Two exact lattice propagators

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Exact Schrödinger and heat propagators are given for a particle hopping on a one-dimensional rectangular lattice, assuming a uniform field $V_{nn}=\lambda n$ and a δ-function potential $V_{nn}=\lambda\delta_{n0}$. In its quantum form, the uniform-field propagator is the general solution of the Wannier-Stark problem for a discrete lattice, describing a particle moving in the superposition of a homogeneous field and a discrete periodic potential created by the lattice. A disentangled form for the uniform-field propagator is obtained by using the transformation properties of the Hamiltonian under the Lie algebra iso(1,1). Using this result, it is shown that the expected position and spatial extension of a lattice wave packet oscillate in phase with equal amplitudes. The discrete δ-function heat propagator is related by a Lyapunov transformation to the solution of the lattice Smoluchowski equation for the cusp potential $V_{nn}\propto|n|$. It is shown that the implied discrete-time Smoluchowski evolution operator generates a Markov process in which a pair of nonsymmetric random walks on the right and left half-axes are coupled at cell 0 by a partly reflecting, partly transmitting, sticky barrier. The interaction term in the lattice δ-function heat propagator is a Poisson weighted superposition of nonsymmetric random walks.

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I. INTRODUCTION

There are few known exact time-dependent propagators for quantum or classical particles "hopping" on discrete lattices [1]. Such processes play important quantum roles in exciton and semiconductor physics [2]. Classical analogs of these quantum hopping processes have recently been found in hard core lattice diffusion as well as random adsorption and desorption [3]. There are also related applications to quantum spin chains [4], reaction-diffusion systems [5], and diffusion in the presence of partial traps [6]. Here, I add to the inventory of exact time-dependent solutions for hopping processes with a pair of one-dimensional propagators that satisfy the lattice Schrödinger equation

$$\dot{\mathbf{K}}(t)=(\mathbf{Q}-\mathbf{I}-\mathbf{V})\mathbf{K}(t)\ . \tag{1.1}$$

In (1.1), **I** is the identity matrix;

$$\mathbf{Q}=\frac{1}{2}\begin{bmatrix} \cdots & \cdots & & & & \\ \cdots & 0 & 1 & & & \\ & 1 & 0 & 1 & & \\ & & 1 & 0 & 1 & \\ & & & 1 & 0 & \cdots \\ & & & & \cdots & \cdots \end{bmatrix} \tag{1.2}$$

is the generator of a discrete-time, symmetric random walk on a doubly infinite lattice; and $\mathbf{V}=\lambda\mathbf{T}$ represents a local time-dependent lattice field with coupling strength λ and diagonal interaction matrix **T**. Unless otherwise stated, the matrices $(\mathbf{Q},\mathbf{I},\mathbf{V})$ are taken to be doubly infinite throughout the discussion.

For the nonsingular lattice potentials considered here, $\mathbf{K}(t)$ is an entire function of complex t. With this simple analytic structure, time t is only a place holder in an algebraic expression for $\exp[(\mathbf{Q}-\mathbf{I}-\mathbf{V})t]$. Given the proper probability interpretation, the propagators derived here therefore describe both classical and quantum systems without any analytic continuation complications.

The technical objective is to disentangle the noncommuting operators $(\mathbf{Q},\mathbf{V})$ in the formal expression for the propagator $\mathbf{K}(t)=\exp[(\mathbf{Q}-\mathbf{I}-\mathbf{V})t]$. The disentangling operation is nontrivial for lattice calculations because one must take full account of the underlying periodic structure. From an algebraic point of view, one is required to treat the complete Baker-Hausdorff expansions, $\exp[-\mathbf{V}t]\mathbf{Q}\exp[\mathbf{V}t],\ldots$, implicit in $\mathbf{K}(t)$. This is done here by using an underlying Lie symmetry to factorize the propagator and by summing the complete perturbation series for the energy Green's function. The first method is used in Sec. II to obtain the lattice propagator for the uniform field. It is shown that this propagator solves the one-band approximation for the $d=1$ (Wannier-Stark) problem of a particle moving in a periodic potential with a superimposed homogeneous external field. Exact expressions for the first and second moments of a lattice wave packet are obtained. The wave packet behaves as a "breather"; its expected position and the variance of the associated probability distribution oscillate in phase with equal amplitudes.

The perturbation theoretic approach is used in Sec. III to solve for the δ-function lattice propagator $\mathbf{K}_\delta(t)$. In heat propagator form, $\mathbf{K}_\delta(t)$ is related by a Lyapunov transformation $e^{-\mathbf{V}_F}\mathbf{K}_\delta(t)$ to the solution of the lattice Smoluchowski equation with the classical potential $V_{F_{nn}}=\lambda|n|$. The same correspondence between the quantum δ-function field and classical cusp potential occurs on the continuum [7]. In the discrete-time version of the lattice Smoluchowski picture, the attractive quantum δ-

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function field maps to a Markov process in which a particle carries out a nonsymmetric random walk biased toward the force center at cell 0. On reaching cell 0, there are equal probabilities p of hopping right or left and probability $1-2p$ of remaining in place. The interaction term in the δ-function heat propagator reflects this Markov structure. In the repulsive case, the interaction term can be represented as a Poisson weighted superposition of nonsymmetric random walks. To check that the discretization used here gives rise to a physically consistent theory, it is shown that the propagators under study properly reduce to the known continuum forms. The interplay exhibited here among an underlying Lie symmetry, a Poisson point process, and a random walk is expected on general grounds [8].

Notation and tools. In the argument to follow, use is made of the known lattice propagators that describe the symmetric random walk

$$K_{0kj}(t)=(e^{(\mathbf{Q}-\mathbf{I})t})_{kj}=e^{-t}I_{k-j}(t) \tag{1.3a}$$

and the free quantum lattice particle

$$K_{0kj}=(-it)=e^{it}e^{i\pi(k-j)/2}J_{k-j}(t)\ . \tag{1.3b}$$

In (1.3), $J_n(t)$ is the ordinary Bessel function and $I_n(t)$ the modified Bessel function of imaginary argument, each of integer order n. The propagators (1.3) are the general classical and quantum solutions of (1.1) for $\mathbf{V}=\mathbf{0}$. Given an arbitrary initial lattice state $\boldsymbol{\varphi}(0)$, the state at time t is the vectorial product $\boldsymbol{\varphi}(t)=\mathbf{K}_0(t)\boldsymbol{\varphi}(0)$.

The random walk solution (1.3a) follows directly from the differential recursion relation $I_n'(z)=\frac{1}{2}[I_{n+1}(z)+I_{n-1}(z)]$. In vectorial form

$$\mathbf{W}'(z)=\mathbf{Q}\mathbf{W}(z)\ , \tag{1.4a}$$

where $\mathbf{W}(z)$ is an infinite vector with components $W_n=I_n(z)$. From (1.4a), we have the matrix generating function $[\exp(\mathbf{Q}t)]_{kn}=I_{k-n}(t)$, and (1.3a) follows. Probability conservation $\sum_{k=-\infty}^{\infty}K_{0kj}(t)=1$ is guaranteed by $e^{-z}\sum_{k=-\infty}^{\infty}I_k(z)=1$.

In the quantum case (1.3b), the analogous relations are $J_n'(z)=\frac{1}{2}[J_{n-1}(z)-J_{n+1}(z)]$, or, defining the vector $Y_n=J_n(z)$,

$$\mathbf{Y}'(z)=\mathbf{Q}^*\mathbf{Y}(z)\ . \tag{1.4b}$$

Quantum probability conservation is enforced by the unitarity condition $\mathbf{K}_0^\dagger\mathbf{K}_0=\mathbf{I}$, which follows from the Bessel sum $\sum_{k=-\infty}^{\infty}J_k^2(z)=1$. In (1.4b),

$$\mathbf{Q}^*=\frac{1}{2}\begin{bmatrix} \cdots & \cdots & & & & \\ \cdots & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & -1 & 0 & 1 & \\ & & & -1 & 0 & \cdots \\ & & & & \cdots & \cdots \end{bmatrix}, \tag{1.5}$$

the generator of ordinary Bessel functions via $[\exp(\mathbf{Q}^*t)]_{kn}=J_{n-k}(t)$.

In the presence of an interaction $\mathbf{V}$, the symmetric random walk generated by (1.3a) is desymmetrized. In general, the perturbed propagator incorporates the generator

$$\mathbf{R}_t(p)=e^{[\mathbf{Q}-(1-2p)\mathbf{Q}^*-\mathbf{I}]t}\ , \tag{1.6}$$

in which $\mathbf{Q}$ in (1.3a) is replaced by the transition matrix

$$\mathbf{Q}-(1-2p)\mathbf{Q}^*=\begin{bmatrix} \cdots & \cdots & & & & \\ \cdots & 0 & p & & & \\ & 1-p & 0 & p & & \\ & & 1-p & 0 & p & \\ & & & 1-p & 0 & \cdots \\ & & & & \cdots & \cdots \end{bmatrix} \tag{1.7}$$

of the doubly infinite, nonsymmetric random walk with step probabilities $(p,1-p)$. In the continuum limit, (1.3a) becomes the $d=1$ heat propagator denoted by

$$G_0(x-y;t)=\frac{e^{-(x-y)^2/2t}}{\sqrt{2\pi t}}\ . \tag{1.8}$$

The argument to follow also uses the free-particle energy Green's function

$$\tilde{K}_{0ij}(k)=\int_0^\infty K_{0ij}(t)e^{-kt}dt=\frac{e^{-|i-j|u}}{\sinh u}\ , \tag{1.9}$$

where $\cosh u=k+1$.

II. UNIFORM FIELD

For the constant field case, take the potential $\mathbf{V}=-\lambda\mathbf{Z}$, with interaction matrix

$$\mathbf{Z}=\begin{bmatrix} \cdots & & & & & & \\ & -2 & & & & & \\ & & -1 & & & & \\ & & & 0 & & & \\ & & & & 1 & & \\ & & & & & 2 & \\ & & & & & & \cdots \end{bmatrix}. \tag{2.1}$$

With the choice of interaction (2.1), the Schrödinger equation $\dot{\boldsymbol{\varphi}}=(\mathbf{Q}-\mathbf{I}+\lambda\mathbf{Z})\boldsymbol{\varphi}$ may be interpreted as describing a particle moving in a left-directed, homogeneous field under the influence of the periodic potential created by the lattice. In the continuum limit, it is known that the constant-field propagator factorizes into a free-particle contribution and a field dependent phase factor that can be interpreted as playing the role of a gauge transformation [9]. Here, we will derive a disentangled expression for $\mathbf{K}_z=\exp(\mathbf{Q}-\mathbf{I}+\lambda\mathbf{Z})t$ that exhibits an analogous factorization on the lattice. It will be shown that with this factorization the external field is encoded in the propagator as a pair of identical hyperbolic rotations, $\exp[\lambda\mathbf{Z}t/2]$, operating on a $(1+1)$ lattice defined by all possible initial and final positions.

The point of the calculation is to evaluate $\exp[(\lambda\mathbf{Z}+\mathbf{Q})t]$ in terms of a product of exponential operators involving $\mathbf{Z}$ and $\mathbf{Q}$ alone. The final result can be derived in two ways: (i) make the strong coupling Lyapunov transformation $\mathbf{K}'=e^{-\lambda t\mathbf{Z}}\mathbf{K}_z$, eliminate the interaction term $\lambda\mathbf{Z}$ from the lattice Hamiltonian $\mathbf{H}=\mathbf{Q}-\mathbf{I}+\lambda\mathbf{Z}$, integrate the time ordered product, and obtain a closed form for the resulting matrix sum, (ii) use the Lie algebraic properties of $\mathbf{H}$ to express $\mathbf{K}_z$ as a product of exponential operators with coefficients $f_i(t)$, and fix the $f_i(t)$ by using the lattice Schrödinger equation (1.1). In parallel with Lie algebraic calculations of path integrals [10], method (ii) is used in this section.

The operators $[\mathbf{Q},\mathbf{Z}]$ in $\mathbf{K}_z$ generate the Lie algebra iso(1,1), which generates in turn the group ISO(1,1) of translations and rotations in the pseudo-Euclidean plane [11]. The iso(1,1) structures emerges if one commutes (1.2) and (2.1) and continues to closure, obtaining the commutation relations

$$[\mathbf{Q},\mathbf{Z}]=\mathbf{Q}^*,[\mathbf{Q}^*,\mathbf{Z}]=\mathbf{Q},[\mathbf{Q},\mathbf{Q}^*]=\mathbf{0}\ . \tag{2.2}$$

The finiteness of the algebra (2.2) allows a closed form solution for the propagator $\mathbf{K}_z$. Let the evolution matrix $\mathbf{M}$ of an infinite linear system $\dot{\mathbf{V}}=\mathbf{M}\mathbf{V}$ be a linear combination of generators $\{\mathbf{G}_i\}$ of a finite Lie algebra $\mathcal{L}$. Then it is known that the fundamental matrix $\mathbf{K}=\exp(\mathbf{M}t)$ that embodies the general solution of $\dot{\mathbf{V}}=\mathbf{M}\mathbf{V}$ may be expressed as a finite product $\mathbf{K}=\prod_i\exp[f_i(t)\mathbf{G}_i]$. The scalar coefficients $f_i(t)$ in general satisfy a set of coupled nonlinear differential equations whose structure is fixed by the commutation relations of the $\mathbf{G}_i$ [12].

Factorization of $\mathbf{K}(t)$ succeeds when the Hamiltonian generates a finite Lie algebra such as (2.2) because the Baker-Hausdorff expansions implicit in $\exp[(\mathbf{Q}-\mathbf{I}-\mathbf{V})t]$ then terminate. In particular, the commutation relations (2.2) imply

$$e^{-\lambda\mathbf{Z}t/2}\mathbf{Q}e^{\lambda\mathbf{Z}t/2}=\cosh(\lambda t/2)\mathbf{Q}+\sinh(\lambda t/2)\mathbf{Q}^*\ , \tag{2.3a}$$

$$e^{f\mathbf{Q}}\mathbf{Z}e^{-f\mathbf{Q}}=\mathbf{Z}+f\mathbf{Q}^*\ , \tag{2.3b}$$

and a further pair of relations in which $\mathbf{Q}$ and $\mathbf{Q}^*$ are interchanged. For the special case $f=1/\lambda$, we have

$$(\mathbf{Q}+\lambda\mathbf{Z})e^{\mathbf{Q}^*/\lambda}=\lambda e^{\mathbf{Q}^*/\lambda}\mathbf{Z}\ , \tag{2.3c}$$

so that $(e^{\mathbf{Q}^*/\lambda})_{kn}=(-1)^{k-n}J_{k-n}(1/\lambda)$ is the nth Schrödinger eigenvector, with eigenvalue $E_n=\lambda n$.

For an easy transition to the continuum case it is helpful to order the exponential operators in the constant-field propagator as

$$\mathbf{K}_z=e^{-t}e^{\lambda\mathbf{Z}t/2}e^{f(t)\mathbf{Q}}e^{\lambda\mathbf{Z}t/2}\ , \tag{2.4}$$

where the function $f(t)$ remains to be determined. The symmetric placement of $\mathbf{Z}$ in (2.4) and the parametrization $\lambda t/2$ are chosen to match the symmetric factor $\exp[\lambda t(x+x')/2]$ in the Feynman constant-field propagator for the continuum [13]. The generator $\mathbf{Q}^*$ is not included in (2.4) because $\exp(\mathbf{Q}^*t)$ is a matrix of oscillatory Bessel functions $J_n(t)$, and given a constant field, symmetric ordering, and imaginary time, one expects no oscillatory factors in $\mathbf{K}_z$.

The ansatz (2.4) is readily checked by solving for the function $f(t)$. Use (2.3a), (2.3b), and (2.4) to obtain the time derivative

$$\dot{\mathbf{K}}_z=[\lambda\mathbf{Z}-\mathbf{I}+g_1(t)\mathbf{Q}+g_2(t)\mathbf{Q}^*]\mathbf{K}_z\ , \tag{2.5}$$

where

$$g_1(t)=\dot{f}(t)\cosh(\lambda t/2)-\tfrac{1}{2}\lambda f(t)\sinh(\lambda t/2)\ , \tag{2.6a}$$

$$g_2(t)=-\dot{f}(t)\sinh(\lambda t/2)+\tfrac{1}{2}\lambda f(t)\cosh(\lambda t/2)\ . \tag{2.6b}$$

From (2.5) and (1.1), $\mathbf{K}_z$ is the correct lattice propagator if $f(t)$ is such that $g_1(t)=1$ and $g_2(t)=0$. From (2.6), these conditions are satisfied uniquely by $f(t)=(2/\lambda)\sinh(\lambda t/2)$. Accordingly, the constant-field lattice propagator takes the form

$$K_{zij}=\{e^{\lambda\mathbf{Z}t/2}\mathbf{K}_0\left[\frac{2}{\lambda}\sinh(\lambda t/2)\right]e^{\lambda\mathbf{Z}t/2}\}_{ij}$$
$$=e^{-t}e^{\lambda t(i+j)/2}\mathbf{I}_{i-j}\left[\frac{\sinh(\lambda t/2)}{\lambda/2}\right]\ . \tag{2.7}$$

The nonlinear time transformation $t\to(2/\lambda)\sinh(\lambda t/2)$ in the argument of the free-particle propagator in (2.7) arises from the bidirectional random walk incorporated in $\mathbf{H}=\mathbf{Q}-\mathbf{I}+\lambda\mathbf{Z}$ when one uses the transform $\exp(-\lambda t\mathbf{Z})\mathbf{H}\exp(\lambda t\mathbf{Z})$ to eliminate the interaction term $\lambda\mathbf{Z}$. An analogous nonlinear time transformation occurs in random sequential adsorption (RSA), where the analog of a random walk in a uniform lattice field is random dimer filling of a $d=1$ lattice in the cumulative probability representation [14]. In the RSA process the underlying space is semi-infinite, the stochastic process is unidirectional, and the associated nonlinear time transformation is $t\to e^{-t}$. An application of (2.7) in its real-time quantum form follows below.

Continuum limit. It is straightforward to derive the continuum propagator from (2.7) by making the replacements $\lambda\to\lambda\Delta^3$, $t\to t/\Delta^2$, $(i,j)\to(x,x')/\Delta^2$, and computing terms that survive for $\Delta\to0$. Observe first that the argument of the exponential factor in (2.7) is $O(\Delta^0)$ in the lattice spacing and so gives directly $\exp[\lambda t(x+x')/2]$. To evaluate the Bessel function $I_{(x-x')/\Delta}((2/\lambda\Delta^2)\sinh(\Delta\lambda t/2))$ for $\Delta\to0$, we require the standard asymptotic result

$$I_n(z)\underset{\mathrm{Re}\,z\to\infty}{\sim}\frac{e^z}{\sqrt{2\pi z}}\sum_{k=0}^{\infty}\frac{(-1)^k}{(2z)^k k!}(n^2-\tfrac{1}{4})(n^2-\tfrac{9}{4})\cdots[n^2-(2k-1)^2/4]\ . \tag{2.8}$$

For this application $z \gg n \gg 1$, and we have the Gaussian limit $e^{-z}I_n(z) \sim [2\pi z]^{-1/2}\exp(-n^2/2z)$, where $n=(x-x')/\Delta$ and $z=t/\Delta^2+\lambda^2 t^3/24+O(\Delta^2)$. To $O(\Delta^0)$, (2.7) and (2.8) then give, omitting an overall normalization factor Δ,

$$\lim_{\Delta\to 0}(K_z)_{x'/\Delta,x/\Delta} = G_0(x-x';t)\exp\left[\frac{\lambda t(x+x')}{2}+\frac{\lambda^2 t^3}{24}\right], \qquad (2.9)$$

which matches the Feynman quantum propagator for $t \to -it$. Analogous arguments based on iso$(1,k)$ may be helpful in characterizing the dynamics of fully discretized $(1+k)$ lattices [15].

Dynamics on the quantum lattice: Wannier-Stark localization. From (2.7) the uniform-field quantum lattice propagator is

$$K_{zkj}(-it)=e^{it}e^{-i\lambda t(k+j)/2}e^{i\pi(k-j)/2}J_{k-j}\left[\frac{\sin(\lambda/2)}{\lambda/2}\right]. \qquad (2.10)$$

Equation (2.10) gives the exact general solution of the discrete lattice variant of the Wannier-Stark problem in which an electron moves in a periodic potential under the additional influence of an external homogeneous electric field [16]. From (2.3c), the energy spectrum implicit in (2.10) is the well-known Stark ladder

$$E_n=\lambda n, \qquad (2.11a)$$

and we may choose phase factors such that the (normalized) lattice eigenvectors take the Toeplitz form

$$\varphi_k^n=J_{n-k}(1/\lambda). \qquad (2.11b)$$

Relations (2.11) also follow from the recursion relation for cylinder functions

$$z\mathbf{Q}\mathbf{Y}(z)=\mathbf{Z}\mathbf{Y}(z) \qquad (2.12)$$

[cf. the definition preceding (1.4b)] or from the requirement that the eigenvectors and spectrum of the infinite linear system

$$(\mathbf{Q}+\lambda\mathbf{Z})\varphi^n=E_n\varphi^n \qquad (2.13)$$

be the smooth limit as $N\to\infty$ of the eigenvectors and spectrum of the finite system with the same form in which $\mathbf{Q}$ and $\mathbf{Z}$ are taken to be $N\times N$.

The results (2.11) match those of the exact one-band calculation for Wannier electrons [17] and also the analogous conclusions from the one-band treatment of the $d=3$ perfect crystal in a homogeneous external field [18]. In particular, (2.11b) is the basis for the known result that a Wannier-Stark particle in ladder state n is localized about cell n, with a spatial extension of order $1/\lambda$.

The exact propagator (2.10) enables us to explore the time behavior of the Wannier-Stark localization analytically. To do so, we shall propagate the zero-momentum lattice wave packet

$$\psi_k(0)=\frac{1}{\sqrt{2N+1}}, \quad -N\le k\le N, \qquad (2.14)$$

which corresponds to an initial uniform distribution centered on lattice site 0 with spatial width $2N+1$ and variance $\frac{1}{3}N(N+1)$. Writing out $\boldsymbol{\psi}(t)=\mathbf{K}_z\boldsymbol{\psi}(0)$, we see that the nth moment of the probability density vector is

$$X_n(t)=\frac{1}{2N+1}\sum_{k=-\infty}^{\infty}k^n\psi_k^*(t)\psi_k(t) =\frac{1}{2N+1}\times\sum_{k=-\infty}^{\infty}k^n\sum_{p=k-N}^{k+N}\sum_{q=k-N}^{k+N}J_p(z)J_q(z)e^{i\xi(p-q)/2}, \qquad (2.15)$$

where $\xi\equiv\lambda t+\pi$ and $z\equiv\sin(\lambda t/2)/(\lambda/2)$. Dropping the noncontributing imaginary parts, reordering the summations, and using the symmetry of the summands, (2.15) becomes

$$X_n(t)=\frac{1}{2N+1}\left\{\sum_{n=-\infty}^{\infty}J_p^2(z)S_n(2N,p-N)+\sum_{l=1}^{2N}\cos\left[\frac{\xi l}{2}\right]\sum_{p=-\infty}^{\infty}J_p(z)J_{p+l}(z)[S_n(2N-l,p+l-N)+S_n(2N-l,p-N)]\right\}, \qquad (2.16)$$

where

$$S_n(K,L)=\sum_{k=0}^{K}(k+L)^n. \qquad (2.17)$$

To evaluate the time behavior of the expected position and spatial extension of the packet, we first carry out the sums

$$S_1(K,L)=(K+1)(K/2+L), \qquad (2.18a)$$

$$S_2(K,L)=(K+1)[L(K+L)+\tfrac{1}{6}K(2K+1)]. \qquad (2.18b)$$

Using (2.18), (2.16) gives

$$X_1(t)=\sum_{-\infty}^{\infty} pJ_p^2(z)+\frac{2N}{2N+1}\cos\left[\frac{\xi}{2}\right]\sum_{p=-\infty}^{\infty} pJ_p(z)J_{p+1}(z)\ , \tag{2.19a}$$

$$X_2(t)=\tfrac{1}{3}N(N+1)+\sum_{p=-\infty}^{\infty} pJ_p^2(z)+\frac{2}{2N+1}\sum_{l=1}^{2}(2N-l+1)\cos\left[\frac{\xi l}{2}\right]\sum_{p=-\infty}^{\infty} p^2J_p(z)J_{p+l}(z)\ . \tag{2.19b}$$

The identities $\cos(\xi)=-\cos(\lambda t)$ and $\cos(\xi/2)=-\sin^2(\lambda t)$ and the Bessel moments following from the Graf addition theorem [19],

$$\sum_{p=-\infty}^{\infty} J_p(z)J_{p+n}(z)=\delta_{n0}\ , \tag{2.20a}$$

$$\sum_{p=-\infty}^{\infty} pJ_p(z)J_{p+n}(z)=\frac{z}{2}[\delta_{n1}+\delta_{n,-1}]\ , \tag{2.20b}$$

$$\sum_{p=-\infty}^{\infty} p^2J_p(z)J_{p+n}(z)=\frac{z^2}{4}[\delta_{n2}+2\delta_{n0}+\delta_{n,-2}]-\frac{z}{2}[\delta_{n1}-\delta_{n,-1}]\ , \tag{2.20c}$$

then give

$$X_1(t)=-\frac{2N}{2N+1}\frac{1-\cos(\lambda t)}{\lambda}\ , \tag{2.21a}$$

$$X_2(t)=\tfrac{1}{3}N(N+1)-X_1(t)+\frac{4N^2-1}{4N^2}X_1^2(t)+\frac{4\sin^2(\lambda t/2)}{\lambda^2(2N+1)}\ . \tag{2.21b}$$

If we fix λ and drop terms of $O(1/N)$, the variance of the distribution becomes

$$X_2(t)-X_1^2(t)\cong X_2(0)-X_1(t)\ . \tag{2.21c}$$

By inspection of (2.21a), the limits of small t and small coupling λ, as well as the continuum limit, all yield the classical path $X_1\cong-\lambda t^2/2$ for sufficiently large N. Equations (2.21a) and (2.21c) show that the wave packet behaves as a "breather"; its position and spatial extension oscillate with equal phase and amplitude. The motion is increasingly localized as the field strength increases. On differentiating (2.21a) one obtains an expected velocity proportional to $\sin(\lambda t)$, consistent with the known result that Wannier-Stark particles carry no current. On differentiating (2.21a) twice, the equation of motion

$$\ddot{X}_1(t)=\lambda\left[\frac{2N}{2N+1}-\lambda X_1(t)\right] \tag{2.22}$$

follows, showing that the Wannier-Stark wave packet performs classical motion subject to the combined effects of the imposed uniform field and the induced harmonic response, $-\lambda^2X_1$, resulting from the periodicity of the lattice.

These results generalize easily to systems in which an arbitrary number of finite size hops is allowed. In particular, consider the Hamiltonian

$$\mathbf{H}=\sum_{j=1}^{L}\alpha_j\mathbf{Q}_j-\mathbf{I}+\lambda\mathbf{Z}\ , \tag{2.23}$$

where the α_j are real coefficients such that $\sum\alpha_j=1$, and $\mathbf{Q}_j$ is the Toeplitz matrix with $\frac{1}{2}$ on the jth super- and subdiagonals and zeros everywhere else. Then the propagator

$$e^{it}e^{-i\lambda t\mathbf{Z}/2}\exp\left[-\frac{2i}{\lambda}\sum_{j=1}^{L}\frac{\alpha_j}{j}\mathbf{Q}_j\sin(j\lambda t/2)\right]e^{-i\lambda t\mathbf{Z}/2} \tag{2.24}$$

solves the discrete lattice problem equivalent to the one-band continuum problem with a periodic potential characterized by the dispersion relation $E(k)=\sum_{j=1}^{L}\alpha_j\cos(jk\Delta)$ (cf. [17]). In this case, the underlying Lie algebra is the L-fold direct sum $\mathrm{iso}(1,1)\oplus\mathrm{iso}(1,1)\oplus\cdots\oplus\mathrm{iso}(1,1)$. The spectrum remains the Stark ladder (2.11a). Further generalization to two-band systems in which odd and even lattice sites have different interaction energies requires consideration of infinite-dimensional Lie algebras.

III. δ-FUNCTION INTERACTION

For the discrete δ-function potential, take $\mathbf{V}_S=-\lambda\boldsymbol{\delta}$, where

$$\boldsymbol{\delta}=\begin{bmatrix}\ddots & & & & & \\ & 0 & & & & \\ & & 0 & & & \\ & & & 1 & & \\ & & & & 0 & \\ & & & & & 0 \\ & & & & & & \ddots\end{bmatrix}\ , \tag{3.1}$$

and the subscript S distinguishes the Schrödinger field $\mathbf{V}_S$ from the Smoluchowski-Fokker-Planck field $\mathbf{V}_F$ introduced below. The propagation problem with the field $-\lambda\boldsymbol{\delta}$ can be interpreted either as a discrete version of the quantum dynamics problem for a particle moving in a periodic potential under the additional influence of a δ function at position 0, or as a classical-stochastic problem in which the δ-function field is the zero-range image of an extended, as yet unspecified lattice potential $\mathbf{V}_F$ under a Lyapunov transformation of the associated classical system. The classical case is discussed here. It will be shown that the implied discrete-time evolution matrix generates a Markov process incorporating two nonsymmetric random walks on the right and left half axes, coupled at cell 0 by a partly reflecting, partly transmitting, sticky barrier.

In general, the imaginary-time lattice Schrödinger equation

$$\dot{\mathbf{K}}=(\mathbf{Q}-\mathbf{I}-\mathbf{V}_S)\mathbf{K} \tag{3.2}$$

does not define a physically feasible process because probability is not conserved in the presence of a nontrivial potential $\mathbf{V}_S$. However, by analogy with the relation between the imaginary-time continuum Schrödinger equation and the Smoluchowski equation on the continuum [7], one can show that probability conservation can be implemented by imposing the Lyapunov transformation $\mathbf{P}=e^{-\mathbf{V}_F}\mathbf{K}\equiv\mathbf{UK}$ in (3.2) and fixing $\mathbf{V}_F$ by variation of parameters. Explicitly, under this transformation (3.2) takes the form

$$\dot{\mathbf{P}}=(\mathbf{UQU}^{-1}-\mathbf{I}-\mathbf{V}_S)\mathbf{P}\ . \tag{3.3}$$

From (3.3), a suitable classical field $\mathbf{V}_F$ must be such that

$$\mathbf{UQU}^{-1}-\mathbf{V}_S=E\mathbf{M}\ , \tag{3.4}$$

where the discrete-time piece of the transformed evolution operator is proportional to a stochastic matrix $\mathbf{M}$, with $1\geq M_{ij}\geq 0$ and $\sum_i M_{ij}=1$. In particular, (3.4) gives

$$EM_{ii}=-V_{Sii}\ , \tag{3.5a}$$

$$EM_{i\pm1,t}=\tfrac{1}{2}U_{ii}^{-1}U_{i\pm1,i\pm1}\ . \tag{3.5b}$$

From (3.5) and probability conservation $\sum_i M_{ij}=1$, it follows that $1>-V_{Sii}/\mathbf{E}>0$ and

$$(\mathbf{Q}-\mathbf{V}_S)\mathbf{u}-E\mathbf{u}, \tag{3.6}$$

a form of the time-independent lattice Schrödinger equation, where $u_n=CU_{nn}$ and C is a normalization constant. Given that $\mathbf{V}_F$ is real and local, Eq. (3.6) implies that the diagonal elements of $\mathbf{U}=\exp(-\mathbf{V}_F)$ can be identified with the components of any Schrödinger (lattice) eigenfunction $\mathbf{u}$ with consistently signed components $u_iu_j>0$. For the discrete δ-function field $-\lambda\boldsymbol{\delta}$, an appropriate solution of (3.6) is therefore given by the quantum state with energy $E=\sqrt{1+\lambda^2}$ and (unnormalized) wave function

$$u_n=(\sqrt{1+\lambda^2}-\lambda)^{|n|}\ . \tag{3.7}$$

Thus, a feasible Smoluchowski field is the cusp potential

$$V_{Fnn}=\ln(\sqrt{1+\lambda^2}-\lambda)|n|\equiv-\rho|n|\ . \tag{3.8}$$

From (3.5) and (3.7), the Markov matrix in (3.4) takes the form

$$\mathbf{M}=\begin{bmatrix} \cdots & \cdots & & & & & \\ \cdots & 0 & p & & & & \\ & 1-p & 0 & p & & & \\ & & 1-p & 1-2p & 1-p & & \\ & & & p & 0 & 1-p & \\ & & & & p & 0 & \cdots \\ & & & & & \cdots & \cdots \end{bmatrix}, \tag{3.9}$$

where

$$p=\frac{\sqrt{1+\lambda^2}-\lambda}{2\sqrt{1+\lambda^2}}\ . \tag{3.10}$$

From (3.9), we see that the discrete Schrödinger δ-function field is mapped in the Smoluchowski picture to a discrete-time Markov process. This process comprises a pair of back to back nonsymmetric random walks coupled at the force center by the rule that a particle at cell 0 moves to the right or left with equal probability p or sticks in place with probability $1-2p$. From (3.9) and (3.10), in the repulsive (attractive) case $\lambda<0$ $(\lambda>0)$, $0<p<\frac{1}{2}$ $(\frac{1}{2}<p<1)$, the coupled walks are both directed outward (inward). The asymptotic equilibrium state associated with (3.9) is given by the doubly infinite probability vector with components $p_n^*=\tanh(\rho)e^{-2|n|\rho}$, $n=\cdots,-2,-1,0,1,2.\ldots$.

The solution of $\dot{\mathbf{K}}_\delta(t)=(\mathbf{Q}-\mathbf{I}+\lambda\boldsymbol{\delta})\mathbf{K}_\delta(t)$ follows immediately from a general property of the evolution equation

$$\dot{\mathbf{K}}=(\mathbf{H}_0+\lambda\mathbf{T})\mathbf{K}\ , \tag{3.11}$$

given time-independent $(\mathbf{H}_0,\mathbf{T})$ and an interaction matrix that factorizes as $\mathbf{T}=\mathbf{W}^2$. In such a case, the Laplace transform of (3.11) reads

$$\begin{aligned}\tilde{\mathbf{K}}&=(\tilde{\mathbf{K}}_0^{-1}-\lambda\mathbf{W}^2)^{-1}\\ &=\tilde{\mathbf{K}}_0+\lambda\tilde{\mathbf{K}}_0\mathbf{W}\mathbf{W}\tilde{\mathbf{K}}_0+\lambda^2\tilde{\mathbf{K}}_0\mathbf{W}\mathbf{W}\tilde{\mathbf{K}}_0\mathbf{W}\mathbf{W}\tilde{\mathbf{K}}_0+\cdots\\ &=\tilde{\mathbf{K}}_0+\lambda\tilde{\mathbf{K}}_0\mathbf{W}(\mathbf{I}-\lambda\mathbf{W}\tilde{\mathbf{K}}_0\mathbf{W})^{-1}\mathbf{W}\tilde{\mathbf{K}}_0\ ,\end{aligned} \tag{3.12}$$

where $\dot{\mathbf{K}}_0=\mathbf{H}_0\mathbf{K}_0$. The identity matrix in (3.12) refers to the sublattice defined by the nonzero elements of $\mathbf{W}\tilde{\mathbf{K}}_0\mathbf{W}$. Equation (3.12) applies, e.g., to idempotent interactions $\mathbf{T}=\mathbf{T}^2$ composed of an arbitrary superposition of equal strength lattice δ functions at different sites and to the oscillator sequence $\mathbf{T}=\mathbf{Z}^{2n}$, $n=1,2,3,\ldots$, of even powers of the uniform field (2.1). Special cases of (3.12) have been derived in treating diffusion in the presence of localized partial traps [5], and a continuum form has recently been used to obtain the δ-function continuum propagators for $d=1,2,3$ [20]. A similar approach applicable to a different class of potentials uses fully summed perturbation series to compute exact propagators for the continuum [21].

The configuration space form of (3.12) can be derived independently by writing $\mathbf{K}(t)$ in Trotter product form. The starting point is the discrete path integral

$$\mathbf{K}(t)=\lim_{N\to\infty}(\mathbf{K}_0(\varepsilon)e^{\varepsilon\mathbf{V}})^N\ ,$$

where $\varepsilon=t/N$. The configuration space evolution operator follows if one keeps leading order terms in ε, so that

$$\mathbf{K}(t)=\lim_{N\to\infty}[\mathbf{K}_0(\varepsilon)(\mathbf{I}+\varepsilon\mathbf{W}^2)]^N\ ,$$

expands in $\varepsilon\mathbf{W}^2$, takes $N\to\infty$, and expresses the result as a sum over products of convolution integrals, one such product for each order in $\varepsilon\mathbf{W}^2$.

In the case at hand, $\mathbf{W}\tilde{\mathbf{K}}_0\mathbf{W}=\delta\tilde{\mathbf{K}}_0\delta$ has only one nonzero element, and the resulting scalar geometric series in (3.12) gives the energy Green's function we seek in the form

$$\tilde{K}_{\delta ij}=\tilde{K}_{0ij}+\lambda\frac{e^{-u(|i|+|j|)}}{\sinh u(\sinh u-\lambda)} . \quad (3.13)$$

In (3.13), the transform (1.4) and definition $\cosh u=k+1$ have been used.

An integral representation for $\mathbf{K}_\delta(t)$ follows from (3.13) if we make the replacement

$$(\sinh u-\lambda)^{-1}=\int_0^\infty e^{-w(\sinh u-\lambda)}dw \quad (3.14)$$

and use the tabulated transform [22]

$$\int_w^\infty \left[\frac{t-w}{t+w}\right]^{n/2} I_n(\sqrt{t^2-w^2})e^{-kt}dt=\frac{e^{-nu-w\sinh u}}{\sinh u} , \quad (3.15)$$

valid for Re $k>1$. Given (3.14) and (3.15), (3.13) yields the representation

$$K_{\delta ij}(t)=K_{0ij}(t)+\lambda e^{-t}\int_0^t e^{\lambda u}\left[\frac{t-u}{t+u}\right]^{(|i|+|j|)/2} \times \mathbf{I}_{|i|+|j|}(\sqrt{t^2-u^2})du . \quad (3.16)$$

An infinite sum over terms with the form of the integrand in (3.16) appears also in the exact Green's function for the second-order, continuum telegraph equation with a partly reflecting boundary [23]. An open question is how to relate in detail the underlying physics of the telegraph equation with partial traps, where the basic equation is known to incorporate a Markov process in which the velocity changes sign at Poisson times [24], with the physics of the combined nonsymmetric lattice walk and Poisson point process discussed here.

The structure $\mathbf{K}_\delta$ emerges more clearly in the form

$$K_{\delta ij}(t)=K_{0ij}(t)+\lambda e^{-t}\int_0^t e^{\lambda u}(e^{tQ-uQ^*})_{0,|i|+|j|}du , \quad (3.17)$$

via the matrix generating function

$$e^{aQ-bQ^*}=\sum_{k=-\infty}^{+\infty}\left[\frac{a-b}{a+b}\right]^{k/2} I_k(\sqrt{a^2-b^2})\mathbf{T}_k . \quad (3.18)$$

The matrices $\mathbf{T}_k$ in (3.18) are the Abelian set of doubly infinite, Toeplitz shift operators, where $k>0$ ($k<0$) labels a Toeplitz matrix $\mathbf{T}_k$ with 1's on the kth super- (sub-) diagonal and zeros elsewhere.

Equations (3.16) and (3.17) show that the lattice propagator shares important features with the corresponding continuum form [25,26]

$$G_\delta(x-y;t)=G_0(x-y;t)+\lambda\int_0^\infty e^{\lambda u}G_0(|x|+|y|+u;t)du . \quad (3.19)$$

In both cases the combinatorial coupling $\lambda e^{\lambda u}$ characterizes the sum over all possible closed loops that begin and end at the force center. Also, on the lattice and the continuum, the dependence $[|i|+|j|,|x|+|y|]$ on the final and initial positions in (3.17) and (3.19) indicates that the path of the propagating particle is decorrelated each time it loops through the force center.

There are also properties of $\mathbf{K}_\delta$ specific to the lattice. In the repulsive case $\lambda\to-\lambda$, a simple transformation of variables allows the second term on the right in (3.17) to be written as a probability integral, so that

$$K_{\delta ij}(t)=K_{0ij}(t)-\int_0^1\left[\mathbf{R}_t\left[\frac{p}{2}\right]\right]_{0,|i|+|j|}\frac{d}{dp}F_t(1-p)dp . \quad (3.20)$$

As anticipated, (3.20) shows that the contribution of the lattice δ-function field to the propagator incorporates a nonsymmetric random walk [cf. (1.6)] over a total distance $|i|+|j|$ from the force center, with step probabilities $(p/2,1-p/2)$. This nonsymmetric walk is averaged over a Poisson process characterized by the probability $F_t(p)=1-e^{-\lambda tp}$ of one or more interactions at the force center in the time interval from 0 to pt, with mean arrival rate λ. The integration over p in (3.20) can also be interpreted as an average over all possible fractional allocations of the total time t among the Poisson loops at the origin and the initial and final random walks from i to 0 and 0 to j, respectively.

Continuum limit. To recover the continuum result, make the replacements $\lambda\to\lambda\Delta$, $t\to t/\Delta^2$, and $(i,j)\to(x,x')/\Delta^2$, in (3.16) and again compute terms that survive for $\Delta\to 0$. We have

$$\lim_{\Delta\to 0}[\mathbf{K}_\delta(t)-\mathbf{K}_0(t)]_{x'/\Delta,x/\Delta}=\lambda e^{-t/\Delta^2}\int_0^{t/\Delta^2}e^{\lambda u-[(|x'|+|x|)u/t]+O(\Delta^2)}I_{(|x'|+|x|)/\Delta}\times\left[\frac{t}{\Delta^2}\left[1-\frac{u^2\Delta^2}{2t^2}\right]+O(\Delta^2)\right]du , \quad (3.21)$$

from which, by (2.8), the continuum result (3.19) follows.

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[1] A reasonably thorough search of the literature has revealed no solutions of the time-dependent lattice Schrödinger equation for the uniform-field and δ-function potentials treated here. For specific probability-conserving choices of the coupling strength of the interaction **V**, general solutions of (1.1) for semi-infinite and finite lattices can be taken over directly from the theory of single-server queues **M/M**/1/*N*, with Poisson arrival and service times. There are also several complete sets of known eigensolutions of the time-dependent lattice Schrödinger equation

$$\Psi(n+1)+\Psi(n-1)-2\Psi(n)-V(n)\Psi(n)=-E\Psi(n) ,$$

for the cusp potential $V_n=\lambda|n|$, the linear harmonic oscillator, and the Coulomb potential on the half-lattice. See, respectively, J.-P. Gallinar and D. C. Mattis, J. Phys. A. **18**, 2583 (1985); E. Chalbaud, J.-P. Gallinar, and G. Mata, J. Phys. A **19**, L385 (1986); A. A. Kvitsinsky, *ibid.* **25**, 65 (1992). The cusp and oscillator problems fall into the class discussed here. But closed form lattice propagators corresponding to these solutions are as yet unknown, and they are not treated here. The singular Coulomb lattice field raises problems beyond the scope of this paper.

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[7] On the continuum, it is well known that the correction factor $\varphi^0(x)=e^{-\mathbf{V}_F(x)}$ transforms the imaginary-time Schrödinger propagator K into the probability conserving solution $P=\varphi^0(x)K$ of Smoluchowski's form of the Fokker-Planck equation $P_t=(V_{Fx}P)_x+P_{xx}$. Here, φ^0 is the ground state quantum wave function, and V_F is a C_2 potential function that is related to the Schrödinger field by the Ricatti equation $\mathbf{V}_F''(x)-\mathbf{V}_F'^2(x)=-\mathbf{V}_S(x)$. This relation appears here in the lattice form (3.4). See, e.g., H. Risken, *The Fokker-Planck Equation* (Springer, Berlin, 1984), Chap. 5. For a discussion of discrete-space techniques for solving infinite tridiagonal systems of the type considered here, see H. Risken, *ibid.*, Chap. 9.

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[15] Consider, for example, the closely related case of a random walk on a rectangular $(1+1)$ space-time lattice with mesh sizes (Δ_x,Δ_t) and a fixed correlation between forward and backward time steps. This model has applications to hydrodynamics [P. Rosenau, Phys. Rev. E **48**, R655 (1993)] and to cellular automata [T. Toffoli, in *Complexity, Entropy, and the Physics of Information,* edited by W. Zurek (Addision-Wesley, Redwood City, CA, 1990), p. 301]. Using the notation introduced here, the dynamics are governed by the double-lattice telegraph equation

$$[\mathbf{Q}_t\otimes\mathbf{I}_x-\mathbf{Q}_x\otimes\mathbf{I}_t+(1-\lambda\Delta_t/2)^{-1}(\lambda\Delta_t/2)\mathbf{Q}_t^*\otimes\mathbf{I}_x]\psi=\mathbf{0} ,$$

where $\psi\equiv\psi_{ij}$ is a second-rank tensor whose indices specify (x,t) lattice coordinates, and the convention is that a generator $\mathbf{A}_q$ operates on the q dimension only. This is a case of the general principle that dynamical lattice equations incorporate the continuous symmetry of the associated continuum forms. See A. Chodos and J. Healy, Phys. Rev. D **16**, 387 (1977). The band structure arising from the lattice emerges easily if one performs a Lyapunov transformation $\psi\rightarrow e^{-\alpha\mathbf{Z}_t}\chi$, with $\exp(2\alpha)=1-\lambda\Delta_t$, which induces a hyperbolic rotation of the form (2.3a). Applying $e^{-\alpha\mathbf{Z}_t}\cdots e^{\alpha\mathbf{Z}_t}$, the field Q_t^* is transformed away, and we obtain a form of the double-lattice Klein-Gordon equation

$$[\mathbf{Q}_t\otimes I_x-\cosh(\alpha)\mathbf{Q}_x\otimes\mathbf{I}_t]\chi=\mathbf{0} ,$$

from which a discrete Fourier transform yields the band structure $\cosh\alpha\cos k_x=\cos k_t$. Here (k_x,k_t) are the transform variables corresponding to the lattice coordinates. I thank T. Toffoli for a helpful discussion of his work.

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