

Exact and Asymptotic Properties of Multistate Random Walks

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A method is presented which allows one to obtain explicit analytical expressions (both exact and asymptotic) for many of the physically interesting quantities related to a multistate random walk (MRW). The exact results include the Laplace-Fourier-transformed probability distribution (continuous time) and generating function (discrete time), and closed evolution equations for the propagators related to each "internal" state of the walker. Analytical expressions for the scattering dynamical structure function and the frequency-dependent diffusion coefficient are given as illustrations. Asymptotic approximations to the single-state propagators are derived, allowing a detailed analysis of the long-time behavior and the calculation of asymptotic properties by single-state random walk standard methods. As an example, analytical expressions for the drift and diffusion coefficients are given.

KEY WORDS: Multistate random walk; exact results; embedded Markov process; asymptotic properties.

1. INTRODUCTION

In recent years considerable interest has arisen in the theory and applications of multistate random walks (MRWs),⁽¹⁻³⁾ based on the great variety of processes that can be described by these models.⁽⁴⁻¹¹⁾ The central idea is that of a random walk (RW) on a lattice, where the walker can be at each site in a number of "internal" states whose properties affect that of the RW.

Although these models have led to a variety of results, it is usually

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difficult or impossible⁽³⁻⁵⁾ to obtain explicit analytical expressions for many quantities of interest (either exact or asymptotic). The difficulty lies in the fact that the evolution equations for MRWs are matricial, and the usual procedures to solve them involve the diagonalization of matrices whose dimension is the number of internal states.^(3,12)

An early approach to this problem was that of Landman and Shlesinger,⁽⁴⁾ but their matrix method, though formally elegant and general, becomes unmanageable as a computing tool even for moderately large matrices. This situation was improved by Roerdink and Shuler,⁽⁵⁾ but their method only avoids the diagonalization for a restricted class of irreducible MRWs, the so-called “locally unbiased” ones. In more general cases (e.g., processes with drift⁽⁵⁾ or Lorentz-gas models^(8,9)), this method still requires the computation of the full set of eigenvalues and eigenvectors of the transition matrix, a task that can be carried out analytically only for some especially simple matrices. Besides, this method only deals with asymptotic properties, and it gives no hint of the *exact* form of the probability distribution, which is needed for a number of applications (calculation of the dynamical structure function for scattering on the walker,^(3,11) of frequency-dependent conductivities,⁽¹¹⁾ etc.). The resolvent matrix⁽¹³⁾ approach only deals with the marginal (summed over internal states) distribution, and analytical calculations can be implemented only for systems with a few internal states.

In this paper we will introduce a method providing analytical expressions for most of the physically interesting quantities. These expressions are derived in a systematic way from the MRW evolution equations, by means of direct algebraic procedures which do not involve the solving of eigenvalue problems nor make any restrictive assumption on the features of the MRW. The method only needs the calculation of the invariants of the Fourier–Laplace-transformed transition matrix, allowing one to obtain analytical results no matter how complex this matrix may be. In Section 2 we derive explicit expressions for the Fourier–Laplace-transformed probability distributions of continuous-time MRWs. For Markovian MRWs we also construct closed evolution equations for the propagators related to each single internal state of the walker. In Section 3 we derive, for Markovian MRWs, long-time asymptotic approximations for the single-state propagators. The number of stationary states of the process summed over the lattice is found to be decisive for the long-time behavior of these propagators. We also construct expressions for some moments of the single-state propagators, and for the drift and diffusion coefficients. As an example, these results are applied to a RW on a sparsely periodic lattice⁽⁵⁾ with drift. All these results are easily extended to discrete-time MRWs. Finally, in Section 4 we summarize and discuss the results obtained.

2. EXACT RESULTS

We begin by considering a continuous-time RW on a Bravais lattice with translational invariance (the detailed lattice structure and dimensionality are immaterial). We assume that the walker can be, at any site \mathbf{s} , in one of a *finite number* N of internal states (labeled by $i = 1, \dots, N$).³

Evolution Equations. Let $P^i(\mathbf{s}, t)$ be the probability for the walker to be at site \mathbf{s} and state i at time t . We assume a description in terms of a system of coupled generalized master equations^(2,14) (GMEs),

$$\partial_t P^i(\mathbf{s}, t) = \sum_{\mathbf{s}'} \sum_{j=1}^N \int_0^t dt' W_{ij}(\mathbf{s} - \mathbf{s}', t - t') P^j(\mathbf{s}', t') \quad (2.1)$$

where $\partial_t \equiv \partial/\partial t$. The spatial convolution can be eliminated by a discrete Fourier transform,⁽²⁾

$$P^i(\mathbf{k}, t) = \sum_{\mathbf{s}} [\exp(i\mathbf{k} \cdot \mathbf{s})] P^i(\mathbf{s}, t)$$

(We will keep track of transformations by explicitly writing the arguments of all functions.) This leads to

$$\partial_t \mathbf{P}(\mathbf{k}, t) = \int_0^t dt' \mathbb{W}(\mathbf{k}, t - t') \mathbf{P}(\mathbf{k}, t') \quad (2.2)$$

where $\mathbf{P}(\mathbf{k}, t)$ is the (column) vector with components $P^i(\mathbf{k}, t)$ and $\mathbb{W}(\mathbf{k}, t)$ the $N \times N$ matrix with elements $W_{ij}(\mathbf{k}, t)$.

Equation (2.2) must be supplemented with suitable initial conditions $\mathcal{P}_0^i(\mathbf{k}) \equiv P^i(\mathbf{k}, t = 0)$. Taking $\mathcal{P}_0^i(\mathbf{s}) = \delta_{ij} \delta(\mathbf{s} - \mathbf{s}_0)$, we get $P^i(\mathbf{s}, t) \equiv P_{1|1}(\mathbf{s}, i, t | \mathbf{s}_0, j, 0)$, the two-times conditional probability⁽¹²⁾; but unless the MRW is Markovian, this is not identical with the propagator for P^i .⁽¹⁵⁾

Probability Distributions. Taking a Laplace transform

$$P^i(\mathbf{k}, u) \equiv \int_0^\infty P^i(\mathbf{k}, t) e^{-ut} dt$$

in Eq. (2.2) and solving for \mathbf{P} , we get

$$\mathbf{P}(\mathbf{k}, u) = [u\mathbb{1} - \mathbb{W}(\mathbf{k}, u)]^{-1} \mathcal{P}_0(\mathbf{k}) \quad (2.3)$$

³ If the internal states stand for different sublattices of a non-Bravais lattice, with \mathbf{a} , the vector connecting the origin with the i th site in a unit cell, then \mathbf{s} must be replaced by $\mathbf{s} + \mathbf{a}_i$ in all subsequent definitions.

where $\mathbb{1}$ is the $N \times N$ identity matrix. However, this is an analytical expression for \mathbf{P} only in a formal sense. What is usually needed is an *explicit* expression for P^i in terms of the elements of \mathbb{W} .

At this point the usual procedure is to diagonalize \mathbb{W} and expand the initial conditions vector $\mathcal{P}_0(\mathbf{k})$ in the eigenvector basis, but this can be done analytically only for some simple forms of \mathbb{W} (which in general is not even guaranteed to be diagonalizable⁽¹²⁾). Nevertheless, it can be shown that

$$\mathbf{P}(\mathbf{k}, u) = \frac{1}{\not\phi_w(u)} \sum_{n=0}^{N-1} u^{N-1-n} \mathcal{S}_n(\mathbf{k}, u) \quad (2.4)$$

where

$$\not\phi_w(\lambda) \equiv \det[\lambda \mathbb{1} - \mathbb{W}(\mathbf{k}, u)] = \sum_{n=0}^N \lambda^{N-n} \alpha_n(\mathbf{k}, u) \quad (2.5)$$

and

$$\mathcal{S}_n(\mathbf{k}, u) = \sum_{m=0}^n \alpha_m(\mathbf{k}, u) \mathcal{P}_{n-m}(\mathbf{k}, u) \quad (2.6)$$

Here $\alpha_m(\mathbf{k}, u)$ are the *invariants* of $\mathbb{W}(\mathbf{k}, u)$, and $\mathcal{P}_m(\mathbf{k}, u) = \mathbb{W}^m(\mathbf{k}, u) \mathcal{P}_0(\mathbf{k})$. (For a Markovian MRW, α_n , \mathcal{S}_n^i , and \mathcal{P}_n^i become independent of u .)

Equation (2.4) can be verified by multiplying both sides from the left by $[\lambda \mathbb{1} - \mathbb{W}(\mathbf{k}, u)]$, noting from (2.6) that $\mathcal{S}_n = \alpha_n \mathcal{P}_0 + \mathbb{W} \mathcal{S}_{n-1}$, and using

$$\mathcal{S}_N = \sum_{n=0}^N \alpha_n \mathbb{W}^{N-n} \mathcal{P}_0 = \not\phi_w(\mathbb{W}) \mathcal{P}_0 \equiv 0$$

since $\not\phi_w(\mathbb{W}) \equiv 0$ by the Cayley–Hamilton theorem.⁽¹⁶⁾ (We have omitted the arguments \mathbf{k} and u , for simplicity.) Since the Cayley–Hamilton theorem is valid for *any* finite-dimensional matrix, Eq. (2.4) is valid independently of the particular MRW being considered.

Single-State Evolution Equations. For Markovian MRWs, $\mathbb{W}(\mathbf{k}, t) = \mathbb{W}(\mathbf{k}) \delta(t^+)$, so Eq. (2.2) reduces to

$$\partial_t \mathbf{P}(\mathbf{k}, t) = \mathbb{W}(\mathbf{k}) \mathbf{P}(\mathbf{k}, t) \quad (2.7)$$

Using again the Cayley–Hamilton theorem, we see that

$$\not\phi_w(\partial/\partial t) \mathbf{P}(\mathbf{k}, t) = \not\phi_w[\mathbb{W}(\mathbf{k})] \mathbf{P}(\mathbf{k}, t) \equiv 0$$

so using Eq. (2.5) we get

$$\sum_{n=0}^N \alpha_n(\mathbf{k}) \partial_t^{N-n} P^i(\mathbf{k}, t) = 0 \quad (2.8)$$

It is worth noting that Eq. (2.8) is exactly the same for each P^i , i.e., they only differ in their initial conditions. Also, though the evolution equation (2.7) for \mathbf{P} is Markovian, that for each P^i is a closed N th-order differential equation, so we have a non-Markovian description⁽¹²⁾ for each P^i taken separately.

Discrete-Time MRWs. If the jumps occur at discrete time intervals, the equation describing the MRW is

$$P^i_{n+1}(\mathbf{s}) = \sum_{\mathbf{s}'} \sum_{j=1}^N M_{ij}(\mathbf{s} - \mathbf{s}') P^j_n(\mathbf{s}') \tag{2.9}$$

where n is the step number. Discrete Fourier transformation leads to

$$\mathbf{P}_{n+1}(\mathbf{k}) = \mathbb{M}(\mathbf{k}) \mathbf{P}_n(\mathbf{k}) \tag{2.10}$$

where we adopted vector notation. The generating function for $P^i_n(\mathbf{k})$ is defined as the i th component of the vector

$$\mathbf{G}(\mathbf{k}, z) = \sum_{n=0}^{\infty} z^n \mathbf{P}_n(\mathbf{k}) \tag{2.11}$$

Multiplying Eq. (2.10) by z^{n+1} , summing over n from 0 to ∞ , and using definition (2.11), we get the known result

$$\left[\frac{1}{z} \mathbb{1} - \mathbb{M}(\mathbf{k}) \right] \mathbf{G}(\mathbf{k}, z) = \mathbf{P}_0(\mathbf{k}) \tag{2.12}$$

Similarly to the continuous-time case, the explicit solution for G^i is

$$G^i(\mathbf{k}, z) = \frac{1}{\not\!/\!_M(1/z)} \sum_{n=0}^{N-1} \left(\frac{1}{z}\right)^{N-n} S^i_n(\mathbf{k}) \tag{2.13}$$

with

$$S^i_n(\mathbf{k}) = \sum_{m=0}^n \alpha_m(\mathbf{k}) P^i_{n-m}(\mathbf{k}) \tag{2.14}$$

where $\alpha_m(\mathbf{k})$ are the invariants of $\mathbb{M}(\mathbf{k})$, $\not\!/\!_M(\lambda) \equiv \det[\lambda \mathbb{1} - \mathbb{M}]$, and $P^i_m(\mathbf{k})$ is the i th component of $\mathbb{M}^m(\mathbf{k}) \mathbf{P}_0(\mathbf{k})$. The corresponding closed recurrence relations for each distribution $P^i_n(\mathbf{k})$ are

$$P^i_n(\mathbf{k}) = - \sum_{l=1}^N \alpha_l(\mathbf{k}) P^i_{n-l}(\mathbf{k}), \quad n \geq N \tag{2.15}$$

As before, Eq. (2.15) is the same for each P_n^i . Also, though the evolution equation (2.10) for \mathbf{P}_n is Markovian, Eq. (2.15) gives a non-Markovian description⁽¹²⁾ for each process P_n^i taken separately, with a memory “depth” of N steps.

Sample Applications. As an illustration, we give the expressions for the dynamical structure function $S(\mathbf{k}, \omega)$ and the frequency-dependent diffusion coefficient $D(\omega)$. From the Kubo–Lax linear response theory⁽¹⁾ we have

$$D(\omega) = \left[-\frac{u^2}{2} \nabla_{\mathbf{k}}^2 \sum_{i=1}^N P^i(\mathbf{k}, u) \right]_{\mathbf{k}=0, u=i\omega}$$

Likewise,⁽³⁾

$$S(\mathbf{k}, \omega) = \frac{1}{\pi} \operatorname{Re} \sum_{i=1}^N P^i(\mathbf{k}, u) \Big|_{u=i\omega}$$

Substitution of Eq. (2.4) then gives explicit expressions for S and D in terms of W_{ij} . Both expressions must be calculated with thermal equilibrium initial conditions $\mathcal{P}_0^i(\mathbf{k}) = 1/N$. A practical example can be found in ref. 11.

3. ASYMPTOTIC APPROXIMATIONS AND PROPERTIES

We will derive here some asymptotic properties for Markovian MRWs (the general non-Markovian case will be treated elsewhere), assuming hereafter that probability is conserved.⁴

General Treatment. We start by finding the lowest-order approximation to (2.4) for small u , still conserving probability.

Let $\mathbb{W}_0 = \mathbb{W}(\mathbf{k}=0)$. We define the embedded Markov process (EMP) as the process obtained by summing Eq. (2.1) over all sites of the lattice [or by evaluating Eq. (2.2) at $\mathbf{k}=0$],

$$\partial_t \mathbf{P}(\mathbf{k}=0, t) = \mathbb{W}_0 \mathbf{P}(\mathbf{k}=0, t) \quad (3.1)$$

This equation describes the evolution of the walker in the internal-state space, regardless of its position on the lattice.

Let us assume that the dimension of the kernel of \mathbb{W}_0 is K , i.e., that \mathbb{W}_0 has K vanishing eigenvalues ($1 \leq K < N$). By Eq. (2.5), this is equivalent to

$$\alpha_{N-K}(\mathbf{k}=0) \neq 0, \quad \alpha_{N-K+1}(\mathbf{k}=0) = \dots = \alpha_N(\mathbf{k}=0) = 0 \quad (3.2)$$

⁴ This implies no real restriction, since a probability-nonconserving MRW can be mapped onto a probability-conserving one by introducing one or more additional internal states, in which the population lost by the original MRW is accumulated.

Evaluating Eq. (2.4) at $\mathbf{k} = 0$, approximating for $u \rightarrow 0$, and using Watson’s lemma,⁽¹⁷⁾ we get for the EMP the asymptotic expansion

$$\mathbf{P}(\mathbf{k} = 0, t) \underset{t \rightarrow \infty}{\sim} \frac{1}{\alpha_{N-K}(\mathbf{k} = 0)} \sum_{m=0}^{K-1} \mathcal{S}_{N-K+m}(\mathbf{k} = 0) \frac{t^m}{m!} \tag{3.3}$$

Now, \mathbb{W}_0 is a W -matrix (in the sense of ref. 12), so the final state of the EMP must be a *finite* vector. Thus, we conclude from Eq. (3.3) that

$$\mathcal{S}_{N-K+1}(\mathbf{k} = 0) = \dots = \mathcal{S}_{N-1}(\mathbf{k} = 0) = 0 \tag{3.4}$$

and Eq. (3.3) (Laplace-transformed) reduces to

$$u\mathbf{P}(\mathbf{k} = 0, u) \underset{u \rightarrow 0}{\sim} \mathcal{S}_{N-K}(\mathbf{k} = 0) / \alpha_{N-K}(\mathbf{k} = 0) \tag{3.5}$$

which gives an expression for the final state of the EMP. Summing over the internal states, and noting that $\sum_{i=1}^N \mathcal{S}_n^i(\mathbf{k} = 0) = \alpha_n(\mathbf{k} = 0)$ ($0 \leq n \leq N - 1$), we see that Eq. (3.5) conserves probability.

We now approximate Eq. (2.4) for arbitrary \mathbf{k} , keeping in both numerator and denominator the lowest possible orders of u allowing one to recover Eq. (3.5) at $\mathbf{k} = 0$ (note that the limits $\mathbf{k} \rightarrow 0$ and $u \rightarrow 0$ cannot be freely exchanged). This leads to

$$u\mathbf{P}(\mathbf{k}, u) \underset{u \rightarrow 0}{\sim} \left(\sum_{n=1}^K u^n \mathcal{S}_{N-n}(\mathbf{k}) \right) \left(\sum_{n=0}^K u^n \alpha_{N-n}(\mathbf{k}) \right)^{-1} \tag{3.6}$$

This is the lowest-order asymptotic approximation for $\mathbf{P}(\mathbf{k}, u)$ still conserving probability, which we call the “minimal” approximation. The value of K fully determines the order of the approximation, and equals the number of independent stationary states of the EMP.⁽¹²⁾

The necessary conditions for Eq. (3.6) to be valid are

$$\alpha_{N-K-1}(\mathbf{k})u \ll \alpha_{N-K}(\mathbf{k}), \quad \mathcal{S}_{N-K-1}(\mathbf{k})u \ll \mathcal{S}_{N-K}(\mathbf{k})$$

or in the time domain

$$t \gg \tau = \text{Max} \left(\frac{\alpha_{N-K-1}(\mathbf{k})}{\alpha_{N-K}(\mathbf{k})}, \frac{\mathcal{S}_{N-K-1}^i(\mathbf{k})}{\mathcal{S}_{N-K}^i(\mathbf{k})} \right) \tag{3.7}$$

with \mathbf{k} in the first Brillouin zone and $i = 1, \dots, N$.

Remark. In the preceding derivation we disregarded the possibility of $\mathbb{W}(\mathbf{k})$ having one or more eigenvalues which *identically* vanish as functions of \mathbf{k} , i.e., that $\alpha_n(\mathbf{k}) \equiv 0$ for some $n \leq N$ [see Eq. (3.2)]. This case

corresponds to MRWs which are reducible^(5,12) *on the lattice*, i.e., where some lattice sites cannot be reached from some others even after an arbitrarily large number of steps. Hence, it is evident that, unless we select very particular initial conditions, the probability distributions will lack the translational invariance assumed for their evolution equations. Although examples of such behavior can be found (e.g., the “collapsed” limit of the Lorentz gas of ref. 8), they are fairly uncommon in usual applications. The theory can be extended to encompass these cases with little effort, rewriting the derivation of Eqs. (3.3)–(3.6) from the corresponding particular form of Eq. (2.4), but we will not do it here.

Particular Case $K = 1$. In this case the EMP has a unique stationary state, i.e., \mathbb{W}_0 is not “decomposable” (we classify W -matrices according to van Kampen⁽¹²⁾). From Eq. (3.6) we get

$$\mathbf{P}(\mathbf{k}, u) \underset{u \rightarrow 0}{\sim} \frac{\boldsymbol{\sigma}(\mathbf{k})}{u + \eta(\mathbf{k})} \equiv \boldsymbol{\Pi}(\mathbf{k}, u) \quad (3.8)$$

where

$$\eta(\mathbf{k}) = \frac{\alpha_N(\mathbf{k})}{\alpha_{N-1}(\mathbf{k})}, \quad \boldsymbol{\sigma}(\mathbf{k}) = \frac{\mathcal{S}_{N-1}(\mathbf{k})}{\alpha_{N-1}(\mathbf{k})} \quad (3.9)$$

Here we defined a distribution $\boldsymbol{\Pi}(\mathbf{k}, u)$, having *precisely* the form given by (3.8) for all u , so $\mathbf{P}(\mathbf{k}, t)$ tends asymptotically to $\boldsymbol{\Pi}(\mathbf{k}, t)$ for long times. Laplace-antitransforming Eq. (3.8) gives the Markovian evolution equation

$$\partial_t \Pi^i(\mathbf{k}, t) = -\eta(\mathbf{k}) \Pi^i(\mathbf{k}, t), \quad \Pi^i(\mathbf{k}, t=0) = \sigma^i(\mathbf{k}) \quad (3.10)$$

[exact for $\Pi^i(\mathbf{k}, t)$ and asymptotic for $P^i(\mathbf{k}, t)$]. The validity condition for (3.10) is given by Eq. (3.7) with $K = 1$.

Note that for $t \gg \tau$ each distribution P^i evolves as a single-state *Markovian* RW, with a lattice structure factor^(1,2) $\eta(\mathbf{k})$. Hence each process $P^i(\mathbf{k}, t)$ shows a non-Markovian *transient*, but eventually sets into a Markovian asymptotic regime. From the definition of η we see, however, that this single-state RW will generally involve jumps to far-lying neighbors, even if the MRW we started with included only jumps to nearest neighbors.

With (3.8) and (3.10), asymptotic properties of each process P^i can be calculated in the usual way for single-state RWs.⁽¹⁾ As an example, we will work out analytical expressions for the mean displacements and variances,

and the drift and diffusion coefficients. We first observe that in general $P^i(\mathbf{s}, t)$ is not normalized. Instead, from (3.10) and (3.2)

$$\sum_{\mathbf{s}} P^i(\mathbf{s}, t) \underset{t \rightarrow \infty}{\sim} \sum_{\mathbf{s}} \Pi^i(\mathbf{s}, t) = \Pi^i(\mathbf{k} = 0, t) = \sigma^i(\mathbf{k} = 0)$$

wherefore we define the mean displacements by⁵

$$\langle \mathbf{s} \rangle^i(t) = \frac{\sum_{\mathbf{s}} \mathbf{s} P^i(\mathbf{s}, t)}{\sum_{\mathbf{s}} P^i(\mathbf{s}, t)} \underset{t \rightarrow \infty}{\sim} \left. \frac{-i \nabla_{\mathbf{k}} \Pi^i(\mathbf{k}, t)}{\sigma^i(\mathbf{k})} \right|_{\mathbf{k} = 0} \tag{3.11}$$

Thus, from Eq. (3.10) [or (3.8) and Watson’s lemma⁽¹⁷⁾] we get

$$\langle \mathbf{s} \rangle^i(t) \underset{t \rightarrow \infty}{\sim} \langle \mathbf{s} \rangle_{\sigma}^i + \mathbf{d}t \tag{3.12}$$

with the drift coefficient \mathbf{d} given by

$$\mathbf{d} = i \nabla_{\mathbf{k}} \eta(\mathbf{k}) \Big|_{\mathbf{k} = 0} = i \left. \frac{\nabla_{\mathbf{k}} \alpha_N(\mathbf{k})}{\alpha_{N-1}(\mathbf{k})} \right|_{\mathbf{k} = 0} \tag{3.13}$$

[we used $\alpha_N(\mathbf{k} = 0) = 0$ in the last step], and

$$\langle \mathbf{s} \rangle_{\sigma}^i = \frac{\sum_{\mathbf{s}} \mathbf{s} \sigma^i(\mathbf{s})}{\sum_{\mathbf{s}} \sigma^i(\mathbf{s})} = -i \left. \frac{\nabla_{\mathbf{k}} \sigma^i(\mathbf{k})}{\sigma^i(\mathbf{k})} \right|_{\mathbf{k} = 0} \tag{3.14}$$

This last term gives the contribution of the non-Markovian transient to the asymptotic value of $\langle \mathbf{s} \rangle^i(t)$. Using similar definitions for the mean square displacements $\langle s^2 \rangle^i(t)$ and $\langle s^2 \rangle_{\sigma}^i(t)$, and defining the variances as usual by $\langle\langle s^2 \rangle\rangle = \langle s^2 \rangle - |\langle \mathbf{s} \rangle|^2$, the same kind of calculation gives

$$\langle\langle s^2 \rangle\rangle^i(t) \underset{t \rightarrow \infty}{\sim} \langle\langle s^2 \rangle\rangle_{\sigma}^i + 2Dt \tag{3.15}$$

with the diffusion coefficient D given by

$$D = \frac{1}{2} \nabla_{\mathbf{k}}^2 \eta(\mathbf{k}) \Big|_{\mathbf{k} = 0} = \frac{1}{2} \left. \frac{\nabla_{\mathbf{k}}^2 \alpha_N(\mathbf{k}) + 2i \mathbf{d} \cdot \nabla_{\mathbf{k}} \alpha_{N-1}(\mathbf{k})}{\alpha_{N-1}(\mathbf{k})} \right|_{\mathbf{k} = 0} \tag{3.16}$$

and

$$\langle\langle s^2 \rangle\rangle_{\sigma}^i = - \left. \frac{\nabla_{\mathbf{k}}^2 \sigma^i(\mathbf{k})}{\sigma^i(\mathbf{k})} \right|_{\mathbf{k} = 0} - |\langle \mathbf{s} \rangle_{\sigma}^i|^2 \tag{3.17}$$

⁵ For “transient” internal states,⁽¹²⁾ which are depopulated for $t \rightarrow \infty$, $\sigma^i(\mathbf{k} = 0) = 0$, so they cannot be normalized by (3.11); a higher-order approximation for $P^i(\mathbf{k}, u)$ must be used. A matrix \mathbb{W}_0 having such states is called⁽¹²⁾ “incompletely reducible.”

which gives the contribution of the non-Markovian transient to the asymptotic value of $\langle\langle s^2 \rangle\rangle^i(t)$.

Case $K \geq 2$. In this case the EMP has several stationary states, i.e., \mathbb{W}_0 is⁽¹²⁾ “decomposable” or “splitting.” We will only analyze the case $K=2$, as the extension to the general case is direct. From Eq. (3.6) we get

$$\mathbf{P}(\mathbf{k}, u) \underset{u \rightarrow 0}{\sim} \frac{\boldsymbol{\sigma}_1(\mathbf{k})u + \boldsymbol{\sigma}_0(\mathbf{k})}{u^2 + \eta_1(\mathbf{k})u + \eta_0(\mathbf{k})} \equiv \boldsymbol{\Pi}(\mathbf{k}, u) \quad (3.18)$$

with $\boldsymbol{\Pi}(\mathbf{k}, u)$ having the same meaning as for $K=1$ and

$$\begin{aligned} \eta_0(\mathbf{k}) &= \frac{\alpha_N(\mathbf{k})}{\alpha_{N-2}(\mathbf{k})}, & \eta_1(\mathbf{k}) &= \frac{\alpha_{N-1}(\mathbf{k})}{\alpha_{N-2}(\mathbf{k})} \\ \boldsymbol{\sigma}_0(\mathbf{k}) &= \frac{\mathcal{L}_{N-1}(\mathbf{k})}{\alpha_{N-2}(\mathbf{k})}, & \boldsymbol{\sigma}_1(\mathbf{k}) &= \frac{\mathcal{L}_{N-2}(\mathbf{k})}{\alpha_{N-2}(\mathbf{k})} \end{aligned} \quad (3.19)$$

Laplace-antitransforming Eq. (3.18), we now get a non-Markovian evolution equation

$$\begin{aligned} \partial_t^2 \Pi^i(\mathbf{k}, t) + \eta_1(\mathbf{k}) \partial_t \Pi^i(\mathbf{k}, t) + \eta_0(\mathbf{k}) \Pi^i(\mathbf{k}, t) &= 0 \\ \Pi^i(\mathbf{k}, t=0) &= \sigma_1^i(\mathbf{k}) \\ \partial_t \Pi^i(\mathbf{k}, t=0) &= \sigma_0^i(\mathbf{k}) - \eta_1(\mathbf{k}) \sigma_1^i(\mathbf{k}) \end{aligned} \quad (3.20)$$

The validity condition for (3.20) is given by Eq. (3.7) with $K=2$.

Now even for arbitrarily long times each P^i evolves as a single-state *non-Markovian* RW (with the definition of η_0 and η_1 inducing jumps to farly neighbors, as for $K=1$). That the processes P^i will not reach a Markovian regime was somehow to be expected, since the time scale for the setup of Markovian evolution in the $K=1$ case turns out to be *infinite* for $K \geq 2$ [for now $\alpha_{N-1}(\mathbf{k}=0) = 0$]. This behavior is general for $K \geq 2$.

Defining $\Pi_0^i(\mathbf{k}) = \Pi^i(\mathbf{k}, t=0)$ and $\dot{\Pi}_0^i(\mathbf{k}) = \partial_t \Pi^i(\mathbf{k}, t=0)$, we find from (3.20) the mean displacements

$$\langle \mathbf{s} \rangle^i(t) \underset{t \rightarrow \infty}{\sim} \langle \mathbf{s} \rangle_{\Pi_0}^i + \langle \mathbf{s} \rangle_{\dot{\Pi}_0}^i t + i \nabla_{\mathbf{k}} \eta_0(\mathbf{k}) \Big|_{\mathbf{k}=0} \frac{t^2}{2} \quad (3.21)$$

with

$$\langle \mathbf{s} \rangle_{\dot{\Pi}_0}^i = -i \frac{\nabla_{\mathbf{k}} \Pi_0^i(\mathbf{k})}{\Pi_0^i(\mathbf{k})} \Big|_{\mathbf{k}=0} \quad (3.22)$$

the contribution of the transient to the mean displacements, and

$$\langle \mathbf{s} \rangle_{\dot{H}_0}^i = -i \frac{\nabla_{\mathbf{k}} \dot{H}_0^i(\mathbf{k})}{\dot{H}_0^i(\mathbf{k})} \Big|_{\mathbf{k}=0} \tag{3.23}$$

its contribution to the mean “velocity.” Similarly, we get

$$\begin{aligned} \langle s^2 \rangle^i(t) \underset{t \rightarrow \infty}{\sim} & \langle s^2 \rangle_{\dot{H}_0}^i + \langle s^2 \rangle_{\dot{H}_0}^i t \\ & + [\nabla_{\mathbf{k}}^2 \eta_0(\mathbf{k}) + 2i \langle \mathbf{s} \rangle_{\dot{H}_0}^i \cdot \nabla_{\mathbf{k}} \eta_0(\mathbf{k})]_{\mathbf{k}=0} \frac{t^2}{2} \end{aligned} \tag{3.24}$$

for the mean-squared displacements, the averages with \dot{H}_0 and \dot{H}_0^i having definitions similar to (3.22) and (3.23), respectively.

In this case, drift and diffusion coefficients cannot be defined as the coefficients of t in the asymptotic expressions for $\langle \mathbf{s} \rangle^i(t)$ and $\langle s^2 \rangle^i(t)$, respectively. Instead, (3.24) shows that the processes P^i will exhibit *enhanced* diffusion. This behavior is general for $K \geq 2$.

Relevance of the EMP. From the preceding analysis, we see that the number K of stationary states of the EMP is the fundamental quantity determining the detailed asymptotic behavior of P^i . The value of K is found by simply counting the number of invariants of $\mathbb{W}(\mathbf{k})$ which vanish at $\mathbf{k} = 0$.

Discrete-Time MRWs. Asymptotic properties for large step number can be obtained by analyzing the generating functions (2.13) near $z = 1$ in a way analogous to the continuous-time case, but this requires rewriting $G^i(\mathbf{k}, z)$ as a ratio of polynomials in $(1 - z)$. We sketch a procedure for exploiting the continuous-time results to obtain asymptotic approximations for G^i and asymptotic properties of P_n^i :

1. Start from a discrete-time MRW (2.10) and artificially introduce an exponential waiting time density $\phi(t) = \tau^{-1} \exp(-t/\tau)$ (the same one for all internal states), passing to a continuous-time description in terms of Markovian GMEs like (2.2), with⁽¹⁴⁾

$$\mathbb{W}(\mathbf{k}) = \frac{1}{\tau} [\mathbb{M}(\mathbf{k}) - \mathbb{I}] \tag{3.25}$$

2. Compute the invariants of $\mathbb{W}(\mathbf{k})$ from its characteristic polynomial by definition (2.5), find the value of K , and construct the corresponding asymptotic approximation for $P^i(\mathbf{k}, u)$ by Eq. (3.6).

3. Find the corresponding asymptotic approximation ($z \rightarrow 1$) for

$G^i(\mathbf{k}, z)$, which for $\phi(u) = 1/(1 + \tau u)$ [the Laplace transform of $\phi(t)$] is given by

$$G^i(\mathbf{k}, z) = \frac{1}{\tau z} P^i \left(\mathbf{k}, u = \frac{1-z}{\tau z} \right) \tag{3.26}$$

4. Finally, either find the asymptotic properties by the usual methods⁽¹⁾ for discrete-time single-state RWs, using (3.26) and Tauberian theorems,⁽¹⁸⁾ or calculate the corresponding continuous-time asymptotic quantities and then make the replacement⁽¹⁾ $t/\tau \rightarrow n$.

To illustrate the above procedure, we present the resulting general asymptotic expression for the $K=1$ case (the EMP having only one stationary state). The asymptotic approximation for $P^i(\mathbf{k}, u)$ is then (3.8), so the result for G^i is

$$G^i(\mathbf{k}, z) \underset{z \rightarrow 1}{\sim} \frac{\sigma^i(\mathbf{k})}{1 - z[1 + \tau\eta(\mathbf{k})]} \tag{3.27}$$

with η and σ^i defined by (3.9). The asymptotic mean displacements and variances are more easily obtained by setting $t \equiv n\tau$ in (3.12) and (3.15); the drift and diffusion coefficients are found from (3.13) and (3.16), multiplying by τ and τ^2 , respectively.

Example. To illustrate the use of the previous results, we will find the drift and diffusion coefficients for a RW on a 1d, sparsely periodic lattice. The model is taken from Roerdink and Shuler,⁽⁵⁾ but the results presented here are more complete.

The model (see Fig. 1) consists of a regular 1d lattice with spacing l , where the walker jumps to the right (left) with probability p (q) at each step ($p + q = 1$). The pausing-time densities are $\phi_1(t) = ae^{-at}$ for the sites marked by dots, and $\phi_2(t) = be^{-bt}$ for the crosses. The unit cell contains N

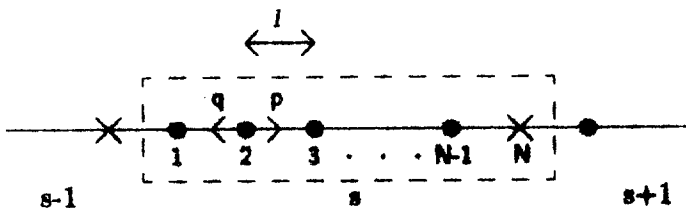


Fig. 1. One-dimensional sparsely periodic lattice. The jump probabilities from each site are p and q , the waiting times a^{-1} (dots) and b^{-1} (crosses). The dashed boxes are the unit cells.

sites (one cross and $N - 1$ dots) or “internal states,” numbered as shown in Fig. 1. The MRW is Markovian, and the matrix $\mathbb{W}(\mathbf{k})$ of Eq. (2.2) reads

$$\mathbb{W}(k) = \begin{pmatrix} -a & aq\varepsilon^* & & & & & & bpe \\ ap\varepsilon & -a & aq\varepsilon^* & & & & & \\ & \dots & \dots & \dots & & & & \\ & & & & ap\varepsilon & -a & bq\varepsilon^* & \\ aq\varepsilon^* & & & & & ap\varepsilon & -b & \end{pmatrix} \quad (3.28)$$

where $\varepsilon = \exp(ikl)$ and the asterisk stands for complex conjugation (elements not shown are zero). It is easily seen that

$$\not\mu_w(u) = \mathcal{F}_N - abpq \mathcal{F}_{N-2}^0 - a^{N-1}b(p^N e^{iNlk} + q^N e^{-iNlk}) \quad (3.29)$$

where

$$\begin{aligned} \mathcal{F}_n &= (a + u)\mathcal{F}_{n-1} - a^2pq\mathcal{F}_{n-2}, \quad 2 \leq n \leq N \\ \mathcal{F}_2 &= (a + u)(b + u) - abpq \\ \mathcal{F}_1 &= (b + u) \end{aligned} \quad (3.30a)$$

and

$$\mathcal{F}_n^0 = \mathcal{F}_n|_{b=a} \quad (3.30b)$$

The recurrence relation for \mathcal{F}_n is readily solved, giving

$$\begin{aligned} \mathcal{F}_n &= \frac{a^{n-1}(pq)^{n/2}}{a + u} \{2(b - a)uT_n(x) + [(2a - b)u + ab] U_n(x)\} \\ \mathcal{F}_n^0 &= a^n(pq)^{n/2} U_n(x) \end{aligned} \quad (3.31)$$

where T_n (U_n) are the n th-degree Chebyshev polynomials of the first (second) kind⁽¹⁹⁾ and $x = (a + u)/[2a(pq)^{1/2}]$. The required invariants are calculated through definition (2.5), substituting (3.31) in Eq. (3.29) and using the recurrence relations for T_n , U_n , and their derivatives.⁽¹⁹⁾ This gives

$$\alpha_{N-1}(k) \equiv \left. \frac{\partial \not\mu_w(u)}{\partial u} \right|_{u=0} = a^{N-2} [a + (N - 1)b] \frac{p^N - q^N}{p - q} \quad (3.32a)$$

$$\alpha_N(k) \equiv \not\mu_w(u)|_{u=0} = a^{N-1}b [p^N(1 - e^{iNlk}) + q^N(1 - e^{-iNlk})] \quad (3.32b)$$

Substituting (3.32) in Eq. (3.13), we get the drift coefficient

$$d = \frac{Nlab(p - q)}{a + (N - 1)b} \quad (3.33)$$

The diffusion coefficient is computed by substituting (3.32) in Eq. (3.16), which gives

$$D = D_0 \Delta \quad (3.34)$$

where

$$D_0 = \frac{1}{2} \frac{N^2 ab}{a + (N-1)b} \quad (3.35)$$

is the zero-drift diffusion coefficient, and

$$\Delta = N(p-q) \frac{p^N + q^N}{p^N - q^N} \quad (3.36)$$

is the correction arising from the drift ($\Delta = 1$ for $p = q$).

The expressions for d and D_0 agree with the results of Roerdink and Shuler.⁽⁵⁾ However, for nonvanishing drift the process is not “locally unbiased.” This prevented Roerdink and Shuler from finding the full expression for D , since in this case their method needs the full set of eigenvalues and eigenvectors of \mathbb{W}_0 to be computed. They argue that the drift corrections to D_0 are small for macroscopic systems; however, from Eq. (3.36) we can see that this is not so, since for p varying from 1/2 to 1 we find that Δ varies from 1 to N , the number of sites in the unit cell.

Any model leading to a form for $\mathbb{W}(\mathbf{k})$ similar to (3.28) can be handled along the same lines. An example is that of multiple-trapping models, in particular the ladder-trapping model.⁽³⁾

4. SUMMARY AND DISCUSSION

As shown in Section 2, the exact expressions obtained for $\mathbf{P}(\mathbf{k}, u)$ and $\mathbf{G}(\mathbf{k}, z)$ allow the analytical calculation of quantities such as the frequency-dependent diffusion coefficient or the incoherent quasielastic dynamical structure function for scattering on the walkers.

The asymptotic approximations derived for each single-state propagator P^i show that they behave for long times as single-state RWs, Markovian if the EMP has a single stationary state and non-Markovian otherwise. The expressions for the first and second moments of P^i show that the single-state propagators exhibit normal diffusion if the EMP has a single stationary state, and enhanced diffusion if it has several. Hence, the number of invariants of $\mathbb{W}(\mathbf{k})$ vanishing at $\mathbf{k} = 0$ fully specifies the qualitative long-time behavior of the single-state propagators.

The evolution equations and the expressions for $G^i(\mathbf{k}, z)$ and $P^i(\mathbf{k}, u)$ (both exact and asymptotic), as well as all quantities therefrom derived, involve only the knowledge of the matrices $\mathbb{M}(\mathbf{k})$ or $\mathbb{W}(\mathbf{k})$ and their invariants (only a few of them for asymptotic properties). So their construction is systematic and does not require the eigenvalue problem for \mathbb{M} or \mathbb{W} to be solved, allowing for fully analytical calculations even in systems having a large number of internal states. Since no restrictive assumptions have been made concerning the properties of the MRW, these results have the widest generality.

It must be noted that for both discrete and continuous time, finding the probability distributions in the space and time domains from $G^i(\mathbf{k}, z)$ or $P^i(\mathbf{k}, u)$ requires finding the zeros of the corresponding characteristic polynomial, i.e., the eigenvalues of $\mathbb{M}(\mathbf{k})$ or $\mathbb{W}(\mathbf{k})$. This can be thought to be a severe drawback, for the eigenvalue problem cannot be analytically solved in the general case. However, as shown in the example given, and in some other applications,^(9,11) most of the physically interesting information can be directly obtained from the expressions for $G^i(\mathbf{k}, z)$ or $P^i(\mathbf{k}, u)$ (or their asymptotic approximations) in the Fourier or Fourier–Laplace domains, respectively. From a practical point of view, this last feature is very useful.

Also, such results as the existence of an asymptotic Markovian regime for the single-state propagators, or analytical expressions for the asymptotic properties, can be obtained after constructing only some invariants of \mathbb{M} or \mathbb{W} , which makes the application to specific problems a systematic matter. This can be seen in the example given, where knowledge of only α_N and α_{N-1} sufficed for computing the drift and diffusion coefficients. (This MRW not being “locally unbiased,” the calculation of the diffusion coefficient by the methods of ref. 5 or by former ones would have required finding the full set of eigenvalues and eigenvectors of large matrices.)

Given the mathematical simplicity of the calculations involved, we think that the general results presented here can be profitably applied to a variety of problems. The extension of the asymptotic analysis to non-Markovian MRWs is in progress.

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