# One-dimensional quantum random walk for fermions and bosons

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With the help of quantum-scattering-theory methods and the approximation of the stationary phase, we propose a one-dimensional quantum-random-walk (QRW) model, which describes for both tunneling and scattering above the potential, the coherent diffusion of independent particles described by wave packets in a periodic one-dimensional lattice. The QRW model describes for each lattice cell the time evolution of modulating amplitudes of two opposite-moving wave packets as they are scattered by periodic potential barriers. Since the QRW model is a coherent process, interference contributions in the probabilities bring about strong departures from classical results. For many identical free particles we obtain the theoretical and graphical Bose and Fermi two-body QRW probability distribution. The result is generalized to $N$ identical free particles and we obtain the $N$-body Bose and Fermi QRW probability distribution.

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## I. INTRODUCTION

Tunneling diffusion for mesoscopic materials has been studied extensively [1]. The diffusion coefficient in a system of noninteracting electrons, which was first found by Landauer [2], has been indirectly studied by several authors. In particular, since diffusion and conductivity are connected by the Einstein relation, the Landauer conductivity has been a fertile ground to *quantum* theoretical calculations [3–5].

It is well known that classical (*incoherent*) random walks have been used as simple mathematical models to study the microscopic theory of diffusion [6,7]. An example of quantum-random-walk theory for a single particle is known in the literature [8]. However, as far as we know, nobody has found a *coherent* random-walk process in position space for a system of identical free particles. The main purpose in this paper is to propose a quantum-random-walk (QRW) model for diffusion of Bose and Fermi free particles in a one-dimensional (1D) periodic lattice. The model is based in the following set of Markovian equations for the *amplitudes* of moving wave packets, which are scattered in a periodic lattice:

$$\begin{bmatrix} B[Ml,N\tau] \\ A[(M+1)l,N\tau] \end{bmatrix} = \begin{bmatrix} \sqrt{R}\,e^{i2kMl} & i\sqrt{T} \\ i\sqrt{T} & \sqrt{R}\,e^{-i2kMl} \end{bmatrix} \times \begin{bmatrix} A[Ml,(N-1)\tau] \\ B[(M+1)l,(N-1)\tau] \end{bmatrix} . \quad (1.1)$$

Here $A(Ml,N\tau)$ and $B(Ml,N\tau)$ are the position- and time-dependent modulating *amplitudes* of two wave packets moving freely in each valley, moving toward the right and left, respectively. With $M$ an integer number $(0,\pm1,\pm2,\ldots)$, $Ml$ denotes the discrete coordinates of any midpoint of a valley in the lattice (lattice constant $l$), and with $N$ a positive integer number, $N\tau$ denotes the *discrete times* at which the centroid of any packet arrives at the coordinates of a midvalley. The parameter $\tau$, called the jump time, is a fixed time associated with the scattering process. Be aware that, in this model, Eq (1.1) describes the amplitudes only at specific discrete coordinates and discrete times. In Eq. (1.1), $R$ and $T$ are the reflection and transmission coefficients of the microscopic potential barriers ($T+R=1$). Depending on the energy of the particle, walk (1.1) describes both a tunneling or scattering above the potential diffusion process in a 1D lattice.

This is a coherent model, with the one-body QRW probability density $P$ at any midvalley, with coordinates $x=Ml$ and time $t=N\tau$ given, respectively, by (for simplicity we will use $l=1$ and $\tau=1$)

$$P(M,N)=|A(M,N)|^2+|B(M,N)|^2 . \quad (1.2)$$

Since $A$ and $B$ are given by the addition of complex numbers, we expect in (1.2) to have interference terms which will produce a strong departure from classical results.

In Secs. II–IV, using the quantum theory of scattering and the approximation of the stationary phase, a heuristic derivation of the above equations will be given. In Sec. V, for some specific initial conditions, we obtain the exact analytic solution for the amplitude equations $A(M,N)$ and $B(M,N)$. In Sec. VI we find that for a system of identical free particles the two-body Bose and Fermi QRW probability distribution is obtained. The result is generalized to the $N$ free-body QRW Bose and Fermi probability distribution.

## II. MICROSCOPIC DIFFUSION OF AMPLITUDES

Let us consider two arbitrary, opposite-moving, plain waves incoming upon a symmetric potential barrier at

 

the origin. This potential barrier may be though of as the boundary between two adjacent cells of lattice constant $l$. In the stationary state for $k \geq 0$, the incoming wave functions are given by

$$\psi_{\pm}^{\text{inc}}(x)=\begin{cases} ae^{+ikx}, & x<0 \\ be^{-ikx}, & x>0, \end{cases} \tag{2.1}$$

where $a$ and $b$ are arbitrary amplitudes. From elementary 1D quantum-scattering theory, the stationary outgoing solutions are given by

$$\psi_{\mp}^{\text{out}}(x)=\begin{cases} [S_{11}(k)a+S_{12}(k)b]e^{-ikx}, & x<0 \\ [S_{21}(k)a+S_{22}(k)b]e^{+ikx}, & x>0. \end{cases} \tag{2.2}$$

Here $S_{ij}(k)$ are the matrix elements of the $2\times 2$ scattering matrix $\mathbb{S}$ of the barrier at the origin.

Assuming the symmetries and invariance properties of (1) conservation of probability, (2) time-reversal invariance, and (3) invariance of the potential barrier under mirror reflections (symmetric about the origin), the $S$ matrix has to be unitary and symmetric, with symmetry $S_{11}=S_{22}$, and $S_{12}=S_{21}$. $\mathbb{S}$ can then be parametrized in the general form [9]

$$\mathbb{S}(k)=e^{i\alpha(k)}\begin{bmatrix} \sqrt{R} & i\sqrt{T} \\ i\sqrt{T} & \sqrt{R} \end{bmatrix}, \tag{2.3}$$

where $T(k)$ and $R(k)$ are the transmission and reflection coefficients, respectively. They satisfy $T+R=1$. The common phase $\alpha(k)$ may be neglected later on in the probability, as we will see in Sec. IV.

The above plane waves (2.1) and (2.2) leave the positions of the particles entirely unspecified. In order to describe a mass transport phenomenon, we need some localization in position. So, instead of plane waves, we choose to describe our diffusion model by localized wave packets which by assumption are scattered only at the cell's boundaries in a 1D lattice.

In the general case, the incoming wave packets are given by

$$\Psi_{\pm}^{\text{inc}}(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(k)e^{-i\omega(k)t}\begin{bmatrix} ae^{+ikx} \\ be^{-ikx} \end{bmatrix} dk, \quad \begin{matrix} x<0 \\ x>0. \end{matrix} \tag{2.4}$$

Here $\omega(k)\equiv\hbar k^2/2m$, and $g(k)$ is an arbitrary peaked function with spreading $\Delta k$, and with the maximum at $k=k_0$ (the average) which is associated with the particle velocities $v_0=\pm\hbar k_0/m$ and energy $\varepsilon_0=\hbar\omega(k_0)$. The incoming packets (2.4), which are valid only for negative times, can be rewritten as

$$\Psi_{\pm}^{\text{inc}}(x,t)=\begin{bmatrix} ae^{+ik_0x} \\ be^{-ik_0x} \end{bmatrix}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(k)e^{-i\omega(k)t}\begin{bmatrix} e^{+i(k-k_0)x} \\ e^{-i(k-k_0)x} \end{bmatrix} dk, \quad \begin{matrix} x<0 \\ x>0, \end{matrix} \tag{2.5}$$

or, in short notation,

$$\Psi_{\pm}^{\text{inc}}(x,t<0)=\begin{cases} ae^{+ik_0x}G(+x,t), & x<0 \\ be^{-ik_0x}G(-x,t), & x>0, \end{cases} \tag{2.6}$$

where we have defined the complex $G$ function as

$$G(x,t)\equiv\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\, g(k)e^{-i\omega(k)t}e^{+i(k-k_0)x}. \tag{2.7}$$

The modulating $G(x,t)$ function depends on the particular form of $g(k)$. It is well known, for example, that if $|g(k)|^2$ is a Gaussian, then $G(x,t)$ is a spreading moving Gaussian [10]. $G(x,t)$ has the property that, if in $k$ space, $|g(k)|^2$ is normalized to 1, then $|G(x,t)|^2$ in $x$ space is also normalized to 1 [Bessel-Parseval relation]. Under time reversal and space reflection $G$ satisfies $G(-x,-t)=G(x,t)^*$.

It is well known in quantum mechanics [10] that for a peaked function $g(k)$, the position of the maximum of the packet [centroid of $G(x,t)$] is well approximated by the requirement of the stationary phase [11] evaluated at $k=k_0$. Using this method of stationary phase for the two incoming waves in Eq. (2.5), we have the two incoming centroids moving according to the relation $x_i=\pm\omega'(k_0)t=\pm\hbar k_0 t/m$ (with $t<0$). If we choose both incoming centroids to be located exactly at the middle of their respective lattice valleys $x_i\equiv\mp l/2$, we have the same initial time $t_i=-lm/2\hbar k_0$. Just there, at the middle of their valleys, the wave functions of the incoming packets are given exactly by

$$\Psi_{\pm}^{\text{inc}}(x,t_i)=\begin{cases} A(x_i<0,t_i)e^{+ik_0x}G(+x,t_i), & x<0 \\ B(x_i>0,t_i)e^{-ik_0x}G(-x,t_i), & x>0, \end{cases} \tag{2.8}$$

where

$$\begin{bmatrix} A(x_i<0,t_i) \\ B(x_i>0,t_i) \end{bmatrix}=\begin{bmatrix} a \\ b \end{bmatrix}. \tag{2.9}$$

Similarly, both outgoing wave packets are given by

$$\Psi_{\mp}^{\text{out}}(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dk\, g(k)e^{-i\omega(k)t}\begin{bmatrix}[aS_{11}(k)+bS_{12}(k)]e^{-ikx} & x<0\\ [aS_{21}(k)+bS_{22}(k)]e^{+ikx} & x>0\end{bmatrix}. \tag{2.10}$$

This integral, valid only for positive times, cannot be done unless an explicit model for the $S$ matrix (or the potential barrier) is given. To avoid this, an approximation will be done. Since $g(k)$ is a sharp-peaked function centered at $k=k_0$, we can proceed to make a Taylor-series expansion of the matrix $\mathbb{S}(k)$ around $k_0$; we write

$$\mathbb{S}(k)=\mathbb{S}(k_0)+\frac{d\mathbb{S}}{dk_0}(k-k_0)+\cdots . \tag{2.11}$$

Next we go one step further in the approximation. Is it possible to make our approximation to zero order? That is, does $\mathbb{S}(k)\simeq\mathbb{S}(k_0)$? This will be true only if

$$|\mathbb{S}(k_0)|\gg|d^n\mathbb{S}/dk_0^n| . \tag{2.12}$$

Certainly, Eq. (2.12) is not true for arbitrary values of $k_0$; however, just looking into any graph of the transmission coefficient $|S_{11}|^2$ vs energy in any particular model [10] will convince us that we can find such points in which Eq. (2.12) holds. Indeed, choosing large values for $k_0$, or points standing about the middle of resonant energies where the transmission coefficient $|S_{11}(k_0)|^2\equiv T(k_0)$ is almost flat, condition (2.12) is well satisfied. Under this smooth varying $S$-matrix condition, and assuming a peaked function $g(k)$, we can approximate the outgoing wave packet (2.10) as

$$\Psi_{\mp}^{\text{out}}(x,t)\simeq\begin{bmatrix}[aS_{11}(k_0)+bS_{12}(k_0)]e^{-ik_0x}\\ [aS_{21}(k_0)+bS_{22}(k_0)]e^{+ik_0x}\end{bmatrix}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}g(k)e^{-i\omega(k)t}e^{\mp i(k-k_0)x}dk\ ,\quad \begin{matrix}x<0\\ x>0\end{matrix}, \tag{2.13}$$

or, in terms of the $G$ function, we have

$$\Psi_{\mp}^{\text{out}}(x,t>0)\simeq\begin{cases}[aS_{11}(k_0)+bS_{12}(k_0)]e^{-ik_0x}G(-x,t)\ , & x<0\\ [aS_{21}(k_0)+bS_{22}(k_0)]e^{+ik_0x}G(+x,t)\ , & x>0 .\end{cases} \tag{2.14}$$

For the outgoing packets, both centroids will arrive at the midvalley positions $x_f=\mp l/2$ at the same time $t_f=+lm/2\hbar k_0=-t_i$ (notice that Wigner's time delay is neglected in this approximation). Therefore the outgoing wave functions at midvalleys will be given by

$$\Psi_{\mp}^{\text{out}}(x,t_f)\simeq\begin{cases}B(x_f<0,t_f)e^{-ik_0x}G(-x,t_f)\ , & x<0\\ A(x_f>0,t_f)e^{+ik_0x}G(+x,t_f)\ , & x>0 .\end{cases} \tag{2.15}$$

According to (2.14), the relation between the new (outgoing) and old (incoming) modulating amplitudes becomes

$$\begin{bmatrix}B(x_f<0,t_f=t_i+\tau)\\ A(x_f>0,t_f=t_i+\tau)\end{bmatrix}=\begin{bmatrix}S_{11}(k_0) & S_{12}(k_0)\\ S_{21}(k_0) & S_{22}(k_0)\end{bmatrix}\begin{bmatrix}A(x_i<0,t_i)\\ B(x_i>0,t_i)\end{bmatrix}, \tag{2.16}$$

where we have defined $\tau$, the jump time, as the time for the round trip $\tau\equiv2|t_i|=l/\omega_0'=lm/\hbar k_0$. Notice that, in this approximation, at each cell the outgoing packets have different amplitudes and directions of motion compared with the incoming packets. However according to (2.15), the outgoing packets have the same form and centroid position (the middle of the valley) as the incoming ones. Thus in turn these outgoing packets will become incoming packets for the next scattering process at the two adjacent barriers, and the whole scattering process repeats itself. A recursive diffusion process will be carried out this way. Equations (2.16) are the basic recursive partial difference equations upon which we will build our quantum-random-walk (QRW) model.

## III. QRW ONE-BODY WAVE FUNCTION

In this section we apply the results of Sec. II to a periodic crystal lattice (Kronig-Penney model), in which free particles described by wave packets move in the potential valleys, and from each valley to the next by quantum tunneling (or scattering above the potential). As in Sec. II, for mathematical simplicity, we have the origin at a potential barrier. In order to discuss our QRW diffusion model for an arbitrary cell, let us denote cell $M$ as the valley bounded by two potential barriers at $(M-1)l$ and $Ml$($M\equiv0,\pm1,\pm2,\ldots$). We also shift the time to $t=N\tau$, such that for arbitrary multiples ($N\equiv0$, 1, 2, . . .) of the jump time $\tau$, the centroids are located at midvalley positions. In this proposed QRW model of diffusion, we generalize the results of Sec. II in such a way that *at every lattice valley $M$* we have both right- and left-moving packets, each of whose wave function at a fixed discrete time $t=N\tau$ is given by

$$\Psi_M(x,N\tau)=[A(Ml,N\tau)e^{+ik_0x} +B(Ml,N\tau)e^{-ik_0x}]G(x,N\tau,M) \quad (3.1)$$

$$\equiv\Psi_M^+(x,N\tau)+\Psi_M^-(x,N\tau) . \quad (3.2)$$

Here the coordinates $(Ml,N\tau)$ denote the cell-position $(Ml)$ and discrete-time $(N\tau)$ dependence of the modulating amplitudes $A$ and $B$ for right- and left-moving packets, respectively.

In this QRW model, by assumption, we neglect more than one cell spreading of the packets. That is, at all times the wave packets are assumed to be bounded to a *single cell.* The function $G(x,N\tau,M)$ is centered at the midvalley $M$, and we assume that $G(x,N\tau,M)\neq 0$, only if $(M-1)l<x<Ml$. Therefore in the QRW model we neglect the time dispersion of the packets beyond a single cell of size $l$. Under this assumption every wave packet has no overlapping to neighboring cells. This assumption limits, for *short times only,* the validity of our solution as a true Schrödinger wave packet. Clearly this prevents us from finding, for long times, the correct stationary solution (Bloch's wave functions).

The normalization requires

$$\int_{\text{cell}M} dx\,|G(x,N,M)|^2=1$$

and

$$\int_{\text{cell}\neq M} dx\,|G(x,N,M)|^2=0 . \quad (3.3)$$

The amplitudes $A$ and $B$ satisfy, for arbitrary lattice valleys $M$ and $M+1$, the same recursive equations (2.16). That is, for a scattering at the potential barrier at $x=Ml$, we have the relations (for simplicity $l=\tau\equiv 1$ from now on)

$$\begin{bmatrix} B[M,N+1] \\ A[M+1,N+1] \end{bmatrix}=\mathbb{S}(k_0,M)\begin{bmatrix} A[M,N] \\ B[M+1,N] \end{bmatrix} . \quad (3.4)$$

Here the right-hand side at time $N$ has incoming amplitudes for right-moving $A(M,N)$ and left-moving $B(M+1,N)$ packets. The left-hand side has the corresponding outgoing amplitudes, one jump time later $N+1$. $\mathbb{S}(k_0,M)$ denotes the $S$ matrix associated with the barrier located at $x=M$. Notice that for the single fact of having the barrier shifted at $x=M$, the $S$ matrix now has the mathematical structure [9]

$$\mathbb{S}(k_0,M)=\mathbb{U}\mathbb{S}(k_0,0)\mathbb{U}^T = \begin{bmatrix} e^{ik_0M} & 0 \\ 0 & e^{-ik_0M} \end{bmatrix} \times\mathbb{S}(k_0,0)\begin{bmatrix} e^{+ik_0M} & 0 \\ 0 & e^{-ik_0M} \end{bmatrix} . \quad (3.5)$$

Therefore the general $S$ matrix located at $x=M$ is parametrized as

$$\mathbb{S}(k_0,M)=e^{i\alpha(k_0)}\begin{bmatrix} \sqrt{R}\,e^{+ik_02M} & i\sqrt{T} \\ i\sqrt{T} & \sqrt{R}\,e^{-ik_02M} \end{bmatrix} . \quad (3.6)$$

Equation (3.4) which *for amplitudes* has the same mathematical structure of a Markovian random-walk process, defines the basic equations of our QRW model.

## IV. ONE-BODY QRW PROBABILITY

We want the conditional, one-body probability of finding a particle at an arbitrary lattice cell $M$. It is conditional because it depends strongly on the initial conditions. Since the packets do not overlap, we can integrate the one-body probability density for a single $\Psi_M(x,N)$ along a cell $M$:

$$P(M,N)\equiv\int_{\text{cell}M}|\Psi_M(x,N)|^2dx = \int_M|\Psi_M^+(x,N)+\Psi_M^-(x,N)|^2dx . \quad (4.1)$$

Substituting from Eq. (3.1), we have

$$P(M,N)=|A(M,N)|^2+|B(M,N)|^2 + \left[\int_M\Psi_M^+(x,N)\Psi_M^-(x,N)^*dx+\text{c.c.}\right] . \quad (4.2)$$

Here the integral is an interference contribution produced by the total superposition, at the same cell $M$, of two packets moving in *opposite* directions. After some elementary integrations the explicit value of this integral is given by

$$\int_M\Psi_M^+(x,N)\Psi_M^-(x,N)^*dx = AB^*\int_M dx\,e^{i2k_0x}|G(x,N,M)|^2 = AB^*\exp(i2\hbar k_0^2t/m)\int_{-\infty}^{\infty}dk\,g(k)g^*(k+2k_0)e^{i\hbar 2k_0kt/m} . \quad (4.3)$$

The last integral has two $g(k)$ functions, $g(k)$ centered at $k_0$ and the other $g(k+2k_0)$ centered at $-k_0$. Since by hypothesis we have a sharp distribution of momenta around $k_0$ so that $\Delta k\ll k_0$, the two $g$ functions do not overlap in $k$ space and the integral is negligible. Two wave packets traveling in opposite directions are orthogonal. The only interference will come from packets superposing in the same valley and traveling in the *same* direction. The final result for (4.2) is that the total probability at each lattice cell is an incoherent superposition of two wave packets moving in opposite directions:

$$P(M,N)=|A(M,N)|^2+|B(M,N)|^2 \equiv P_+(M,N)+P_-(M,N) . \quad (4.4)$$

So far this looks like a classical result. However, notice that according to Eq. (3.4) both $A(M,N)$ and $B(M,N)$ are made of a coherent superposition of two amplitudes, currently traveling in the *same* direction, but evaluated at a previous time. This will produce quantum interference, as we show next. Substituting Eq. (3.4) into Eq. (4.4), we find

$$P_+(M,N)\equiv|A(M,N)|^2 = TP_+(M-1,N-1)+RP_-(M,N-1) + \sqrt{TR}\,[iA(M-1,N-1)B^*(M,N-1) \times e^{+ik_0 2M}+\text{c.c.}] , \quad (4.5a)$$

$$P_-(M,N)\equiv|B(M,N)|^2 = RP_+(M,N-1)+TP_-(M+1,N-1) + \sqrt{TR}\,[iA^*(M,N-1)B(M+1,N-1) \times e^{-ik_0 2(M+1)}+\text{c.c.}] . \quad (4.5b)$$

The existence of these interference terms makes the great difference between classical (incoherent) and quantum (coherent) random processes. Notice that if we arbitrarily neglect the interference terms in Eqs. (4.5), we recover the classical (incoherent) correlated walk equations of Ref. [7], namely

$$P_+(M,N)=TP_+(M-1,N-1)+RP_-(M,N-1) , \quad (4.6a)$$

$$P_-(M,N)=RP_+(M,N-1)+TP_-(M+1,N-1) . \quad (4.6b)$$

From these classical (incoherent) equations, the Landauer diffusion coefficient $D_1=(v_0 l)T/2R$ has been readily derived [7]. However, in Ref. [8] it was proved that if the full interference contributions are taken into account, then we have an additive quantum correction to the diffusion coefficient $D_2=(v_0 l)\sqrt{T/R}$.

## V. ONE-BODY QRW ANALYTIC SOLUTION FOR AN INFINITE LATTICE

The set of finite difference Eqs. (3.4) can, in principle, be solved for any arbitrary set of initial and boundary conditions. For simplicity we take an infinite lattice, and choose an initial single wave packet at arbitrary cell $m$ moving to the right:

$$A(M,N=0)=\delta_{M,m} , \quad B(M,N=0)=0 . \quad (5.1)$$

Given these initial conditions, the solution of Eq. (3.4) is obtained as follows: we first define the characteristic functions $\tilde{A}(s,N)$ and $\tilde{B}(s,N)$ by a finite Fourier transform

$$\begin{bmatrix}\tilde{A}(s,N)\\ \tilde{B}(s,N)\end{bmatrix}\equiv\sum_{M=-\infty}^{\infty} e^{isM}\begin{bmatrix}A(M,N)\\ B(M,N)\end{bmatrix} . \quad (5.2)$$

Neglecting common phases $[\alpha(k)]$ and Fourier transforming Eq. (3.4), we obtain a Markov chain equation

$$\begin{bmatrix}\tilde{A}(s,N)\\ \tilde{B}(s-2k,N)\end{bmatrix}=\begin{bmatrix}i\sqrt{T}e^{is} & \sqrt{R}\\ \sqrt{R}e^{i2k} & i\sqrt{T}e^{-i(s-2k)}\end{bmatrix} \times\begin{bmatrix}\tilde{A}(s,N-1)\\ \tilde{B}(s-2k,N-1)\end{bmatrix} , \quad (5.3)$$

where for simplicity we have dropped the subindex from $k_0$. From now on, every equation which depends on the central momentum of the packet will be denoted just by $k$

Equation (5.3) is a first-order difference equation in variable $N$, and has the formal solution

$$\begin{bmatrix}\tilde{A}(s,N)\\ \tilde{B}(s-2k,N)\end{bmatrix}=\mathbb{P}(s,k)^N\begin{bmatrix}\tilde{A}(s,0)\\ \tilde{B}(s-2k,0)\end{bmatrix} , \quad (5.4)$$

where we have defined the $\mathbb{P}(s,k)$ matrix as

$$\mathbb{P}(s,k)\equiv\begin{bmatrix}i\sqrt{T}e^{is} & \sqrt{R}\\ \sqrt{R}e^{i2k} & i\sqrt{T}e^{-i(s-2k)}\end{bmatrix} . \quad (5.5)$$

Using the standard methods of linear algebra, we obtain

$$\mathbb{P}(s,k)^N=g(s,N)\mathbb{P}(s,k)+g(s,N-1)e^{i2k}\mathbb{I} . \quad (5.6)$$

Here the scalar function $g(s,N)$ is the Green's function of the problem, and is given by

$$g(s,N)\equiv\frac{\lambda_+^N-\lambda_-^N}{\lambda_+-\lambda_-} , \quad (5.7)$$

where $\lambda_+$ and $\lambda_-$ are the unitary eigenvalues of the $\mathbb{P}$ matrix, given by

$$\lambda_\pm=ie^{ik}e^{\mp i\theta(s,k)} \quad \text{with } \tan\theta\equiv\frac{\sqrt{1-T\cos^2(s-k)}}{\sqrt{T}\cos(s-k)} . \quad (5.8)$$

Substituting Eqs. (5.6), (5.7), and (5.1) into Eq. (5.4), we obtain

$$\begin{bmatrix}\tilde{A}(s,N)\\ \tilde{B}(s-2k,N)\end{bmatrix}=g(s,N)\begin{bmatrix}i\sqrt{T}e^{is(m+1)}\\ \sqrt{R}e^{i(2k+sm)}\end{bmatrix} +g(s,N-1)\begin{bmatrix}e^{i(2k+s)}\\ 0\end{bmatrix} . \quad (5.9)$$

Next, taking the inverse Fourier series

$$\mathcal{G}(M,N)=\frac{1}{2\pi}\int_{-\pi}^{\pi}e^{-isM}g(s,N)ds , \quad (5.10)$$

we finally arrive at

$$A(M,N)=i\sqrt{T}\,\mathcal{G}(M-m-1,N)+e^{2ik}\mathcal{G}(M-m,N-1)\ , \tag{5.11a}$$

$$B(M,N)=\sqrt{R}\,e^{2ik(M+1)}\mathcal{G}(M-m,N)\ . \tag{5.11b}$$

In Appendix A we explicitly calculate the Green's function $\mathcal{G}(M,N)$, and the result is given by

$$\mathcal{G}(M,N+1)=i^N e^{i(N-M)k}\sum_{j=0}^{[(N-M)/2]}(-1)^j\left[\sqrt{T}\,\right]^{N-2j}\frac{(N-j)!}{j!\left[\frac{N-M-2j}{2}\right]!\left[\frac{N+M-2j}{2}\right]!}\ . \tag{5.12}$$

This Green's function is different from zero only if the coordinate $M$ has the same parity as $N$.

Finally the one-body QRS probability distribution (4.4) then becomes

$$P(M,N)=T|\mathcal{G}(M-1,N)|^2+R|\mathcal{G}(M,N)|^2+|\mathcal{G}(M,N-1)|^2+\left[i\sqrt{T}e^{-2ik}\mathcal{G}^*(M,N-1)\mathcal{G}(M-1,N)+\text{c.c.}\right]\ . \tag{5.13}$$

In Fig. 1 we show an example of the one-body QRW probability distribution as a function of cell position $M$, and compare it with the classical probability distribution obtained with Eqs. (4.6) in Ref. [7]. From Fig. 1 we notice that the most important distinction between QRW and classical distributions is that the QRW shows the following:

(a) At any arbitrary time, there are well defined destructive and constructive interference points.

(b) There is an unexpected localization of the probability. The probability is conserved, so almost all probability lost in destructive interference points appears to be concentrated in the neighborhood of a single point where the probability has a big spike. This spike is a consequence of initially having the particle moving toward the right; see Eq. (5.1).

(c) The position of this localization overshoots by far the classical average value. Interference makes quantum particles diffuse faster.

(d) At fixed times, the QRW probability fluctuates very strongly between neighboring points, and also for fixed points the probability fluctuates very strongly between successive times. The cause of these fluctuations is nothing but interference.

(e) Notice also that, in clear distinction with classical diffusion theory, in the QRW diffusion process the values of the first few moments lose any physical meaning.

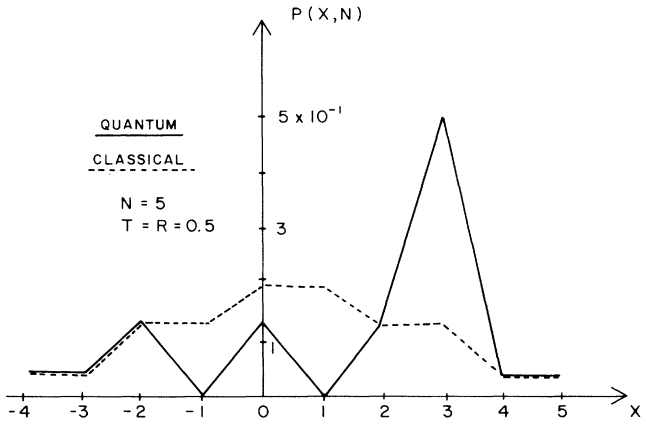


FIG. 1. Quantum and classical one-body probability distribution $P(M,t=5)$. Initial conditions: $A(M,0)=\delta_{M,0}$ and $B(M,0)=0$. The continuous line is a coherent QRW theory; the dashed line is incoherent.

## VI. $N$-BODY QRW PROBABILITY FOR FERMIONS AND BOSONS

From Sec. III we have obtained, neglecting the spin wave function, for discrete times $t=N(N=1, 2, \ldots)$, a one-particle QRW wave function $\phi^{(1)}(x_1,t)$. The superindex is to denote the initial condition (1) of that particle:

$$\phi^{(1)}(x_1,t)=\sum_{M=-\infty}^{+\infty}[A(M,t)e^{ik_0x_1}+B(M,t)e^{-ik_0x_1}]G(x_1,t,M)\ . \tag{6.1}$$

For our QRW function (6.1) with bounded packets, the state of the single free particle is determined at every cell $M$ by the specification of the two central values $\pm k_0$ (times $2s+1$ for spin $s$). In the same cell $M$, two fermions with the same spin can only occupy two states of different central momentum $\pm k_0$. Full constructive (destructive) statistical interference for bosons (fermions) will come, at the same cell, only by having the same central momentum $k_0$. We choose the case of maximum statistical interference to present in this section.

As previously proved in (5.4), the modulating amplitudes $[A(M,t),B(M,t)]$ depend strongly on the specific initial conditions $[A(M,0),B(M,0)]$. Having a second particle with the same energy, if different initial condi-

tions are given, QRW equations (3.4) generate different amplitudes, say $[C(M,t),D(M,t)]$, and therefore a different one-particle QRW wave function $\phi^{(2)}(x_2,t)$:

$$\phi^{(2)}(x_2,t)=\sum_{M=-\infty}^{+\infty}[C(M,t)e^{ik_0x_2} +D(M,t)e^{-ik_0x_2}]G(x_2,M,t) . \tag{6.2}$$

In the case of two *identical* free particles diffusing in the same lattice, we have to introduce the correct symmetry under permutation operators [10]. For bosons and fermions we have the two-body QRW wave function, having one particle described by $\phi^{(1)}$ and the other by $\phi^{(2)}$:

$$\Psi(x_1,x_2,t)\equiv\tfrac{1}{2}[\phi^{(1)}(x_1,t)\phi^2(x_2,t) \pm\phi^{(1)}(x_2,t)\phi^2(x_1,t)] . \tag{6.3}$$

The + sign is for bosons, the − for fermions.

Using this wave function we can obtain the *conditional* two-body QRW probability density $P(m,n,t|)$ for finding particle 1 on cell $m$ and particle 2 simultaneously on cell $n$:

$$P(m,n,t|\phi^{(1)}(0),\phi^{(2)}(0)) =\int_{\text{cell }m}dx_1\int_{\text{cell }n}dx_2|\Psi(x_1,x_2,t)|^2 . \tag{6.4}$$

Since we have a particle permutation symmetry (antisymmetry), we clearly have $P(n,m,t|)=P(m,n,t|)$. The quantum probability $\mathcal{P}(m,n,t|)$ of finding one (any) particle at cell $m$ and the other one simultaneously at cell $n\neq m$ is

$$\mathcal{P}(m,n,t|)=P(m,n,t|)+P(n,m,t|)=2P(m,n,t|) . \tag{6.5}$$

Normalization demands that

$$\sum_m\sum_n P(m,n,t|)=1 . \tag{6.6}$$

Symmetry and antisymmetry are conserved over time [10]. So for simplicity we neglect time notation, and from (6.3) and (6.4) we have

$$P(m,n|\phi^{(1)},\phi^{(2)})=\frac{1}{2}\left[\int_m dx_1|\phi^{(1)}(x_1)|^2\int_n dx_2|\phi^{(2)}(x_2)|^2+\int_m dx_1|\phi^{(2)}(x_1)|^2\int_n dx_2|\phi^{(1)}(x_2)|^2 \pm\left[\int_m dx_1\phi^{(1)}(x_1)\phi^{(2)*}(x_1)\int_n dx_2\phi^{(2)}(x_2)\phi^{(1)*}(x_2)+\text{c.c.}\right]\right] . \tag{6.7}$$

Since wave packets centered at different cells do not overlap, we have

$$P(m,n|\phi^{(1)},\phi^{(2)})=\tfrac{1}{2}\{[|A(m)|^2+|B(m)|^2]\times[|C(n)|^2+|D(n)|^2]+[|C(m)|^2+|D(m)|^2]\times[|A(n)|^2+|B(n)|^2]\} \pm\{[A(m)C^*(m)+B(m)D^*(m)]\times[C(n)A^*(n)+D(n)B^*(n)]+\text{c.c.}\} . \tag{6.8}$$

Defining the row-vector amplitudes $\phi_m^{(1)}$ and $\phi_m^{(2)}$ for each lattice cell $m$,

$$\phi_m^{(1)}(t)\equiv[A(m,t),B(m,t)] , \quad \phi_m^{(2)}(t)\equiv[C(m,t),D(m,t)] , \tag{6.9}$$

we have finally a condensed notation for (6.8):

$$P(m,n,t|\phi^{(1)},\phi^{(2)}) =\tfrac{1}{2}\{|\phi_m^{(1)}|^2|\phi_n^{(2)}|^2+|\phi_m^{(2)}|^2|\phi_n^{(1)}|^2 \pm[\phi_m^{(1)}\phi_m^{(2)\dagger}\times\phi_n^{(2)}\phi_n^{(1)\dagger}+\text{c.c.}]\} , \tag{6.10}$$

where $\phi_m^{(1)\dagger}$ defines the adjoint of the vector $\phi_m^{(1)}$.

As an example, consider two identical particles having different initial conditions $\phi^{(1)}(0)$ and $\phi^{(2)}(0)$. Suppose the case in which, at some time later and at the *same* cell $(m=n)$, we have the two particles with different amplitudes but the same (right) direction of motion:

$$\phi_m^{(1)}=[A(m),0], \quad \phi_m^{(2)}=[C(m),0] . \tag{6.11}$$

Substituting (6.11) into (6.10), we have

$$P(m,m|\phi^{(1)},\phi^{(2)}) =\tfrac{1}{2}\{|A(m)|^2|C(m)|^2+|A(m)|^2|C(m)|^2 \pm[A(m)C^*(m)C(m)A^*(m)+\text{c.c.}]\} \tag{6.12}$$

or

$$P(m,m|\phi^{(1)},\phi^{(2)})=\begin{cases}2|A(m)|^2|C(m)|^2 , & \text{Bose}\\ 0, & \text{Fermi} .\end{cases} \tag{6.13}$$

As expected, the example shows that no matter what the values of the amplitudes $A(m)$ and $C(m)$, as long as $A(m)$ or $C(m)$ are not zero, two bosonic wave packets with the same position and momentum will have maximum constructive interference. This is the well known tendency for bosons to clump together in position. On the other hand, two fermionic packets with the same position and momentum will have, in space, maximum destructive interference (statistical repulsion). The 3D plot

of Eq. (6.10) is shown in Fig. 2.

In the case of $N$ *identical* free particles having the same energy and diffusing in the same lattice, the generalization is straightforward. We have now $N$ initial conditions, and therefore $N$ one-body QRW wave functions $\phi^{(j)}(j=1,2,\ldots,N)$. The $N$-body wave function $\Psi$ is given by

$$\Psi(x_1,x_2,\ldots,x_N,t) = \frac{1}{\sqrt{N!}}\sum_P (\pm 1)^P P\phi^{(1)}(x_1,t) \times \phi^{(2)}(x_2,t)\cdots\phi^{(N)}(x_N,t) , \quad (6.14)$$

where $P$ is the permutation operator of the states $(1),(2),\ldots,(N)$. If we define, for the one-body wave function $j$, the row vector $\phi_m^{(j)}(t)$ at cell $m$,

$$\phi_m^{(j)}(t) \equiv [A^{(j)}(m,t), B^{(j)}(m,t)] , \quad (6.15)$$

then the conditional $N$-body QRW probability density of finding particle 1 at cell $s_1$, particle 2 at cell $s_2$, etc., is given by

$$P(s_1,s_2,\ldots,s_N,t|) = \frac{1}{N!}\sum_{PP'} (\pm 1)^{P+P'} PP' \phi_{s_1}^{(1)}\phi_{s_2}^{(2)}\cdots\phi_{s_N}^{(N)}\phi_{s_1}^{(1')\dagger}\phi_{s_2}^{(2')\dagger}\cdots\phi_{s_N}^{(N')\dagger} . \quad (6.16)$$

For symmetry in (6.16), all permutations of $\{s_1,s_2,\ldots,s_N\}$ give the same probability. The quantum probability $\mathcal{P}(s_1,s_2,\ldots,s_N,t|)$ of finding one (any) particle at cell $s_1$, any other particle simultaneously at cell $s_2$, etc., is given by

$$\mathcal{P}(s_1,s_2,\ldots,s_N,t|) = N!P(s_1,s_2,\ldots,s_N,t|) . \quad (6.17)$$

Normalization demands that

$$\sum_{s_1}\sum_{s_2}\cdots\sum_{s_N} P(s_1,s_2,\ldots,s_N,t|) = 1 . \quad (6.18)$$

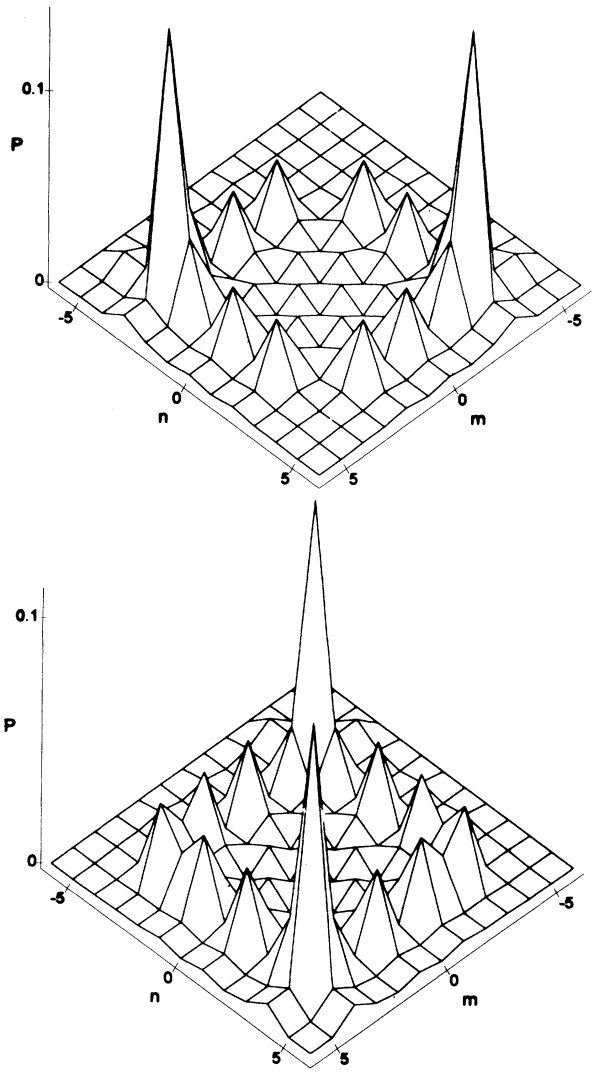


FIG. 2. Two-body QRW probability distribution $P(m,n,t=6)$. (a) is for fermions, (b) is for bosons. Initial conditions: $A(m,0)=\delta_{m,0}$, $B(m,0)=0$, $C(n,0)=0$, and $D(n,0)=\delta_{n,1}$. Notice the region $m=n$; fermions show statistical repulsion, bosons show clumping.


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## APPENDIX: ANALYTIC EXPRESSIONS FOR GREEN'S FUNCTION

In this appendix we derive an exact expression for the Green's function $\mathcal{G}(x,t)$ defined in (5.7) and (5.10):

$$\mathcal{G}(x,t) \equiv \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-isx} g(s,t)\,ds \quad \text{with } g(s,t) \equiv \frac{\lambda_+^N - \lambda_-^N}{\lambda_+ - \lambda_-} . \quad (A1)$$

We want the exact solution. First we note that the function $g(s,t)$ is proportional to a Chebyshev polynomial of the second kind, $U_{t-1}(z)$. This is so because we can rewrite the eigenvalues $\lambda$ as follows:

$$\lambda_\pm = ie^{ik}e^{\mp i\theta(s,k)} \quad \text{with } \tan\theta(s,k) \equiv \frac{\sqrt{1-T\cos^2(s-k)}}{\sqrt{T}\cos(s-k)} . \quad (A2)$$

Substituting Eq. (A2) into Eq. (A1), we obtain [12]

$$g(s,t)=i^{t-1}e^{ik(t-1)}\frac{\sin(t\theta)}{\sin\theta}$$
$$=(i)^{t-1}e^{ik(t-1)}\begin{cases}0, & t=0\\ U_{t-1}(z), & t\geq 1\end{cases}. \quad \text{(A3)}$$

Next the Chebyshev polynomial $U_t(z)$ can be written as [13]

$$U_t(z)=\sum_{j=0}^{[t/2]}\frac{(-1)^j(t-j)!}{j!(t-2j)!}(2z)^{t-2j}, \quad \text{(A4)}$$

and using the binomial theorem

$$(2z)^{t-2j}=\left[\sqrt{T}\right]^{t-2j}[e^{i(s-k)}+e^{-i(s-k)}]^{t-2j}$$
$$=(\sqrt{T})^{t-2j}\sum_{n=0}^{t-2j}\frac{(t-2j)!}{n!(t-2j-n)!}$$
$$\times e^{i(s-k)(t-2j-2n)}. \quad \text{(A5)}$$

If we substitute Eqs. (A4) and (A5) into Eq. (A1), and make an elementary integration, we have an expression for the Green's function as follows:

$$\mathcal{G}(x,t+1)=(i)^t\sum_{j=0}^{[t/2]}(-1)^j\left[\sqrt{T}\right]^{t-2j}\sum_{n=0}^{t-2j}\frac{e^{ik(2j+2n)}(t-j)!\delta(t-x,2j+2n)}{j!t!(t-2j-n)!}. \quad \text{(A6)}$$

Kronecker's delta implies that $\mathcal{G}(x,t+1)$ is different from zero only if $t-x=2(j+n)$. Since $j$ and $n$ are positive integers, then $t-x$ must be a positive even integer. Therefore $t$ and $x$ must have the same parity. Under these conditions $n=(t-x-2j)/2$ will be a positive integer only if $2j<t-x$. Therefore from (A6) we have the final result for $G(x,t+1)$:

$$\mathcal{G}(x,t+1)=(i)^t e^{i(t-x)k}\sum_{j=0}^{[(t-x)/2]}(-1)^j\left[\sqrt{T}\right]^{t-2j}\frac{(t-j)!}{j!\left[\frac{t-x-2j}{2}\right]!\left[\frac{t+x-2j}{2}\right]!}. \quad \text{(A7)}$$

Notice that $\mathcal{G}(x,t+1)$ has even parity in the $x$ variable.


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