d^3k \tag{66}$$

If we let $x_j = \tau^{1/2}k_j$ and let $\tau \to \infty$, the term of order τk_1^3 become $x_1\tau^{-1/2}$, which can be neglected. Then

$$\begin{aligned}\tilde{P}(l, t) &\sim (2\pi)^{-3}\tau^{-3/2} \iiint_{-\infty}^{\infty} \exp\{i\tau^{-1/2}[x \cdot l + p\tau(1 - 2\eta)x_1]\} \\ &\quad \times \exp(-qx_2^2) \exp(-qx_3^2) \exp(-px_1^2)\, d^3x \\ &\sim (4\pi\alpha t)^{-3/2} (pq^2)^{-1/2} \\ &\quad \times \exp -\{[(l_2^2 + l_3^2)/4\alpha qt] + [l_1 + p\alpha t(1 - 2\eta)]^2/4\alpha tp\}\end{aligned} \tag{67}$$

This is a three-dimensional Gauss distribution whose peak travels in the x direction with a velocity

$$dl/dt = 2p\alpha(2\eta - 1) \tag{68}$$

The asymptotic Gauss distribution is also observed for other members of the class of $\psi(t)$ given by (38a) and in fact for other $\psi(t)$'s for which all moments

$$\mu_n = \int_0^\infty t^n \psi(t)\, dt$$

exist (and indeed even for those for which only the first two moments exist).[3]

The central limit theorem for the distribution of a sum of random variables states that if the first three moments of each of the random variables is finite, then the probability distribution of the sum becomes Gaussian as the number of variables becomes large.[13,14] Actually the necessary and sufficient condition for this result is somewhat weaker than the existence

[3] Shlesinger[12] relates the asymptotic behavior of $\psi(t)$ to $\tilde{P}(l, t)$.

of third moments.[13] The theorem also applies to the sum of random three-component space vectors.[13] Since the final position of our walker after time t is a vector sum of the individual step vectors, we see that as t (and therefore the number of individual steps) becomes large the central limit theorem implies that $\tilde{P}(l, t)$ becomes Gaussian. This Gaussian distribution function is completely specified when the first and second moments of $\tilde{P}(l, t)$ become known. The conditions that $\tilde{P}(l, t)$ becomes Gaussian for large t are satisfied when the pausing time distribution $\psi(t)$ has the form (38a) but are not for the forms (39a) and (40a).

When $\tilde{P}(l, t)$ is Gaussian and $\lambda(k)$ is given by (20) the center of the moving Gaussian packet is at $l_2 = l_3 = 0$ and

$$\langle l_1 \rangle = i[\partial\gamma(k, t)/\partial k_1]_{k=0} = i[\partial\gamma/\partial\lambda]_{\lambda=1}\, [\partial\lambda/\partial k_1]_{k=0} \tag{69a}$$

$$= \bar{l}_1[\partial\gamma/\partial\lambda]_{\lambda=1} \tag{69b}$$

where $\bar{l}_1$ is given by (50b); it has the value $2p(2\eta - 1)$ in the nearest-neighbor jump case for $\lambda(k)$ given by (20). When we successively let $\gamma(k, t)$ be given by (56), (57), and (58) we find as t becomes large

$$(\partial\gamma/\partial\lambda)_{\lambda=1} = \begin{Bmatrix} \frac{1}{2}\tau = \frac{1}{2}\alpha t \\ \tau = \alpha t \\ 2\tau = 2\alpha t \end{Bmatrix} = t/\bar{t}, \qquad \begin{matrix} \bar{\tau} = 2 \\ \bar{\tau} = 1 \\ \bar{\tau} = \frac{1}{2} \end{matrix} \tag{70}$$

Generally the velocity of propagation of the Gaussian packet which results from $\psi(t)$ of form similar to (38a) is

$$d\langle l_1 \rangle/dt = \bar{l}_1/\bar{t} \tag{71}$$

the ratio of the mean distance per step to the mean time between steps, a result which is generally valid when the Gaussian distribution develops after a long time.

The dispersion is given by

$$\sigma^2 = \langle l_1^2 \rangle - \langle l_1 \rangle^2 \tag{72a}$$

From (47)

$$\langle l_1^2 \rangle = -(\partial^2\gamma/\partial k_1^2)_{k=0} \tag{72b}$$

But

$$\partial^2\gamma/\partial k_1^2 = (\partial\gamma/\partial\lambda)_{\lambda=1}\, (\partial^2\lambda/\partial k^2)_{k=0} + (\partial\lambda/\partial k)^2_{k=0}\, (\partial^2\gamma/\partial\lambda^2)_{\lambda=1} \tag{73}$$

Hence, from (46), (72a), 72b), and (73)

$$\begin{aligned} \sigma_1^2 &= \{(\partial\gamma/\partial\lambda)(\partial^2\lambda/\partial k^2) + (\partial\lambda/\partial k)^2\, [(\partial^2\gamma/\partial\lambda^2) - (\partial\gamma/\partial\lambda)^2]\}_{k=0} \\ &= \overline{l_1^2}(\partial\gamma/\partial\lambda)_{\lambda=1} + l_1^2[(\partial^2\gamma/\partial\lambda^2) - (\partial\gamma/\partial\lambda)^2]_{\lambda=1} \end{aligned} \tag{74}$$

The dispersions for the cases $\bar{\tau} = 2$, $\bar{\tau} = 1$, and $\bar{\tau} = \frac{1}{2}$, are, respectively, as $t \to \infty$

$$\sigma_1^2 = (\overline{l_1^2} - \bar{l}_1^2)(t/\bar{t}) \qquad \text{if} \quad \bar{\tau} = 2 \tag{75a}$$

$$\sigma_1^2 = \overline{l_1^2}(t/\bar{t}) \qquad \text{if} \quad \bar{\tau} = 1 \tag{75b}$$

$$\sigma_1^2 = \overline{l_1^2}(t/\bar{t}) \qquad \text{if} \quad \bar{\tau} = \tfrac{1}{2} \tag{75c}$$

Since in continuum diffusion theory

$$\sigma^2 = 4Dt \tag{76}$$

not all cases have the same diffusion constant.

The more interesting examples of $\psi(t)$ are those which do not lead to the traditional Gaussian packets which with increasing time propagate with a constant velocity and have a dispersion proportional to $t^{1/2}$. Let us first consider the form (39a) for $\psi(t)$. Then from (46) and (60) we find that

$$\langle l_1 \rangle = 2a\bar{l}_1(t/\pi)^{1/2} \tag{77}$$

so that

$$d\langle l_1 \rangle/dt = a\bar{l}_1(t\pi)^{-1/2} \to 0 \qquad \text{as} \quad t \to \infty \tag{78}$$

Also, from (47) and (56)

$$\sigma_1^2 = 2a^2\bar{l}_1^2\, t\{1 - (2/\pi)\} + 2a\overline{l_1^2}(t/\pi)^{1/2} \tag{79a}$$

$$\sim 2a^2\bar{l}_1^2\, t\{1 - (2/\pi)\} \qquad \text{as} \quad t \to \infty \tag{79b}$$

We see then that the dispersion at time t, $\sigma \sim a\bar{l}_1(2t)^{1/2}$, is of the same order as the distance of travel of the mean of the propagating packet. Since the velocity becomes so small as t becomes large, we hardly have a propagating packet at all, but merely one that is slowly spreading. This is to be expected because $\psi(t)$ is so broad that a walker has a good chance of being hung up for a long time at some traps. In a packet of many walkers those trapped for long times become stragglers and are responsible for the spreading of the packet.

Similar results are observed for $\psi(t)$ of the form (40a). In that case

$$\langle l_1 \rangle = \tfrac{1}{2}\bar{l}_1[2a(t/\pi)^{1/2} - \tfrac{1}{2} + \tfrac{1}{2}\exp(4a^2t)\,\mathrm{Erfc}(2at^{1/2})] \tag{80}$$

with

$$d\langle l_1 \rangle/dt = a^2\bar{l}\exp(4a^2t)\,\mathrm{Erfc}(2at^{1/2}) \sim \tfrac{1}{2}a\bar{l}(\pi t)^{1/2} \tag{81}$$

and

$$\sigma_1^2 = \overline{l_1^2}\langle l_1\rangle/\bar{l}_1 - \tfrac{3}{2}\langle l_1\rangle\bar{l}_1 - \langle l_1\rangle^2 + ta^2\bar{l}_1^2[\pi^{-1/2} + \exp(4a^2t)\,\mathrm{Erfc}(2at^{1/2})] \sim a^2\bar{l}^2t(1 - \pi^{-1/2})\pi^{-1/2} \tag{82}$$

If we are concerned with only the x component of the position of our walkers, then we can sum over the y and z components of the various lattice points, l_2 and l_3, in Eq. (42):

$$\tilde{P}(l_1, t) = \sum_{l_2, l_3 = 1}^{N} P(l_1, l_2, l_3; t)$$
$$= (1/N_1) \sum_{s=1}^{N_1} \gamma(2\pi s/N_1, 0, 0) \exp(2\pi i s l_1/N_1) \tag{83}$$

The subscript 1 on some of our variables can now be dropped without incurring confusion. In the numerical work to be reviewed in the remainder of this section we restrict ourselves to the special case in which steps are taken only to nearest-neighboring points as prescribed by (18) and (19). The form for $\lambda(k)$ which is required in (44a) is found from (20) by setting $k_2 = k_3 = 0$:

$$\begin{aligned} \lambda(k, 0, 0) &= 4q + 2pC - 2p(2\eta - 1)\, iS \\ &= 1 - 2p\{1 - C + (2\eta - 1)\, iS\} \end{aligned} \tag{84}$$

with

$$k = 2\pi s/N, \qquad C \equiv \cos k, \qquad S \equiv \sin k \tag{85}$$

We have calculated $\tilde{P}(l, t)$ from (83) for the following selection of forms of $\psi(t)$: the exponential form (38b), the forms (39a) and (39b) with no finite positive integer moments, and the form

$$\psi_4(t) = 96a^2[\exp(ta^2) i^4 \operatorname{Erfc}(at^{1/2}) \tag{86}$$

which has a finite first moment but no finite higher integer moments. A discussion of repeated complementary error function distributions is given in Appendix A. Examples are exhibited with the first j moments finite and all higher moments infinite for $j = 1, 2, 3, \ldots$.

The finite Fourier series summations required in (83) have been performed with the Cooley–Tukey[15] algorithm, which is especially effective when N is a power of 2. Our calculations were made with $N = 2^8 = 256$ and $2^9 = 512$. The first case considered was the exponential $\psi(t)$, since in that case the closed-form expression for the limit as $N \to \infty$,

$$\tilde{P}(l, t) = [(1 - \eta)/\eta]^{l/2} e^{-2p\alpha t} I_l(4p\alpha t[\eta(1 - \eta)]^{1/2}) \tag{87}$$

was available for checking the accuracy of programs for computation based on (83).

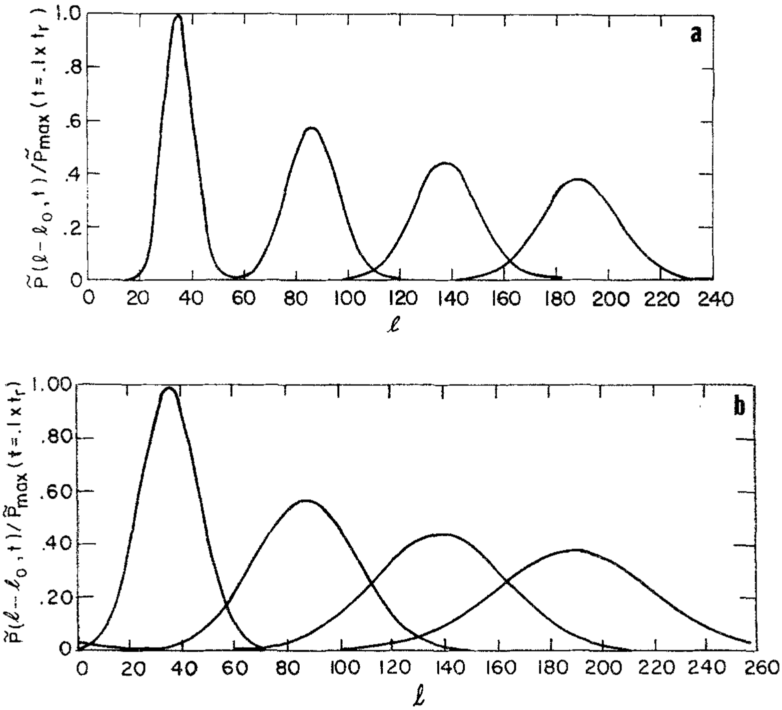

Fig. 1. Plot of the propagator or probability distribution $P(l - l_0, t)$ vs. l for a random walk based on $\psi(t) = \alpha \exp - \alpha t$ for a range of t. $t = (2n + 1)t_r/10$, $n = 0$, 1, 2, 3, where t_r is the "transit time," $\bar{l}(t_r) = N$. The plot is scaled by the peak value of $\tilde{P}(l - l_0, t)$ at the earliest time. $N = 256$. The velocity of the peak is a constant and the dispersion proportional to $t^{1/2}$. The bias factor η of the walk is (a) $\eta = 0.9$, (b) $\eta = 0.6$.

We have plotted $\tilde{P}(l, t)$ [as determined from (83)] as a function of l for various values of t in Fig. 1. The values of η chosen in Fig. 1(a) is 0.9 while that in Fig. 1(b) is 0.6. The pulse is propagated to the right with the velocity given by (71). The dispersion is given by (75c); since

$$\bar{l} = 2p(2\eta - 1) \qquad \text{and} \qquad \overline{l^2} = 2p \tag{88}$$

$$dl/dt = 2p(2\eta - 1)\alpha \qquad \text{and} \qquad \sigma^2 = 2p\alpha t \tag{89}$$

The data used to plot the curves which correspond to the first four time periods shown in Fig. 1 agree with the exact results obtained from (87) to at least four significant figures. At the time at which the distribution is represented by curve 4 in Fig. 1b the effect of the periodic boundary condition becomes apparent since a significant probability has built up for a walker to

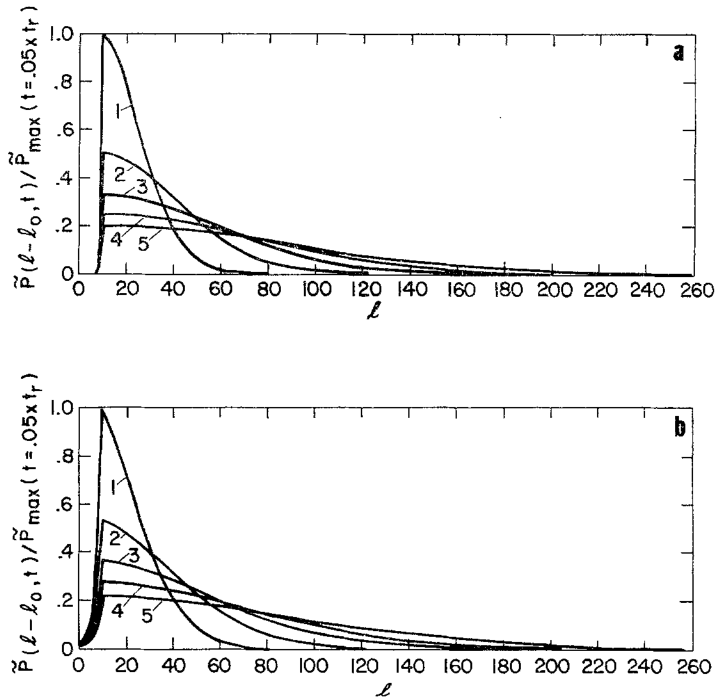

Fig. 2. Plot of the propagator or probability distribution $P(l - l_0, t)$ vs. l for a random walk based on $\psi(t) = 4a^2[\exp(ta^2)]\, i^2\, \mathrm{Erfc}(at^{1/2})$ for a range of $t^{1/2}$. $t^{1/2} = nt_r^{1/2}/20$, $n = 1, 2, 3, 4, 5$, where t_r is the "transit time," $\bar{l}(t_r) = N$. The plot is scaled by the peak value of $\tilde{P}(l - l_0, t)$ at the earliest time. $N = 256$. The velocity of the mean value decreases as $t^{-1/2}$ and the dispersion is proportional to $t^{1/2}$. The bias factor η of the walk is (a) $\eta = 0.9$, (b) $\eta = 0.6$.

be at a point represented by small integers.[4] It is to be emphasized in the Gaussian case since the distance reached by a pulse by the time t is proportional to t while the dispersion is only of order $t^{1/2}$, the pulse propagates as a packet and the probability of a walker being left at the starting point for a long time is neglible.

The data plotted in Fig. 2 are derived from walks in which the pausing time distribution at each point is of the form $\psi_2(t)$ given by Eq. (40a):

$$\psi_2(t) = 4a^2[\exp(ta^2)]i^2\, \mathrm{Erfc}(at^{1/2})$$

[4] The analytic expressions for $\langle l_t \rangle$ in (70), (77), and (80) do not exhibit effects of the periodic behavoir of $\tilde{P}(l, t)$ (for finite N). This limitation can be traced to the step where we differentiate with respect to k, i.e., we assume k to be a continuous variable which implies $N \rightarrow \infty$. Therefore the derivation is valid for the packet before it encounters the boundary at finite N (see the end of Sec. 3).

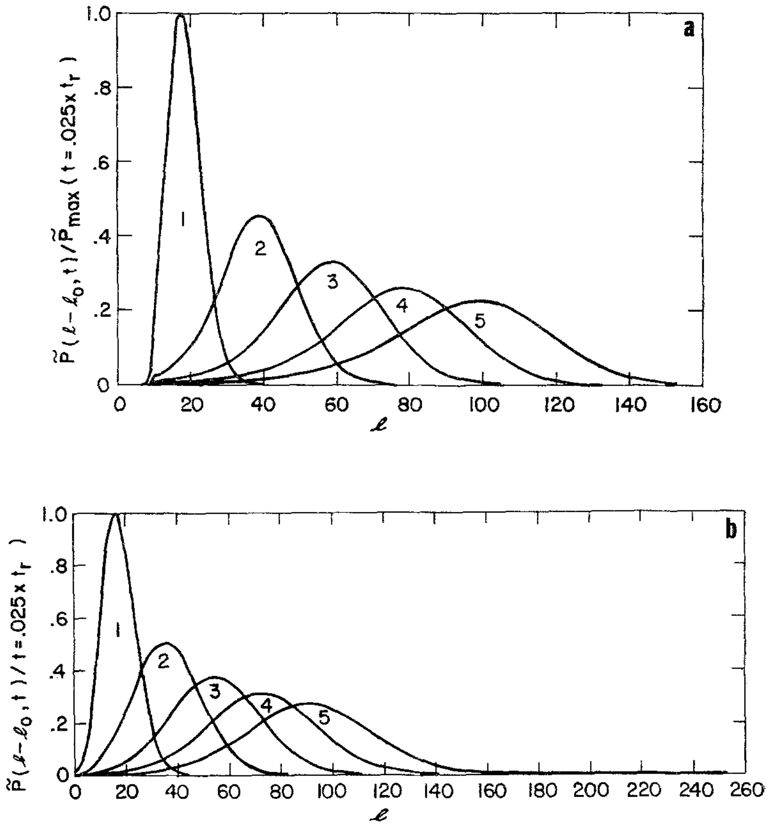

Fig. 3. Plot of the propagator or probability distribution $P(l - l_0, t)$ vs. l for a random walk based on $\psi(t) = 4!\, 4a^2[\exp(ta^2)]\, i^4 \operatorname{Erfc}(at^{1/2})$ for a range of t. $t = (2.75n - 1.75)t_r/40$, $n = 1, 2, 3, 4, 5$, where t_r is the "transit time," $(t_r) = N$. The plot is scaled by the peak value of $\tilde{P}(l - l_0, t)$ at the earliest time. $N = 256$. The velocity of the peak is constant and the dispersion varies as t. The bias factor η of the walk is (a) $\eta = 0.9$, (b) $\eta = 0.6$.

The sharp drops to the left of the initial position l_0 in Fig. 2 are related to the bias of the walk. However, the asymmetry of the spreading distribution function is actually less than the Gaussian packets in Fig. 1. For comparable times (the unit of time is always the "transit" time t_r, i.e., the time at which $\langle l \rangle = N$) the value of $\tilde{P}(l, t)$ for $l < l_0$ in Fig. 2(a, b) is larger than in Fig. 1(a, b), respectively. In other words, the Gaussian packets "move away" from l_0; thus the probability for the walker to be *at* $l < l_0$ is very small, in contrast to the anomalously spreading $\tilde{P}(l, t)$ in Fig. 2, which always stays peaked at l_0.

In Fig. 3 the distribution function is plotted for walks derived from

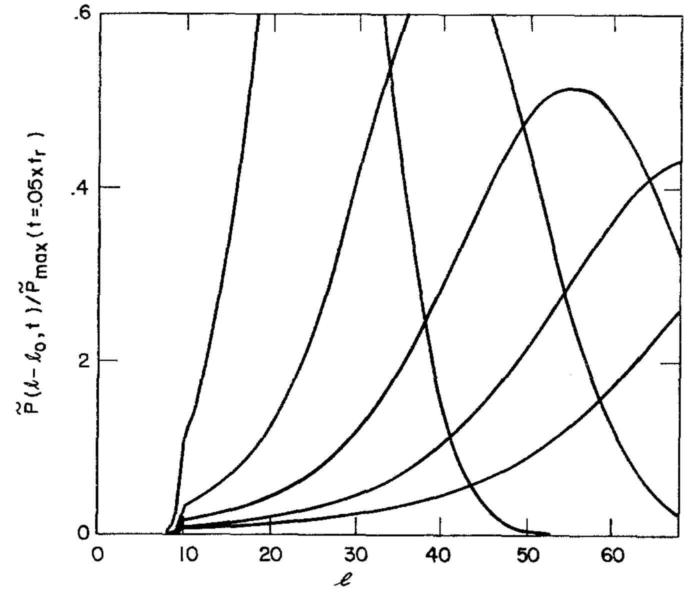

Fig. 4. A closeup of the region $l \approx l_0$ for the plot in Fig. 3(a). $\eta = 0.9$.

$\psi_4(t)$ in (86) and for $\eta = 0.9$ and 0.6. The properties of $\psi_4(t)$ are discussed in Appendix B; in particular, from (B.17), we have

$$\langle l_1 \rangle = (a^2\bar{l}_1/3)\{t + (16t^{1/2}/3a\pi^{1/2}) + (8/9)[\exp(9ta^2)\ \mathrm{Erfc}(3at^{1/2}) - 1]\} \tag{90}$$

i.e., for large t the mean position moves linearly with t. However, we can observe in Fig. 3 that a walk derived from $\psi_4(t)$ represents an interesting transition between the situation shown in Fig. 2, where the waiting time distribution did not have a mean, and the Gaussian packets in Fig. 1. In Fig. 3 the peak moves with the mean, but the value of $\tilde{P}(l, t)$ at l_1 remains finite throughout as in Fig. 2. A closeup of the behavior at l_0 for Fig. 3a is shown in Fig. 4. We can clearly see a residue of the "straight edge" characteristic of the distributions in Fig. 2(a). The dispersion in Fig. 3 as a result of this behavior is more complicated (*eventually* $\sigma \to t^{1/2}$, $t \to \infty$).

3. EFFECT OF TRAPS ON LATTICE WALKS[2,5,16]

In this section we apply ideas developed in Ref. 2 to random walks in the presence of lines or planes of traps.[5] We consider a periodic lattice in n

[5] K. Lakatos-Lindenberg has also considered the effect of absorbing boundaries on random walks in Ref. 17.

dimensions (with $n = 3$ being the case of most interest) with periodic boundary conditions so that the lattice forms a ring in one dimension, a torus in two, etc. We assume that in the absence of traps the probability of a transition from lattice point l' to l depends only on the displacement $l - l'$. Finally we characterize the trapping points as $l_1, l_2, ..., l_i$, members of a set $\mathscr{L}$.

If the lattice point l is not a trap, then the probability of a walker being at l after n steps is

$$P_n(l) = \sum_{l' \notin \mathscr{L}} p(l - l')\, P_{n-1}(l') \tag{91}$$

The trapping points are omitted from the summation because transitions from a trapping point to l are forbidden by definition of a trap. It is convenient to rewrite (91) as

$$P_n(l) = \sum_{l'} p(l - l') P_{n-1}(l') - \sum_{l_j \in \mathscr{L}} p(l - l_j) P_{n-1}(l_j) \tag{92}$$

Now let l be a trapping point, say, that located at l_k. Then, since a walker trapped at l_k remains there forever,

$$P_n(l_k) = P_{n-1}(l_k) + \sum_{l' \notin \mathscr{L}} p(l_k - l')\, P_{n-1}(l') \tag{93}$$

$$= \sum_{l'} p(l_k - l')\, P_{n-1}(l') - \sum_{l_j \in \mathscr{L}} [p(l_k - l_j) - \delta_{l_j, l_k}]\, P_{n-1}(l_j) \tag{94}$$

A single equation which is valid for all l, being equivalent to both (92) and (94), is

$$P_n(l) = \sum_{l'} p(l - l')\, P_{n-1}(l') - \sum_{l_j \in \mathscr{L}} [p(l - l_j) - \delta_{l, l_j}]\, P_{n-1}(l_j) \tag{95}$$

The generating function for our random walk,

$$P(l, z) = \sum_{n=0}^{\infty} P_n(l) z^n \tag{96}$$

is the solution of a difference equation which can be constructed by multiplying both sides of (95) by z^n and summing from $n = 1$ to ∞. Then

$$P(l, z) - z \sum_{l'} p(l - l')\, P(l', z) = F(l) \tag{97a}$$

where

$$F(l) \equiv P_0(l) - z \sum_{l_j \in \mathscr{L}} [p(l - l_j) - \delta_{l, l_j}]\, P(l_j, z) \tag{97b}$$

with $P_0(l)$ being the distribution function of walker initial locations.

If a walker is initially at l_0, then

$$P_0(l) = \delta_{l,l_0} \tag{98}$$

Otherwise it can generally be expressed as

$$P_0(l) = \sum_{l'} p_{l'} \delta_{l,l'} \qquad \text{with} \quad \sum_{l} p_l = 1 \tag{99}$$

Then by superposition the generating function for this initial distribution can be obtained from the solution of (97) with initial conditions of the form of (98).

Let $G(l, z)$ be the Green's function solution of

$$G(l, z) - z \sum_{l'} p(l - l') \, G(l', z) = \delta_{l,0} \tag{100}$$

which is the equation for the generating function of a walk which starts at the origin of a lattice without traps. The solution of (97a) is then

$$P(l, z) = \sum_{l'} G(l - l', z) F(l'), \tag{101}$$

so that when $F(l)$ has the form (97b) and the initial distribution has the form (98)

$$\begin{aligned} P(l, z) &- G(l - l_0, z) \\ &= -z \sum_{l'} G(l - l', z) \sum_{l_j \in \mathscr{L}} [p(l' - l_j) - \delta_{l',l_j}] \, P(l_j, z) \\ &= z \sum_{l_j \in \mathscr{L}} G(l - l_j, z) \, P(l_j, z) \\ &\quad - z \sum_{l_j \in \mathscr{L}} P(l_j, z) \sum_{l'} G(l - l', z) \, p(l' - l_j) \end{aligned} \tag{102}$$

The summation over l' on the right-hand side of this equation can be expedited by introducing the definition of $G(l, z)$, Eq. (100):

$$z \sum_{l''} p(l - l'') \, G(l'', z) = G(l, z) - \delta_{l,0} \tag{103}$$

Clearly, since $G(l, z)$ is translation invariant,

$$\begin{aligned} z \sum_{l'} G(l - l', z) \, p(l' - l_j) &= z \sum_{l'} G(l - l', z) \, p[(l - l_j) - (l - l')] \\ &= z \sum_{l''} G(l'', z) \, p[(l - l_j) - l''] \\ &= G(l - l_j, z) - \delta_{l,l_j} \end{aligned} \tag{104}$$

Hence (102) becomes

$$P(l, z) = G(l - l_0, z) - \sum_{l_j \in \mathscr{L}} [(1 - z) \, G(l - l_j, z) - \delta_{l,l_j}] \, P(l_j, z) \tag{105}$$

When l is a normal nontrapping point

$$P(l, z) = G(l - l_0, z) - (1 - z) \sum_{l_j \in \mathscr{L}} G(l - l_j, z) P(l_j, z) \tag{106}$$

The values of $P(l, z)$ at trapping points which are required in the summation are obtained by successively letting $l = l_1, l_2, ..., l_t$ in (105) and solving the set of t linear equations for $P(l_j, z)$ with $l_j \in \mathscr{L}$:

$$(1 - z) \sum_{l_j \in \mathscr{L}} G(l_k - l_j, z) P(l_j, z) = G(l_k - l_0, z) \tag{107}$$

As a first example, let us consider the case of a single trap at l_1. Then from (106) and (107),

$$(1 - z)G(0, z)P(l_1, z) = G(l_1 - l_0, z) \tag{108a}$$

$$P(l, z) = G(l - l_0, z) - G(l - l_1, z)G(l_1 - l_0, z)/G(0, z) \quad \text{if} \quad l \neq l_1 \tag{108b}$$

This equation, which was first derived in Ref. 5, has a simple physical interpretation. The quantity

$$F(l_1 - l_0, z) \equiv G(l_1 - l_0, z)/G(0, z) \tag{109}$$

is the generating function of all walks which start at l_0 and reach l_1 for the first time at the nth step ($n = 1,..., \infty$), while $G(l - l_0, z)$ is the generating function which corresponds to the sum over all paths which start at l_0 and end at l_1. Hence the difference on the right-hand side of (108b) represents the sum over all paths which never go through the trap at l_1.

The influence of a line of traps can be considered in a similar manner. We choose a two-dimensional square lattice with traps at (0, 1), (0, 2), (0, 3),..., (0, N_2) as a prototype for our calculation. On a torus of $N_1 \times N_2$ points a cut along this line would allow one to open the torus into the form of a cylinder. We write a typical lattice point as (l_1, l_2) and the generating function at that point as $P(l_1, l_2; z)$. Then (107) has the form [with $l_0 \equiv (l_1^0, l_2^0)$]

$$(1 - z) \sum_{j=1}^{N_2} G(0, k - j; z) P(0, j; z) = G(-l_1^0, k - l_2^0; z), \qquad k = 1, 2,..., N_2 \tag{110}$$

Since our line of traps forms a closed ring on our two-dimensional periodic lattice on a torus, this equation can be solved for $P(0, j; z)$ through the aid of finite Fourier series. Let us define $g_s(l, z)$ and $p_s(l, z)$ by

$$\begin{Bmatrix} g_s(l, z) \\ p_s(l, z) \end{Bmatrix} = \sum_{k=1}^{N_2} \begin{Bmatrix} G(l, k; z) \\ P(l, k; z) \end{Bmatrix} e^{-2\pi isk/N_2} \tag{111a}$$

Then by finite Fourier series inversion

$$\begin{Bmatrix} G(l, k; z) \\ P(l, k; z) \end{Bmatrix} = \frac{1}{N_2} \sum_{s=1}^{N_2} \begin{Bmatrix} g_s(l, z) \\ p_s(l, z) \end{Bmatrix} e^{2\pi i s k/N_2} \tag{111b}$$

In view of the Faltung form of the left-hand side of (110), we find

$$(1 - z) g_s(0, z) p_s(0, z) = g_s(-l_1{}^0, z) \exp(-2\pi i s l_2{}^0/N_2) \tag{112}$$

When (l_1, l_2) is a normal trapping point (106) has the following form:

$$P(l_1, l_2, z) = G(l_1 - l_1{}^0, l_2 - l_2{}^0; z) - (1 - z) \sum_{j=1}^{N_2} G(l_1, l_2 - j; z) P(0, j; z) \tag{113}$$

If we Fourier-invert this expression, use the definition (111a), and apply the Faltung factorization and Eq. (112), we find

$$p_s(l_1, z) = \{g_s(l_1 - l_1{}^0, z) - g_s(l_1, z) g_s(-l_1{}^0, z)/g_s(0, z)\} \times \exp(-2\pi i s l_2{}^0/N_2) \tag{114a}$$

which upon application of (111b) yields for nontrapping points (l_1, l_2)

$$P(l_1, l_2; z) = \frac{1}{N_2} \sum_{s=1}^{N_2} \{g_s(l_1 - l_1{}^0, z) - g_s(l_1, z)\, g_s(-l_1{}^0, z)/g_s(0, z)\} \times \exp[2\pi i s (l_2 - l_2{}^0)/N_2] \tag{114b}$$

Equation (114a) is the prototype basic equation for extended lines and planes of traps in any number of dimensions. It is structurally similar to the one-trap equation (118b). When the points $(0, s_2, s_3)$ with $s_2 = 1, 2, 3, \ldots, N_2$ and $s_3 = 1, 2, 3, \ldots, N_3$ are traps on a $3D$ simple cubic lattice the analog of (114a) is (with $k_j \equiv 2\pi s_j/N_j$)

$$p_{s_2 s_3}(l_1, z) = \{g_{s_2 s_3}(l_1 - l_1{}^0, z) - g_{s_2 s_3}(l_1, z) g_{s_2 s_3}(-l_1{}^0, z)/g_{s_2 s_3}(0, z)\} \times \exp - i(k_2 l_2 + k_3 l_3) \tag{115}$$

where, for a lattice function $F(l_1, l_2, l_3; z)$,

$$f_{s_2 s_3}(l, z) = \sum_{l_2=1}^{N_2} \sum_{l_3=1}^{N_3} F(l, l_2, l_3; z) \exp - i(k_2 l_2 + k_3 l_3) \tag{116}$$

and

$$F(l; z) = (1/N_2 N_3) \sum_{s_1} \sum_{s_2} f_{s_2 s_3}(l, z) \exp i(k_2 l_2 + k_3 l_3) \tag{117}$$

The $3D$ analog of (114b),

$$P(l_1, l_2, l_3; z) = \frac{1}{N_2 N_3} \sum_{s_2=1}^{N_2} \sum_{s_3=1}^{N_3} p_{s_2 s_3}(l_1, z) \exp i(k_2 l_2 + k_3 l_3) \quad (118)$$

then gives the probability generating function for walks in the presence of a plane of traps.

If we are concerned only with the x component of a walker's position, we can sum over all values of l_2 and l_3 in (118) to obtain

$$P(l_1, z) = g_{00}(l_1 - l_1^0, z) - g_{00}(l_1, z) g_{00}(-l_1^0, z)/g_{00}(0, z) \quad (119)$$

The quantities $g_{s_2 s_3}(l, z)$ are related to the Green's function of the unperturbed lattice walk which, as was noted in Eq. (12), has the form

$$G(l_1, l_2, l_3; z) = \frac{1}{N_1 N_2 N_3} \sum_{s_1 s_2 s_3} \frac{\exp 2\pi i[(s_1 l_1/N_1) + (s_2 l_2/N_2) + (s_3 l_3/N_3)]}{1 - z\lambda(s_1, s_2, s_3)} \quad (120)$$

where $\lambda(s_1, s_2, s_3)$ is the structure function which characterizes the unperturbed walk. By comparing this expression with the 3D analog of (111b), we note that

$$G(l_1, l_2, l_3; z) = (1/N_2 N_3) \sum_{s_2 s_3} g_{s_2 s_3}(l_1, z) \exp 2\pi i[(s_2 l_2/N_2) + (s_3 l_3/N_3)] \quad (121)$$

where

$$g_{s_2 s_3}(l, z) = \frac{1}{N_1} \sum_{s_1=1}^{N_1} \frac{\exp 2\pi i(s_1 l/N_1)}{1 - z\lambda(s_1 s_2 s_3)} \quad (122)$$

In particular the $g_{0,0}(l, z)$ is given by

$$g_{0,0}(l, z) = \frac{1}{N_1} \sum_{s_1=1}^{N_1} \frac{\exp 2\pi i(s_1 l_1/N_1)}{1 - z\lambda(s_1, 0, 0)} \quad (123)$$

In the special case in which only jumps to nearest neighboring-points are permitted according to (18) we find from (20)

$$\lambda(k_1, 0, 0) = 4q + 2pC_1 + 2i(1 - 2\eta)pS_1 \quad (124)$$

which corresponds to the structure function for a 1D walk in which the walker has a probability $2p\eta$ of going to the right at a given step, a probability of $2(1 - \eta)p$ of going to the left, and a probability $4q$ of pausing and waiting until the next opportunity to take a step. This is to be expected because jumps in the $\pm y$ or $\pm z$ directions (which have total probability $4q$) do not affect the x component of the walk.

When (123) and (124) are compared with the 1D analog of (102) it is clear that (119) becomes

$$P(l_1, z) = G(l_1 - l_1^0, z) - G(l_1, z)G(-l_1^0, z)/G(0, z) \tag{125}$$

which is the same form as (108b) with a single trap at the origin when the structure function is the 1D walk described above.

The quantity $g_{0,0}(l, z) \equiv G(l, z)$, which has the following form for the choice (124) for $\lambda(s, 0, 0)$:

$$g_{0,0}(l, z) = \frac{1}{N} \sum_{s=1}^{N} \frac{e^{2\pi i s l/N}}{(1 - 4qz) - 2pz[\eta e^{-2\pi i s/N} + (1 - \eta)e^{+2\pi i s/N}]} \tag{126}$$

$$= \frac{1}{N(1 - 4qz)} \sum_{s=1}^{N} \frac{e^{2\pi i s l/N}}{1 - Pe^{2\pi i s/N} - Qe^{-2\pi i s/N}} \tag{127}$$

where

$$Q = 2pz\eta/(1 - 4qz) \qquad \text{and} \qquad P = 2pz(1 - \eta)/(1 - 4qz). \tag{128}$$

The sum in (127) is evaluated in Appendix C. It is found that

$$g_{00}(l, z) = [2pz(1 - \eta)(\alpha_2 - \alpha_1)]^{-1} [\alpha_1^l(1 - \alpha_1^N)^{-1} - \alpha_2^l(1 - \alpha_2^N)^{-1}] \tag{129}$$

where

$$\left.\begin{matrix}\alpha_2\\ \alpha_1\end{matrix}\right\} = (1/2P)[1 \pm (1 - 4PQ)^{1/2}] \tag{130}$$

The derivation of (129) is based on the assumption that $|\alpha_2| > 1 > |\alpha_1|$. Also, if $N > l > 0$,

$$g_{00}(-l, z) = g_{00}(N - l, z) \tag{131}$$

A quantity which can be obtained directly from $P(l, z)$ as defined by (125) is the probability that a walker survives for a time t. Clearly, if a walker has survived without being trapped, he must be at a typical non-trapping lattice point. Hence the probability of surviving after n steps is

$$S_n = \sum_{l \notin N} P_n(l) \tag{132}$$

Hence the generating function for S_n is

$$S = \sum_n S_n z^n = \sum_{l \notin N} P(l, z) \tag{133}$$

so that in the presence of our absorbing barrier (or plane of traps) at $l_1 = 0$ we have from the definition (118) of $P(l, z)$

$$S(z) = \sum_{l=1}^{N-1} P(l, z)$$
$$= \sum_{l=1}^{N-1} [G(l - l_0, z) - G(l, z)G(-l_0, z)/G(0, z)] \tag{134}$$

Now from (131), since $g_{00}(l, z) \equiv G(l, z)$,

$$\sum_{l=1}^{N} G(l, z) = [2pz(1 - \eta)(\alpha_2 - \alpha_1)]^{-1} \{[\alpha_1/(1 - \alpha_1)] - [\alpha_2/(1 - \alpha_2)]\}$$
$$= [2pz(1 - \eta)(\alpha_2 - 1)(1 - \alpha_1)]^{-1} \tag{135}$$

Also,

$$\sum_{l=1}^{N} G(l - l_0, z) = \sum_{l=1}^{l_0-1} G(l - l_0, z) + \sum_{l=l_0}^{N} G(l - l_0, z)$$
$$= \sum_{l=1}^{l_0-1} G(N - l_0 + l, z) + \sum_{l=l_0}^{N} G(l - l_0, z)$$
$$= \sum_{l=1}^{N} G(l, z) = [2pz(1 - \eta)(\alpha_2 - 1)(1 - \alpha_1)]^{-1} \tag{136}$$

Since $G(-l^0, z) \equiv G(N - l_0, z)$ and $G(N, z) \equiv G(0, z)$, the summand in (134) vanishes when $l = N$. Hence no error is committed in extending the summation in (134) to include the $l = N$ term. Hence from (134)–(136) and

$$\alpha_1\alpha_2 = \eta/(1 - \eta), \qquad \alpha_1 + \alpha_2 = (1 - 4qz)/2pz(1 - \eta) \tag{137}$$

we see that

$$S(z) = (1 - z)^{-1}\{1 - [\Delta(N - l_0) - (\alpha_1\alpha_2)^N \Delta(-l_0)]/\Delta(N)\} \tag{138a}$$

where

$$\Delta(j) \equiv \alpha_1{}^j - \alpha_2{}^j \tag{138b}$$

The mean life of a walker before being trapped can be obtained directly from $S(z)$. Since S_n was defined to be the fraction of untrapped walkers surviving at the beginning of the nth time interval, the fraction of original walkers trapped during the nth time interval is

$$T_n \equiv S_{n+1} - S_n \tag{139}$$

The generating function for this quantity is

$$T(z) = \sum z^n T_n = \sum (S_{n+1} - S_n) z^n = z^{-1}(1 - z)S(z) \tag{140}$$

The mean life of a walker is then

$$\bar{n} = -(\partial T/\partial z)_{z=1} \tag{141}$$

The required coefficient is

$$\lim_{z \to 1} \partial[(1 - z)S(z)]/\partial z = -\bar{n} \tag{142}$$

Since

$$\alpha_2 = [\eta/(1 - \eta)](1 + \epsilon) \qquad \text{and} \qquad \alpha_1 = 1 - \epsilon \tag{143}$$

where

$$\epsilon = [(1 - z)/2p(2\eta - 1)] + O[(1 - z)^2] \tag{144}$$

we see that

$$\Delta(j) = (1 - \kappa^j) - \epsilon j(1 + \kappa^j) + O(\epsilon^2) \tag{145}$$

where

$$\kappa = \eta/(1 - \eta) \tag{146}$$

Hence

$$(1 - z)S(z) = \epsilon\left[(N - l_0) - N\frac{\kappa^{N-l_0} - 1}{\kappa^N - 1}\right] + O(\epsilon^2) \tag{147}$$

From (140), (143), and (147) one finds

$$\bar{n} = [2p(2\eta - 1)]^{-1}\left[(N - l_0) - N\frac{\kappa^{N-l_0} - 1}{\kappa^N - 1}\right] \tag{148}$$

The first term, proportional to $(N - l)$, represents loss of walkers by collision with the absorbing barrier at $l = N$, while the term proportional to $N\kappa^{-l_0}$ for large N represents capture at $l = 0$.

Let us assume that l_0 is large so that terms in the fraction in (148) can be neglected. Then, since $2p(2\eta - 1)$ is the speed of propagation of a pulse of walkers in our lattice and $\bar{n}$ represents the mean life of a walker before being trapped by the boundary at N, we see that (148) implies the reasonable result that the mean life is the distance the pulse travels before being trapped divided by the speed with which it approaches the trapping plane.

This result could also have been derived from Eq. (II.2a) in Ref. 4.

The mean first passage time for a random walker on a ring of N points periodically spaced to reach a point $N - l$ after starting from the origin is

$$\langle n(N - l)\rangle = N\{G(0, 1) - G(N - l, 1)\} \tag{149}$$

Here $G(l)$ is the random walk Green's function for the lattice,

$$G(l, z) = \frac{1}{N} \sum_{s=1}^{N} \frac{\exp(2\pi i s l/N)}{1 - z\lambda(2\pi s/N)} \tag{150}$$

If the form (124) is used for $\lambda(2\pi s/N)$ and if the sum is given by (129) as derived in Appendix C, then (149) becomes

$$\langle n(N - l)\rangle = N \lim_{z\to 1}[2p(1 - \eta)(\alpha_2 - \alpha_1)]^{-1} \left(\frac{1 - \alpha_1^{N-l}}{1 - \alpha_1^{N}} - \frac{1 - \alpha_2^{N-l}}{1 - \alpha_2^{N}}\right) \tag{151}$$

When the forms (143), (144), and (146) are substituted into this equation and the limit is taken one obtains exactly Eq. (148).

The above ideas can be extended to the case in which the waiting time between steps is the general function $\psi(t)$. The generalization of (125) is, analogous to the connection between (37) and (12),

$$\tilde{P}(l, t) = (1/2\pi i) \int_{c-i\infty}^{c+i\infty} (du/u)\, e^{ut}[1 - \psi^*(u)] \times [G(l - l_0, \psi^*(u)) - G(l, \psi^*(u))G(N - l_0, \psi^*(u))/G(0, \psi^*(u))] \tag{152}$$

where now the function $\tilde{P}(l, t)$ is the probability of a walker being at l at time t in the presence of the absorbing boundary at $l = N$. The probability function in (37) will now be denoted by $\tilde{G}(l, t)$, i.e., the unperturbed propagator. We further define the inverse transform of (109) [with $z = \tilde{\psi}^*(u)$]

$$\tilde{F}(l, t) = (1/2\pi i) \int_{c-i\infty}^{c+i\infty} du\, e^{ut} G(l, \psi^*(u))/G(0, \psi^*(u)) \tag{153}$$

where $\tilde{F}(l, t)$ is the probability density for reaching l for the first time at time t [see discussion in Section V in Ref. 4, especially Eq. (V.7)]. With (37) and (153) one can perform the inverse transform in (152) and obtain

$$\tilde{P}(l, t) = \tilde{G}(l - l_0, t) - \int_0^t d\tau\, \tilde{F}(N - l_0, \tau)\, \tilde{G}(l, t - \tau) \tag{154}$$

The interpretation of (154) is quite simple: The probability for a walker starting at l_0 at $t = 0$ to be found at l at time t, $\tilde{P}(l, t)$, is equal to the unperturbed propagator $l_0 \to l$ minus the contribution of all paths that have crossed the boundary [the second term on the right-hand side of (154)]. All the paths that cross the boundary at $l = N$ can be characterized by first grouping them according to the probability per unit time of reaching N from l_0 for the first time at some earlier time τ, $\tilde{F}(N - l_0, \tau)$, and then propagating back to l with an arbitrary number of crossings through the boundary in the remaining time $t - \tau$, $\tilde{G}(l, t - \tau) = \tilde{G}(-[N - l], t - \tau)$. For the total of the above paths one sums over all times τ up to the time of observation t.

In Figs. 1–4 we have shown the results of a computation of the unperturbed propagator [designated $\tilde{P}(l, t)$ in Section 2] for various $\psi(t)$ and bias conditions. Thus to calculate $\tilde{P}(l, t)$ in (154) one must now determine $\tilde{F}(l, \tau)$ and then perform the τ integration. We will pursue this in another paper.

As a final point, one can get some information about numerical effects of the boundary by examining the time dependence of the mean $\langle l \rangle$ of $\tilde{P}(l, t)$ in (152), which is proportional to the transient current $J(t)$ [i.e., $J(t) \propto d\langle l \rangle / dt$] in the experiments alluded to in the beginning of Section 1.

For the large-time behavior of $\tilde{P}(l, t)$ we examine the small-u behavior of the integrand in (152). Such asymptotic behavior can be discussed quite rigorously.[12] However, it is our purpose to simply examine how the boundary at $l = N$ manifests itself in the expression (152). The small-u behavior in (152) is characterized by

$$1 - \tilde{\psi}^*(u) \to cu^\alpha \tag{155}$$

where we have given examples in Section 2 of $\tilde{\psi}^*(u)$ with $\alpha = 1/2$ and $\alpha = 1$ [in general if the first moment of $\psi(t)$ exists, then one always obtains $\alpha = 1$, $c = \bar{t}$]. Analogous to (144), let us define $1 - \psi^*(u) \equiv \bar{l}_1 \epsilon$. With the limit $\epsilon \to 0$ it is apparent that only singular terms (i.e., terms containing inverse powers of ϵ) in the second set of brackets in (152) give rise to anything other than contributions to $\tilde{P}(l, t)$ falling off with increasing t. Therefore for a qualitative understanding of

$$\langle l \rangle \equiv \sum_{l=1}^{N} l\tilde{P}(l, t) \tag{156}$$

we investigate the singular structure of

$$L(z) \equiv \sum_{l=1}^{N} l\{G(l - l_0, z) - G(l, z)G(N - l_0, z)/G(0, z)\} \tag{157}$$

where now $z = \tilde{\psi}^*(u)$. One can compute the sums in (157) and write

$$G(N - l_0, z)/G(0, z) = 1 - (1 - z)S(z) \tag{158}$$

with $S(z)$ defined in 138a,

$$\sum_{l=1}^{N} lG(l-l_0, z) = \sum_{l=1}^{N} lG(l, z) + l_0 \sum_{l=1}^{N} G(l, z) - N \sum_{l=N-l_0+1}^{N} G(l, z)$$
$$= \bar{l}(z) + [l_0/1-z] - N[2pz(1-\eta)(\alpha_2-\alpha_1)]^{-1}$$
$$\times \left[\frac{\alpha_1}{1-\alpha_1} \frac{\alpha_1^{N-l_0} - \alpha_1{}^N}{1-\alpha_1{}^N} - (\alpha_2 \leftrightarrow \alpha_1)\right] \tag{159}$$

where

$$\bar{l}(z) \equiv \sum_{l=1}^{N} lG(l, z) = [2pz(1-\eta)(\alpha_2-\alpha_1)]^{-1}$$
$$\times \left[\frac{\alpha_1}{(1-\alpha_1)^2} - \frac{N\alpha_1^{N+1}}{(1-\alpha_1)(1-\alpha_1{}^N)} - (\alpha_2 \leftrightarrow \alpha_1)\right] \tag{160}$$

Recalling (143), i.e., $\alpha_1 = 1-\epsilon$ and $\alpha_2 = \kappa(1+\epsilon)$ for $\epsilon \to 0$ ($\kappa > 1$), one observes two types of singular terms in (157)–(160). They are proportional to $(1-\alpha_1)^{-1}$ and $(1-\alpha_1{}^N)^{-1}$, respectively. Now although $\alpha_1 \gg 1$, the term $\alpha_1{}^N$ could be very small:

$$\alpha_1{}^N \simeq e^{-N\epsilon}, \qquad \epsilon \ll 1 \tag{161}$$

and for $N\epsilon \gg 1$, $\alpha_1{}^N \to 0$. Thus the singular structure of $L(z)$ is determined by $\epsilon \to 0$; however, even for small ϵ one has two regions to consider: (i) $N\epsilon > 1$ and (ii) $N\epsilon < 1$. Hence the presence of a boundary in (152) is manifested through the $(1-\alpha_1{}^N)^{-1}$ terms. In region (i) one can show

$$G(N-l_0, z)/G(0, z) \simeq \alpha_1^{N-l_0} + \alpha_2^{-l_0} \simeq e^{-(N-l_0)\epsilon} + \kappa^{-l_0} e^{-l_0\epsilon} \tag{162}$$

The right-hand side of (162) is much less than one if $(ln\ \kappa)^{-1} < l_0 \ll N$ (which we assume) and one can approximate $L(z)$ by the expression in (159). Thus in region (i), $\langle l \rangle$ is essentially identical to that calculated in Section 2 for various $\psi(t)$. In region (ii)

$$G(N-l_0, z)/G(0, z) \to 1 - \epsilon(N - l_0 - N\kappa^{-l_0}) \tag{163}$$

This is essentially the result obtained in (147) with the assumption $\kappa^N \gg 1$ (e.g., for $\kappa = 1.5$ and $N = 256$, $\kappa^N = 1.2 \times 10^{45}$). Inserting (163) in the right-hand side of (157), we find a cancellation of $\bar{l}(z)$ between the first and second terms. Further, in the limit $\alpha_1{}^N \to 1$ there is a cancellation of the second term in (159) with the ϵ^{-1} term in the third term. Thus,

$$L(z) \simeq \epsilon(N - l_0 - N\kappa^{-l_0})\,\bar{l}(z) + \text{const} \tag{164}$$

Now, the limit of $\bar{l}(z)$ for $\alpha_1{}^N \to 1$ is very interesting. The ϵ^{-2} terms in (160) cancel and

$$\bar{l}(z) \approx (1/\bar{l}_1\epsilon)(N+1)/2 \tag{165}$$

One thus arrives at the final result that in region (ii)

$$\langle l \rangle \to 0 \tag{166}$$

and since $l = N$ and $l = 0$ are equivalent,[6] one simply has the mean position coinciding with the position of a totally absorbing boundary for $t \to \infty$. The condition for the transition between region (i) and region (ii) can be expressed [using (155)] as

$$1 \sim N\epsilon = Ncu^\alpha/\bar{l}_1 \sim (Nc/\bar{l}_1)t_r^{-\alpha} \tag{167}$$

or t_r the "transit time" is

$$t_r \sim (Nc/\bar{l}_1)^{1/\alpha} \tag{168}$$

for $0 < \alpha < 1$ and

$$t_r \sim N\bar{t}/\bar{l}_1 \tag{169}$$

for $\tilde{\psi}^*(u) \to 1 - \bar{t}u$.

If one considers *only* the "free propagator" [i.e., the $G(l - l_0, z)$ term in (157)] in region (ii), one determines

$$\langle l \rangle \to (N+1)/2 \tag{170}$$

where use has been made of the result in (165). The meaning of this limiting value for $\langle l \rangle$ for the free propagation is apparent if one considers

$$\langle l \rangle = \sum_{l=1}^{N} l\tilde{G}(l, t) \underset{t\to\infty}{\to} \sum_{l=1}^{N} (l/N) = (N+1)/2 \tag{171}$$

The fact that $\tilde{G}(l, t) \to 1/N$ is a consequence of the periodic boundary condition, i.e., propagation around a "ring." Transport around the ring become stationary, $d\langle l \rangle/dt \to 0$, as $t \to \infty$. We have determined the correct $(t \to \infty)$ limit in (171) as we did not differentiate with respect to k (see footnote 4). The results for $\langle l \rangle$ in Section 2 are valid for $N \to \infty$, i.e., before the packet encounters the boundary.

APPENDIX A. LAPLACE TRANSFORM OF REPEATED INTEGRALS OF THE COMPLIMENTARY ERROR FUNCTION

We shall consider the Laplace transform of the function

$$f_n(t) = C_n a^2[\exp(a^2 t)] i^n \operatorname{Erfc}(at^{1/2}) \tag{A.1}$$

[6] We have used the periodic property of $G(l, z)$ in (159).

where $i^n \operatorname{Erfc}(z)$ is the nth repeated integral of the complimentary error function defined in (41) by

$$i^n \operatorname{Erfc}(z) = (2/\pi^{1/2}n!) \int_z^\infty (y - z)^n \exp(-y^2)\, dy \tag{A.2}$$

and C_n is a normalizing constant. Inserting (A.2) into (A.1) and changing the variable of integration, we have

$$f_n(t) = (C_n a^2 2/\pi^{1/2}n!) \int_0^\infty ds\, s^n \exp(-s^2 - 2at^{1/2}s) \tag{A.3}$$

The Laplace transform

$$\begin{aligned} \mathscr{L}(f_n(t)) \equiv F_n(u) &= \int_0^\infty dt\, e^{-ut} f_n(t) \\ &= (C_n a^2 2/\pi^{1/2}n!) \int_0^\infty dt\, e^{-ut} \int_0^\infty ds\, s^n \exp(-s^2 - 2at^{1/2}s) \end{aligned} \tag{A.4}$$

can be calculated by interchanging the order of integration in (A.4) to obtain

$$\begin{aligned} F_n(u) &= (C_n a^2 2/\pi^{1/2}n!) \int_0^\infty ds\, s^n(\exp -s^2) \int_0^\infty dt \exp(-ut - 2ast^{1/2}) \\ &= (C_n a^2/\pi^{1/2}n!)\, u^{(n-1)/2} \\ &\quad \times \int_0^\infty dx\, e^{-ux} x^{n/2}[x^{-1/2} - \pi^{1/2} a \exp(a^2 x) \operatorname{Erfc}(ax^{1/2})] \end{aligned} \tag{A.5}$$

where $s^2 \equiv ux$. Now considering only even integers for n and using the well known property[10]

$$\mathscr{L}\{x^m f(x)\} = (-)^m\, d^m g(u)/du^m \tag{A.6}$$

where

$$g(u) = \mathscr{L}\{f(x)\} \tag{A.7}$$

we derive

$$F_{2m}(u) = \frac{C_{2m}}{(2m)!} (-)^m s^{m-(1/2)} \frac{d^m}{ds^m} (s^{1/2} + 1)^{-1} \tag{A.8}$$

where $s \equiv u/a^2$. In general the form of $F_{2m}(u)$ can easily be seen to be

$$F_{2m}(u) = \frac{P_{m-1}(s^{1/2})}{(s^{1/2} + 1)^{m+1}} \tag{A.9}$$

where $P_{m-1}(x)$ is a polynomial of degree $m - 1$ and $P_{m-1}(0) = 1$. Using an expansion of (A.4) in powers of $u^{1/2}$, one can show

$$C_{2m}/(2m)! = 2\Gamma(\tfrac{1}{2})/\Gamma(m - \tfrac{1}{2}) \tag{A.10}$$

The first five explicit expressions for $F_{2m}(u)$ are

$$F_2(u) = 1/(s^{1/2} + 1)^2 \tag{A.11}$$

$$F_4(u) = (3s^{1/2} + 1)/(s^{1/2} + 1)^3 \tag{A.12}$$

$$F_6(u) = (5s + 4s^{1/2} + 1)/(s^{1/2} + 1)^4 \tag{A.13}$$

$$F_8(u) = [7s^{3/2} + (47/5)s + 5s^{1/2} + 1]/(s^{1/2} + 1)^5 \tag{A.14}$$

$$F_{10}(u) = [9s^2 + (122/7)s^{3/2} + (102/7)s + 6s^{1/2} + 1]/(s^{1/2} + 1)^6 \tag{A.15}$$

The rational functions $F_{2m}(u)$ have the fascinating property that the derivatives

$$\mu_j^{(m)} \equiv \left.\frac{d^j F_{2m}(u)}{du^j}\right|_{u=0} \tag{A.16}$$

only exist for $j < m$. Now for distribution functions $\psi_{(m)}(t) = f_{2m}(t)$ the $\mu_j^{(m)}$ are equal to the jth moment of $\psi_{(m)}(t)$. Thus the functions $\{\psi_{(m)}(t)\}$ represent a particularly versatile set of distributions. One can choose a $\psi(t)$ [from $\psi_{(m)}(t)$] with a finite number of moments and one can vary this number from zero to any arbitrary value. In the text we have derived the characteristic function for $\psi(t) = f_2(t)$. In the next appendix we shall derive $\gamma(k, t)$ for $\psi(t) = f_4(t)$.

APPENDIX B. CHARACTERISTIC FUNCTION $\gamma(k, t)$ FOR $\psi(t) = f_4(t)$

For

$$f_4(t) = 4!\, 4a^2[\exp(a^2t)]i^4 \operatorname{Erfc}(at^{1/2}) \tag{B.1}$$

[denoted $\psi_4(t)$ in (86)] the first moment $\mu_1^{(4)}$ exists and all higher moments are infinite. In this appendix we shall derive the characteristic function corresponding to $\psi(t) = f_4(t)$. From (52) and (53)

$$\gamma(k, t) = 1 - [1 - \lambda(k)]\, I\{h(s)\} \tag{B.2}$$

$$I\{h(s)\} = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{e^{s\tau}\, ds}{s\{h(s) - \lambda(k)\}} \tag{B.3}$$

with $\tau \equiv a^2t$ and $h(s) \equiv [\psi^*(u/a^2)]^{-1}$. The Laplace transform of $f_4(t)$ is given in (A.12). Therefore we must compute

$$I\{h(s)\} = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{e^{s\tau}\, ds}{s\{(s^{1/2} + 1)^3/(3s^{1/2} + 1) - \lambda(k)\}}$$

$$= \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{ds}{s}\, \frac{e^{s\tau}(3s^{1/2} + 1)}{(s^{1/2} + 1)^3 - 3\lambda(k)(s^{1/2} + 1) + 2\lambda(k)} \tag{B.4}$$

We determine the roots z_i that satisfy the equation

$$z_i^3 - 3\lambda z_i + 2\lambda = 0 \tag{B.5}$$

We have

$$z_1 = s_1 + s_2 \tag{B.6}$$

$$z_2 = -e^{-i\pi/3}s_1 - e^{i\pi/3}s_2 \tag{B.7}$$

$$z_3 = -e^{-i\pi/3}s_2 - e^{i\pi/3}s_1 \tag{B.8}$$

where

$$\left.\begin{matrix} s_1 \\ s_2 \end{matrix}\right\} = [-\{1 \mp [1 - \lambda(k)]^{1/2}\}\lambda(k)]^{1/3} \tag{B.9}$$

For $\lambda(k) \to 1$

$$\left.\begin{matrix} s_1 \\ s_2 \end{matrix}\right\} \to e^{\pm i\pi/3} \tag{B.10}$$

and $z_1 \to 1$, $z_2 \to 1$, $z_3 \to -2$. To correctly obtain the limiting values of z_i for $\lambda(k) \to 1$, we choose the cut in the complex z-plane along the negative real axis ($-\pi < \arg z \leqslant \pi$). The denominator in (B.5) is factored and the integrand is expanded into partial fractions, with the result

$$\gamma(k, t) = 1 - [1 - \lambda(k)] \sum_{i=1}^{3} \frac{z_i - 2/3}{[z_i^2 - \lambda(k)](1 - z_i)} \{1 - F([1 - z_i]\tau^{1/2})\} \tag{B.11}$$

where $F(z) \equiv (\exp z^2) \operatorname{Erfc}(z)$. The roots $\{z_i\}$ satisfy the following:

$$z_1 + z_2 + z_3 = 0 \tag{B.12}$$

$$z_1 z_2 + z_1 z_3 + z_2 z_3 = -3\lambda(k) \tag{B.13}$$

$$z_1 z_2 z_3 = -2\lambda(k) \tag{B.14}$$

in addition to the defining equation (B.6). With the use of (B.6) and (B.13)–(B.15) and some algebraic manipulation we can simplify $\gamma(k, t)$ in Eq. (B.12) to the following:

$$\gamma(k, t) = \sum_{i=1}^{3} (z_i^2 + 2z_i)F([1 - z_i]\tau^{1/2})/6\lambda(k) \tag{B.15}$$

To calculate $\langle l_1 \rangle$, we calculate $\partial\gamma/\partial\lambda$ and take the limit $\lambda \to 1$,

$$\left.\frac{\partial\gamma}{\partial\lambda}\right|_{\lambda\to 1+i\epsilon} \to \frac{\tau}{3} + \frac{16\tau^{1/2}}{9\sqrt{\pi}} + \frac{8}{27}[F(3\tau^{1/2}) - 1] \tag{B.16}$$

so that

$$\langle l \rangle \propto \tau \qquad \text{for large} \quad \tau \tag{B.17}$$

in contrast to (77) and (80).

APPENDIX C. EVALUATION OF THE SUM IN EQ. (127)

$$S(l) \equiv \frac{1}{N} \sum_{s=1}^{N} \frac{e^{2\pi isl/N}}{1 - Pe^{2\pi is/N} - Qe^{-2\pi is/N}} \tag{C.1}$$

we write

$$1 - Px - Qx^{-1} = -(P/x)(x - \alpha_1)(x - \alpha_2) \qquad \text{with } x \equiv e^{2\pi is/N} \tag{C.2}$$

where

$$\left.\begin{matrix}\alpha_2\\ \alpha_1\end{matrix}\right\} = (1/2P)[1 \pm (1 - 4PQ)^{1/2}] \tag{C.3}$$

We will be concerned with the case in which $|\alpha_2| > 1 \geqslant |\alpha_1|$. Then, since $|x| = 1$, when $l > 0$

$$S(l) = -(NP)^{-1} \sum_{s=1}^{N} \frac{e^{2\pi i(l+1)/N}}{\alpha_1 - \alpha_2} \left(\frac{1}{x - \alpha_1} - \frac{1}{x - \alpha_2}\right) \tag{C.4}$$

$$= [NP(\alpha_2 - \alpha_1)]^{-1} \sum_{s=1}^{N} e^{2\pi i(l+1)s/N} \{x^{-1}[1 + (\alpha_1/x) + (\alpha_1/x)^2 + \cdots]$$

$$+ \alpha_2{}^1[1 + (x/\alpha_2) + (x/\alpha_2)^2 + \cdots]\} \tag{C.5}$$

$$[NP(\alpha_2 - \alpha_1)]^{-1} [\alpha_1{}^l(1 + \alpha_1{}^N + \alpha_1^{2N} + \cdots)$$

$$+ \alpha_2{}^l(\alpha_2^{-N} + \alpha_2^{-2N} + \alpha_2^{-3N} + \cdots)] \tag{C.6}$$

since

$$N^{-1} \sum_{s=1}^{N} e^{2\pi ils/N} = \begin{cases} 1 & \text{if } \; l = 0, \pm N, \pm 2N, \pm 3N, \ldots \\ 0 & \text{for } \; \text{other integral } N \end{cases} \tag{C.7}$$

Hence

$$S(l) = [P(\alpha_2 - \alpha_1)]^{-1} [\alpha_1{}^l(1 - \alpha_1{}^N)^{-1} - \alpha_2{}^l(1 - \alpha_2{}^N)^{-1}] \tag{C.8}$$

Note also from (4) that if $N > l > 0$

$$S(-l) = S(N - l) = [P(\alpha_2 - \alpha_1)]^{-1} [\alpha_1^{N-l}(1 - \alpha_1{}^N)^{-1} - \alpha_2^{N-l}(1 - \alpha_2{}^N)^{-1}] \tag{C.9}$$

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