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Transitional probabilities for the four-state random walk on a lattice in the presence of partially reflecting boundaries

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The four-state random walk (4RW) model, wherein the particle is endowed with two states of spin and two states of directional motion in each space coordinate, permits a stochastic solution of the Schrödinger equation (or the equivalent parabolic equation) without resorting to the usual analytical continuation in complex space of the particle trajectories. Analytical expressions are derived here for the various transitional probabilities in a 4RW by employing generating functions and eigenfunction expansions when the particle moves on a 1+1 space-time lattice with two-point boundary conditions. The most general case of dissimilar boundaries with partially reflecting boundary conditions is treated in this paper. The transitional probabilities are all expressed in terms of a finite summation involving trigonometric functions and/or Chebyshev polynomials of the second kind that are characteristics of diffusion and Schrödinger equations, respectively, in the 4RW model. Results for the special case of perfectly absorbing boundaries are compared to numerical values obtained by directly counting paths in the random walk simulations. © 2009 American Institute of Physics. [DOI: [10.1063/1.3122768](https://doi.org/10.1063/1.3122768)]

I. INTRODUCTION

The four-state random walk (4RW) model, wherein a particle undergoing random walk is endowed with two states of direction (in a one-dimensional case) and two states of spin or parity, was considered by Ord and Deakin¹ to arrive at a macroscopic model for the Schrödinger equation and physically interpret its wavelike solutions. It was shown in that paper that both the traditional diffusion equation as well as the Schrödinger equation were embedded in the same physical model. The usual diffusion process is contained in the overall sum of all particle paths irrespective of their direction and parity, while the wavelike behavior of the Schrödinger equation is contained in the differences in densities of the right-going particles or left-going particles with opposite parity. The 4RW model owes its existence to the Feynman chessboard model as elaborated in Ref. 2 and is also useful in solving practical electromagnetic, acoustic, and optical boundary value problems for the complex field amplitude when a stochastic approach is used to treat the governing *parabolic equation*. (In the applied sciences area, the parabolic equation is sometimes referred to as the parabolic wave equation.) The standard parabolic equation used in such time-harmonic problems contains partial derivatives with respect to the spatial coordinates only, where the spatial coordinate along the axial direction takes the place of the time variable in the time-dependent Schrödinger equation. Furthermore, the potential function present in the Schrödinger equation is replaced by the medium refractive-index term in the parabolic equation. The parabolic equation is obtained when the Helmholtz equation describing the true field is subject to a one-way propagation with a subsequent application of the paraxial approximation.^{3,4} Normally one needs to resort to analytical continuation of boundary data, as is done in Ref. 5, when the parabolic equation is

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solved numerically using a stochastic approach. The resulting random walks will then traverse a complex-valued space, which, in turn, calls for analytical continuation of boundary data and the spatial geometry.⁶ However, the 4RW model permits a solution to these problems without such analytical continuations.

In a previous paper,⁷ the author developed expressions for the various transitional probabilities for the 4RW on a discrete lattice for spatially unbounded case. In addition to detailing a method for arriving at the transitional probabilities, the results presented therein could also be useful in determining other stochastic quantities of interest such as the first passage time probabilities, expected number of visits to a given site, and maximum excursions of a random walk on a line for various linear combinations of these probabilities. In developing numerical schemes for solving boundary value problems with complex geometries, it is desirable to have analytical solutions for simpler geometries to facilitate validation against benchmark problems.⁸ The traditional way to discretize the Schrödinger equation or the diffusion equation for numerical treatment by the finite difference method is to employ a central difference formula in the spatial coordinates. An example of this is the implicit Crank–Nicolson scheme, which, for the diffusion equation, can be identified with the traditional two-state random walk, where the particle is endowed with two directions of motion only. Analytical results for the traditional two-state random walk with perfectly absorbing and/or reflecting boundaries have been treated in number of works including Refs. 9 and 10. Separately, the case of the telegraph equation with partially reflecting boundaries is studied in Ref. 11. No such analytical results are yet available for the 4RW model and it is the purpose of the present paper to provide analytical results for a benchmark initial-boundary-value problem in 1 + 1 space-time dimension for the model. To this end, we extend the results in Ref. 7 by considering two-point boundary conditions for the 4RW model and derive analytical expressions for various transitional probabilities. Setting aside the fact that the 4RW model has a physical basis in the Feynman chessboard model and that various transitional probabilities are related to the solution of the continuous Schrödinger equation, it is not at all obvious at the outset from the governing difference equations that an analytical solution is possible for the said boundary value problem, particularly for the wavelike solutions. The transform approach utilized in this paper will reveal the presence of the discrete Laplacian operator that is embedded in these equations and will clearly demonstrate why such a solution is still possible, while paving the way for eigenfunction expansion. This will be elaborated in Secs. II and III. The most general case of partially absorbing and dissimilar boundaries is considered in this paper. Results for the special cases of perfectly absorbing and perfectly reflecting boundaries are also provided in the paper. The results presented here correspond to the solution of the discrete form of the diffusion equation as well as to the real and imaginary parts of the discrete Schrödinger equation.

In Sec. II, the 4RW model is briefly reviewed, and the problem under investigation is defined. In Sec. III, the solution to the 4RW model subject to the general boundary conditions is developed using the concept of generating functions and eigenfunction expansion. Expressions are provided for the special cases of perfectly reflecting and perfectly absorbing boundaries and the results for the latter are compared to numerical simulations obtained by directly counting paths. Finally, conclusions and topics of further research are given in Sec. IV. It may be noted parenthetically that it is not our purpose here to evaluate other various models that have been put forward to physically interpret the Schrödinger equation, a topic that is immensely interesting in its own right.

II. 4RW MODEL

For a particle moving on a discrete lattice and subject to random collisions, the transitional probabilities considered in Ref. 7 at the discrete space-time point $(x=m\Delta, t=s\epsilon)$ are of the form

$$E_t \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} (E_x + E_x^{-1}) & - (E_x - E_x^{-1}) \\ 0 & 0 \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}, \quad (1)$$

$$E_t \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} E_x^{-1} & -E_x \\ E_x^{-1} & E_x \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}, \quad (2)$$

where $q_1(m\Delta, s\epsilon) = 2^{s/2}[p_1(m\Delta, s\epsilon) - p_3(m\Delta, s\epsilon)]$, $q_2(m\Delta, s\epsilon) = 2^{s/2}[p_2(m\Delta, s\epsilon) - p_4(m\Delta, s\epsilon)]$, $w_1(m\Delta, s\epsilon) = [p_1(m\Delta, s\epsilon) + p_2(m\Delta, s\epsilon) + p_3(m\Delta, s\epsilon) + p_4(m\Delta, s\epsilon)]$, $w_2(m\Delta, s\epsilon) = [p_1(m\Delta, s\epsilon) + p_3(m\Delta, s\epsilon)] - [p_2(m\Delta, s\epsilon) + p_4(m\Delta, s\epsilon)]$, and $p_\mu(m\Delta, s\epsilon)\Delta$, $\mu = 1, \dots, 4$, is the probability that a particle is in state μ at the space-time point $(m\Delta, s\epsilon)$, $m = 0, \pm 1, \pm 2, \dots$, $s = 0, 1, \dots$. The particle changes its direction of motion with every collision, but changes its parity or spin at every other collision. The combination of two directions of motion and two states of spin constitute the four states in the model. It has been shown in Refs. 1 and 12 that such a four-state random walk simultaneously encompasses the diffusion as well as Schrödinger equations. The quantities w_1 and w_2 pertain to the diffusion process, while q_2 and q_1 correspond to the real and imaginary parts of the Schrödinger wave function in the discrete case. We will refer to (1) as the diffusion equation and to (2) as the Schrödinger equation even though they are really the respective discrete counterparts of the traditional diffusion and Schrödinger equations. The operators E_x and E_t are, respectively, the spatial and temporal advancing operators and are defined mathematically as $E_x^{\pm 1} p_\mu(m\Delta, s\epsilon) = p_\mu[(m \pm 1)\Delta, s\epsilon]$ and $E_t p_\mu(m\Delta, s\epsilon) = p_\mu[m\Delta, (s+1)\epsilon]$. It is assumed in Eqs. (1) and (2) that the probability that a particle maintains its direction at the next time step remains the same as the probability that it will change its direction at the next time step and that the probability of remaining at the same location at the next time step is zero. If the number of right-going particles is the same as those going to the left at time $t=0$, then $w_2 \equiv 0$ and Eq. (1) reduces to the simpler equation

$$E_t w_1 = D_x w_1, \quad (3)$$

where $D_x = (E_x + E_x^{-1})/2$ is the discrete averaging operator. The averaging operator in (3) owes its existence to the presence of the Laplacian operator in the continuous diffusion equation $\partial w_1 / \partial t = D_1 \partial^2 w_1 / \partial x^2$ when the spatial and temporal step sizes are subject to the condition $\Delta = \sqrt{2\epsilon} D_1$. As such, most of the well-posed issues that pertain to the continuous case¹³ will be carried over to the discrete case. In particular, Eq. (3) will be well posed with two-point Robin type of boundary conditions and the solution will exist.

The difference equations (1) and (2) are assumed to be valid in the region $0 < m < \ell$ and $s > 0$ and they are supplemented by an initial condition at $s=0$ and boundary conditions at $m=0, \ell$. We will adopt the abbreviation $v(m, s)$ to denote the discrete function $v(m\Delta, s\epsilon)$. The boundary conditions we are interested in are of the form

$$p_j(0, s) - \alpha_1 p_j(1, s) = 0 \quad \text{and} \quad p_j(\ell, s) - \alpha_2 p_j(\ell - 1, s) = 0, \quad j = 1, \dots, 4, \quad (4)$$

where the constants α_1 and α_2 are assumed to be real and positive. These are the discrete versions of the general Robin type of boundary conditions for the continuous case. The case of purely absorbing boundaries at $m=0, \ell$ is characterized by $\alpha_i=0$, $i=1, 2$, while the purely reflecting case is characterized by $\alpha_i=1$, $i=1, 2$.^{9,14} The general case corresponds to partially absorbing and partially reflecting boundaries with different degrees of absorption at the two ends. Our interest is to obtain analytical solutions to (1) and (2) on a discrete space-time lattice $(m\Delta, s\epsilon)$ subject to the boundary conditions in (4). In contrast to the diffusion equation (3), it is not clear at the outset whether a solution will exist for (2) under the boundary condition (4), setting aside the fact that it is tied to the Schrödinger equation. This is because of the presence of the spatial shift operators that are neither symmetric (as in the operator D_x) nor asymmetric (as in an operator of the form $V_x = [E_x - E_x^{-1}]$). Recall, for instance, that the diffusion equation with a drift term, whose discrete counterpart will have neither a symmetric nor an asymmetric spatial operator, will not always have a solution even with Neumann type of boundary conditions. However, we will demonstrate in Sec. III that the temporally transformed equation corresponding to (2) will indeed contain the averaging operator and the existence question will be set to rest. Because of the linearity of Eqs. (1) and (2),

a convenient solution can be obtained by using generating function and integral transform techniques as outlined in Refs. 7 and 15.

III. SOLUTION BY GENERATING FUNCTIONS

In the following, we assume complete symmetry between the right-moving and left-moving particles so that $w_2 \equiv 0$. Consider a function $v(m\Delta, s\epsilon)$ and its temporal transform $\hat{v}(m\Delta, z)$ as defined in Ref. 7,

$$\hat{v}(m\Delta, z) = \sum_{s=0}^{\infty} v(m\Delta, s\epsilon) z^s \equiv \mathcal{T}v. \quad (5)$$

The quantity $\hat{v}(m\Delta, z)$ may be thought of as the discrete version of the Laplace transform of v and is simply referred to as the z -transform. The inverse relation is defined as

$$v(m\Delta, s\epsilon) = \frac{1}{2\pi i} \oint_{C_z} \frac{\hat{v}(m\Delta, z)}{z^{s+1}} dz \equiv \mathcal{T}^{-1}\hat{v}, \quad (6)$$

where C_z is a closed contour around the origin in the complex z -plane that encloses only the singularities at the origin, $i=\sqrt{-1}$, and the symbol $\mathcal{T}$ denotes the temporal transform. The transformed variable $\hat{v}(m\Delta, z)$ is also referred to as the *generating function* within the random walk community.⁹ Applying the temporal transform to (2) and (3) and making use of the shift property of the $\mathcal{T}$ transform ($\mathcal{T}[E_x v_1] = z^{-1}[\hat{v}_1(m\Delta, z) - v_1(m, 0)]$) and carrying out some simplifications, we arrive at the following equations for various generating functions in terms of the initial conditions:

$$[1 - zD_x]\hat{w}_1(m\Delta, z) = w_1(m, 0), \quad (7)$$

$$[1 - \sqrt{2}zD_x + z^2]\hat{q}_1(m\Delta, z) = q_1(m, 0) - \frac{z}{\sqrt{2}}E_x[q_2(m, 0) + q_1(m, 0)], \quad (8)$$

$$[1 - \sqrt{2}zD_x + z^2]\hat{q}_2(m\Delta, z) = q_2(m, 0) - \frac{z}{\sqrt{2}}E_x^{-1}[q_2(m, 0) - q_1(m, 0)]. \quad (9)$$

The characteristic operators that appear on the left hand sides of (7)–(9) are generic to the diffusion and the Schrödinger equations under the 4RW model and are seen to be completely independent of the boundary conditions. A remarkable feature of the spatial dependence of these operators, which is not entirely evident in the initial Eq. (2) describing the transitional probabilities, is that they all involve only the averaging operator D_x that is the discrete counterpart of the Laplacian operator in the continuous case. Such a relation has already been alluded to in Sec. II. Both the diffusion and the Schrödinger equations contain the Laplacian operator as far as the spatial variables are concerned, and the transformation from the continuous case to the discrete case for a given order of accuracy is not unique. Employing a central difference formula for the spatial operator will lead to Crank–Nicolson type of discrete equations,⁸ which, like the 4RW model, result in a spatially second order accurate schemes. The important point to note from (9) is that the unknown variable contains only the averaging operator D_x and that any other asymmetries that arise from E_x or E_x^{-1} alone are contained only on the right hand side, operating on the known initial conditions. A formal solution to Eqs. (7)–(9) can be affected by using the inverse relation (6) and evaluating the integrals in the complex z -plane after expanding the reciprocal of the characteristic operators in a Maclaurin series. [Recall that the contour integral in the inverse operator in (6) is a closed loop of vanishing size around the origin]. The procedure is similar to that outlined in Ref. 7 and will involve Chebyshev polynomials of the second kind for the wave functions q_1 and q_2 . The result is

$$w_1(m, s) = D_x^s w_1(m, 0), \quad (10)$$

$$q_1(m, s) = U_s\left(\frac{D_x}{\sqrt{2}}\right)q_1(m, 0) - \frac{1}{\sqrt{2}}U_{s-1}\left(\frac{D_x}{\sqrt{2}}\right)E_x[q_2(m, 0) + q_1(m, 0)], \quad (11)$$

$$q_2(m, s) = U_s\left(\frac{D_x}{\sqrt{2}}\right)q_2(m, 0) - \frac{1}{\sqrt{2}}U_{s-1}\left(\frac{D_x}{\sqrt{2}}\right)E_x^{-1}[q_2(m, 0) - q_1(m, 0)], \quad (12)$$

where $U_s(x)$ is Chebyshev polynomial of the second kind of order s and argument x . The formal solution given in (10)–(12) are general enough and are valid for all appropriate boundary conditions. The presence of the operator D_x^s in the diffusion variable $w_1(m, s)$ is not surprising at all. Indeed, in free space, (10) directly generates the *characteristic function* $\cos^s \theta$ of the probability w_1 when $w_1(m, 0)$ is expanded in a Fourier series with transform variable θ . By the same token, the appearance of the polynomials $U_s(\cdot)$ and $U_{s-1}(\cdot)$ is intrinsic to the Schrödinger equation in the 4RW model, as already indicated previously. Note that the operators D_x (or any power of it) and E_x commute and the order of these terms on the right hand sides of (11) and (12) is not important. To complete the solution, we must now expand the unknown functions in terms of eigenfunctions of the D_x operator that are consistent with the boundary conditions at $m=0, \ell$. In free space, the appropriate eigenfunctions are plane waves with a continuous wavenumber as adopted in Ref. 7 (or said in other words, the unknown function is represented in terms of its Fourier transform or series).

For the boundary conditions indicated as in (4), we seek an expansion of a spatial function $v(m)$ in terms of exponential and/or trigonometric functions. An exponential function of the form $v_0(m) = r^m$ is a valid eigenfunction provided that the base $r = \alpha_1^{-1} = \alpha_2$. Clearly this is only possible in the special case of $\sqrt{\alpha_1 \alpha_2} := \alpha_g = 1$, where α_g denotes the geometric mean of α_1 and α_2 . In such a case, $D_x v_0(m) = 0.5(\alpha_1 + \alpha_2)v_0(m) := \alpha_a \cdot v_0(m)$, where α_a , being the arithmetic mean of α_1 and α_2 , is the eigenvalue pertaining to $v_0(m)$. When $\alpha_g \neq 1$, such an exponential function will not exist. We will denote the presence of this exponential function by employing the Kronecker symbol $\delta_{\alpha_g}^1$. A harmonic function of the form

$$u_j(m) = A_j \sin(k_j m) + B_j \cos(k_j m), \quad j = 1, 2, \dots \quad (13)$$

is also a valid eigenfunction provided that

$$B_j(1 - \alpha_1 \cos k_j) = A_j \alpha_1 \sin k_j \quad (14)$$

with the spatial frequency k_j given by

$$\sin(k_j \ell) - 2\alpha_a \sin[k_j(\ell - 1)] + \alpha_g^2 \sin[k_j(\ell - 2)] = 0. \quad (15)$$

Equations (14) and (15) are obtained by enforcing the boundary condition (4) at the two ends. A trivial solution of Eq. (15) is $k_j = 0$. There will be a total of $(\ell - 1)$ nontrivial solutions of (15), thus constituting a total of ℓ distinct eigenfunctions [including the function $v_0(m)$] to represent the solution of (9) and (12) at the points $m = 0, \dots, \ell$. Making use of (14) in (13) allows us to extract a bare eigenfunction $v_j(m)$ (i.e., without the coefficient A_j and other common factors) in the form

$$v_j(m) = \sin(k_j m) - \alpha_1 \sin[k_j(m - 1)], \quad (16)$$

with the spatial frequency set by (15) for a given α_1 , α_2 , and ℓ . It can be easily verified that $D_x v_j(m) = \cos k_j \cdot v_j(m)$ so that the eigenvalue of $v_j(m)$ with respect to the averaging operator is $\cos k_j$. Furthermore, the eigenfunctions $v_j(m)$ with distinct k_j as well as $v_j(m)$ and $v_0(m)$ are mutually orthogonal, i.e.,

$$\sum_{m=1}^{\ell-1} v_i(m)v_j(m) = 0, \quad i, j = 1, \dots, \ell-1, \quad i \neq j, \quad (17)$$

$$\sum_{m=1}^{\ell-1} v_j(m)v_0(m) = 0, \quad j = 1, \dots, \ell-1. \quad (18)$$

The following normalization results can also be readily established for the functions $v_0(m)$ and $v_j(m)$:

$$\sum_{m=1}^{\ell-1} v_0^2(m) = \frac{\alpha_1^{-2(\ell-1)} - 1}{1 - \alpha_1^2} := 1/a_0 \quad (19)$$

and

$$\begin{aligned} \sum_{m=1}^{\ell-1} v_j^2(m) &= \frac{\sin(k_j \ell)}{\sin k_j} \left[\alpha_1 \cos[k_j(\ell-2)] - \frac{1}{2}(1 + \alpha_1^2) \cos[k_j(\ell-1)] \right] + \frac{\ell(1 + \alpha_1^2)}{2} - \alpha_1 \ell \cos k_j \\ &\quad - \alpha_1^2 \sin^2[k_j(\ell-1)] := 1/a_j. \end{aligned} \quad (20)$$

Gathering all of the above results, an arbitrary function $v(m)$ satisfying the boundary condition (4) will admit a spectral representation of the form

$$v(m) = A_0 v_0(m) \delta_{\alpha_g}^1 + \sum_{j=1}^{\ell-1} A_j v_j(m), \quad (21)$$

where the coefficients A_0 and A_j of the basis functions $v_0(m)$ and $v_j(m)$ can be obtained in terms of the function $v(m)$ via the orthogonality conditions and normalization relations (17)–(20),

$$A_0 = a_0 \sum_{m=1}^{\ell-1} v_0(m)v(m), \quad (22)$$

$$A_j = a_j \sum_{m=1}^{\ell-1} v_j(m)v(m), \quad j = 1, \dots, \ell-1. \quad (23)$$

With this spectral representation, it is clear that

$$D_x v(m) = A_0 \alpha_a \cdot v_0(m) \delta_{\alpha_g}^1 + \sum_{j=1}^{\ell-1} A_j \cos k_j \cdot v_j(m). \quad (24)$$

Hence, the presence of D_x in the spatial domain is accounted for by multiplying the spectral basis function term by its respective eigenvalue. In particular,

$$D_x^s v(m) = A_0 \alpha_a^s \cdot v_0(m) \delta_{\alpha_g}^1 + \sum_{j=1}^{\ell-1} A_j \cos^s k_j \cdot v_j(m) \quad (25)$$

and

$$U_s \left(\frac{D_x}{\sqrt{2}} \right) v(m) = A_0 U_s \left(\frac{\alpha_a}{\sqrt{2}} \right) \cdot v_0(m) \delta_{\alpha_g}^1 + \sum_{j=1}^{\ell-1} A_j U_s \left(\frac{\cos k_j}{\sqrt{2}} \right) \cdot v_j(m). \quad (26)$$

Having laid out the formulation for the general case, we will now consider two interesting special cases which will merit a separate discussion.

A. Totally absorbing boundaries

In this case $\alpha_1 = \alpha_2 = 0$, which precludes the exponential solution $v_0(m)$. Equation (15) implies a solution $k_j = \pi j / \ell$, $j = 1, \dots, \ell - 1$. The eigenfunctions $v_j(m)$ will be reduced to $\sin(\pi j m / \ell)$ and $a_j = 2 / \ell$ from (20). In this case, one gets the discrete sine transform¹⁶ representation for a function satisfying Dirichlet boundary conditions,

$$v(m) = \sum_{j=1}^{\ell-1} A_j \sin\left(\frac{j\pi m}{\ell}\right), \quad A_j = \frac{2}{\ell} \sum_{m=1}^{\ell-1} v(m) \sin\left(\frac{j\pi m}{\ell}\right), \quad j = 1, \dots, \ell - 1. \quad (27)$$

B. Totally reflecting boundaries

For totally reflecting boundaries at both ends, $\alpha_1 = \alpha_2 = 1$, which dictate that $\alpha_g = \alpha_a = 1$. Equation (15) indicates a solution $k_j = j\pi / (\ell - 1)$, $j = 1, \dots, \ell - 1$. The exponential function now reduces to a constant function $v_0(m) = 1$. The normalization constants a_0 and a_j are obtained from (19) and (20) as

$$1/a_0 = (\ell - 1), \quad 1/a_j = 2(\ell - 1) \sin^2\left(\frac{\pi j}{2(\ell - 1)}\right). \quad (28)$$

An unknown function $v(m)$ satisfying perfectly reflecting conditions at the two ends can then be expressed as

$$\begin{aligned} v(m) &= A_0 + \sum_{j=1}^{\ell-1} A_j \left[\sin\left(\frac{\pi j m}{\ell - 1}\right) - \sin\left(\frac{\pi j (m - 1)}{\ell - 1}\right) \right] = A_0 + \sum_{j=1}^{\ell-1} 2A_j \sin\left(\frac{\pi j}{2(\ell - 1)}\right) \cos\left(\frac{\pi j (m - \frac{1}{2})}{\ell - 1}\right) \\ &:= A_0 + \sum_{j=1}^{\ell-1} C_j \cos\left(\frac{\pi j (m - \frac{1}{2})}{\ell - 1}\right) \end{aligned} \quad (29)$$

with the coefficients given by

$$A_0 = \frac{2}{\ell - 1} \sum_{m=1}^{\ell-1} v(m), \quad C_j = \frac{2}{\ell - 1} \sum_{m=1}^{\ell-1} \cos\left(\frac{\pi j (m - \frac{1}{2})}{\ell - 1}\right) v(m), \quad j = 1, \dots, \ell - 1. \quad (30)$$

Equations (29) and (30) constitute the discrete-cosine-transform (Ref. 16) representation of a function satisfying Neumann type of boundary conditions at the end points.

C. Solution for general case

The results given in (25) and (26) will now be used to determine the Green's function¹³ of the diffusion equation (10) and the Schrödinger equations (11) and (12). The linearity of the governing equations with respect to the initial conditions enables the solution to arbitrary initial conditions in terms of this Green's function. To this end we consider initial conditions of the form $p_\mu(m, 0)\Delta = P_{\mu 0} \delta_m^{m_0}$, $1 \leq m_0 \leq \ell - 1$, where $\sum_{\mu=1}^4 P_{\mu 0} = 1$. This initial condition corresponds to the case where the particles are released from the location m_0 in a state μ with probability $P_{\mu 0}$. Letting $\Gamma_1 = (P_{10} - P_{30}) / \Delta$ and $\Gamma_2 = (P_{20} - P_{40}) / \Delta$, it is clear from the definitions that $w_1(m, 0) = \delta_m^{m_0}$, $q_1(m, 0) = \Gamma_1 \delta_m^{m_0}$, and $q_2(m, 0) = \Gamma_2 \delta_m^{m_0}$. Using the spectral representation given in (21)–(23) for the functions $w_1(m, 0)$, $q_1(m, 0)$, and $q_2(m, 0)$, we arrive at

$$w_1(m, 0) = a_0 v_0(m_0) v_0(m) \delta_{\alpha_g}^1 + \sum_{j=1}^{\ell-1} a_j v_j(m_0) v_j(m), \quad (31)$$

$$q_1(m, 0) = a_0 \Gamma_1 v_0(m_0) v_0(m) \delta_{\alpha_g}^1 + \Gamma_1 \sum_{j=1}^{\ell-1} a_j v_j(m_0) v_j(m), \quad (32)$$

$$q_2(m, 0) = a_0 \Gamma_2 v_0(m, 0) v_0(m) \delta_{\alpha_g}^1 + \Gamma_2 \sum_{j=1}^{\ell-1} a_j v_j(m_0) v_j(m). \quad (33)$$

Substituting (31)–(33) into (10) and (11) and recalling relations (25) and (26), we arrive at the solution for the general boundary conditions as

$$w_1(m, s) = a_0 \alpha_a^s v_0(m_0) v_0(m) \delta_{\alpha_g}^1 + \sum_{j=1}^{\ell-1} a_j \cos^s(k_j) v_j(m_0) v_j(m) \quad (34)$$

and

$$\begin{aligned} q_1(m, s) = & a_0 v_0(m_0) \delta_{\alpha_g}^1 \left[\Gamma_1 U_s \left(\frac{\alpha_a}{\sqrt{2}} \right) v_0(m) - \frac{\Gamma_2 + \Gamma_1}{\sqrt{2}} U_{s-1} \left(\frac{\alpha_a}{\sqrt{2}} \right) v_0(m+1) \right] + \sum_{j=1}^{\ell-1} a_j v_j(m_0) \\ & \times \left[\Gamma_1 U_s \left(\frac{\cos k_j}{\sqrt{2}} \right) v_j(m) - \frac{\Gamma_2 + \Gamma_1}{\sqrt{2}} U_{s-1} \left(\frac{\cos k_j}{\sqrt{2}} \right) v_j(m+1) \right], \end{aligned} \quad (35)$$

$$\begin{aligned} q_2(m, s) = & a_0 v_0(m_0) \delta_{\alpha_g}^1 \left[\Gamma_2 U_s \left(\frac{\alpha_a}{\sqrt{2}} \right) v_0(m) - \frac{\Gamma_2 - \Gamma_1}{\sqrt{2}} U_{s-1} \left(\frac{\alpha_a}{\sqrt{2}} \right) v_0(m-1) \right] + \sum_{j=1}^{\ell-1} a_j v_j(m_0) \\ & \times \left[\Gamma_2 U_s \left(\frac{\cos k_j}{\sqrt{2}} \right) v_j(m) - \frac{\Gamma_2 - \Gamma_1}{\sqrt{2}} U_{s-1} \left(\frac{\cos k_j}{\sqrt{2}} \right) v_j(m-1) \right]. \end{aligned} \quad (36)$$

D. Solution for totally absorbing case

We will now provide some numerical results for the special case of totally absorbing boundaries at the two ends. In this case, Eqs. (34)–(36) will be reduced to

$$w_1(m, s) = \frac{2}{\ell} \sum_{j=1}^{\ell-1} \sin \left(\frac{\pi j m_0}{\ell} \right) \sin \left(\frac{\pi j m}{\ell} \right) \cos^s \left(\frac{\pi j}{\ell} \right), \quad (37)$$

$$\begin{aligned} q_1(m, s) = & \frac{2}{\ell} \sum_{j=1}^{\ell-1} \sin \left(\frac{\pi j m_0}{\ell} \right) \left[\Gamma_1 U_s \left(\frac{\cos \left(\frac{\pi j}{\ell} \right)}{\sqrt{2}} \right) \sin \left(\frac{\pi j m}{\ell} \right) \right. \\ & \left. - \frac{\Gamma_2 + \Gamma_1}{\sqrt{2}} U_{s-1} \left(\frac{\cos \left(\frac{\pi j}{\ell} \right)}{\sqrt{2}} \right) \sin \left(\frac{\pi j (m+1)}{\ell} \right) \right], \end{aligned} \quad (38)$$

FIG. 1. Comparison of analytical solution for $w_1(m\Delta, s\epsilon)\Delta$ with that obtained from counting paths in random walk simulations for totally absorbing boundary conditions.

$$q_2(m, s) = \frac{2}{\ell} \sum_{j=1}^{\ell-1} \sin\left(\frac{\pi j m_0}{\ell}\right) \left[\Gamma_2 U_s \left(\frac{\cos\left(\frac{\pi j}{\ell}\right)}{\sqrt{2}} \right) \sin\left(\frac{\pi j m}{\ell}\right) - \frac{\Gamma_2 - \Gamma_1}{\sqrt{2}} U_{s-1} \left(\frac{\cos\left(\frac{\pi j}{\ell}\right)}{\sqrt{2}} \right) \sin\left(\frac{\pi j (m-1)}{\ell}\right) \right]. \quad (39)$$

Because the Green's functions satisfy reciprocity conditions, it is permissible to interchange m and m_0 in the above expressions without changing the field values. The solution for a continuous space can be obtained by carrying out the same limiting process as outlined in Ref. 7. For example, Eq. (37) reduces to the expression for the probability density function of the diffusion process with a diffusion constant D with two totally absorbing points at $x=0$ and $x=L$ and an impulsive initial condition at $x=x_0$,

$$p(x, t) = \frac{2}{L} \sum_{j=1}^{\infty} \sin\left(\frac{\pi j x_0}{L}\right) \sin\left(\frac{\pi j x}{L}\right) \exp\left(-\frac{\pi^2 j^2 D t}{2 L^2}\right), \quad (40)$$

a result that is found in many texts including Ref. 9. The results given in (34)–(39) are exact, and as such, no validation is necessary. Nevertheless, it is interesting to compare the numerical data they generate with those generated through direct random walk simulations, as the latter will more likely be employed for more complicated time-dependent boundaries. In such cases, the analytical results developed here will serve more as a validation check for the numerical results generated through random walk simulations. The analytical results (labeled “Ana” in the figures) and the results obtained by counting the fractional number of paths (labeled “Num” in the figures) in the 4RW simulations with initial conditions set at $P_{10}=0.5=P_{20}$ from the location $m_0=4$ are shown in Figs. 1 and 2 at $s=16$ and for $\ell=32$. For reference, the solution for Schrödinger equation in free space is also shown in Fig. 2. For the parameters chosen in Fig. 2, the solution with boundaries will differ from the free-space case only for $0 \leq m \leq 12$, as is clearly seen in the figure. A large number of realizations (about 10^8) was needed to arrive at numerically converging results, particularly for the Schrödinger equation whose solution involves difference in probabilities. Both

FIG. 2. (Color online) Comparison of the exact solution of Schrödinger equation with that obtained through counting paths in random walk simulations.

figures reveal that the numerical simulated results closely mimic the analytical formulas derived here. The numerical results also underscore the importance of a good numerical random number generator, particularly needed for large s , as the sample size grows exponentially with s . The use of entwined paths described in Ref. 17 is a possible means of getting around this difficulty, although details have only been demonstrated there for the relativistic case of bounded particle speed.

E. Appropriateness of the 4RW model to wave propagation problems

It might be worthwhile to comment a little on the relationship between the 4RW model and the continuous parabolic equation for which the former is being targeted in numerical computations. For the parabolic equation encountered in a number of wave propagation problems such as in underwater acoustics, radio wave propagation, and optical wave propagation in fibers, the governing equation for the field variable ψ in a homogeneous medium with time-harmonic excitation is of the form

$$\frac{\partial \psi}{\partial t} = \frac{i}{2k_0} \frac{\partial^2 \psi}{\partial x^2}, \quad (41)$$

where the independent variable t denotes the axial spatial coordinate and the variable x denotes the lateral spatial coordinate, $k_0 = 2\pi/\lambda$ is the wavenumber in the medium, and λ is the wavelength of the time-harmonic excitation. Equation (41) describes two-dimensional wave propagation in the t - x -plane subject to the approximation that all waves travel within an angle of $\theta = \pm 15^\circ$ about the axial direction.³ It can be shown that the maximum step size Δ in the lateral direction is restricted by $\Delta \lesssim \lambda/(2 \sin \theta_{\max})$, where $\theta_{\max}$ is the maximum angle of propagation with respect to the t -axis. As θ is restricted to a value less than 15° for the parabolic approximation to be valid, we may take $\sin \theta_{\max} \approx \tan \theta_{\max} \approx \Delta/\epsilon$. We then get the approximate relation

$$\pi\epsilon \gtrsim k_0\Delta^2. \quad (42)$$

It may be remarked parenthetically that the inequality (42) translates to the condition that the Schrödinger equation is valid for describing particle motion for nonrelativistic particle speeds with the normalized speed $v/c \lesssim \tan \theta_{\max} \approx 0.27$ for $\theta_{\max} = 15^\circ$, where c is the speed of light in free space. In the 4RW model, the relation between the step sizes of the form $\epsilon = k_0\Delta^2$ is implied and this is consistent with the inequality (42) If $\Delta = \lambda/\sqrt{2}$, then this relation implies that $\epsilon = \pi\lambda$. Both of these values are well within the maximum values permitted by the parabolic equation approximation and it is believed that the 4RW model constitutes a very appropriate discretization scheme for numerically handling the parabolic equation.

IV. CONCLUSIONS

Analytical expressions have been provided for the transitional probabilities of a 4RW model on a lattice constrained in space with dissimilar boundaries and subject to partially reflecting boundary conditions. Special cases of perfectly absorbing boundaries and perfectly reflecting boundaries have been treated. Solution for the transitional probabilities evaluated at time s to the diffusion process is shown to involve s th power of the averaging operator D_x , whereas those of the Schrödinger equation involve Chebyshev polynomials of the second kind of order s and $s-1$ with argument $D_x/\sqrt{2}$. These are the general characteristics of diffusion and Schrödinger processes in the 4RW model irrespective of the boundary conditions. Different boundary conditions will dictate different choices of the eigenfunctions in which the initial probabilities at $s=0$ are expanded. The eigenfunctions in the most general case will involve exponential function as well as harmonic functions. The exponential function will only exist when the parameters present in the boundary conditions satisfy certain relationship. While the results presented in this paper should have a significance of their own for random walk with dissimilar boundaries, it is hoped that they will also serve as benchmark cases for numerical stochastic methods designed to solve more complicated situations. Although it had not been the major focus of the current paper, numerical implementation of the random walk solution necessitates the availability of an effective random number generator to sufficiently populate all portions of the sample space. This is particularly critical for field evaluated at large times. Extension of these results to higher dimensions and to situations with a potential field is a topic worthy of further study and will be taken up in the future.

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- ¹G. N. Ord and A. S. Deakin, *J. Phys. A* **30**, 819 (1997).
- ²G. N. Ord and J. A. Gualtieri, *Phys. Rev. Lett.* **89**, 250403 (2002).
- ³F. B. Jensen, W. A. Kuperman, M. B. Porter, and H. Schmidt, *Computational Ocean Acoustics* (Springer, New York, 1994).
- ⁴J. R. Kuttler and R. Janaswamy, *Radio Sci.* **37**, 5-1 (2002).
- ⁵R. Janaswamy, IEEE Applied Electromagnetics Conference, Kolkata, India, 2007, Vol. 1, Paper No. AEMC.2007.4638046, pp. 1-4; available online at <http://ieeexplore.ieee.org/arnumber=4638046&isnumber=4637999&punumber=4629478>.
- ⁶B. V. Budaev and D. B. Bogy, *Q. J. Mech. Appl. Math.* **55**, 209 (2002).
- ⁷R. Janaswamy, *J. Phys. A: Math. Theor.* **41**, 155306 (2008).
- ⁸J. C. Strikwerda, *Finite Difference Schemes and Partial Differential Equations*, 2nd ed. (Society of Industrial and Applied Math, Philadelphia, PA, 2004).
- ⁹G. H. Weiss, *Aspects and Applications of the Random Walk* (North-Holland, New York, NY, 1994).
- ¹⁰F. B. Knight, *Essentials of Brownian Motion and Diffusion* (American Mathematical Society, New York, NY, 1981).
- ¹¹J. Masoliver, J. M. Porra, and G. H. Weiss, *Phys. Rev. E* **48**, 939 (1993).
- ¹²G. N. Ord, *Ann. Phys.* **250**, 51 (1996).
- ¹³G. Barton, *Elements of Green's Functions and Propagation* (Oxford University Press, New York, NY, 1989).
- ¹⁴W. Feller, *An Introduction to Probability Theory and Its Applications*, 2nd ed. (Wiley, New York, NY, 1970), Vol. 2.
- ¹⁵E. W. Montroll, *J. Math. Phys.* **6**, 167 (1965).
- ¹⁶S. A. Martucci, *IEEE Trans. Signal Process.* **42**, 1038 (1994).
- ¹⁷G. N. Ord, J. A. Gualtieri, and R. B. Mann, *Found. Phys. Lett.* **19**, 471 (2006).