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Transitional probabilities for the 4-state random walk on a lattice

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Abstract

The diffusion and Schrödinger propagators have been known to coexist on a lattice when a particle undergoing random walk is endowed with two states of spin in addition to the two states of direction in a 1+1 spacetime dimension. In this paper we derive explicit expressions for the various transitional probabilities by employing generating functions and transform methods. The transitional probabilities are all expressed in terms of a one-dimensional integral involving trigonometric functions and/or Chebyshev polynomials of the first and second kind from which the spacetime continuum limits of the diffusion equation and Schrödinger equation follow directly.

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1. Introduction

There has been a lot of interest in the recent past to understand quantum mechanics in the context of classical statistical mechanics. On the one hand, Brownian motion provides a microscopic model of diffusion and provides an unambiguous interpretation of the diffusion equation. On the other hand, a similar physical interpretation is lacking for the Schrödinger equation, whose wave solution is a complex quantity without a physical reality. Because classical diffusion cannot account for the self-interference pattern that is so intrinsic to quantum behavior, several theories have been put forward recently to understand the microphysics of quantum behavior. Nelson [1] derived the Schrödinger equation starting from Newtonian mechanics and by assuming that a particle is subject to an underlying Brownian motion described by a combined forward-in-time and a backward-in-time Wiener processes. A detailed account of Nelson's original idea of stochastic mechanics and its subsequent refinement is given in [2–5]. Nottale [6] and Ord [7] advanced the idea that spacetime is not differentiable but is of a fractal nature, suggesting that an infinity of geodesics lie between any two points and, thereby, providing a fundamental and universal origin for the double

Wiener process of Nelson. These ideas are elaborated in the monograph [8]. El Naschie [9] too considered a fractal spacetime with a Cantorial structure and argued that quantum behavior could be mimicked by combining this fractal spacetime with a diffusion process. A totally different paradigm was recently introduced by Ord [10], who by considering a symmetric random walk on a lattice, showed that both the diffusion equation and the Schrödinger equation occur as approximate descriptions of different aspects of the same classical probabilistic system. By considering a 4-state random walk (4RW) on a discrete lattice, wherein a particle is endowed with two states of direction and two states of spin, Ord [10–12] has shown that both diffusion and Schrödinger propagators coexist on a lattice and that either can be obtained from a distinct projection of the same random walk. It is too early to speculate as to which of Nelson's or Ord's model will duplicate the true quantum behavior under a variety of situations. This can only be ascertained through additional work on both models. It may be mentioned that the combination of displacement and spin have also been used previously in [13, 14] to study dynamics of a quantum particle in spacetime. However, the important distinction between the Ord model and the one considered in [13, 14] is that the states describing the direction of motion are independent of those describing the spin states in the former model. There is also an intrinsic notion of *memory* embedded in the Ord's model.

The Schrödinger type of equation is encountered under the guise of *parabolic wave equation*, or simply parabolic equation in the solution of boundary-value problems in several branches of applied physics such as acoustics [15], optics and classical electromagnetic wave propagation [16]. In such boundary-value problems, inhomogeneities of the propagating medium caused by the varying index of refraction of the intervening material take the place of the potential field experienced by a quantum particle. The standard parabolic equation is resulted when one extracts paraxial propagation along a preferred direction from the full Helmholtz equation. In addition to providing a microscopic model for the Schrödinger equation, the 4RW model considered by Ord is also attractive in the solution of stochastic differential equations associated with these parabolic type of equations, carried out by employing only real random processes. Because walks modeling the Schrödinger equation in the 4RW model traverse only real space, no analytical continuation of boundary data into complex space is required that would otherwise be demanded [17, 18] when solving these boundary-value problems.

Ord does not provide explicit expressions for the various transitional probabilities, but, instead, discusses the continuum limits directly from the governing difference equations. For a variety of reasons, it is desirable to obtain closed-form expressions (or those involving integrals) for these transitional probabilities. In this paper, we provide analytical expressions for the transitional probabilities associated with the 4-state random walk in 1+1 dimension in spacetime by using a transform approach. Our work here is partly motivated by the desire to have expressions for the transitional probabilities while solving the aforementioned boundary-value problems using the parabolic equation in a homogeneous medium. Using these expressions, it is further shown that in the continuum limits as the mesh size shrinks to zero in both space and time, one directly recovers the diffusion equation and the Schrödinger equation. Thus, the main contributions of the paper are to (i) elucidate methodology for obtaining the closed-form expressions for the various transitional probabilities of the 4RW, and (ii) establish the continuum limits of the diffusion and Schrödinger equations describing the dynamics of particles obeying the 4RW. The methodology presented in this paper is most suitable for describing quantum dynamics of a free-particle, although the 4RW model itself has been extended in the presence of a potential field [19]. The paper is organized as follows: section 2 gives a brief introduction of the random walks considered in [10, 12]. Section 3 introduces the generating functions and the 2D transforms considered in this paper.

Table 1. Various states in random walk.

State	Direction	Spin
1	Right	+1
2	Left	+1
3	Right	−1
4	Left	−1

Section 4 provides expressions for the various transitional probabilities as well as discusses the derivation of the diffusion equation and the Schrödinger equation as continuum limits of these probabilities.

2. Multistate random walks

Consider the 4RW model proposed by Ord and Deakin [12], where a particle undergoes random motion in discrete spacetime $(x = m\Delta, t = s\epsilon)$, with x denoting space and t denoting time, and Δ and ϵ denoting the spatial and temporal steps, respectively. At every point the particle is endowed with two independent binary properties, its direction of motion (right or left) and its spin or parity (± 1). The particle is assumed to change its direction with every collision, but change its spin only every other collision. The four states of the particle corresponding to the four combinations of direction and spin are indicated in table 1. Note that the particle can execute any direction of motion irrespective of the spin, in contrast to the model used in [13, 14]. However, there is an intrinsic assumption of *memory* in Ord's model that arises from keeping track of the parity of collisions. If $p_\mu(m\Delta, s\epsilon)\Delta$, $\mu = 1, \ldots, 4$, is the probability that a particle is in state μ at the spacetime point $(m\Delta, s\epsilon)$, $m = 0, \pm 1, \pm 2, \ldots, s = 0, 1, \ldots,$ then the transitional relations considered in [12] were of the form

$$\begin{aligned}
p_1[m\Delta, (s+1)\epsilon)] &= \alpha p_1[(m-1)\Delta, s\epsilon] + \beta p_4[(m+1)\Delta, s\epsilon] \\
p_2[m\Delta, (s+1)\epsilon)] &= \alpha p_2[(m+1)\Delta, s\epsilon] + \beta p_1[(m-1)\Delta, s\epsilon] \\
p_3[m\Delta, (s+1)\epsilon)] &= \alpha p_3[(m-1)\Delta, s\epsilon] + \beta p_2[(m+1)\Delta, s\epsilon] \\
p_4[m\Delta, (s+1)\epsilon)] &= \alpha p_4[(m+1)\Delta, s\epsilon] + \beta p_3[(m-1)\Delta, s\epsilon],
\end{aligned} \tag{1}$$

where $\alpha + \beta = 1$. Here, α is the probability that a particle maintains its direction at the next time step, whereas β is the probability that it will change its direction at the next time step. The Markov-chain character of the transitional probabilities is evident from definitions in (1). From the total probability theorem, the probability that a particle is somewhere on the lattice at a given time is equal to 1 and is represented mathematically by

$$\sum_{\mu=1}^{4} \sum_{m=-\infty}^{\infty} p_\mu(m\Delta, s\epsilon)\Delta = 1. \tag{2}$$

Ord [10] has shown that the diffusion and Schrödinger propagators coexist on the lattice and that both behaviors are embedded in equations (1). To affect a separation of the diffusive behavior from the wave-like behavior, the following linear transformation is used: $q_1(m\Delta, s\epsilon) = 2^{s/2}[p_1(m\Delta, s\epsilon) - p_3(m\Delta, s\epsilon)]$, $q_2(m\Delta, s\epsilon) = 2^{s/2}[p_2(m\Delta, s\epsilon) - p_4(m\Delta, s\epsilon)]$, $w_1(m\Delta, s\epsilon) = [p_1(m\Delta, s\epsilon) + p_2(m\Delta, s\epsilon) + p_3(m\Delta, s\epsilon) + p_4(m\Delta, s\epsilon)]$, and $w_2(m\Delta, s\epsilon) = [p_1(m\Delta, s\epsilon) + p_3(m\Delta, s\epsilon)] - [p_2(m\Delta, s\epsilon) + p_4(m\Delta, s\epsilon)]$. The quantity $q_1\Delta$ (without the weight factor $2^{s/2}$) indicates the expected difference in the number of particles of opposite spin arriving at $(m\Delta, s\epsilon)$ while moving to the right. Similarly, $q_2\Delta$ refers to the expected number of particles arriving at $(m\Delta, s\epsilon)$ while moving to the left. Also, $w_1(m\Delta, s\epsilon)\Delta$ is the probability that a particle leaves $(m\Delta, s\epsilon)$ in either direction and in any spin state, and $w_2(m\Delta, s\epsilon)\Delta$ is the difference in the probabilities that a particle leaves $(m\Delta, s\epsilon)$ to the right and the left. Introducing the shift operator $E_x^{\pm 1} p_\mu(m\Delta, s\epsilon) = p_\mu[(m \pm 1)\Delta, s\epsilon]$, a time-advancing operator $E_t p_\mu(m\Delta, s\epsilon) = p_\mu[m\Delta, (s+1)\epsilon]$, and the vector $\mathbf{p} = [p_1, p_2, p_3, p_4]^T$, where the superscript T denotes transpose, the transitional relations in (1), which are of the form $E_t\mathbf{p} = \mathbf{S}_x\mathbf{p}$, get transformed into

$$E_t \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \left(E_x + E_x^{-1}\right) & -\left(E_x - E_x^{-1}\right) \\ (\alpha - \beta)\left(E_x - E_x^{-1}\right) & (\alpha - \beta)\left(E_x + E_x^{-1}\right) \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}, \tag{3}$$

$$E_t \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 2\alpha E_x^{-1} & -2\beta E_x \\ 2\beta E_x^{-1} & 2\alpha E_x \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}. \tag{4}$$

Thus the variables (w_1, w_2) get decoupled from (q_1, q_2). Essentially, this decoupling results from block-diagonalizing the matrix $\mathbf{S}_x$ and describing the system in terms of its eigenstates. The physical significance of this transformation is touched upon in [11, 12]. Note that w_j and q_j need not strictly be probabilistic quantities (meaning $\geqslant 0$), but we will continue to describe them as 'transitional probabilities' with the understanding that the actual probabilistic quantities, namely, p_μ, can be easily recovered from these using the inverse relations.

3. Generating functions and transforms

We are interested in the solutions of (3) and (4) for the special case of a symmetric random walk with $\alpha = \beta = 0.5$. In this case we have a set of linear difference equations and the solution can be obtained conveniently using transform methods [20, 21] and appropriate generating functions. The key step here is to pick a suitable transform consistent with the nature and domain of definition of the problem. We denote the 2D transform $\mathcal{L}$, consisting of a Fourier transform in space (owing to the unbounded nature of the spatial coordinate) and the z-transform [22] in time (the z-transform can be arrived from the discretized version of a Laplace transform and is suitable for discrete functions defined on a half-line), of a discrete function $v(m\Delta, s\epsilon)$ as $V(k_x, z)$ and define

$$V(k_x, z) = \Delta \sum_{m=-\infty}^{\infty} \sum_{s=0}^{\infty} v(m\Delta, s\epsilon) z^s \,\mathrm{e}^{-\mathrm{i}mk_x\Delta} \equiv \mathcal{L}v(m\Delta, s\epsilon). \tag{5}$$

The inverse relation can then be obtained as

$$v(m\Delta, s\epsilon) = \frac{1}{4\pi^2\mathrm{i}} \int_{k_x=-\pi/\Delta}^{\pi/\Delta} \oint_{C_z} \frac{V(k_x, z)}{z^{s+1}} \,\mathrm{e}^{\mathrm{i}mk_x\Delta} \,\mathrm{d}k_x \,\mathrm{d}z \equiv \mathcal{L}^{-1} V(k_x, z), \tag{6}$$

where the identities

$$\int_{k_x\Delta=-\pi}^{\pi} \mathrm{e}^{\mathrm{i}(n-m)k_x\Delta} \,\mathrm{d}k_x\Delta = 2\pi\delta_m^n \tag{7}$$

$$\oint_{C_z} z^{r-s-1} \,\mathrm{d}z = 2\pi\mathrm{i}\delta_s^r \tag{8}$$

are used to derive (6). Here δ_m^n is the Kronecker's delta and C_z is a closed contour around the origin in the complex z-plane that encloses only the singularities at the origin. The present analysis, consisting of the z-transform along the time axis and Fourier transform along the spatial axis, is most suitable for studying linear difference equations with constant coefficients such as encountered in the study of free-Schrödinger equation by the 4RW model. Other suitable methods must be devised for studying particle motion in the presence of a potential field. Note that $V(k_x, z)$ is periodic in k_x with a period $2\pi/\Delta$. Using the definition in (5), it can also be shown that

$$\mathcal{L}v[m\Delta, (s+1)\epsilon] = z^{-1}[V(k_x, z) - V_0(k_x)] \tag{9}$$

$$\mathcal{L}v[(m \pm 1)\Delta, s\epsilon] = \mathrm{e}^{\pm \mathrm{i}k_x\Delta} V(k_x, z), \tag{10}$$

where $V_0(k_x)$ is the Fourier transform of the initial distribution $v(m\Delta, 0)$:

$$V_0(k_x) = \Delta \sum_{m=-\infty}^{\infty} v(m\Delta, 0)\,\mathrm{e}^{-\mathrm{i}mk_x\Delta}. \tag{11}$$

Note that the periodicity property of $V_0(k_x)$ implies that $V_0(\pi/\Delta) = V_0(-\pi/\Delta)$.

4. Transitional probabilities

Having defined the required transforms, we will now derive expressions for the transitional probabilities w_1, w_2, q_1 and q_2. Because of the decoupling afforded in (3) and (4), it is sufficient to consider the diffusive and wave-like behaviors separately.

4.1. Diffusive behaviour

The diffusive part of the particle motion is governed by the discrete functions w_1 and w_2 as will be evident shortly. Let $W_1(k_x, z)$ and $W_2(k_x, z)$ be the 2D transforms of $w_1(m\Delta, s\epsilon)$ and $w_2(m\Delta, s\epsilon)$ and $\Upsilon_1(k_x)$ and $\Upsilon_2(k_x)$ be the transforms of the initial distributions $w_1(m\Delta, 0)$ and $w_2(m\Delta, 0)$, respectively. From the definition of w_1 in terms of $p_\mu, \mu = 1, \ldots, 4$, and relation (2), it is seen that $\Upsilon_1(0) = 1$. On applying the transform $\mathcal{L}$ to the set (3) and making use of the properties (9) and (10), it is easy to see that $W_2(k_x, z) = \Upsilon_2(k_x)$ and

$$W_1(k_x, z) = \frac{\Upsilon_1(k_x) - \mathrm{i}z\sin(k_x\Delta)\Upsilon_2(k_x)}{1 - z\cos(k_x\Delta)} \tag{12}$$

$$= \sum_{n=0}^{\infty} z^n \cos^n(k_x\Delta)\,[\Upsilon_1(k_x) - \mathrm{i}z\sin(k_x\Delta)\Upsilon_2(k_x)] \tag{13}$$

where (13) has been obtained by using the series expansion of $[1 - z\cos(k_x\Delta)]^{-1}$. Such a series converges uniformly provided that $|z\cos(k_x\Delta)| < 1$ and this can always be insured by choosing an appropriate C_z in (6). In other words, the contour C_z is chosen such that the zeroes of the function $1 - z\cos(k_x\Delta)$ lie outside it. Substituting this into (6) and making use of (8), we finally arrive at

$$w_1(m\Delta, s\epsilon) = \frac{1}{2\pi}\int_{-\pi/\Delta}^{\pi/\Delta} \cos^s(k_x\Delta)[\Upsilon_1(k_x) - \mathrm{i}\Theta(s-1)\tan(k_x\Delta)\Upsilon_2(k_x)]\,\mathrm{e}^{\mathrm{i}mk_x\Delta}\,\mathrm{d}k_x, \tag{14}$$

where $\Theta(\cdot)$ is the Heaviside step function. For a given $\Upsilon_1(k_x)$ and $\Upsilon_2(k_x)$, integral (14) may be computed efficiently by the application of the inverse fast Fourier transform (iFFT) algorithm [22]. However, for special values of $\Upsilon_1(k_x)$ and $\Upsilon_2(k_x)$, the integral may be evaluated in

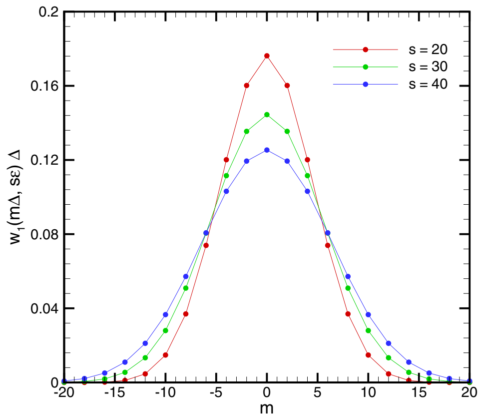


Figure 1. Calculated values of $w_1(m\Delta, s\epsilon)$ for $\Upsilon_1(k_x) = 1$, $\Upsilon_2(k_x) = 0$.

a closed form. For example, with $w_1(m\Delta, 0) = \frac{1}{\Delta}\delta_m^0$, $w_2(m\Delta, 0) = 0 (\Longrightarrow \Upsilon_1(k_x) = 1, \Upsilon_2(k_x) = 0)$ and m and s even, (14) reduces to ([23], 3.631–17)

$$w_1(m\Delta, s\epsilon)\Delta = \frac{1}{2^s}\binom{s}{(s-m)/2}, \qquad m \leqslant s. \tag{15}$$

The right-hand side of (15) gives the probability of finding a particle at m in s steps, given that it started at the origin at $s = 0$, in a symmetric, discrete-time, 1D random walk. The result can be obtained directly from combinatorial analysis and is available in standard texts ([24], p 75), ([25], p 16). Figure 1 shows a plot of $w_1(m\Delta, s\epsilon)\Delta$ for $s = 20$, 30 and 40, where the data at discrete m has been connected by smooth lines for the sake of visual clarity. The plots clearly exhibit the diffusive behavior of w_1, wherein w_1 spreads out in space with a diminishing peak value as s increases. Using the identity $\sum_{m=-\infty}^{\infty} \exp(\pm \mathrm{i} m x) = 2\pi\delta(x)$, $-\pi \leqslant x \leqslant \pi$, where $\delta(\cdot)$ is the delta function, it may be easily verified from (14) that $\sum_{m=-\infty}^{\infty} w_1(m\Delta, s\epsilon)\Delta = 1$. Also note that $w_1 > 0$. Hence $w_1\Delta$ behaves like a true probability mass function.

We are also interested in the continuum limits $\Delta \to 0, \epsilon \to 0, m \to \infty$, and $s \to \infty$ such that $\Delta^2/2\epsilon = D > 0, m\Delta \to x, s\epsilon \to t$. Using the results $\lim_{\substack{\Delta\to 0\\ s\to\infty}} [\cos^s(k_x\Delta)] = \exp\left(-k_x^2 Dt\right)$, $\lim_{\substack{\Delta\to 0\\ s\to\infty}} [\cos^s(k_x\Delta)\tan(k_x\Delta)] = 0$ in (14), we arrive at

$$w_1(x, t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \Upsilon_1(k_x)\, \mathrm{e}^{-k_x^2 Dt}\, \mathrm{e}^{\mathrm{i}k_x x}\, \mathrm{d}k_x. \tag{16}$$

This is the well-known solution of the diffusion equation $\partial w_1/\partial t = D\partial^2 w_1/\partial x^2$ in an unbounded medium with an initial spectral content $\Upsilon_1(k_x)$ (see, for example, [26]). For an impulsive initial condition, $\Upsilon_1(k_x) = 1$, and one recovers the Green's function $w_1(x, t) = \exp(-x^2/4Dt)/\sqrt{4\pi Dt}$. The function $w_1(m\Delta, s\epsilon)$ given in equation (14) is the discrete version of $w_1(x, t)$ and is seen to depend not only on $\Upsilon_1(k_x)$, but also on $\Upsilon_2(k_x)$. The latter contribution arises entirely from the discrete nature of space and vanishes in the continuum limit. To summarize, the quantity $w_1(m\Delta, s\epsilon)\Delta$ that describes the probability that a particle leaves $(m\Delta, s\epsilon)$ in either direction and in any spin state describes the diffusion process for a symmetric 4RW.

4.2. Wave-like behaviour

The wave-like behavior of the particle motion is governed by the discrete functions q_1 and q_2. The governing equations in this case are repeated below from (4):

$$E_t\begin{pmatrix}q_1\\q_2\end{pmatrix}=\frac{1}{\sqrt{2}}\begin{pmatrix}E_x^{-1} & -E_x\\E_x^{-1} & E_x\end{pmatrix}\begin{pmatrix}q_1\\q_2\end{pmatrix}. \tag{17}$$

Our objective here is to derive closed-form expressions for the transitional probabilities q_1 and q_2. Let $Q_j(k_x, z)$ be the $\mathcal{L}$ transforms of $q_j(m\Delta, s\epsilon)$, and let $\Gamma_j(k_x)$ be the Fourier transforms of the initial distribution $q_j(m\Delta, 0)$, $j = 1, 2$. On applying the $\mathcal{L}$ transform to (17) and making use of properties (9) and (10) and carrying out some algebraic manipulations, we get

$$\begin{bmatrix}Q_1(k_x,z)\\Q_2(k_x,z)\end{bmatrix}=\frac{1}{(1-\sqrt{2}z\cos(k_x\Delta)+z^2)}\begin{bmatrix}1-\frac{z}{\sqrt{2}}\,\mathrm{e}^{\mathrm{i}k_x\Delta} & -\frac{z}{\sqrt{2}}\,\mathrm{e}^{\mathrm{i}k_x\Delta}\\ \frac{z}{\sqrt{2}}\,\mathrm{e}^{-\mathrm{i}k_x\Delta} & 1-\frac{z}{\sqrt{2}}\,\mathrm{e}^{-\mathrm{i}k_x\Delta}\end{bmatrix}\begin{bmatrix}\Gamma_1(k_x)\\\Gamma_2(k_x)\end{bmatrix}. \tag{18}$$

To permit evaluation of the integral with respect to z in the inverse transform, we need to express Q_1 and Q_2 in a separable form with respect to k_x and z. To this end, we make use of the identity ([23], 8.945.2)

$$\frac{1}{1-2tx+t^2}=\sum_0^\infty U_n(x)t^n, \tag{19}$$

where $U_n(\cdot)$ is the Chebyshev polynomial of the second kind of order n, in (18) to arrive at

$$Q_1(k_x,z)=\sum_{n=0}^\infty U_n\left(\frac{\cos k_x\Delta}{\sqrt{2}}\right)z^n\left[\left(1-\frac{z}{\sqrt{2}}\,\mathrm{e}^{\mathrm{i}k_x\Delta}\right)\Gamma_1(k_x)-\frac{z}{\sqrt{2}}\,\mathrm{e}^{\mathrm{i}k_x\Delta}\Gamma_2(k_x)\right] \tag{20}$$

$$Q_2(k_x,z)=\sum_{n=0}^\infty U_n\left(\frac{\cos k_x\Delta}{\sqrt{2}}\right)z^n\left[\frac{z}{\sqrt{2}}\,\mathrm{e}^{-\mathrm{i}k_x\Delta}\Gamma_1(k_x)+\left(1-\frac{z}{\sqrt{2}}\,\mathrm{e}^{-\mathrm{i}k_x\Delta}\right)\Gamma_2(k_x)\right]. \tag{21}$$

As with the diffusive case, the contour C_z in the inverse transform is chosen such that the zeroes of the denominator function $(1-\sqrt{2}z\cos(k_x\Delta)+z^2)$ lie outside it. Equations (20) and (21) may be substituted into the definition of the inverse transform (6) and the integral with respect to z evaluated by making use of (8). For reasons that will become clear shortly, we are interested in the composite discrete function $\psi_d(m\Delta, s\epsilon) = q_2(m\Delta, s\epsilon) + \mathrm{i}q_1(m\Delta, s\epsilon)$, which will be compared directly with the solution of the Schrödinger equation. The expression for ψ_d is

$$\begin{aligned}\psi_d(m\Delta,s\epsilon)=\frac{1}{2\pi}\int_{-\pi/\Delta}^{\pi/\Delta}\Bigg\{&U_s\left(\frac{\cos k_x\Delta}{\sqrt{2}}\right)[\Gamma_2+\mathrm{i}\Gamma_1(k_x)]\\&+U_{s-1}\left(\frac{\cos k_x\Delta}{\sqrt{2}}\right)[(\mathrm{e}^{-\mathrm{i}\pi/4}\Gamma_1(k_x)-\mathrm{e}^{\mathrm{i}\pi/4}\Gamma_2(k_x))\cos(k_x\Delta)\\&+(\mathrm{e}^{-\mathrm{i}\pi/4}\Gamma_1(k_x)+\mathrm{e}^{\mathrm{i}\pi/4}\Gamma_2(k_x))\sin(k_x\Delta)]\Bigg\}\,\mathrm{e}^{\mathrm{i}mk_x\Delta}\,\mathrm{d}k_x.\end{aligned} \tag{22}$$

As in section 4.1, the integral in (22) may be evaluated efficiently by employing the iFFT algorithm. In the special case of $\Gamma_1(k_x) = 0, \Gamma_2(k_x) = K_2$, a constant, the expression provided in (22) can be further simplified. Making a change of variable $y = \cos(k_x\Delta)$

and using $\mathrm{d}y/\sqrt{1-y^2} = -\mathrm{d}k_x\Delta$, $\cos(m\cos^{-1}y) = T_m(y)$, where $T_m(\cdot)$ is the Chebyshev polynomial of the first kind of order m, we can show that

$$\psi_d(m\Delta, s\epsilon)\Delta = \frac{K_2}{\pi}\int_{-1}^{1}\frac{1}{\sqrt{1-y^2}}\left\{U_s\left(\frac{y}{\sqrt{2}}\right)T_m(y) - \frac{1}{\sqrt{2}}U_{s-1}\left(\frac{y}{\sqrt{2}}\right)\right.$$
$$\left.\times\,[T_{m-1}(y) + \mathrm{i}T_{m+1}(y)]\right\}\mathrm{d}y. \tag{23}$$

From the even and odd properties of Chebyshev polynomials, it can be deduced that for $s = 2r$ and $m = 2n-1$ (or vice versa), the integral in (23) vanishes implying that $\psi_d[(2n-1)\Delta, 2r\epsilon] = 0$ in this special case.

Other interesting identities can be derived starting from (22). Using the relation $U_s(1/\sqrt{2}) = U_s[\cos(\pi/4)] = \sin(s\pi/4) + \cos(s\pi/4)$, one can readily see that

$$\sum_{m=-\infty}^{\infty}\psi_d(m\Delta, s\epsilon)\Delta = \mathrm{e}^{-\mathrm{i}\pi s/4}[\Gamma_2(0) + \mathrm{i}\Gamma_1(0)]\,. \tag{24}$$

Hence, unlike $w_1\Delta$, the quantities $q_1\Delta$ and $q_2\Delta$ can be of alternating signs and do not represent true probability mass functions.

Ord [11] has shown that eight different continuous functions are embedded into the discrete functions q_1 and q_2. We will focus on the continuous function that would result from choosing $x = 2n\Delta, n = 0, \pm1, \pm2, \ldots,$ and $t = 8r\epsilon, r = 0, 1, 2, \ldots,$ in the discrete functions q_1 and q_2. We show that ψ_d satisfies the Schrödinger equation for $m = 2n$, $s = 8r$ in the limit as $\Delta \to 0, \epsilon \to 0, n \to \infty, r \to \infty$ such that $\Delta^2/2\epsilon = D$. The following identities [23, 27] involving Chebyshev polynomials will be utilized in subsequent development:

$$zU_{s-1}(z) = U_s(z) - T_s(z) \tag{25}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}T_s(z) = sU_{s-1}(z) \tag{26}$$

$$T_s\left(\frac{1}{\sqrt{2}}\right) = \cos\left(\frac{\pi s}{4}\right), \qquad (1-z^2)T_s''(z) - zT_s'(z) + s^2T_s(z) = 0 \tag{27}$$

$$U_{s-1}\left(\frac{1}{\sqrt{2}}\right) = \sqrt{2}\sin\left(\frac{\pi s}{4}\right), \qquad (1-z^2)U_s''(z) - 3zU_s'(z) + s(s+2)U_s(z) = 0, \tag{28}$$

where a prime denotes differentiation with respect to the argument. For the purpose of investigating the continuum limits, we would like to cast (22) in a form more suitable for asymptotic analysis. The last term in (22) involving $U_{s-1}(\cdot)$ can be replaced with $\mathrm{d}T_s(\cdot)/\mathrm{d}k_x$ on using the second relation (26) to yield

$$\frac{\sin k_x\Delta}{\sqrt{2}}U_{s-1}\left(\frac{\cos k_x\Delta}{\sqrt{2}}\right) = \frac{-1}{s\Delta}\frac{\mathrm{d}}{\mathrm{d}k_x}T_s\left(\frac{\cos k_x\Delta}{\sqrt{2}}\right). \tag{29}$$

This term is then integrated by parts and simplified using the periodicity condition $\Gamma_j(\pi/\Delta) = \Gamma_j(-\pi/\Delta)$, $j = 1, 2$. A convenient expression for the evaluation of $\psi_d(m\Delta, s\epsilon)$ is then obtained as

$$\psi_d(m\Delta, s\epsilon) = \frac{1}{2\pi}\int_{-\pi/\Delta}^{\pi/\Delta}\mathrm{e}^{\mathrm{i}mk_x\Delta}\left\{[\Gamma_1(k_x) - \mathrm{i}\Gamma_2(k_x)]U_s\left(\frac{\cos k_x\Delta}{\sqrt{2}}\right)\right.$$
$$+ (1+\mathrm{i})\left(\left[1 + \mathrm{i}\frac{m}{s}\right]\Gamma_2(k_x) + \left[\mathrm{i} + \frac{m}{s}\right]\Gamma_1(k_x)\right)T_s\left(\frac{\cos k_x\Delta}{\sqrt{2}}\right)$$
$$\left.+ \frac{1+\mathrm{i}}{s\Delta}[\Gamma_2'(k_x) - \mathrm{i}\Gamma_1'(k_x)]T_s\left(\frac{\cos k_x\Delta}{\sqrt{2}}\right)\right\}\mathrm{d}k_x, \tag{30}$$

which is also more amenable to asymptotic analysis than (22). In the special case of $\Gamma_1(k_x) = 0, \Gamma_2(k_x) = K_2$ and for $m/s \to 0$ (small spatial locations and large times) we move on using (25) that

$$\psi_d(m\Delta, s\epsilon) = \frac{K_2}{2\pi}\int_{-\pi/\Delta}^{\pi/\Delta} \mathrm{e}^{\mathrm{i}mk_x\Delta}\left[T_s\left(\frac{\cos k_x\Delta}{\sqrt{2}}\right) - \mathrm{i}\frac{\cos k_x\Delta}{\sqrt{2}}U_{s-1}\left(\frac{\cos k_x\Delta}{\sqrt{2}}\right)\right]\mathrm{d}k_x. \tag{31}$$

We now perform an asymptotic analysis for small $k_x\Delta$ in (31) and show that $\psi_d(2n\Delta, 8r\epsilon)$ satisfies the Schrödinger equation. To this end, we note the following Taylor series expansions which are obtained by making use of (26)–(28):

$$\cos k_x\Delta \sim 1 - \frac{k_x^2\Delta^2}{2} + \frac{(k_x\Delta)^4}{4!} + \cdots \tag{32}$$

$$T_s\left(\frac{\cos k_x\Delta}{\sqrt{2}}\right) \sim \cos\left(\frac{\pi s}{4}\right) - \frac{k_x^2\Delta^2 s}{2}\sin\left(\frac{\pi s}{4}\right) - \frac{(k_x\Delta)^4 s^2}{4!}$$
$$\times\left[3\cos\left(\frac{s\pi}{4}\right) - \frac{4}{s}\sin\left(\frac{s\pi}{4}\right)\right] + \cdots \tag{33}$$

$$\frac{1}{\sqrt{2}}U_{s-1}\left(\frac{\cos k_x\Delta}{\sqrt{2}}\right) \sim \sin\left(\frac{\pi s}{4}\right) + \frac{k_x^2\Delta^2 s}{2}\left[\cos\left(\frac{\pi s}{4}\right) - \frac{1}{s}\sin\left(\frac{\pi s}{4}\right)\right]$$
$$+ \frac{(k_x\Delta)^4}{4!}\left[(10 - 3(s^2-1))\sin\left(\frac{\pi s}{4}\right) - 10s\cos\left(\frac{\pi s}{4}\right)\right] + \cdots \tag{34}$$

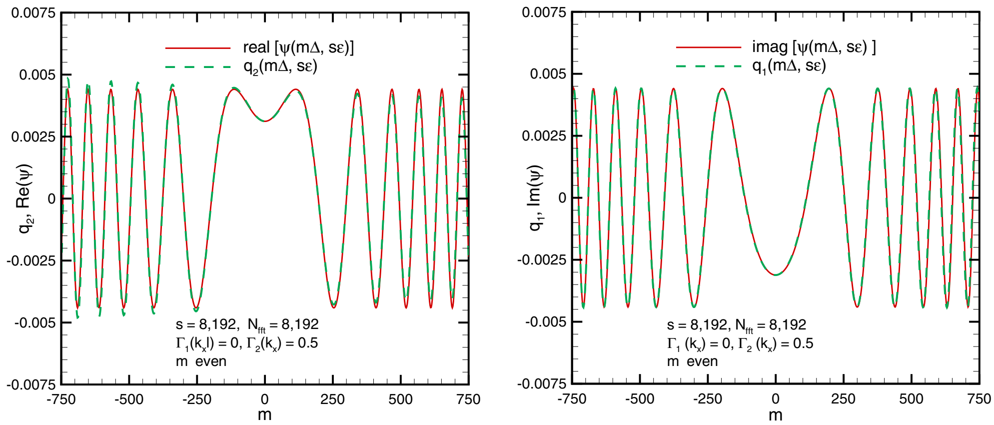
Inserting (32)–(34) into (31) and choosing $s = 8r, \Delta^2 = 2D\epsilon, s\epsilon = t, m\Delta = x, s \to \infty$, $m \to \infty, \Delta \to 0, \epsilon \to 0$, we arrive at the desired result:

$$\psi_d(x,t) = q_2(x,t) + \mathrm{i}q_1(x,t) \sim \frac{K_2}{2\pi}\int_{-\infty}^{\infty}\left(1 - \mathrm{i}Dk_x^2 t - \frac{k_x^4 D^2 t^2}{2!} + \cdots\right)\mathrm{e}^{\mathrm{i}k_x x}\,\mathrm{d}k_x$$
$$= \frac{K_2}{2\pi}\int_{-\infty}^{\infty}\mathrm{e}^{-\mathrm{i}Dk_x^2 t}\mathrm{e}^{\mathrm{i}k_x x}\,\mathrm{d}k_x. \tag{35}$$

Equation (35) is the spectral representation of the Green's function corresponding to the Schrödinger equation $\partial\psi/\partial t = \mathrm{i}D\partial^2\psi/\partial x^2$ with the impulsive initial condition $\psi(x, t = 0^+) = K_2\delta(x)$. It has the exact solution

$$\psi(x,t) = \frac{K_2}{\sqrt{4\pi\mathrm{i}Dt}}\mathrm{e}^{\mathrm{i}x^2/4Dt}. \tag{36}$$

To reinforce to the reader that the plots of the transitional probabilities (q_1, q_2) do resemble the solutions of the free Schrödinger equation, we show in figure 2*a* comparison of the real, $\Re$, and imaginary, $\Im$, parts of the exact solution (36) of the Schrödinger equation with the partial solution (q_1, q_2) of the 4RW. The numerical solutions shown in the figure for ψ_d are on a discrete spacetime $(x = m\Delta, t = s\epsilon)$ and have been computed using (31) with the iFFT algorithm [22] with size $s = 2^{13} = 8192$. It is seen that the 4RW produces solutions of oscillatory type with both positive and negative excursions for the expectations q_1 and q_2, which are in excellent agreement with the analytical results for small $\frac{m}{s}$. This is in contrast to the quantity w_1 shown in figure 1, which, behaving like the solution of the diffusion equation, decays exponentially in space and always remains positive.



(*a*) (*b*)

Figure 2. Comparison of the exact solution of Schrödinger equation with the discrete solution of a 4RW for an impulsive initial condition. (*a*) $q_2(m\Delta, s\epsilon)$, $\Re\{\psi(m\Delta, s\epsilon)\}$ and (*b*) $q_1(m\Delta, s\epsilon)$, $\Im\{\psi(m\Delta, s\epsilon)\}$.

5. Summary

By considering a multistate random walk on a discrete lattice, expressions have been derived for the various transitional probabilities using the concept of generating functions. A 2D transform involving Fourier transformation in space and the z-transformation in time is employed to accomplish this. The transitional probabilities governing particle motion are expressed in terms of integrals involving trigonometric functions in the case of the diffusion equation, and involving Chebyshev polynomials of the first and second kinds in the case of the Schrödinger equation. Closed-form expressions have been given for particular cases of the initial conditions. The continuum limits of the diffusion equation and Schrödinger equation have been shown to follow directly from these transitional probabilities through the performance of appropriate asymptotic analysis. The present analysis consisting of the z-transform along the time axis and Fourier transform along the spatial axis is most suitable for studying linear difference equations with constant coefficients. In the 4RW model, this would correspond to the free Schrödinger equation. The important extension of this analysis to higher dimensions is worth exploring and would be taken up in the future. The incorporation of a smooth potential field in the Schrödinger equation into the 4RW model has already been addressed by Ord in [19] and the study of its transitional probabilities will be taken up in a separate paper using a different approach.

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