Asymptotic Properties of Multistate Random Walks. I. Theory

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A calculation is presented of the long-time behavior of various random walk properties (moments, probability of return to the origin, expected number of distinct sites visited) for *multistate* random walks on periodic lattices. In particular, we consider inhomogeneous periodic lattices, consisting of a periodically repeated unit cell which contains a finite number of internal states (sites). The results are identical to those for perfect lattices except for a renormalization of coefficients. For walks without drift, it is found that all the asymptotic random walk properties are determined by the diffusion coefficients for the multistate random walk. The diffusion coefficients can be obtained by a simple matrix algorithm presented here. Both discrete and continuous time random walks are considered. The results are not restricted to nearest-neighbor random walks but apply as long as the single-step probability distributions associated with each of the internal states have finite means and variances.

KEY WORDS: Multistate random walks; embedded Markov chain; inhomogeneous periodic lattices.

1. INTRODUCTION

Considerable interest has developed recently in the theory of multistate random walks because of the variety of physical and chemical processes which can be modeled by such random walks (for a review see, e.g., Ref. 1). The basic concept is that the walker, while moving on a lattice, can be in a number of internal states; and the properties of the random walk depend on the nature of these states. Such internal states can be different energy

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levels or spin states, but we will be concerned here only with the case of *configurational internal states*. That is, we consider random walks on lattices which are built up by periodically repeated unit cells. The unit cells themselves contain several nonequivalent sites which are now considered as internal states. Such constructs can be termed *inhomogeneous periodic lattices*; for succinctness, we will refer to them simply as inhomogeneous lattices. Because such lattices are globally translation invariant, the time dependence of the random walk properties is the same as for perfect lattices (i.e., periodic lattices with one site per unit cell), and only a renormalization of coefficients occurs. The question to be answered is how the presence of internal states affects these coefficients.

The main motivation for this study arose out of a series of papers by Silver, Shuler, and Lindenberg[2]; Shuler[3]; and Seshadri, Lindenberg, and Shuler.[4] These studies were concerned with nearest-neighbor random walks on so-called sparsely periodic or random lattices. Such lattices are obtained from a regular lattice by periodically (or randomly) removing a number of vertical columns. A two-dimensional example is shown in Fig. 1. On this lattice, motion in the y direction is possible only at a subset of points, the so-called intersection sites. The case shown in Fig. 1 represents a sparsely periodic lattice with horizontal periodicity k, i.e., there is one vertical connection for every kth site along the horizontal direction. Random walk properties for such lattices have been obtained by rather complicated
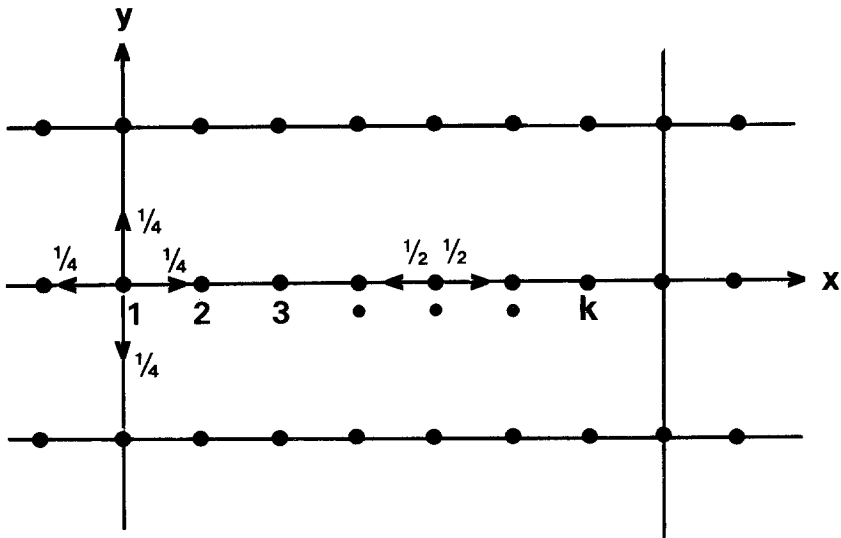

Fig. 1.   Sparsely periodic two-dimensional lattice with periodicities $k_x = k$, $k_y = 1$.

generating function techniques[2,4] as well as by probabilistic methods.[5,6] On the other hand, a set of simple assumptions has been proposed[3] [called the bond enumeration method (B.E.M)], which reproduce the correct asymptotic random walk properties and which are based on counting the number of bonds in the unit cell in the various space directions.

In order to investigate the range of validity of the B.E.M., we derive in this paper simple expressions for various properties [occupation probabilities, moments, probability of return to the origin, expected number of distinct sites visited] of multistate random walks in the long-time limit. In this way a quick comparison of such properties for different types of inhomogeneous lattices becomes possible without the need of computing the generating functions for each different case. The explicit question of the range of validity of the B.E.M. will be reserved for another paper.[7]

In paper II of this series[8] we will touch upon another important theme in the work cited above,[2–6] namely, the question under which conditions the properties of the random walk do not depend upon the spatial arrangement of the nonequivalent sites within the unit cell but only upon their density. For the sparsely periodic lattices mentioned above, it has been shown that for a fixed density of vertical columns the random walk properties are identical for periodic and nonperiodic or random distributions of vertical columns,[3] provided that certain asymptotic uniformity conditions are satisfied.[5,6] We will present additional examples for which this is the case as well as examples where the detailed spatial arrangements cannot be ignored.

Among earlier approaches to random walks with internal states, we mention those of Landman, Montroll, and Shlesinger,[10] and of Landman and Shlesinger[11,12] in the context of continuous time random walks (CTRW's). The latter authors present two different and lengthy prescriptions to calculate the asymptotic behavior of the moments of the walk. In this paper we present an algorithm to obtain these moments which is much simpler, especially for walks for which the average single-step displacement from each site of the lattice in each direction is zero.[4] The probability of return to the origin and the expected number of distinct sites visited were not discussed in the papers cited above. The simple relations we establish in this paper between these properties and the moments of the walk permit us to include these properties in calculations of specific examples without additional effort.

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[3] A similar result has been found in the one-dimensional waiting time Lorentz model, where the diffusion coefficient is identical for lattices with fixed and with random intervals between scatterers for a given density of scatterers.[9]

[4] We will call such walks "locally unbiased"; see Section 2.2.

The organization of this paper is as follows. Section 2 is devoted to the case of discrete time random walks with internal states. The main mathematical tool in the derivations is Darboux' method,[13] applied to the matrix generating functions for the various random walk properties. The case of continuous time random walks is considered in Section 3, where Darboux' method is replaced by the Hardy–Littlewood–Karamata theorem,[14] applied to the Laplace transforms of the random walk properties. In Section 4 we present a summary of this paper and draw some conclusions.

We stress that the method developed here is not restricted to nearest-neighbor random walks. We only require that the means and variances of the distributions of jump distances for every site of the unit cell be finite.

2. DISCRETE TIME RANDOM WALKS

2.1. Introduction

Consider a d-dimensional lattice with fundamental translation vectors $\mathbf{a}_1, \mathbf{a}_2,..., \mathbf{a}_d$, i.e., the arrangement of all the sites as seen from a position $\mathbf{r}$ is the same as that seen from a position

$$\mathbf{r}' = \mathbf{r} + \sum_{i=1}^{d} l_i \mathbf{a}_i \tag{2.1.1}$$

where $l_i = 0, \pm 1, \pm 2,...$.[15] The vectors $\{\mathbf{a}_i\}$ define a d-dimensional parallelopipid, which is called a unit cell. We will use primitive translation vectors so that the resulting unit cell is the smallest possible one. The translation vectors are not necessarily orthogonal.

The unit cell contains a number of inequivalent sites or "internal states." These will be referenced by an index α, where $\alpha = 1, 2,..., m$. The position of a particular unit cell is labeled by a vector l, where the components of l are integers, as in (2.1.1). Accordingly, we will indicate the position of a random walker on an inhomogeneous periodic lattice by the symbol (l, α). In the following we will always indicate internal states by Greek indices $(\alpha, \beta, \gamma,...)$ and the various space directions by Latin indices $(i, j, k,...)$.

Now consider a discrete time random walk (DTRW) on such a lattice. A basic quantity of interest is $P_{\alpha\beta}^{(n)}(l \mid l_0)$, the probability that the walker is at site (l, α) after n steps, having started from (l_0, β). By the global translation invariance of the lattice, $P_{\alpha\beta}^{(n)}(l \mid l_0)$ depends only on the difference

$l - l_0$, hence we will take $l_0 = 0$ in what follows and write $P_{\alpha\beta}^{(n)}(l)$ for $P_{\alpha\beta}^{(n)}(l \mid 0)$, etc. Conservation of probability is expressed by

$$\sum_{\alpha} \sum_{l} P_{\alpha\beta}^{(n)}(l) = 1 \tag{2.1.2}$$

The evolution of the random walk is described by the Chapman–Kolmogorov equation for Markov chains,

$$P_{\alpha\beta}^{(n+1)}(l) = \sum_{l',\gamma} T_{\alpha\gamma}(l - l') \, P_{\gamma\beta}^{(n)}(l') \tag{2.1.3}$$

Here $T_{\alpha\gamma}(l - l')$ is the single-step transition probability from site (l', γ) to site (l, α), which again only depends on the difference $l - l'$. It is convenient to use the matrix representation

$$P_{\alpha\beta}^{(n)}(l) = [\mathsf{P}^{(n)}(l)]_{\alpha\beta}$$

etc., so that (2.1.3) becomes the matrix equation

$$\mathsf{P}^{(n+1)}(l) = \sum_{l'} \mathsf{T}(l - l') \, \mathsf{P}^{(n)}(l') \tag{2.1.4}$$

The dimension of all the matrices in (2.1.4) is $m \times m$, where m is the number of internal states.

The derivation of many random walk properties is facilitated by introducing the *matrix generating function*

$$\mathsf{G}(l, z) = \sum_{n=0}^{\infty} z^n \mathsf{P}^{(n)}(l) \tag{2.1.5}$$

It can be shown that[16]

$$\mathsf{G}(l, z) = (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\boldsymbol{\theta} \, \boldsymbol{\Gamma}(\boldsymbol{\theta}, z) \, e^{-il \cdot \boldsymbol{\theta}} \tag{2.1.6}$$

where

$$\boldsymbol{\Gamma}(\boldsymbol{\theta}, z) = [1 - z\boldsymbol{\Lambda}(\boldsymbol{\theta})]^{-1} \tag{2.1.7}$$

and

$$\boldsymbol{\Lambda}(\boldsymbol{\theta}) = \sum_{l} \mathsf{T}(l) \, e^{il \cdot \boldsymbol{\theta}} \tag{2.1.8}$$

Here $\mathsf{T}(l)$ is the matrix of transition probabilities occurring in (2.1.4).

The basic assumption we will make is that the random walk is irreducible, i.e., each site of the lattice can be reached from every other site

after a sufficient number of steps.[5] The class of irreducible Markov chains can be subdivided into aperiodic (or primitive) walks and periodic (or cyclic) walks.[17,18] The transition matrix associated with an irreducible (aperiodic, periodic) walk is called irreducible (aperiodic, periodic). An irreducible stochastic matrix is defined as follows:

Definition.   A nonnegative matrix Q is called irreducible if for every α and β there exists an integer $\mathcal{M}(\alpha, \beta)$ such that $(Q^n)_{\alpha\beta} > 0$ if $n \geqslant \mathcal{M}(\alpha, \beta)$.

If an $\mathcal{M}$ can be found which does not depend on α and β, Q is aperiodic. If in addition $\sum_\alpha Q_{\alpha\beta} = 1$, the matrix is called a stochastic irreducible matrix (periodic or aperiodic).

At this point we make the following observation, which will play an important role in what follows. The probability $P_{\alpha\beta}^{(n)} = \sum_l P_{\alpha\beta}^{(n)}(l)$ that the walker is in internal state α after n steps, having started in state β, irrespective of the particular unit cell which the walker occupies after the nth step, obeys the equation [we use (2.1.4)]

$$\mathsf{P}^{(n+1)} = \mathsf{T}\mathsf{P}^{(n)} \qquad\qquad (2.1.9)$$

where the matrix T is defined by

$$\mathsf{T} = \sum_l \mathsf{T}(l) \qquad\qquad (2.1.10)$$

In view of the normalization of the transition probabilities, we have

$$\sum_\alpha T_{\alpha\beta} = 1 \qquad\qquad (2.1.11)$$

so T is a stochastic matrix. Hence, we see that by ignoring the position of the unit cell, one obtains an embedded Markov chain on the finite set of internal states. If the original random walk on the infinite inhomogeneous lattice (or finite lattice with periodic boundary conditions) is irreducible, the embedded Markov chain is also irreducible. Hence T is a finite irreducible stochastic matrix. Such matrices have in general a number, say p, of simple eigenvalues, of the form

$$\lambda_\alpha = \exp\left(\frac{2\pi i}{p}\,\alpha\right), \qquad \alpha = 0, 1, 2,\dots, p-1 \quad (p \leqslant m) \qquad (2.1.12)$$

The integer p is called the period. Aperiodic matrices have only a single eigenvalue $\lambda_0 = 1$ with absolute value 1; thus, the period $p = 1$. If the matrix

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[5] We follow the terminology of Seneta[17]; unfortunately, there is no agreement as to terminology in the vast literature on this subject.

T in (2.1.9) is aperiodic, the ergodic theorem for primitive Markov chains[17] leads to the asymptotic result

$$P_{\alpha\beta}^{(n)} \to \pi_\alpha \qquad (n \to \infty) \tag{2.1.13}$$

independent of the starting site β. The vector $\pi = \mathrm{Col}\{\pi_1, \pi_2,..., \pi_m\}$ is the normalized right eigenvector of T corresponding to the maximal eigenvalue $\lambda_0 = 1$. The components $\pi_1, \pi_2,..., \pi_m$ represent the equilibrium occupation probabilities of the walker to be in internal state $1, 2,..., m$. In the periodic case the limit (2.1.13) no longer exists, but the eigenvector π continues to play an important role, as will become clear below.

We now turn to the determination of the asymptotic behavior as n, the number of steps, goes to infinity of various random walk properties, in particular the moments of $P_{\alpha\beta}^{(n)}(l)$, the probability of return to the origin and the expected number of distinct sites visited. It should be noted that the only restriction made up to this point is that the random walk on the inhomogeneous periodic lattice (i.e., the multistate random walk) is irreducible. The results presented below are thus very general and are valid regardless of any assumed lattice structure, as long as a unit cell can be defined which generates the lattice.

2.2. Moments

2.2.1. Moments of $P_{\alpha\beta}^{(n)}(l)$.   The first moment of $P_{\alpha\beta}^{(n)}(l)$ is defined by

$$\langle l_j(n) \rangle_{\alpha\beta} \equiv \sum_l l_j P_{\alpha\beta}^{(n)}(l) \qquad (j = 1, 2,..., d) \tag{2.2.1}$$

The corresponding generating function $L_{\alpha\beta}^{(j)}(z) \equiv \sum_{n=0}^{\infty} z^n \langle l_j(n) \rangle_{\alpha\beta}$ is given by

$$L_{\alpha\beta}^{(j)}(z) = \sum_l l_j G_{\alpha\beta}(l, z) = -i \left[\frac{\partial}{\partial \theta_j} \Gamma_{\alpha\beta}(\boldsymbol{\theta}, z) \right]_{\boldsymbol{\theta}=0} \tag{2.2.2}$$

where $\Gamma(\boldsymbol{\theta}, z)$ is given by (2.1.7). Similarly, the generating function $L_{\alpha\beta}^{(jk)}(z)$ of the second moments $\langle l_j(n) l_k(n) \rangle_{\alpha\beta} \equiv \sum_l l_i l_j P_{\alpha\beta}^{(n)}(l)$ is

$$L_{\alpha\beta}^{(jk)}(z) = \sum_{n=0}^{\infty} z^n \langle l_j(n) l_k(n) \rangle_{\alpha\beta} = -\left[\frac{\partial}{\partial \theta_j} \frac{\partial}{\partial \theta_k} \Gamma_{\alpha\beta}(\boldsymbol{\theta}, z) \right]_{\boldsymbol{\theta}=0} \tag{2.2.3}$$

The large-n behavior of the moments can now be obtained by applying Darboux' method[13,19] to the respective generating functions. That is, one expands the generating functions around the singularities in the complex z plane. The dominant contribution comes from the singularities closest to

the origin, which for the cases considered here lie on the unit circle. The singularities outside it (if present) correspond to contributions which are exponentially small for large n. The coefficient of z^n in the part of the generating function which contains the dominant singularity (henceforth referred to as the singular part of the generating function) then yields the asymptotic behavior as $n \to \infty$ of the quantity considered.

As a first step, we introduce here the matrix H which diagonalizes the transition matrix T defined in (2.1.10) (or brings it into Jordan form if T is not diagonalizable), i.e.,[6]

$$H^{-1}TH \equiv \tilde{T} = \begin{bmatrix} \lambda_0 & | & \\ - - - & | & - - - \\ & | & \Omega \end{bmatrix} \tag{2.2.4}$$

We assume that T is irreducible, so that the eigenvalue $\lambda_0 = 1$ is simple and the submatrix Ω in (2.2.4) contains all the eigenvalues of T smaller than 1 on its diagonal. We use here the notation

$$\tilde{A} \equiv H^{-1}AH \tag{2.2.5}$$

for an arbitrary matrix A. The indices of all the matrices are labeled as $0, 1, \ldots, m-1$, so that $\tilde{T}_{00} = \lambda_0 = 1$, etc. The first column of H is identical to the eigenvector π as defined in the previous section, and the first row of H^{-1} is the corresponding left eigenvector which has all components equal to 1, so that

$$H_{\alpha 0} = \pi_\alpha, \qquad (H^{-1})_{0\beta} = 1 \tag{2.2.6}$$

Now we write the function $\Gamma_{\alpha\beta}(\mathbf{\theta}, z)$ in (2.2.2) and (2.2.3) as

$$\Gamma_{\alpha\beta}(\mathbf{\theta}, z) = \sum_{\alpha'\beta'} H_{\alpha\alpha'} \tilde{\Gamma}_{\alpha'\beta'}(\mathbf{\theta}, z)(H^{-1})_{\beta'\beta} \tag{2.2.7}$$

where, from (2.1.7)

$$\tilde{\Gamma}_{\alpha'\beta'}(\mathbf{\theta}, z) = \{[1 - z\tilde{\Lambda}(\mathbf{\theta})]^{-1}\}_{\alpha'\beta'} \tag{2.2.8}$$

and[7]

$$\tilde{\Lambda}(\mathbf{\theta}) \sim \tilde{T} + i\sum_j \theta_j \langle \tilde{l}_j \rangle - \frac{1}{2}\sum_{j,k} \theta_j\theta_k \langle \widetilde{l_j l_k} \rangle \qquad (\mathbf{\theta} \to \mathbf{0}) \tag{2.2.9}$$

We always write the single-step averages without argument, e.g., $\langle l_i \rangle_{\alpha\beta} \equiv \langle l_i(1) \rangle_{\alpha\beta} = \sum_l l_i T_{\alpha\beta}(l)$, etc. Notice that single-step transitions between the sites within the same unit cell do not contribute to the moments $\langle l_i \rangle_{\alpha\beta}$ and $\langle l_i l_j \rangle_{\alpha\beta}$.

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[6] Empty positions in matrices denote zeros.
[7] By $f(x) \sim g(x)$ as $x \to c$ we mean $\lim_{x \to c} [f(x)/g(x)] = 1$.

The singularities in (2.2.8) for $\theta = 0$ are located at the points in the z plane where $1 - z\lambda_\alpha = 0$, where $\{\lambda_\alpha\}$ are the eigenvalues of T. Hence the only singularity on the unit circle for an *aperiodic* matrix T occurs at $z = 1$, corresponding to the maximal eigenvalue $\lambda_0 = 1$. Thus the singular part $\Gamma_{\alpha\beta}^{(s)}(\theta, z)$ of $\Gamma_{\alpha\beta}(\theta, z)$ comes solely from the term with $\alpha' = \beta' = 0$ in (2.2.7),

$$\Gamma_{\alpha\beta}^{(s)}(\theta, z) = \pi_\alpha \tilde{\Gamma}_{00}(\theta, z) \qquad (2.2.10)$$

where we have used (2.2.6). By making use of the relation

$$\{[A + \varepsilon B + \varepsilon^2 C + O(\varepsilon^3)]^{-1}\}_{00}$$

$$= \left\{ A_{00} + \varepsilon B_{00} + \varepsilon^2 \left[C_{00} - \sum_{\beta,\gamma}{}' B_{0\beta}(A^{-1})_{\beta\gamma} B_{\gamma 0} \right] + O(\varepsilon^3) \right\}^{-1} \qquad (2.2.11)$$

for arbitrary matrices A, B, and C, where A is diagonal or of Jordan form (2.2.4) and ε a small parameter, we derive the following expansion:

$$\tilde{\Gamma}_{00}(\theta, z) \sim \left[1 - z \left\{ 1 + i \sum_j \theta_j m_j - \tfrac{1}{2} \sum_{j,k} \theta_j \theta_k s_{jk} \right\} \right]^{-1} \qquad (\theta \to 0) \qquad (2.2.12)$$

where

$$m_j = [\langle \tilde{l}_j \rangle]_{00} \qquad (2.2.13a)$$

and

$$s_{jk} = [\langle \widetilde{l_j l_k} \rangle]_{00} + \sum_{\beta,\gamma}{}' \{ [\langle \tilde{l}_j \rangle]_{0\beta} [(1 - \Omega)^{-1}]_{\beta\gamma} [\langle \tilde{l}_k \rangle]_{\gamma 0} + j \leftrightarrow k \} \qquad (2.2.13b)$$

Here Ω is the same as in (2.2.4), the prime on the summation signs indicates that $\beta \neq 0$ and $\gamma \neq 0$, and the symbol $j \leftrightarrow k$ denotes the same term as the preceding one, but with j and k interchanged. In fact, the matrix $(1 - \Omega)^{-1}$ in (2.2.13b) should be $(1 - z\Omega)^{-1}$, but we are interested in the behavior as $z \to 1$ and therefore have already put $z = 1$ in this factor. The error thus made is of order $(1 - z)^{-1}$ in $L_{\alpha\beta}^{(jk)}(z)$, i.e., of order unity in (2.2.17).

From (2.2.2), (2.2.3), and (2.2.10)–(2.2.13) we find

$$L_{\alpha\beta}^{(j)}(z) \sim \pi_\alpha m_j z(1 - z)^{-2} \qquad (z \to 1) \qquad (2.2.14)$$

and

$$L_{\alpha\beta}^{(jk)}(z) \sim \pi_\alpha \{ s_{jk} z(1 - z)^{-2} + 2z^2(1 - z)^{-3} m_j m_k \} \qquad (z \to 1) \qquad (2.2.15)$$

The large-n behavior of the moments is found by determining the coefficient of z^n in these expressions. The first moment is found as

$$\langle l_j(n) \rangle_{\alpha\beta} \sim \pi_\alpha n \cdot m_j \qquad (n \to \infty) \qquad (2.2.16a)$$

After summing over final states α and averaging over the (arbitrary) initial distribution $\{p_\beta^{(0)}\}$ of the internal states, we obtain

$$\langle l_j(n) \rangle \equiv \sum_{\alpha\beta} \langle l_j(n) \rangle_{\alpha\beta}\, p_\beta^{(0)} \sim m_j n \qquad (n \to \infty) \qquad (2.2.16\text{b})$$

Similarly we find from (2.2.15)

$$\langle l_j(n)\, l_k(n) \rangle_{\alpha\beta} \sim \pi_\alpha \{ n s_{jk} + n(n-1)\, m_j m_k \} \qquad (2.2.17)$$

Finally, the covariance, defined by

$$\langle\!\langle l_j(n)\, l_k(n) \rangle\!\rangle \equiv \left[\sum_{\alpha\beta} \langle l_j(n)\, l_k(n) \rangle_{\alpha\beta}\, p_\beta^{(0)} \right] - \langle l_j(n) \rangle \langle l_k(n) \rangle$$

is given by

$$\langle\!\langle l_j(n)\, l_k(n) \rangle\!\rangle \sim n \{ s_{jk} - m_j m_k \} \qquad (n \to \infty) \qquad (2.2.18)$$

The quantities m_j and s_{jk} in (2.2.16) and (2.2.18) are defined in (2.2.13) and can be expressed in terms of the moments of $T_{\alpha\beta}(l)$ and the eigenvalues and eigenvectors of T by using (2.2.5), e.g.,

$$m_j = \sum_{\alpha\beta} \langle l_j \rangle_{\alpha\beta}\, \pi_\beta \qquad (2.2.19)$$

If the matrix T is periodic, there are additional contributions in (2.2.10), corresponding to other singularities on the unit circle,

$$\Gamma_{\alpha\beta}^{(s)}(\boldsymbol{\theta}, z) = \sum_{\gamma=0}^{p-1} H_{\alpha\gamma}\, \tilde{\Gamma}_{\gamma\gamma}(\boldsymbol{\theta}, z)(H^{-1})_{\gamma\beta} \qquad (2.2.20)$$

where p is the period of T. However, since $\sum_\alpha H_{\alpha\gamma} = \delta_{\gamma,0}$,[8] the generating function (2.2.20), *summed over final states* α, involves only $\tilde{\Gamma}_{00}(\boldsymbol{\theta}, z)$. Hence in the periodic case the results (2.2.16b) and (2.2.18) remain valid.

    2.2.2. Moments of the Displacement. The moments of the actual displacement $\mathbf{r}(n)$ after n steps can be related to the moments (2.2.16) and (2.2.18). This is done in Appendix A. We give the results for the components $r_i(n) = \mathbf{r}(n) \cdot \mathbf{e}_i$, where $\{\mathbf{e}_i\}$ is a complete set of unit vectors, which span the d-dimensional space $\mathbb{R}^d$. The first moment is found to be

$$\langle r_i(n) \rangle \sim n V_i \qquad (n \to \infty) \qquad (2.2.21)$$

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[8] This follows from the fact that $(H^{-1})_{0\beta} = 1$ and $H^{-1}H = 1$.

where the factor V_i, called the "drift velocity" in direction $\mathbf{e}_i$, is given by

$$V_i = \sum_{k=1}^{d} m_k A_{ki} \tag{2.2.22}$$

For the covariances the result is[9]

$$\langle\!\langle r_i(n)\, r_j(n) \rangle\!\rangle \sim 2D_{ij}n \qquad (n \to \infty) \tag{2.2.23}$$

where D_{ij} is the (ij)th element of the matrix of diffusion coefficients

$$D_{ij} = \tfrac{1}{2} \sum_{k,l} \{ s_{kl} - m_k m_l \} A_{ki} A_{lj} \tag{2.2.24}$$

The quantities m_k and s_{kl} in (2.2.22) and (2.2.24) are defined in (2.2.13), while

$$A_{ki} = \mathbf{a}_k \cdot \mathbf{e}_i \tag{2.2.25}$$

Here $\mathbf{a}_k$ is the kth translation vector as defined in Section 2.1.

It should be emphasized that the quantities m_k and s_{kl} depend only on the *connectivity* of the lattice (or more precisely, of the random walk defined on it), but not on the length and direction of the steps.[10] The geometrical factors A_{ki} in the expressions for the moments of $\mathbf{r}(n)$ take account of the size and shape of the unit cell.

From (2.2.19) and (2.2.22) one notes that the asymptotic means of $l_j(n)$ or $r_j(n)$ only involve the eigenvector $\boldsymbol{\pi}$ of T belonging to the maximal eigenvalue $\lambda_0 = 1$. The asymptotic second moments, however, involve all eigenvalues and eigenvectors of T [see (2.2.13)], which in general are hard to calculate,[11] with the exception of the equilibrium eigenvector $\boldsymbol{\pi}$ which can often be obtained by physical arguments, such as detailed balance. It would thus be desirable to have an expression for the diffusion coefficients which involves only this vector $\boldsymbol{\pi}$. Such an expression does exist for the special class of walks for which the average single-step displacement from every site of the lattice in every space direction is zero. We will refer to such walks as *locally unbiased* (the term *symmetric walks* is avoided here since the matrix T for the class of walks just defined is not necessarily symmetric.) If we define $p_{\alpha\beta}(\mathbf{r})$ as the probability that the walker makes a step from internal state β to internal state α with corresponding displacement $\mathbf{r}$,

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[9] The factor $\tfrac{1}{2}$ in the definition of D_{ij} is customary in the physical and chemical literature.

[10] In paper II we will use this fact to calculate the diffusion coefficient of a locally biased walk by constructing an associated locally unbiased walk with the same connectivity properties as the original walk.

[11] The one-dimensional case is still tractable (see Ref. 20).

then the average single-step displacement in direction e_j from site β is defined by

$$\langle r_j \rangle_\beta \equiv \sum_r r_j \, p_\beta(\mathbf{r}) = \sum_\alpha \langle r_j \rangle_{\alpha\beta} \qquad (2.2.26)$$

where

$$p_\beta(\mathbf{r}) = \sum_\alpha p_{\alpha\beta}(\mathbf{r}), \qquad \langle r_j \rangle_{\alpha\beta} \equiv \sum_r r_j \, p_{\alpha\beta}(\mathbf{r}) \qquad (2.2.27)$$

For locally unbiased walks, we thus have that $\langle r_j \rangle_\beta = 0$, $\beta = 0, 1,..., m - 1$; $j = 1, 2,..., d$.[12]

If we define $P_{\alpha\beta}^{(n)}(\mathbf{r})$ as the probability that after n steps the displacement of the walker is $\mathbf{r}$, given initial state β and final state α, then again the Chapman–Kolmogorov equation holds,

$$P_{\alpha\beta}^{(n+1)}(\mathbf{r}) = \sum_{\mathbf{r}',\gamma} p_{\alpha\gamma}(\mathbf{r} - \mathbf{r}') \, P_{\gamma\beta}^{(n)}(\mathbf{r}') \qquad (2.2.28)$$

This equation has the same form as (2.1.3). Obviously, $p_{\alpha\beta}(\mathbf{r})$ and $T_{\alpha\beta}(l)$ are related; to be precise, if the transition from state β in unit cell l' to state α in unit cell $l' + l$ corresponds to a displacement $\mathbf{r}$, then $p_{\alpha\beta}(\mathbf{r}) = T_{\alpha\beta}(l)$.

Since (2.1.3) and (2.2.28) have the same form, the derivation of the moments of $P_{\alpha\beta}^{(n)}(l)$ can be repeated for those of $P_{\alpha\beta}^{(n)}(\mathbf{r})$, with the result that in the expressions (2.2.13a) and (2.2.13b) we only have to replace l_j by r_j. Hence, for the drift velocity (2.2.22) and the diffusion coefficient (2.2.24), we have the alternative results

$$V_i = \sum_\beta \langle r_i \rangle_\beta \, \pi_\beta \qquad (2.2.29a)$$

and

$$D_{ij} = \tfrac{1}{2} \sum_\beta \langle r_i r_j \rangle_\beta \, \pi_\beta + \tfrac{1}{2} \left[\sum_{\beta,\gamma}' \{ \langle \tilde{r}_i \rangle_{0\beta} [(1 - \Omega)^{-1}]_{\beta\gamma} \langle \tilde{r}_j \rangle_{\gamma 0} + i \leftrightarrow j \} \right]$$
$$- \tfrac{1}{2} V_i V_j \qquad (2.2.29b)$$

where

$$\langle r_i r_j \rangle_\beta \equiv \sum_r r_i r_j \, p_\beta(\mathbf{r}) \qquad (2.2.30)$$

is the single-step covariance from internal state β.

For *locally unbiased walks* $V_i = 0$ and the diffusion coefficient is given by

$$D_{ij} = \tfrac{1}{2} \sum_\beta \langle r_i r_j \rangle_\beta \, \pi_\beta \qquad (2.2.31)$$

---

[12] If $\langle r_j \rangle_\beta = 0$ for all β, but not necessarily all j, we will refer to the walk as "locally unbiased in the direction e_j."

To derive (2.2.31) we have used the fact that for locally unbiased walks the quantity $\langle \tilde{r}_j \rangle_{0\beta}$ in (2.2.29b) vanishes:

$$\langle \tilde{r}_j \rangle_{0\beta} = \sum_{\alpha\gamma} (H^{-1})_{0\alpha} \langle r_j \rangle_{\alpha\gamma} H_{\gamma\beta} = \sum_{\gamma} \langle r_j \rangle_{\gamma} H_{\gamma\beta} = 0$$

The corresponding quantity $\langle \tilde{l}_j \rangle_{0\beta}$ in (2.2.13b) is in general nonzero, even for locally unbiased walks.

It should be noted that there are walks which are not locally unbiased, but for which nevertheless $V_i = 0$. Such walks will be called *globally unbiased* or *without drift* (in the direction $\mathbf{e}_i$). An example will be discussed in paper II.

2.2.3. Summary. The main results of this section are the following. We have established that the mean and (co)variances of the displacement of a multistate random walk grow linearly with n, the number of steps, as $n \to \infty$ [Eqs. (2.2.21) and (2.2.23)]. The coefficients, called the drift velocity and diffusion coefficient, respectively, have been expressed in terms of the eigenvalues and eigenvectors of the stochastic matrix T, which describes the embedded Markov chain defined on the set of internal states. The relevant formulas are Eq. (2.2.22) or, alternatively, Eq. (2.2.29a), for the drift velocity and Eq. (2.2.24) or Eq. (2.2.29b) for the diffusion coefficient. An important class of random walks is formed by the so-called "locally unbiased walks," for which the single-step averages $\langle r_j \rangle_\beta$ of the displacement are identically zero for all β and j. For such walks the drift velocity vanishes and the diffusion coefficient is given by Eq. (2.2.31) which involves only the eigenvector π of equilibrium occupation probabilities, i.e., the right eigenvector of T belonging to the maximal eigenvalue $\lambda_0 = 1$.

2.2.4. Example. Consider the random walk on the sparsely periodic lattice of Fig. 1. Since every site can be reached from every other site, the walk is irreducible. However, it is not aperiodic, since the walker can only return to his starting site after an even number of steps. The matrix T describing the embedded k-state Markov chain is

$$T = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & & & & & \frac{1}{2} \\ \frac{1}{4} & & \ddots & & & & \\ & \frac{1}{2} & & \ddots & & & \\ & & \frac{1}{2} & & & \frac{1}{2} & \\ & & & \ddots & & & \\ \frac{1}{4} & & & & \frac{1}{2} & & \end{bmatrix} \qquad (2.2.32)$$

Here dots denote repetitions of the same element and blank positions denote zeros. This matrix is aperiodic [a sufficient condition for

aperiodicity is that $T_{\alpha\alpha} > 0$ for some $\alpha^{(17)}$], hence the embedded Markov chain is aperiodic, although the original random walk is not. The vector π of equilibrium occupation probabilities is easily checked to be

$$\pi = (k+1)^{-1} \mathrm{Col}\{2, 1, 1,..., 1\} \qquad (2.2.33)$$

So the equilibrium occupation probability of the intersection sites is twice as large as those of the nonintersection sites, as already noted by one of us on the basis of the B.E.M.[3] In this example detailed balance is satisfied, i.e.,

$$T_{\alpha\beta}\pi_\beta = T_{\beta\alpha}\pi_\alpha \qquad \text{(all } \alpha, \beta) \qquad (2.2.34)$$

The significance of this property in relation to the questions raised in the introduction will be discussed in Ref. 7.

Now we calculate the moments. Since the walk is locally unbiased, the drift velocities in the x and y direction are zero, and the formula (2.2.31) for the diffusion coefficients applies. For the intersection site 1, $\langle x^2 \rangle_1 = \langle y^2 \rangle_1 = \frac{1}{2}$, while for the nonintersection sites $\langle x^2 \rangle_\alpha = 1$, $\langle y^2 \rangle_\alpha = 0$, $\alpha = 2, 3,..., k$; and $\langle xy \rangle_\beta = 0$, all β. So

$$2D_{xx} = \frac{1}{2} \cdot \frac{2}{k+1} + (k-1)\frac{1}{k+1} = \frac{k}{k+1} \qquad (2.2.35)$$

$$2D_{yy} = \frac{1}{2} \cdot \frac{2}{k+1} = \frac{1}{k+1} \qquad (2.2.36)$$

in agreement with the results obtained by the *ansatz* of Ref. 3. An alternative derivation of Eqs. (2.2.35) and (2.2.36) was given in Ref. 4 by first constructing *exact* expressions for the generating functions for this example and subsequently applying Darboux' method, whereas we apply Darboux' method to the *general* problem of obtaining moments before specializing to a particular random walk. A glance at Appendix C of that paper readily shows the great simplification which has been achieved by the method presented here.

2.3. Probability of Return to the Origin

In this section we investigate the probability of return to the original site on an infinite d-dimensional lattice when the walker can traverse several internal states. For the particular case of the two-dimensional sparsely periodic lattice discussed in the preceding section, this quantity was obtained by Silver *et al.*[2] and Seshadri *et al.*[4] using involved generating

function techniques. Apart from the fact that the calculations are quite complicated, there is the additional disadvantage that the results thus obtained are not general, i.e. the derivation has to be repeated for each particular lattice.

It is the aim of this section to show that, starting from the matrix generating function for the multistate random walk, a *general* expression for the asymptotic behavior of the probability of return to the origin can be derived. By a careful comparison with the known results for perfect lattices, we conclude that the only effect of the internal states is a renormalization of the one-step covariances occurring in the perfect lattice results. For the purpose of later comparison, we present first a short derivation of the perfect lattice results.

The probability $p_n(\mathbf{0})$ of returning to the origin $\mathbf{0}$ after n steps on an infinite perfect d-dimensional lattice is given by[1]

$$p_n(\mathbf{0}) = (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\mathbf{0} \, \lambda^n(\mathbf{0}) \tag{2.3.1}$$

where the characteristic (or structure) function $\lambda(\mathbf{0})$ is defined as

$$\lambda(\mathbf{0}) = \sum_l e^{il \cdot \mathbf{0}} p(l) \tag{2.3.2}$$

and where $p(l)$ is the one-step probability distribution. The summation in (2.3.2) is over vectors l with *integer* components, as in Section 2.1. The reason is that $p_n(\mathbf{0})$ is invariant under a change of length and orientation of the individual steps, i.e., it depends only on the *connectivity* of the lattice.

The large n-behavior of $p_n(\mathbf{0})$ can be determined by Laplace's method,[19] i.e., one expands $\lambda(\mathbf{0})$ around all points $\mathbf{0}^*$ where $|\lambda(\mathbf{0}^*)| = 1$. The result, for symmetric walks $[p(l) = p(-l)]$, which always have zero drift, is

$$p_n(\mathbf{0}) \sim (\det \boldsymbol{\sigma})^{-1/2} (2\pi n)^{-d/2} \{ w_+ + w_-(-)^n \} \tag{2.3.3}$$

where the matrix $\boldsymbol{\sigma}$ has elements

$$\sigma_{ij} = \sum_l l_i l_j \, p(l) \tag{2.3.4}$$

and $w_\pm$ are certain weight factors [there can be several points where $\lambda(\mathbf{0}^*) = \pm 1$]. We will always assume that $w_+ = 1$. This is true if one uses so-called *primitive* characteristic functions,[21] i.e., the unit cell is as small as possible. The factor w_- in (2.3.3) appears for so-called loosely packed lattices[22] where the walker can only return to the origin after an even

number of steps. Examples are the s.c. and b.c.c. lattices. As soon as we assign a nonzero probability for the walker to pause at every site, the oscillatory contribution of the form $w_-(-)^n$ in (2.3.3) disappears. This is *a fortiori* the case for CTRW's.

We now consider the case of multistate random walks. To find the asymptotic behavior of $P_{\alpha\beta}^{(n)}(\mathbf{0})$, the probability that the walker returns to the original unit cell after n steps, with initial and final internal states given by β and α, respectively, we apply Darboux' method to the corresponding generating function, which from (2.1.6) and (2.1.7) is given by

$$G_{\alpha\beta}(\mathbf{0}, z) = (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\mathbf{\theta} \, \Gamma_{\alpha\beta}(\mathbf{\theta}, z) \qquad (2.3.5)$$

with

$$\Gamma_{\alpha\beta}(\mathbf{\theta}, z) = \{[1 - z\Lambda(\mathbf{\theta})]^{-1}\}_{\alpha\beta} \qquad (2.3.6)$$

As in the previous section, we expand $G_{\alpha\beta}(\mathbf{0}, z)$ around the singularities in the complex z plane. One singularity is always at $z = 1$, and accordingly we have to expand $\Gamma_{\alpha\beta}(\mathbf{\theta}, z)$ around $\mathbf{\theta} = \mathbf{0}$. But this was already done above; hence we immediately conclude that the singular part $G_{\alpha\beta}^{(s)}(\mathbf{0}, z)$ near $z = 1$ is given by

$$G_{\alpha\beta}^{(s)}(\mathbf{0}, z) = \pi_\alpha \tilde{G}_{00}(\mathbf{0}, z) \qquad (2.3.7)$$

where

$$\tilde{G}_{00}(\mathbf{0}, z) = (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\mathbf{\theta} \, \tilde{\Gamma}_{00}(\mathbf{\theta}, z) \qquad (2.3.8)$$

with $\tilde{\Gamma}_{00}(\mathbf{\theta}, z)$ given by (2.2.12). Expanding (2.3.8) in powers of z and evaluating the coefficient of z^n by Laplace's method, as in the perfect lattice case, we obtain, again for the case of zero drift $[m_j = 0$ in (2.2.12)$]$,

$$P_{\alpha\beta}^{(n)}(\mathbf{0}) \sim \pi_\alpha (\det \mathbf{s})^{-1/2} (2\pi n)^{-d/2} \qquad (n \to \infty) \qquad (2.3.9)$$

where the matrix elements of s are given by (2.2.13b).[13] For walks without drift considered here, we have from (2.2.24)

$$\det \mathbf{s} = (\det 2\mathbf{D})(\det \mathbf{A})^{-2} \qquad (2.3.10)$$

---

[13] If the random walk is periodic, there can be oscillatory contributions to $P_{\alpha\beta}^{(n)}(\mathbf{0})$ involving multiplication of the right-hand side of (2.3.9) by a factor $\exp(2\pi i/p)j$, $j = 1, 2,..., p - 1$, where p is the period [see examples (i) and (ii) below]. We note that in many practical applications such oscillatory terms can be determined by inspection. For CTRW's such contributions do not occur.

The right-hand side of (2.3.10) is especially simple to calculate for locally unbiased walks, where the matrix elements of D can be found by using Eq. (2.2.31), which involves only the eigenvector π of T. The matrix elements of A, as defined in (2.2.25), follow from the geometry of the unit cell.

For comparison with previous results in the literature, we also give the result for the probability of return to the original unit cell and original internal state, averaged over a uniform distribution of all m initial states,

$$p^{(n)}(\mathbf{0}) \equiv \frac{1}{m} \sum_{\alpha=0}^{m-1} P_{\alpha\alpha}^{(n)}(\mathbf{0}) \sim \frac{1}{m} (\det 2\mathbf{D})^{-1/2}(\det \mathbf{A})(2\pi n)^{-d/2} \quad (2.3.11)$$

It is clear from Eq. (2.3.11) that the asymptotic probability of return to the origin in a multistate random walk can indeed be readily obtained, through a simple renormalization of the diffusion coefficients, from the perfect lattice result [Eq. (2.3.3)].

The derivation given in this section can easily be extended to derive the probability of *first* return to the origin by applying the same method to the generating function $f_{\alpha\beta}(\mathbf{0}, z) = \sum_{n=0}^{\infty} z^n f_{\alpha\beta}^{(n)}(l_0 \mid l_0)$, where $f_{\alpha\beta}^{(n)}(l \mid l_0)$ is the probability that the walker visits site (l, α) for the first time, given that he started at (l_0, β). From Eq. (2.4.1) of the next section, one can derive that $f_{\alpha\beta}(\mathbf{0}, z)$ is related to $G_{\alpha\beta}(\mathbf{0}, z)$ of Eq. (2.3.5) by

$$f_{\alpha\beta}(\mathbf{0}, z) = [G_{\alpha\alpha}(\mathbf{0}, z)]^{-1}\{G_{\alpha\beta}(\mathbf{0}, z) - \delta_{\alpha\beta}\} \quad (2.3.12)$$

Examples. (i) As a first example we consider the sparsely periodic two-dimensional lattice of Fig. 1, treated in the previous section. The diffusion coefficients were obtained in (2.2.35) and (2.2.36) as

$$2D_{xx} = \frac{k}{k+1}, \qquad 2D_{yy} = \frac{1}{k+1}, \qquad D_{xy} = D_{yx} = 0 \quad (2.3.13a)$$

Furthermore, since we take the lattice spacing to be unity,

$$A_{xx} = k, \qquad A_{yy} = 1, \qquad A_{xy} = A_{yx} = 0 \quad (2.3.13b)$$

So from (2.3.11) the asymptotic probability of return to the origin in n steps averaged over initial states is

$$p^{(n)}(\mathbf{0}) \sim \frac{k+1}{2\sqrt{k}} \frac{1}{\pi n} \qquad (n \to \infty) \quad (2.3.14)$$

In fact, it is immediately clear from Fig. 1 that the walker can only return

to the original site after an even number of steps, so (2.3.14) should be modified to

$$p^{(n)}(\mathbf{0}) \sim \frac{k+1}{2\sqrt{k}} \frac{1}{\pi n} [1 + (-)^n] \qquad (2.3.15)$$

This result is in agreement with Eq. (4.9) of Ref. 2, derived by generating function techniques, and also with Eq. (27) of Ref. 3.

(ii) Secondly, we consider the hexagonal lattice of Fig. 2. This lattice can be constructed from a unit cell or, more precisely, an irreducible lattice fragment with two nonequivalent sites, labeled 1 and 2 in Fig. 2. These sites differ in that, along the horizontal bonds, the walker can step only to the left from sites 2 and only to the right from sites 1. The fundamental translation vectors chosen here are, with the lattice constant equal to unity,

$$\mathbf{a}_1 = (3, 0), \qquad \mathbf{a}_2 = (\tfrac{3}{2}, \tfrac{1}{2}\sqrt{3}) \qquad (2.3.16a)$$

The basic vectors are $\mathbf{e}_1 = (1, 0)$ and $\mathbf{e}_2 = (0, 1)$. The matrix T is

$$\mathsf{T} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \pi = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad (2.3.16b)$$

The matrix T is cyclic, and the second eigenvalue is $\lambda_1 = -1$. Hence

$$P_{\alpha\alpha}^{(n)} \sim \pi_\alpha (\det 2\mathsf{D})^{-1/2} (\det \mathsf{A}) (2\pi n)^{-1} \{1 + (-)^n\} \qquad (2.3.17)$$
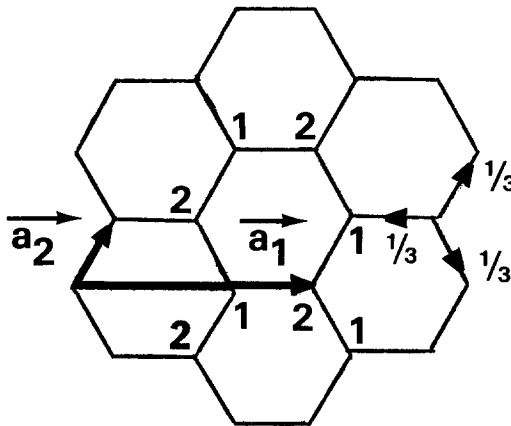

Fig. 2. Hexagonal lattice with two sites per unit cell. The fundamental translation vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are as indicated. Jump probabilities are $\tfrac{1}{3}$ in each direction from each site.

The determinants are easily calculated on the basis $\{\mathbf{e}_1, \mathbf{e}_2\}$. We find from (2.2.25) and (2.2.31),

$$2D_{11} = 2D_{22} = \tfrac{1}{2}; \qquad D_{12} = D_{21} = 0;$$
$$A_{11} = 3, \quad A_{22} = \tfrac{1}{2}\sqrt{3}; \qquad A_{12} = 0; \qquad A_{21} = \tfrac{3}{2} \tag{2.3.18}$$

So

$$\det 2D = \tfrac{1}{4}, \qquad \det A = \tfrac{3}{2}\sqrt{3} \tag{2.3.19}$$

and

$$P_{\alpha\alpha}^{(n)} \sim \pi_\alpha \frac{3\sqrt{3}}{2\pi n}[1 + (-)^n], \qquad \pi_\alpha = \tfrac{1}{2} \tag{2.3.20}$$

We have verified this result by explicitly inverting the matrix $1 - z\Lambda(\boldsymbol{\theta})$ in (2.3.6), expanding the diagonal elements $G_{\alpha\alpha}(\mathbf{0}, z)$ in powers of z and evaluating the coefficient of z^n for large n by Laplace's method. For unit cells with many sites, the latter approach becomes too cumbersome to be useful.

2.4. Expected Number of Distinct Sites Visited

We now turn to a determination of the asymptotic behavior of $S_{\alpha\beta}^{(n)}$, the expected (i.e., mean) number of distinct sites visited after n steps, with initial state β and final state α. Again the result is derived by expanding the generating function $S_{\alpha\beta}(z)$ of $S_{\alpha\beta}^{(n)}$ around $z = 1$. Comparison with the perfect lattice case enables us to conclude immediately that the functional dependence of $S_{\alpha\beta}^{(n)}$ on n is the same as for the perfect lattice, but with modified coefficients. This modification again involves only the diffusion coefficients in dimension $d < 3$, but it is more complicated in $d \geqslant 3$. This is a consequence of the fact (see Ref. 1) that the matrix generating function $G(\mathbf{0}, z)$ diverges at $z = 1$ if $d < 3$, but is finite at $z = 1$ for $d \geqslant 3$. We again assume that the walk has zero drift velocities in all directions.

Define $f_{\alpha\beta}^{(n)}(\mathbf{l})$ as the probability that the walker arrives for the first time in unit cell $\mathbf{l}$ in state α after n steps, given that he started at $(\mathbf{0}, \beta)$. This probability is related to $P_{\alpha\beta}^{(n)}(\mathbf{l})$, as defined before, by

$$P_{\alpha\beta}^{(n)}(\mathbf{l}) = \delta_{n,0}\delta_{\alpha\beta}\delta_{\mathbf{l},0} + \sum_{j=1}^{n} P_{\alpha\alpha}^{(n-j)}(\mathbf{l} \mid \mathbf{l}) f_{\alpha\beta}^{(j)}(\mathbf{l}) \tag{2.4.1}$$

where, from translational invariance, $P_{\alpha\alpha}^{(n-j)}(\mathbf{l} \mid \mathbf{l}) = P_{\alpha\alpha}^{(n-j)}(\mathbf{0})$. Equation (2.4.1) is based on the assumption that different internal states with the

same *l*, visited by the walker, are counted as distinct. In the case considered here of *configurational* internal states which represent different sites on an inhomogeneous periodic lattice, this is a natural choice. If the lattice itself is perfect, i.e., all sites are identical, but the walker can be in different internal states *at a given lattice site* (e.g., spin 1/2 or −1/2), so that (l, α) and (l, β) represent different states at the same site, then (2.4.1) has to be replaced by

$$P_{\alpha\beta}^{(n)}(l) = \delta_{n,0}\delta_{\alpha\beta}\delta_{l,0} + \sum_{j=1}^{n} \sum_{\gamma} P_{\alpha\gamma}^{(n-j)}(0)\, f_{\gamma\beta}^{(j)}(l) \qquad (2.4.2)$$

In the following we will only consider the case described by (2.4.1). The second case, (2.4.2), can be worked out in an analogous manner.[24]

Starting from Eq. (2.4.1), one can derive an expression for the generating function $S_{\alpha\beta}(z) = \sum_{n=0}^{\infty} z^n S_{\alpha\beta}^{(n)}$ along the same lines as followed by Montroll and Weiss[23] for perfect lattices. The result is

$$S_{\alpha\beta}(z) = (1-z)^{-1}[G_{\alpha\alpha}(0, z)]^{-1}[(1-zT)^{-1}]_{\alpha\beta} \qquad (2.4.3)$$

as the relation between $S_{\alpha\beta}(z)$ and the Green's function $G_{\alpha\beta}(0, z)$.

To find the behavior of $S_{\alpha\beta}^{(n)}$ for large n we again apply Darboux' method to the generating function (2.4.3). The dominant contribution now comes solely from the singularity at $z = 1$, corresponding to the eigenvalue $\lambda_0 = 1$ of T. This is true even if T is periodic, owing to the presence of an extra factor $(1-z)^{-1}$ in (2.4.3).[14] From the identity

$$[(1-zT)^{-1}]_{\alpha\beta} = \sum_{\gamma,\delta} H_{\alpha\gamma}[(1-z\tilde{T})^{-1}]_{\gamma\delta}(H^{-1})_{\delta\beta}$$

[see (2.2.4)], one can see that the main contribution again comes from the term with $\gamma = \delta = 0$. Hence,

$$S_{\alpha\beta}(z) \overset{z \to 1}{\sim} \pi_{\alpha}(1-z)^{-2}[G_{\alpha\alpha}(0, z)]^{-1} \qquad (2.4.4)$$

In dimensions $d = 1, 2$, $G_{\alpha\alpha}(0, z)$ diverges as $z \to 1$, hence the dominant contribution as $z \to 1$ is given by

$$G_{\alpha\alpha}(0, z) = \sum_{\gamma\delta} H_{\alpha\gamma}[\tilde{G}(0, z)]_{\gamma\delta}(H^{-1})_{\delta\alpha} \overset{z \to 1}{\sim} \pi_{\alpha}\tilde{G}_{00}(0, z)$$

It thus follows from (2.4.4) that

$$S_{\alpha\beta}(z) \overset{z \to 1}{\sim} (1-z)^{-2}[\tilde{G}_{00}(0, z)]^{-1} \qquad (d = 1, 2) \qquad (2.4.5)$$

---

[14] The singularities at other points of the unit circle, if present, have to be taken into account when higher order corrections are calculated.[25]

where $\tilde{G}_{00}(\mathbf{0}, z)$ is given by (2.3.8). In dimensions $d \geqslant 3$, $G_{\alpha\alpha}(\mathbf{0}, 1)$ is finite, hence to leading order

$$S_{\alpha\beta}(z) \overset{z \to 1}{\sim} \pi_\alpha (1 - z)^{-2} [G_{\alpha\alpha}(\mathbf{0}, 1)]^{-1} \qquad (d \geqslant 3) \qquad (2.4.6)$$

Note that if the walk has a nonzero drift, $G_{\alpha\alpha}(\mathbf{0}, 1)$ is finite even in $d = 1, 2$, so $S_{\alpha\beta}(z)$ is given by (2.4.6) in that case.

For walks on perfect lattices, the generating functions $S(z)$ and $G(\mathbf{0}, z)$ are related by[23]

$$S(z) = (1 - z)^{-2} G^{-1}(\mathbf{0}, z) \qquad (2.4.7)$$

where the expansions of $G(\mathbf{0}, z)$ around $z = 1$ are given by

$$G(\mathbf{0}, z) \overset{z \to 1}{\sim} (\sigma^2)^{-1/2} [2(1 - z)]^{-1/2} \qquad (d = 1) \qquad (2.4.8a)$$

$$G(\mathbf{0}, z) \overset{z \to 1}{\sim} -\frac{1}{2\pi} (\det \boldsymbol{\sigma})^{-1/2} \log(1 - z) \qquad (d = 2) \qquad (2.4.8b)$$

$$G(\mathbf{0}, z) \overset{z \to 1}{\sim} G(\mathbf{0}, 1) - \frac{1}{\pi} (\det \boldsymbol{\sigma})^{-1/2} \left[\frac{1}{2} (1 - z) \right]^{1/2} \qquad (d = 3) \qquad (2.4.8c)$$

where the matrix $\boldsymbol{\sigma}$ is defined in (2.3.4). For the one-dimensional case, we define $\sigma^2 \equiv \sum_l l^2 p(l)$.

For diagonal matrices $\boldsymbol{\sigma}$ these results can be found in Ref. 1 ($d = 1, 2$) and Ref. 23 ($d = 3$).[15] In dimension $d \geqslant 3$ there is a constant term in the expansion of $G(\mathbf{0}, z)$ since $G(\mathbf{0}, 1)$ is finite in this case, but according to Darboux' theorem only the *singular* part of $G(\mathbf{0}, z)$ contributes to the asymptotic behavior of the various random walk properties. For the s.c. and b.c.c. lattices there are similar expressions for $G(\mathbf{0}, z)$ as $z \to -1$. Using (2.4.7) and (2.4.8) it has been shown that[23]

$$S^{(n)} \sim (\sigma^2)^{1/2} \left(\frac{8n}{\pi} \right)^{1/2} \qquad (d = 1) \quad (n \to \infty) \qquad (2.4.9a)$$

$$S^{(n)} \sim (\det \boldsymbol{\sigma})^{1/2} \left(\frac{2\pi n}{\log n} \right) \qquad (d = 2) \quad (n \to \infty) \qquad (2.4.9b)$$

$$S^{(n)} \sim n/G(\mathbf{0}, 1) \qquad (d \geqslant 3) \quad (n \to \infty) \qquad (2.4.9c)$$

We have found in Section 2.3 that the expansion of the function $\tilde{G}_{00}(\mathbf{0}, z)$ in (2.4.5) around $z = 1$ is the same as for perfect lattices, with

---

[15] Note that Eq. (D.8a) of Ref. 23 is in error since a nonprimitive characteristic function was used and the weight factor $w_+ = 4$ for the b.c.c. lattice was omitted.[25]

det $\boldsymbol{\sigma}$ replaced by $(\det 2\mathsf{D})(\det \mathsf{A})^{-2}$. It can readily be seen by comparing (2.4.5) with (2.4.7) that for $d = 1, 2$ the same replacement of det $\boldsymbol{\sigma}$ by $(\det 2\mathsf{D})(\det \mathsf{A})^{-2}$ holds also for $S_{\alpha\beta}^{(n)}$. Thus,

$$S_{\alpha\beta}^{(n)} \overset{n \to \infty}{\sim} \frac{(\det 2\mathsf{D})^{1/2}}{\det \mathsf{A}} \times \begin{cases} \left(\dfrac{8n}{\pi}\right)^{1/2} & (d=1) \\[2mm] \dfrac{2\pi n}{\log n} & (d=2) \end{cases} \tag{2.4.10a}$$

where in one dimension det $2\mathsf{D}$ equals $2D$, i.e., twice the diffusion coefficient, and det $\mathsf{A} = L$, where L is the length of the unit cell. The diffusion matrix D and the matrix A are defined by (2.2.23) and (2.2.25), respectively. In dimension $d \geqslant 3$,

$$S_{\alpha\beta}^{(n)} \sim \pi_\alpha n [G_{\alpha\alpha}(\mathbf{0}, 1)]^{-1} \qquad (n \to \infty) \tag{2.4.10b}$$

and there is no simple dependence of $S_{\alpha\beta}^{(n)}$ on the diffusion coefficients in this case. Such a dependence would only appear in the first correction to the leading order result. For this reason the ansatz of Eq. (51) for $d = 3$ in Ref. 3 is invalid. This will be discussed in more detail in Ref. 8.

The expected number of distinct sites visited, averaged over the initial distribution $p_\beta^{(0)}$ of the walker on the internal states and summed over all final states is obtained from (2.4.10) as

$$S^{(n)} \equiv \sum_{\alpha=0}^{m-1} \sum_{\beta=0}^{m-1} S_{\alpha\beta}^{(n)} p_\beta^{(0)} \tag{2.4.11}$$

Example. For the example (i) of a sparsely periodic two-dimensional lattice with horizontal periodicity k discussed in the previous section, we find from (2.3.13) and (2.4.10a)

$$S_{\alpha\beta}^{(n)} \sim \frac{1}{(k+1)\sqrt{k}} \left(\frac{2\pi n}{\log n}\right) \qquad (n \to \infty)$$

and

$$S^{(n)} \sim \frac{\sqrt{k}}{k+1} \cdot \left(\frac{2\pi n}{\log n}\right) \qquad (n \to \infty) \tag{2.4.12}$$

in agreement with Eq. (4.11) of Ref. 2 and Eq. (20) of Ref. 3.

3. CONTINUOUS TIME RANDOM WALKS

3.1. Introduction

The results of the previous sections can be extended without difficulty to continuous time random walks (CTRW's).[23] The basic quantity which describes the random walk is now the function $\psi_{\alpha\gamma}(l-l', \tau)$, where $\psi_{\alpha\gamma}(l-l', \tau)\,d\tau$ is the probability that the walker jumps from unit cell l' and internal state γ to unit cell l and internal state α in a time interval $(\tau, \tau+d\tau)$. We will restrict ourselves to so-called *separable* walks, for which the function $\psi_{\alpha\gamma}$ has the space and time factorized form

$$\psi_{\alpha\gamma}(l-l', \tau) = T_{\alpha\gamma}(l-l')\,\psi_{\gamma}(\tau) \tag{3.1.1}$$

The function $T_{\alpha\gamma}(l-l')$ is the same as in (2.1.3) and $\psi_{\gamma}(\tau)$ is the waiting time density in state γ, i.e., $\psi_{\gamma}(t)\,d\tau$ is the probability that the walker makes a transition from state γ in the time interval $(\tau, \tau+d\tau)$. The normalization condition is now

$$\int_0^\infty d\tau \sum_{\alpha,l} \psi_{\alpha\gamma}(l, \tau) = 1$$

The random walk described by (3.1.1) is a *Markov process* with continuous time parameter if and only if the functions $\psi_{\gamma}(\tau)$ are exponentials for all γ,[26]

$$\psi_{\gamma}(\tau) = \tau_{\gamma}^{-1} e^{-\tau/\tau_{\gamma}} \tag{3.1.2}$$

The quantity τ_{γ} is called the mean waiting time in internal state γ. We will, however, not restrict ourselves here to waiting time densities of the form (3.1.2). As in the discrete time case, we assume that the random walk is irreducible.

Since we are interested in the asymptotic behavior as $t \to \infty$ of functions $f(t)$, we must examine the properties of the Laplace transformed functions $\hat{f}(u) \equiv \int_0^\infty dt\, e^{-ut}f(t)$ in the limit as $u \to 0$. We consider here two different cases for the waiting time density $\psi_{\gamma}(t)$:

(a) $\psi_{\gamma}(t)$ has finite first and second moments $\langle t_{\gamma} \rangle$ and $\langle t_{\gamma}^2 \rangle$, where

$$\langle t_{\gamma}^l \rangle = \int_0^\infty dt\, \psi_{\gamma}(t)\, t^l \qquad (l = 1, 2,...) \tag{3.1.3}$$

Then

$$\hat{\psi}_{\gamma}(u) = 1 - u\langle t_{\gamma} \rangle + \tfrac{1}{2}u^2\langle t_{\gamma}^2 \rangle + O(u^3) \qquad (u \to 0) \tag{3.1.4}$$

(b) $\psi_\gamma(t)$ has an infinite mean for all γ, in which case

$$\hat{\psi}_\gamma(u) = 1 - u^q B_\gamma + \tfrac{1}{2} u^{2q} C_\gamma + O(u^{3q}) \qquad (u \to 0) \tag{3.1.5}$$

where B_γ and C_γ are constants, and $0 < q < 1$.

Other cases, such as when only the first moment of $\psi_\gamma(t)$ is finite or when the constants in (3.1.5) are slowly varying functions of u, can also be worked out [see, e.g., the work of Shlesinger[27] on perfect lattices]. These and several other possible models involving internal states with both finite and infinite waiting times will not be considered here.

Let $P_{\alpha\beta}(l, t)$ be the probability that the walker is in unit cell l in state α at time t, having started in unit cell 0 in state β. Then the Laplace transform of $P(l, t)$ for the case of separable CTRW's is[28]

$$\hat{P}(l, u) = u^{-1}[1 - \hat{\psi}(u)] \hat{G}[l, u] \tag{3.1.6}$$

Here $\hat{\psi}(u)$ is a diagonal matrix with elements $\hat{\psi}_\gamma(u)$, which are the Laplace transforms of the waiting time density functions $\psi_\gamma(t)$, $\gamma = 0, 1,..., m - 1$. The matrix $\hat{G}$ in (3.1.6) is given by

$$\hat{G}[l, u] = (2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\theta [1 - \Lambda(\theta) \hat{\psi}(u)]^{-1} e^{-il \cdot \theta} \tag{3.1.7}$$

We note that $\hat{G}(l, u)$ would be identical to the generating function $G(l, z)$ of (2.1.6) if $\hat{\psi}(u)$ were replaced by z.

We now turn to the calculation of the asymptotic properties of CTRW's as $t \to \infty$. Since most of the results can be obtained by investigating the discrete time generating function $G(0, z)$ already discussed, we dispense with most of the details of the calculation.

3.2. Moments

3.2.1. Occupation Probabilities.   The Laplace transform $\hat{P}_{\alpha\beta}(u)$ of $P_{\alpha\beta}(t) \equiv \sum_l P_{\alpha\beta}(l, t)$, the probability that the walker is in internal state α at time t, starting from internal state β, irrespective of the unit cell occupied at time t, is given by [using (3.1.6) and (3.1.7)],

$$\hat{P}_{\alpha\beta}(u) = u^{-1}[1 - \hat{\psi}_\alpha(u)]\{[1 - T\hat{\psi}(u)]^{-1}\}_{\alpha\beta} \tag{3.2.1}$$

From (3.1.4) and (3.1.5) we have, as $u \to 0$,

$$u^{-1}[1 - \hat{\psi}_\alpha(u)] = \begin{cases} \langle t_\alpha \rangle + O(u) & \text{(case a)} \tag{3.2.2a} \\ u^{q-1}B_\alpha + O(u^{2q-1}) & \text{(case b)} \tag{3.2.2b} \end{cases}$$

and, as shown in Appendix B,

$$\{[1 - T\hat{\psi}(u)]^{-1}\}_{\alpha\beta} \overset{u \to 0}{\sim} \pi_\alpha \cdot \begin{cases} (u\bar{t})^{-1} + O(1) & \text{(case a)} & (3.2.3a) \\ (u^q\bar{B})^{-1} + O(1) & \text{(case b)} & (3.2.3b) \end{cases}$$

where cases a and b correspond to finite or infinite mean waiting times, respectively. We define $\bar{t}$ and $\bar{B}$ as

$$\bar{t} = \sum_\alpha \pi_\alpha \langle t_\alpha \rangle \qquad (3.2.4a)$$

$$\bar{B} = \sum_\alpha \pi_\alpha B_\alpha \qquad (3.2.4b)$$

with $\langle t_\alpha \rangle$ and B_α defined in (3.1.3)–(3.1.5). Hence, as $u \to 0$,

$$\hat{P}_{\alpha\beta}(u) = \begin{cases} \pi_\alpha \dfrac{\langle t_\alpha \rangle}{\bar{t}} u^{-1} + O(1) & \text{(case a)} & (3.2.5a) \\[2mm] \pi_\alpha \dfrac{B_\alpha}{\bar{B}} u^{-1} + O(u^{q-1}) & \text{(case b)} & (3.2.5b) \end{cases}$$

and thus, in the limit as $t \to \infty$,[16]

$$P_{\alpha\beta}(t) \xrightarrow{t \to \infty} \begin{cases} \pi_\alpha \dfrac{\langle t_\alpha \rangle}{\bar{t}} & \text{(case a)} & (3.2.6a) \\[2mm] \pi_\alpha \dfrac{B_\alpha}{\bar{B}} & \text{(case b)} & (3.2.6b) \end{cases}$$

The limit is again independent of the initial state β. The approach to equilibrium of the embedded Markov chain defined on the internal states may, however, be extremely slow in case b as q approaches zero (see 3.2.5b).

3.2.2. Means and Variances.

The Laplace transforms of the means $\langle l_j(t) \rangle$ and covariances $\langle\!\langle l_j(t) l_k(t) \rangle\!\rangle$ can be obtained by differentiation of the function

$$K(\theta, u) = u^{-1}[1 - \hat{\psi}(u)][1 - \Lambda(\theta) \hat{\psi}(u)]^{-1} \qquad (3.2.7)$$

which is the spatial Fourier transform of (3.1.6). Again we are interested in the small-u behavior of (3.2.7). The analysis is straightforward but

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[16] We use the Hardy–Littlewood–Karamata theorem; see Refs. 14 and 27.

somewhat tedious and the details are given in Appendix B. From the expressions for the moments of $I(t)$, we obtain the following results for the mean $\langle r_i(t) \rangle$ and the covariances $\langle\!\langle r_i(t)\, r_j(t) \rangle\!\rangle$ of the actual displacement of the walker:

$$\langle r_i(t) \rangle \overset{t \to \infty}{\sim} V_i \begin{cases} \dfrac{t}{\bar t} & \text{(case a)} \qquad (3.2.8\text{a}) \\[3mm] \dfrac{t^q}{\Gamma(1+q)} \dfrac{1}{\bar B} & \text{(case b)} \qquad (3.2.8\text{b}) \end{cases}$$

where $\Gamma(\cdot)$ denotes the gamma function, $\bar t$ and $\bar B$ are defined in (3.2.4), and V_i can be obtained from the formulas (2.2.22) or (2.2.29a). The expressions for the covariances are rather complicated [see Eq. (B.15) of Appendix B], and we therefore quote here only the results in the case of *zero drift* (i.e., $V_i = 0$, all $i = 1, 2,..., d$):

$$\langle r_i(t)\, r_j(t) \rangle \overset{t \to \infty}{\sim} 2D_{ij} \begin{cases} \dfrac{t}{\bar t} & \text{(case a)} \qquad (3.2.9\text{a}) \\[3mm] \dfrac{t^q}{\Gamma(1+q)} \cdot \dfrac{1}{\bar B} & \text{(case b)} \qquad (3.2.9\text{b}) \end{cases}$$

where, for the case of zero drift considered here, the discrete time diffusion coefficient D_{ij} can be calculated from (2.2.24) with $m_k = m_l = 0$ or from (2.2.29b) with $V_i = V_j = 0$.

Comparison of the result in (3.2.8) with the discrete time result (2.2.21), and of (3.2.9) with (2.2.23) for the case of zero drift, shows that the only modification is the replacement of the discrete step variable n by $t/\bar t$ and $[t^q/\Gamma(1+q)] \cdot (\bar B)^{-1}$ for cases a and b, respectively. In the case of nonzero drift, this simple replacement no longer holds for the covariances.

Example. Consider the one-dimensional random walk on the lattice with periodically spaced internal states x and 0 depicted in Fig. 3. We assume that the waiting time densities are of the form (3.1.2). The sum of
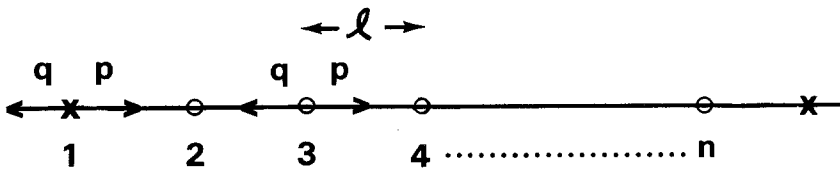

Fig. 3.   One-dimensional random walk with jump probabilities p and q from each site, and waiting times a^{-1} (0 sites) and b^{-1} (x sites).

the jump rates from a site, which is the inverse of the mean waiting time, is a for the 0 sites and b for the x sites. The unit cell contains m sites. The $m \times m$ matrix T for this case is

$$
T = \begin{pmatrix} q & & & & p \\ p & \ddots & & & \\ & \ddots & \ddots & & \\ & & \ddots & \ddots & q \\ q & & & p & \end{pmatrix} \tag{3.2.10}
$$

The fact that the dimension of this matrix can be large prompted Landman and Shlesinger to replace their matrix method[11] for calculating the moments of the displacement by another method using defect generating functions.[12] However, in the symmetric case ($p = q = \frac{1}{2}$), we only need the components π_β of the right eigenvector π of T corresponding to $\lambda_0 = 1$, which are trivially found to be $1/m$, and substitute this in the expression for the variance, which is

$$
\langle x^2(t) \rangle \sim \frac{t}{\bar{t}} \sum_\beta \langle x^2 \rangle_\beta \pi_\beta = \frac{t}{\bar{t}} l^2 \tag{3.2.11}
$$

where l is the lattice spacing and where we have used $\langle x^2 \rangle_\beta = l^2$ for all β for the single-step variance. The mean waiting time $\bar{t}$ is

$$
\bar{t} = \sum_{\alpha=1}^m \langle t_\alpha \rangle \pi_\alpha = m^{-1} \{ b^{-1} + (m-1) a^{-1} \} \tag{3.2.12}
$$

since $\pi_\alpha = m^{-1}$ and $\sum_\alpha \langle t_\alpha \rangle$ is the sum of $m-1$ contributions a^{-1} from 0 sites and one contribution b^{-1} from the x site. The asymptotic variance is thus found to be

$$
\langle x^2(t) \rangle \sim \frac{tl^2 mab}{a + (m-1)b} \tag{3.2.13}
$$

This result is in agreement with Eq. (2.52) of Ref. 12(a).

In the asymmetric case ($p \neq q$) the eigenvector π of (3.2.10) is the same as for the symmetric case, i.e., $\pi_\beta = m^{-1}$. The mean displacement follows from (3.2.8a),

$$
\langle x(t) \rangle \sim \frac{t}{\bar{t}} \sum_\beta \langle x_\beta \rangle \pi_\beta = \frac{t}{\bar{t}} l(p-q) = \frac{tl(p-q) mab}{a + (m-1)b} \tag{3.2.14}
$$

where we have used (3.2.12). The result (2.59) of Ref. 12(a) for $\langle x(t) \rangle$ is in error since for $a = b$ the perfect lattice result $tl(p-q)a$ is not recovered.

The variance of the displacement in the asymmetric case is harder to obtain. In general we need all the eigenvalues and eigenvectors of T [see Eq. (B.15)].[17] The diffusion coefficient $D(E)$ in the presence of a field E (which causes the asymmetry of jump probabilities) differs from that in zero field only by terms of order $(E/\Omega)^2$, where Ω is a measure for the size of the system.[29,30] Hence, in physical applications one usually calculates the drift velocity in the presence of the field and the diffusion coefficient in zero field. Both quantities can be obtained from the expressions (2.2.29a) and (2.2.31) *which involve only the equilibrium occupation probabilities.*

Virtually all examples given by Landman and Shlesinger[12] are of the simple type just studied, i.e., the different configurational sites within the unit cell are distinguished merely by different waiting time distributions. In all these cases the occupation probabilities π_β of the associated discrete time walk are equal to m^{-1}, and the desired results can be written down immediately.

3.3. Probability of Return to the Origin

The long-time behavior of $P_{\alpha\beta}(\mathbf{0}, t)$, which is the probability that the walker will return to state α in the initial unit cell at time t, having started his walk from state β in that cell, is determined by the small-u behavior of $\hat{P}_{\alpha\beta}(\mathbf{0}, u)$, as defined in (3.1.6). The singular part as $u \to 0$ in (3.1.7) is again determined by the eigenvalue $\lambda_0 = 1$ of the matrix T which occurs in $\Lambda(\mathbf{0})$ [see Eq. (2.2.9)].

In the case of finite mean waiting times and again assuming zero drift, we thus obtain, in analogy to (2.3.7),

$$\hat{P}_{\alpha\beta}(u) \overset{u \to 0}{\sim} \langle t_\alpha \rangle \, \pi_\alpha \tilde{\tilde{G}}_{00}[\mathbf{0}, u] \tag{3.3.1a}$$

where (see Appendix B),

$$\tilde{\tilde{G}}_{00}[\mathbf{0}, u] \overset{u \to 0}{\sim} (\bar{t})^{-1}(2\pi)^{-d} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} d^d\boldsymbol{\theta} \left[u + \tfrac{1}{2}(\bar{t})^{-1} \sum_{k,m} \theta_k \theta_m s_{km} \right]^{-1} \tag{3.3.1b}$$

and where s_{km} is given by (2.2.13b). The inverse Laplace transformation yields for $P_{\alpha\beta}(\mathbf{0}, t)$,

$$P_{\alpha\beta}(\mathbf{0}, t) \sim \frac{\langle t_\alpha \rangle \, \pi_\alpha}{\bar{t}} \, (\det 2\mathbf{D})^{-1/2}(\det \mathbf{A})(2\pi t/\bar{t})^{-d/2} \qquad (t \to \infty) \tag{3.3.2}$$

---

[17] The one-dimensional case can still be worked out explicitly.[20]

where (2.3.10) has been used, and the diffusion matrix D is the discrete time matrix appearing in Eq. (2.3.11). Finally, we average again over a uniform initial distribution of the walker over the m internal states to obtain

$$p(\mathbf{0}, t) \equiv \frac{1}{m} \sum_\alpha P_{\alpha\alpha}(\mathbf{0}, t) \sim \frac{1}{m} (\det 2\mathbf{D})^{-1/2} (\det \mathbf{A})(2\pi t/\bar{t})^{-d/2} \quad (3.3.3)$$

where $p(\mathbf{0}, t)$ is the probability that the walker returns to the starting site at time t. Note that (3.3.3) is identical to the discrete-time result (2.3.11) when the discrete step variable n is replaced by $t/\bar{t}$. The weighted average $\bar{t}$ in (3.3.3) of the mean waiting times $\{\langle t_\alpha \rangle\}$ is the same as that encountered in the previous sections. If the mean waiting times $\{\langle t_\alpha \rangle\}$ are infinite, only the time dependence in the last parenthesis of (3.3.3) is changed, in the same way as for perfect lattices.

3.4. Expected Number of Distinct Sites Visited

The generating function for the expected number $S_{\alpha\beta}(t)$ of distinct sites visited after a time t with initial and final states β and α, respectively, can be derived in a way analogous to that in Ref. 23 for perfect lattices. First we write

$$S_{\alpha\beta}(t) = \sum_l \int_0^t d\tau \, f_{\alpha\beta}(\mathbf{l}, \tau) \quad (3.4.1)$$

where $f_{\alpha\beta}(\mathbf{l}, \tau)$ is the probability per unit time that the walker arrives for the first time in unit cell $\mathbf{l}$ and internal state α precisely after a time τ, having started in unit cell $\mathbf{0}$ and internal state β. This probability can be related to the probability $P_{\alpha\beta}(\mathbf{l}, t)$ as defined in Section 3.1 by

$$P_{\alpha\beta}(\mathbf{l}, t) = \delta_{\alpha\beta} \delta_{\mathbf{l}, 0} \Gamma_\beta(t) + \int_0^t d\tau \, P_{\alpha\alpha}(\mathbf{l} - \mathbf{l}, \tau) f_{\alpha\beta}(\mathbf{l}, t - \tau) \quad (3.4.2)$$

which is the CTRW analog of Eq. (2.4.1). Here $\Gamma_\beta(t)$ is the probability that the walker who is initially in state β and unit cell $\mathbf{0}$ has not made a jump after a time t, so

$$\Gamma_\beta(t) = 1 - \int_0^t \psi_\beta(t) \, dt \quad (3.4.3)$$

where $\psi_\beta(t)$ is the waiting time density in state β. Upon Laplace transformation of (3.4.2) and (3.4.3), we obtain

$$\hat{f}_{\alpha\beta}(\mathbf{l}, u) = \frac{\hat{P}_{\alpha\beta}(\mathbf{l}, u) - \delta_{\alpha\beta} \delta_{\mathbf{l}, 0} \hat{\Gamma}_\alpha(u)}{\hat{P}_{\alpha\alpha}(\mathbf{0}, u)} = \frac{\hat{G}_{\alpha\beta}[\mathbf{l}, u] - \delta_{\alpha\beta} \delta_{\mathbf{l}, 0}}{\hat{G}_{\alpha\alpha}[\mathbf{0}, u]} \quad (3.4.4)$$

where $\hat{\mathsf{G}}[l, u]$ is given by (3.1.7). To obtain (3.4.4) we have used Eq. (3.1.6) and the fact that the Laplace transform of $\Gamma_\alpha(t)$ is precisely given by $u^{-1}[1 - \hat{\psi}_\alpha(u)]$, so that the first equality in (3.4.4) can be simplified by dividing out a common factor $\hat{\Gamma}_\alpha(u)$.

Making use of the fact that $\sum_l \hat{\mathsf{G}}[l, u] = [1 - \mathsf{T}\hat{\psi}(u)]^{-1}$, we finally arrive at

$$\hat{S}_{\alpha\beta}(u) = \frac{1}{u} \sum_l \hat{f}_{\alpha\beta}(l, u)$$

$$= \frac{1}{u} [\hat{G}_{\alpha\alpha}[\mathbf{0}, u]]^{-1}[\{[1 - \mathsf{T}\hat{\psi}(u)]^{-1}\}_{\alpha\beta} - \delta_{\alpha\beta}] \qquad (3.4.5)$$

The factor $\delta_{\alpha\beta}$ in (3.4.5) appears because the starting site is not counted as a visited site [in contrast to (2.4.3)] but for the long-time behavior of $S_{\alpha\beta}(t)$ this is of course irrelevant.

Making use of (3.2.3a) we find for the case of finite mean waiting times,

$$\hat{S}_{\alpha\beta}(u) \overset{u \to 0}{\sim} \pi_\alpha(u^2 \bar{t})^{-1}[\hat{G}_{\alpha\alpha}[\mathbf{0}, u]]^{-1} \qquad (3.4.6)$$

The Laplace transform $\hat{G}_{\alpha\alpha}[\mathbf{0}, u]$ approaches the discrete time generating function $G_{\alpha\alpha}(\mathbf{0}, 1)$ as $u \to 0$. In dimension $d \geqslant 3$, $G_{\alpha\alpha}(\mathbf{0}, 1)$ is finite, as noted before, and thus

$$\hat{S}_{\alpha\beta}(u) \overset{u \to 0}{\sim} \pi_\alpha(u^2 \bar{t})^{-1}[G_{\alpha\alpha}(\mathbf{0}, 1)]^{-1} \qquad (d \geqslant 3)$$

Applying the Tauberian theorem cited in Appendix B, we find then for the expected number of distinct sites visited, summed over final states and averaged over the distribution of the walker over the initial states,

$$S(t) \sim \frac{t}{\bar{t}} \sum_\alpha \pi_\alpha[G_{\alpha\alpha}(\mathbf{0}, 1)]^{-1} \qquad (d \geqslant 3) \quad (t \to \infty) \qquad (3.4.7)$$

For $d = 1, 2$, $G_{\alpha\alpha}(\mathbf{0}, 1)$ diverges (assuming zero drift), so

$$\hat{G}_{\alpha\alpha}[\mathbf{0}, u] \sim \pi_\alpha \tilde{\hat{G}}_{00}[\mathbf{0}, u] \qquad (u \to 0) \qquad (3.4.8)$$

where $\tilde{\hat{G}}_{00}[\mathbf{0}, u]$ is given by (3.3.1b), which is identical to (2.3.8) with z replaced by $1 - u\bar{t}$. After inverse Laplace transforming (3.4.6), one obtains the discrete time results (2.4.10a) with the variable n replaced by $\bar{t}$. Summing over final states α and averaging over the initial states β then leads to

$$S(t) \overset{t \to \infty}{\sim} m \frac{(\det 2\mathsf{D})^{1/2}}{\det \mathsf{A}} \begin{cases} \left(\dfrac{8}{\pi} t/\bar{t}\right)^{1/2} & (d = 1) \qquad (3.4.9a) \\[3mm] \dfrac{2\pi t/\bar{t}}{\log(t/\bar{t})} & (d = 2) \qquad (3.4.9b) \end{cases}$$

For case b of infinite mean waiting times, the corresponding results are, with $\bar{B}$ defined in (3.2.4b),

$$S(t) \overset{t \to \infty}{\sim} m \frac{(\det 2D)^{1/2}}{\det A} \begin{cases} \sqrt{2}\,(\bar{B})^{-1/2}\,\dfrac{t^{q/2}}{\Gamma(1+q/2)} & (d=1) \qquad (3.4.10a) \\[3mm] (\bar{B})^{-1}\,\dfrac{2\pi t^q}{\Gamma(1+q)} \Big/ \log[t^q/\bar{B}] & (d=2) \qquad (3.4.10b) \end{cases}$$

and

$$S(t) \overset{t \to \infty}{\sim} m \left\{ \sum_\alpha \pi_\alpha [G_{\alpha\alpha}(\mathbf{0}, 1)]^{-1} \right\} \frac{t^q}{\Gamma(1+q)} \cdot \frac{1}{\bar{B}} \qquad (d \geqslant 3) \quad (3.4.10c)$$

These results reduce to those of Shlesinger[27] for perfect lattices if there is only one internal state ($m=1$).

4. SUMMARY AND CONCLUSIONS

We have considered multistate random walks on inhomogeneous periodic lattices, which are globally translation invariant, and have determined the long-time asymptotic behavior of the occupation probabilities of the internal states, the means and covariances, of the probability of return to the origin, and the expected number of distinct sites visited. The crux of the method is to focus attention on the embedded Markov chain which is obtained by projecting the random walk on the set of internal states and to use asymptotic properties of Markov chains to show that, under the assumption that the walk is irreducible and aperiodic, the distribution of the walker over the internal states evolves toward a unique equilibrium distribution.

It was shown that the random walk properties mentioned above are identical to those for perfect lattices except for a renormalization of coefficients. In the case of the moments, explicit expressions for the modified coefficients (drift velocities and diffusion coefficients) were developed in terms of the eigenvalues and eigenvectors of the transition matrix of the embedded Markov chain. The calculation of the drift velocity and, for the case of locally unbiased walks, the diffusion coefficients, involves only a determination of the equilibrium distribution of the walker among the internal states. In the asymptotic expressions for the probability of return to the origin and the expected number of distinct sites visited (the latter only in dimension $d < 3$), the renormalized coefficients are precisely the diffusion coefficients of the multistate walk as modified by a geometrical scaling factor.

In the case of separable continuous time random walks (CTRW's) with finite mean waiting times and zero drift, the results are identical to those for discrete time walks with the discrete step variable n replaced by $t/\bar{t}$ where t is the time and $\bar{t}$ is a weighted sum of mean waiting times in each internal state. If the mean waiting times are infinite, the time dependence of the asymptotic results is different, but the coefficients still involve the discrete-time diffusion coefficients. If the drift velocity is nonzero, the expressions for the second moments are more complicated.

We therefore conclude that, in the case of walks with zero drift (not necessarily locally unbiased), the calculation of the asymptotic random walk properties for inhomogeneous periodic lattices studied here reduces to: (i) a calculation of the diffusion coefficients in discrete time for such lattices, using the formalism developed in Section 2.2, and (ii) The additional calculation of the quantities $\bar{t}$ and $\bar{B}$, as defined in (3.2.4), for the case of CTRW's.

ACKNOWLEDGMENTS

APPENDIX A

In this appendix, we derive Eqs. (2.2.21)–(2.2.24). The relation between the actual position $[\mathbf{r}(n)]_{\alpha\beta}$ of the walker after n steps, given initial and final states β and α, and $[\mathbf{l}(n)]_{\alpha\beta}$, which is the position of the unit cell which the walker occupies after n steps, is given by $[\mathbf{l}(0) = \mathbf{0}]$:

$$[\mathbf{r}(n)]_{\alpha\beta} = \sum_{i=1}^{d} [l_i(n)]_{\alpha\beta}\, \mathbf{a}_i + \boldsymbol{\rho}_{\alpha\beta} \tag{A1}$$

Here $\boldsymbol{\rho}_{\alpha\beta} = \boldsymbol{\rho}_\alpha - \boldsymbol{\rho}_\beta$, where $\boldsymbol{\rho}_\alpha$ denotes the relative position of the internal state α (which defines a particular site within the unit cell) with respect to the point which is used to indicate the position of the unit cell. The vectors $\{\mathbf{a}_i\}$ are the fundamental translation vectors of the lattice (see Section 2.1). The components of $[\mathbf{r}(n)]_{\alpha\beta}$ with respect to a coordinate system defined by the unit vectors $\mathbf{e}_1,...,\mathbf{e}_d$, are defined by

$$[r_i(n)]_{\alpha\beta} = \mathbf{r}_{\alpha\beta}(n) \cdot \mathbf{e}_i \tag{A2}$$

The average of (A2) is for large n given by

$$\langle r_i(n) \rangle_{\alpha\beta} \sim n\pi_\alpha \sum_i m_i A_{ij} + \pi_\alpha \mathbf{\rho}_{\alpha\beta} \cdot \mathbf{e}_j \tag{A3}$$

where we have used (2.1.13) and (2.1.16a), and where A_{ij} is defined in (2.2.25). Summing over α and the initial distribution $p_\beta^{(0)}$ we obtain (2.2.21) and (2.2.22) (now we omit all terms of order unity). The expressions (2.2.23) and (2.2.24) are derived similarly if one observes that for large n all terms of $O(n)$ in $\langle r_i(n) r_j(n) \rangle$ which depend on $\mathbf{\rho}_{\alpha\beta}$ cancel against the corresponding contributions from the product $-\langle r_i(n) \rangle \langle r_j(n) \rangle$.

APPENDIX B

Here we present an outline of the derivation of (3.2.3), (3.2.8), and (3.2.9). To derive the first result, we need the singular part as $u \to 0$ of $\Gamma_{\alpha\beta}(\mathbf{0}, u) = \{[1 - \mathsf{T}\hat{\psi}(u)]^{-1}\}_{\alpha\beta}$, which, by the same argument as in Section 2.2, is given by

$$\Gamma_{\alpha\beta}^{(s)}(\mathbf{0}, u) = \pi_\alpha \tilde{\Gamma}_{00}(\mathbf{0}, u) \tag{B1a}$$

where

$$\tilde{\Gamma}_{00}(\mathbf{0}, u) = \{[1 - \tilde{\mathsf{T}}\tilde{\hat{\psi}}(u)]^{-1}\}_{00} \tag{B1b}$$

Now,

$$1 - \tilde{\mathsf{T}}\tilde{\hat{\psi}}(u) = 1 - \tilde{\mathsf{T}} + u^q \tilde{\mathsf{B}} - \tfrac{1}{2}u^{2q}\tilde{\mathsf{C}} + O(u^{3q}) \qquad (u \to 0) \tag{B2}$$

The matrices B and C are diagonal, with diagonal elements B_γ and C_γ [see (3.1.5)]. The case of finite mean waiting times is obtained by replacing B_γ by $\langle t_\gamma \rangle$ and C_γ by $\langle t_\gamma^2 \rangle$, and letting $q \to 1$.

In order to apply (2.2.11) we replace $\tilde{\mathsf{T}}$ by $\eta(u)\tilde{\mathsf{T}}$, where the auxiliary parameter $\eta(u) \to 1$ as $u \to 0$. At the end of the calculation this parameter therefore disappears again. Taking $\mathsf{A} = 1 - \eta\tilde{\mathsf{T}}$ in (2.2.11), where ε now indicates the variable u^q, we find

$$\tilde{\Gamma}_{00}(\mathbf{0}, u) \overset{u \to 0}{\sim} u^q \bar{B} - \tfrac{1}{2}u^{2q}\bar{C}' + O(u^{3q}) \tag{B3}$$

where

$$\bar{C}' = \bar{C} + 2 \sideset{}{'}\sum_{\beta,\gamma} \widetilde{(TB)}_{0\beta}[(1 - \Omega)^{-1}]_{\beta\gamma} \widetilde{(TB)}_{\gamma 0} \tag{B4}$$

and

$$\bar{C} = \sum_\alpha \pi_\alpha C_\alpha \tag{B5}$$

The quantity $\bar{B}$ is defined in (3.2.4), and the matrix Ω in (2.2.4). From (B1) and (B3) the result (3.2.3) is immediate (remember that $q = 1$ and $\bar{B} = \bar{t}$ in case a).

To derive the moments of $P_{\alpha\beta}(l, t)$ we have to look at the singular part of (3.2.7), which is

$$K_{\alpha\beta}^{(s)}(\boldsymbol{\theta}, u) = u^{-1}[1 - \hat{\psi}_\alpha(u)] \, \pi_\alpha \tilde{\Gamma}_{00}(\boldsymbol{\theta}, u) \tag{B6}$$

where

$$\tilde{\Gamma}_{00}(\boldsymbol{\theta}, u) = \{ [1 - \tilde{\Lambda}(\boldsymbol{\theta}) \, \tilde{\psi}(u)]^{-1} \}_{00} \tag{B7}$$

We again invoke (2.2.11) with A the same matrix as above, where we retain all terms linear or quadratic in $\{\theta_i\}$ and u or u^q (in case a or case b, respectively). The result is

$$\tilde{\Gamma}_{00}(\boldsymbol{\theta}, u) \sim \left[\tilde{\Gamma}_{00}(\mathbf{0}, u) - i \sum_j \theta_j m_j(u) + \tfrac{1}{2} \sum_{jk} \theta_j \theta_k s_{jk}(u) \right]^{-1} \qquad (\boldsymbol{\theta} \to \mathbf{0}) \tag{B8}$$

where $\tilde{\Gamma}_{00}(\mathbf{0}, u)$ is given in (B3), and

$$m_j(u) = m_j - u^q m_j' + O(u^{2q}) \qquad (u \to 0) \tag{B9a}$$

$$s_{jk}(u) = s_{jk} + O(u^q) \qquad (u \to 0) \tag{B9b}$$

Here m_j and s_{jk} are defined in (2.2.13) and

$$m_j' = (\widetilde{\langle l_j \rangle} B)_{00} + \sideset{}{'}\sum_{\beta,\gamma} [\widetilde{\langle l_j \rangle}_{0\beta} \{(1 - \Omega)^{-1}\}_{\beta\gamma} (\widetilde{TB})_{\gamma 0}$$

$$+ (\widetilde{TB})_{0\beta} \{(1 - \Omega)^{-1}\}_{\beta\gamma} \langle l_j \rangle_{\gamma 0}] \tag{B10}$$

The generating function (B6), summed over final states α and averaged over the initial distribution $\{p_\beta^{(0)}\}$ is

$$K^{(s)}(\boldsymbol{\theta}, u) = (\bar{B} u^{q-1} - \tfrac{1}{2} u^{2q-1} \bar{C} + \cdots) \tilde{\Gamma}_{00}(\boldsymbol{\theta}, u) \qquad (u \to 0) \tag{B11}$$

The Laplace transform of $\langle l_j(t) \rangle$ is given by

$$\langle l_j(u) \rangle = -i \left[\frac{\partial}{\partial \theta_j} K^{(s)}(\mathbf{0}, u) \right]_{\boldsymbol{\theta} = \mathbf{0}} \tag{B12}$$

Using (B11), (B8), and (B3) we find

$$\langle l_j(u) \rangle \overset{u \to 0}{\sim} u^{-(1+q)}(\bar{B})^{-1} m_j + u^{-1} \left[m_j \left(\frac{\bar{C}' - \tfrac{1}{2}\bar{C}}{\bar{B}^2} \right) - \frac{m_j'}{\bar{B}} \right] \tag{B13}$$

from which (3.2.8) follows by the Hardy–Littlewood–Karamata theorem.

The Laplace transform of the second moments is

$$\langle l_j(u)\, l_k(u)\rangle = -\left[\frac{\partial}{\partial\theta_j}\frac{\partial}{\partial\theta_k}K^{(s)}(\mathbf{0},u)\right]_{\boldsymbol{\theta}=\mathbf{0}} \tag{B14}$$

Carrying out the differentiations, inverting the Laplace transform and subtracting the product $\langle l_j(t)\rangle\langle l_k(t)\rangle$ we arrive at

$$\langle\!\langle l_j(t)\, l_k(t)\rangle\!\rangle \overset{t\to\infty}{\sim} \left\{\frac{2t^{2q}}{\Gamma(1+2q)}-\frac{t^{2q}}{\Gamma^2(1+q)}\right\}\frac{m_j m_k}{\bar{B}^2}$$

$$+\frac{t^q}{\Gamma(1+q)}\left\{\frac{s_{jk}}{\bar{B}}+\frac{m_j m_k}{\bar{B}}\left(\frac{\bar{C}'}{\bar{B}^2}\right)-\frac{1}{\bar{B}^2}(m_j m'_k+m_k m'_j)\right\} \tag{B15}$$

For the case of driftless walks $(m_j = 0, j = 1, 2,..., d)$ this expression reduces to (3.2.9).

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