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Exact transition operators for Markov and lattice Schrödinger processes constrained by a boundary

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A closed form is given for a three-parameter family of transition matrices describing continuous-time nonsymmetric random walks on a $d=1$ semi-infinite lattice. The boundary conditions are general, allowing for an arbitrary mixture of reflection, trapping, and sojourn. Special cases give the quantum propagator for the half-lattice, and transition matrices for the random walk on the Bethe lattice and the single-server queue $M/M/1/\infty$.

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Continuous-time random walks on a $d=1$ lattice in the presence of a partly sticky, partly reflecting, or partly trapping boundary have many biological, physical, and chemical applications. A master transition matrix is derived here that simultaneously incorporates these features. The method of solution is to transform the boundary condition into a local interaction, so that the problem is unfolded onto the full lattice. The lattice energy Green's function is then obtained by summing the complete perturbation series. In configuration space, the final result is a convolution of generators of biased and symmetric random walks.

The approach used here provides an independent, compact way to derive exact transition matrices for an array of quantum and classical lattice problems. One such is the imaginary-time Schrödinger propagator for a lattice particle hopping on the half-lattice—the discrete-space generalization of the known continuum solution [1]. Also included here is the complete transition matrix for the random walk on the Bethe lattice, for which the discrete-time return probability has recently been obtained using the method of generating functions [2]. In turn, the Bethe lattice return probability follows from the complete Green's function for the discrete-time walk in a constant field in the presence of a reflecting barrier, obtained many years ago by deriving the complete set of eigenvectors and eigenvalues of the evolution matrix [3]. The continuous-time solution of the general problem treated in [3] is also a special case of the result given below. The present result includes the exact lattice transition matrix for a symmetric $d=1$ random walk in the presence of a reflecting and trapping boundary, a standard mixed boundary condition problem on the continuum [4]. Also incorporated here is an independent matrix-algebraic derivation of the transition matrix for the infinite single-server queue $M/M/1/\infty$ with Poisson arrival and service times [5]. The algebraic technique used here can be applied generally to quantum problems in which there are highly localized eigenstates. For example, it has recently been used in the context of the discrete value representation to obtain an approximate density of states for a model of resonant quantum tunneling [6].

The problems of interest can be formulated in terms of the semi-infinite stochastic system

$$\dot{\mathbf{P}}(t)=\mathbf{E}\cdot\mathbf{P}(t). \tag{1}$$

The objective is to derive a closed form expression for $\mathbf{P}_{jm}(t)$, $(j,m) = 0,1,2,3,\ldots$, the probability that a random walker moves from cell m to cell j in elapsed time t, given the evolution operator $\mathbf{E}$. The walk is taken to be nonsymmetric, so that Eq. (1) describes the continuous-time limit of a Markov process with nearest neighbor transitions. Admissible evolution operators $\mathbf{E}$ are therefore tridiagonal, with column sums $\Sigma_m \mathbf{E}_{jm}=0$, and one can write $\mathbf{E}=\mathbf{M}-\mathbf{I}$, where $\mathbf{M}$ is a stochastic matrix, $0\leqslant\mathbf{M}_{jm}\leqslant 1$, $\Sigma_m\mathbf{M}_{jm}=1$, describing the underlying Markov process. The stochastic matrix with the general boundary conditions of interest is

$$\mathbf{M}=\begin{pmatrix} q\sigma & p & & & \\ 1-q & 0 & p & & \\ & 1-p & 0 & p & \\ & & 1-p & 0 & \cdots \\ & & & \cdots & \cdots \end{pmatrix}. \tag{2}$$

It is convenient to define the reduced transition matrix $\mathbf{K}\equiv\mathbf{P}e^{t}$, and to replace (1) by

$$\dot{\mathbf{K}}(t)=\mathbf{M}\cdot\mathbf{K}(t). \tag{3}$$

In (2), $(p,\ 1-p)$ are the (right, left) step probabilities of a free nonsymmetric random walk, $(q,\ 1-q)$ are the sojourn and reflection probabilities at the (cell 0) boundary, and $1-\sigma$ is the conditional probability that the walker is trapped at the boundary, given a sojourn there. The choice $q=0$ corresponds to pure reflection, or equivalently to the random walk on an infinite Cayley tree or Bethe lattice with coordination number $J=1/p$. The choice $q=1$ makes the boundary a certain trap, while $\sigma=1$, $q\neq 0$ leads to the random walk in the presence of an elastic barrier and to imaginary-time quantum mechanics on the half-lattice. The case $q=p$, $\sigma=1$ gives the problem of the infinite single-server queue $M/M/1/\infty$.

Discrete-space path sum. That there is a closed form solution for (2) and (3) follows from three observations. First, as shown explicitly below, one may decompose the evolution operator in (3) as $\mathbf{M}=\mathbf{M}_0+\mathbf{V}$, where $\mathbf{M}_0$ generates the free nonsymmetric lattice walk and $\mathbf{V}$ is an "interaction" incorporating the boundary conditions at cell 0. One can then

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time-slice and formally write the transition matrix as the Trotter product $\mathbf{K}(t)=\exp(\mathbf{M}t)=\lim_{N\to\infty}(e^{\varepsilon\mathbf{M}_0}e^{\varepsilon\mathbf{V}})^N$, where $\varepsilon=t/N$. Second, because the boundary conditions are equivalent to a point interaction, $\mathbf{V}^2\propto\mathbf{V}$, and therefore $e^{\varepsilon\mathbf{V}}=I+[\varepsilon+O(\varepsilon^2)]\mathbf{V}$. In the Trotter limit the probability of every path from m to j thus factorizes as $(mx)(xx)(xx)\cdots(xx)(xj)$, where (mx) is the probability of a path segment from m to the boundary, and (xx) represents the probability of a closed path with initial and final, but no other, boundary points. Third, because of the pointwise interaction the transition matrix can be expressed as the double sum over (1) all possible allocations of total time t, given a path containing a fixed number, k, of closed loops (xx), and (2) over all path lengths $k\geqslant 0$. The sum over path lengths evaluates the perturbation series in $\mathbf{V}$ and in general results in an exponential function of the effective coupling constant. Given the sum over path lengths, the time allocation sum becomes a k-fold convolution integral. Below, I evaluate the Laplace transform of this multiple convolution and show that the inverse transform gives $\mathbf{K}(t)$ in the form of a single, time-weighted convolution of generators of biased and symmetric random walks.

Unfolding. For algebraic simplicity, it is helpful to follow previous treatment of the Bethe lattice walk [7] and to unfold (2) and (3) into a doubly infinite lattice system. To do so, one decomposes the evolution operator (2) into the free particle operator

$$\mathbf{M}_0(p)=\begin{pmatrix} \cdots & \cdots & \cdots & & & & \\ \cdots & \cdots & p & & & & \\ & \cdots & 0 & p & & & \\ & & 1-p & 0 & p & & \\ & & & 1-p & 0 & \cdots & \\ & & & & 1-p & \cdots & \cdots \\ & & & & \cdots & \cdots & \cdots \end{pmatrix} \tag{4}$$

and the "interaction"

$$\mathbf{V}(p,q,\sigma)=\begin{pmatrix} \cdots & \cdots & \cdots & \cdots & & & \\ \cdots & \cdots & 0 & 0 & \cdots & & \\ \cdots & \cdots & 0 & -p & 0 & & \\ \cdots & \cdots & 0 & q\sigma & 0 & \cdots & \cdots \\ & \cdots & 0 & p-q & 0 & \cdots & \cdots \\ & & \cdots & 0 & 0 & \cdots & \cdots \\ & & & \cdots & \cdots & \cdots & \cdots \end{pmatrix}. \tag{5}$$

The choice $\mathrm{Prob}(0\to -1)=0$ implemented in (4) and (5) preserves the dynamics of paths with initial points on the positive half-lattice.

Dimensionless form. Rescale time by $\tau\equiv 2\sqrt{p(1-p)}t$, and define the parameters $\gamma\equiv\sqrt{p/(1-p)}$, $\beta\equiv q/[2\sqrt{p(1-p)}]$. Then (3) becomes

$$\dot{\mathbf{K}}(\tau)=(\mathbf{Q}+\mathbf{W})\cdot\mathbf{K}(\tau), \tag{6}$$

with

$$\mathbf{Q}=\frac{1}{2}\begin{pmatrix} \cdots & \cdots & & & & & \\ \cdots & \cdots & \gamma & & & & \\ \cdots & \cdots & 0 & \gamma & & & \\ \cdots & \cdots & \frac{1}{\gamma} & 0 & \gamma & \cdots & \cdots \\ & & & \frac{1}{\gamma} & 0 & \cdots & \cdots \\ & & & & \frac{1}{\gamma} & \cdots & \cdots \\ & & & & & \cdots & \cdots \end{pmatrix}, \tag{7}$$

$$\mathbf{W}=\frac{1}{2}\begin{pmatrix} \cdots & \cdots & & & & & \\ \cdots & \cdots & 0 & 0 & & & \\ \cdots & \cdots & 0 & -\gamma & 0 & & \\ \cdots & \cdots & 0 & \beta\sigma & 0 & \cdots & \cdots \\ & & 0 & \gamma-\beta & 0 & \cdots & \cdots \\ & & & 0 & 0 & \cdots & \cdots \\ & & & & & \cdots & \cdots \end{pmatrix}. \tag{8}$$

Summing the perturbation series. The Laplace transform of Eq. (6) can be solved algebraically for $\tilde{\mathbf{K}}(k)=\int_0^\infty\mathbf{K}(\tau)e^{-k\tau}d\tau$, which can be expressed as

$$\tilde{\mathbf{K}}(k)=[k\mathbf{I}-\mathbf{Q}-\mathbf{W}]^{-1}=(\tilde{\mathbf{K}}_0^{-1}-\mathbf{W})^{-1}$$
$$=\tilde{\mathbf{K}}_0+\tilde{\mathbf{K}}_0(\mathbf{W}+\mathbf{W}\tilde{\mathbf{K}}_0\mathbf{W}+\cdots)\tilde{\mathbf{K}}_0\equiv\tilde{\mathbf{K}}_0+\tilde{\mathbf{K}}_0\mathbf{S}\tilde{\mathbf{K}}_0. \tag{9}$$

In (9), $\mathbf{I}$ is the (doubly infinite) unit matrix, and

$$[\tilde{\mathbf{K}}_0(k)]_{jm}=\frac{\gamma^{m-j}e^{-u|j-m|}}{\sinh u},\quad k=\cosh u \tag{10}$$

is the transform of the free random walk transition matrix

$$[\mathbf{K}_0(\tau)]_{jm}=\gamma^{m-j}I_{j-m}(\tau). \tag{11}$$

In (11), $I_m(\tau)$ is the modified Bessel function of order m.

The matrix sum $\mathbf{S}$ in (9) may be evaluated easily because the one-column form of $\mathbf{W}$ results in

$$\mathbf{WAW}=(\mathbf{AW})_{00}\mathbf{W}$$
$$=\frac{1}{2}[\gamma(\mathbf{A}_{01}-\mathbf{A}_{0,-1})+\beta\sigma\mathbf{A}_{00}-\beta\mathbf{A}_{01}]\mathbf{W} \tag{12}$$

for any matrix $\mathbf{A}$. In particular, from (12) the sum $\mathbf{S}$ in (9) is a geometric series with expansion parameter

$$(\tilde{\mathbf{K}}_0\mathbf{W})_{00}=\frac{1}{2\ \sinh u}[(\gamma^2-\gamma\beta-1)e^{-u}+\beta\sigma], \quad (13)$$

and we have

$$\mathbf{S}=\frac{\mathbf{W}}{1-(\tilde{\mathbf{K}}_0\mathbf{W})_{00}}. \quad (14)$$

To complete the evaluation of (9), observe that for any $\mathbf{A}$ we also have

$$(\mathbf{AWA})_{jm}=\frac{1}{2}[\gamma(\mathbf{A}_{j1}-\mathbf{A}_{j,-1})+\beta\sigma\mathbf{A}_{j0}-\beta\mathbf{A}_{j1}]\mathbf{A}_{0m}. \quad (15)$$

Using (15) and (10), the full "interaction term" in (9) is

$$[\tilde{\mathbf{K}}_0\mathbf{S}\tilde{\mathbf{K}}_0]_{jm}=\frac{\gamma^{m-j}}{\sinh u}\left[\frac{(\gamma^2-\beta\gamma)e^{-u|j-1|-u|m|}-e^{-u|j+1|-u|m|}+\beta\sigma e^{-u|j|-u|m|}}{2\cosh u-(1+\gamma^2-\gamma\beta)e^{-u}-\beta\sigma}\right]. \quad (16)$$

A check on (16) follows from setting $\gamma=\beta$ and expanding the bracketed expression as a power series in e^{-u}, obtaining, with the proper rescaling of time, the series expansion Eq. (4.32) of [5] for the transition matrix that describes the birth-death process with fixed birth and death rates, or equivalently the single-server queue $M/M/1/\infty$.

To evaluate the real-time transition matrix corresponding to (16), one may use the tabulated transform [8]

$$\int_0^\infty\left(\frac{t+2z}{t}\right)^{-N/2}I_N(\sqrt{t^2+2zt})e^{-kt}dt=\frac{1}{\sinh u}e^{-Nu+ze^{-u}},$$

$$N>-1,\quad \mathrm{Re}k>1,\quad |\arg z|<\pi \quad (17)$$

and the convolution theorem to obtain the inverse transform

$$L^{-1}\left[\int_0^\infty\frac{e^{-2y\cosh u+(1+\gamma^2-\gamma\beta)ye^{-u}+\beta\sigma y-Ku}}{\sinh u}dy\right]$$

$$=\frac{1}{2}\int_0^\tau e^{\beta\sigma s/2}\left[\frac{\tau-s}{\tau+\gamma(\gamma-\beta)s}\right]^{K/2}$$

$$\times I_K(\sqrt{(\tau-s)[\tau+\gamma(\gamma-\beta)s]})ds\equiv N_K(\tau). \quad (18)$$

From (10), (16), and (18), the transition matrix we seek is

$$K_{jm}(\tau)=\gamma^{m-j}I_{j-m}(\tau)+\gamma^{m-j}[-N_{|j+1|+|m|}(\tau)$$

$$+\gamma(\gamma-\beta)N_{|j-1|+|m|}(\tau)+\beta\sigma N_{|j|+|m|}(\tau)]. \quad (19)$$

It is straightforward to check that in the case $\gamma=1$, $\beta=0$ the continuum limit of (18) and (19) gives the correct heat propagator $G_0(x'+x;\tau)+G_0(x'-x;\tau)$, $G_0(x;\tau)\equiv(2\pi\tau)^{-1/2}\exp(-x^2/2\tau)$, for diffusion in the presence of a reflecting barrier.

Configuration space form. Equations (18) and (19) show the structure outlined above. The sum over all orders in $\mathbf{V}$ results in the factor $e^{\beta\sigma s/2}$ in (18). The broken paths indicated by the position indices in (19) arise from the Feynman-Kac path average over the interaction $\mathbf{W}=\mathbf{w}\delta$, where δ is the discrete δ-function interaction matrix with a single nonzero unit entry at (0,0), and $\mathbf{w}$ is the Toeplitz generalization of (8). The remainder of the integrand in (18) is the final result of the multiple convolution representing the allocation of total time τ among the boundary loops discussed above. A physical interpretation of these factors in the integrand follows from the matrix generating function

$$e^{a\mathbf{M}_0(1/2)-b\mathbf{X}}=\sum_{j=-\infty}^{\infty}\left(\frac{a-b}{a+b}\right)^{j/2}I_j(\sqrt{a^2-b^2})\mathbf{T}_j, \quad (20)$$

where $\mathbf{T}_j$, $j\geqslant 0$ $(j<0)$ is the elementary Toeplitz matrix with 1's on the jth super- (sub-)diagonal and 0's elsewhere,

$$\mathbf{X}=\frac{1}{2}\begin{pmatrix} \cdots & \cdots & & & & & \\ \cdots & \cdots & 1 & & & & \\ \cdots & \cdots & 0 & 1 & & & \\ \cdots & \cdots & -1 & 0 & 1 & \cdots & \cdots \\ & & & -1 & 0 & \cdots & \cdots \\ & & & & -1 & \cdots & \cdots \\ & & & & & \cdots & \cdots \end{pmatrix}, \quad (21)$$

and $\mathbf{M}_0(1/2)$ generates the symmetric walk, as implied by (4). Equation (20) follows from the Graf addition theorem [9]. If we set $a=\tau+[\gamma(\gamma-\beta)-1]s/2$, $b=[\gamma(\gamma-\beta)+1]s/2$ in (20), (18) can be written as

$$N_K(\tau)=\tau\int_0^{1/2}e^{\beta\sigma\tau u}$$

$$\times(e^{[1+2\gamma(\gamma-\beta)u]\tau\mathbf{M}_0(1/2)-[1+\gamma(\gamma-\beta)]\tau u\mathbf{M}_0(1)})_{0,K}du, \quad (22)$$

showing that the signature of this class of boundary processes is a weighted convolution of nonsymmetric random walks, biased toward the boundary, with symmetric walks on different time scales. A similar form for the (nonprobability-conserving) discrete δ-function propagator is derived in [10].

Applications. The approach used here can in principle be applied to other continuous-time random walks, those with idempotent interactions $\mathbf{V}\propto\mathbf{V}^2$, including interaction matrices with diagonal elements that have periodic binary structures or are generated by binary walks, and those with discrete versions of singular interactions $\delta^{(n)}$. Solution of the latter set of problems would generalize known $d=1$ continuum solutions for $n=1,2$ [11] to include a periodic field in the tight binding approximation. A further possible extension is to processes with second-order time derivatives, such as variants of the discrete telegraph equation [12]. The present approach may also be useful for approximating time-dependent Green's functions for chemical and molecular systems such as those discussed in [6], in which the states of the system are highly localized.

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