Representation of electrons on symmetric electron-wave stub-filters by waves and particles

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Abstract: This paper presents a method of computing sample trajectories of particle models of electrons on symmetric electron-wave stub-filters. The time-independent Schrödinger equation describing the electron-wave filters is transformed to a system of linear algebraic equations. The Fourier series expansion transforms the eigenvalues of the system to continuous and differentiable eigenfunctions. A electron wave packet is constructed from the obtained smooth eigenfunctions and a nonlinear stochastic ordinary differential equation (NSODE) which governs the behavior of the electron particle model is established by applying the stochastic quantization to the wave packet. Sample trajectories of the particles are computed by integrating the NSODE. Numerical experiments have shown that the statistical behavior of the particles is almost equal to that of the wave packets.

Key Words: electron wave filter, stub, stochastic differential equation, stochastic quantization

1. Introduction

Waveguides transporting electrons ballistically have been researched actively in recent years [1–4]. They have a possibility to be utilized as couplers and splitters instead of optical counterparts in fiber-optic communication since they can be approximately a hundred times shorter than the optical counterparts [1]. For the same reason, they might be used as front-end filters in the receivers in optical sensing and space optical communication systems [5].

In these fiber and space optical communication systems, the passive electron waveguides and wave filters are accompanied with active quantum effect devices such as single-electron transistors. In circuit simulator models of the active quantum effect devices, electrons are represented by probabilistic particles [6]. On the other hand, in the research of the passive waveguides and filters, electrons have been depicted as quantum waves. For integrated simulation of circuits built of both passive and active quantum devices, it is necessary to unify the representation of electrons. Since the circuit simulator models of the active quantum effect devices are available today [6, 7], electrons in waveguides should be modeled as probabilistic particles.

Let a conditional probability distribution of an electron at the interface between active and passive
quantum devices be denoted by $p_{cnd}(x_1, \cdots, x_{Ns}, t)$. The distribution is obtained from a quantum wave $\psi(x_1, \cdots, x_N, t)$, $N_s < N$, on the passive device. For the integrated simulation, it is necessary to generate samples $(x_1, \cdots, x_{Ns}, t)$ that follow $p_{cnd}$ statistically. However, $p_{cnd}$ might be a complicated distribution. In addition, when multiple electrons exist in a waveguide, dimension $N_s$ is large. In such cases, it is difficult to generate the samples. To solve the difficulty, we represent an electron on whole the passive device by a probabilistic particle. A nonlinear stochastic ordinary differential equation (NSODE) that governs the behavior of the probabilistic particle is derived by the Nelson's stochastic quantization \[8\]. It guarantees that the probability distribution of the sample solutions to the NSODE coincides with that determined from the quantum wave. The equivalence between the probabilistic particles and the quantum wave was confirmed by numerical experiments \[5, 9, 10\].

Several types of electron wave splitters and filters have been proposed. A type of electron wave filter has periodic potential structure \[11\]. Trajectories of electrons modeled as probabilistic particles on this type of filters were computed \[5\] by applying the transfer-matrix method (TMM) \[11, 12\] and the stochastic quantization. Another type of electron wave filter consists of several waveguides coupled by evanescent waves. A method of computing sample trajectories of electrons modeled as probabilistic particles on coupled waveguides has been proposed recently \[13\].

In this paper, we will attempt to compute sample trajectories of electrons modeled as probabilistically behaving particles on electron wave filters with stubs. The modeling is based on Nelson's stochastic quantization, which will be explained later in Section 4. Time-evolving wave packets propagating on electron wave stub-filters can not be obtained analytically, which makes it difficult to construct the NSODE. The transfer characteristics of the filters have been analyzed by the combined use of the mode-matching method (MMM) \[11\] and TMM. The combination of MMM and TMM (MMM-TMM) provides analytical expression of plane electron wave propagation. However, it does not provide directly time-evolving electron wave packets in analytical form. In addition, MMM has disadvantages that its mathematical base is weak and its process to determine components of electron waves is heuristic. Time-evolving electron wave packets can be computed by the finite difference method (FDM) \[14\]. Although the wave packets are not obtained in analytical form by FDM, NSODE is determined at which the probabilistic particle locates. However, in building the probabilistic particle model of electrons and conducting numerical experiments to trace the paths of the particle model, we encounter difficulties of large computational cost and higher-order interpolation of the wave packets between lattice points at which the electron waves are computed.

In this paper, we will attempt the following procedure as a method of constructing probabilistic particle models to eliminate the above disadvantages of MMM-TMM and FDM. At first, we will transform the time-independent Schrödinger equation describing the filter to a system of linear algebraic equations and compute its eigenvalues and eigenvectors. They correspond to eigenenergies and eigenfunctions of the Schrödinger equation. In the second step, we will expand the eigenvectors into Fourier series to obtain approximate continuous and differentiable eigenfunctions. In the third step, we will construct electron wave packets from the obtained smooth eigenfunctions and build the particle models by applying the stochastic quantization to the wave packets. In computing the eigenvectors and the eigenfunctions, we will consider to reduce computational complexity by taking the symmetry of the filter into account. In constructing the particle models, wave packet propagation is approximated to single-mode propagation in order to simplify the models. The first and second steps might be replaced by the spectral method (SM) \[15\] and eigenvector computation. If trigonometric functions are adopted as eigenfunctions in SM, the procedure to compute time-evolving wave packets is simpler than the method to be proposed. However, products of two trigonometric functions, e.g. $\sin(x) \cos(2y)$, can not be adopted as eigenfunctions since they do not satisfy boundary conditions imposed on electron wave stub-filters.

### 2. Spatiotemporally discretized Schrödinger equation

The wave nature of an electron in a scalar potential $V(x, y, t)$ is described by the following Schrödinger equation:
$i\hbar \frac{\partial \psi(x, y, t)}{\partial t} = H\psi(x, y, t), \quad H = -\frac{\hbar^2}{2m_e} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + V(x, y, t)$ (1)

where $i^2 = -1$, $\hbar = h/2\pi$ ($h$: The Planck constant), and $m_e$ is the mass of electron. The operator $H$ is referred to as Hamiltonian.

2.1 Time-independent discretized Schrödinger equation

Let $E_n$ and $\phi_n(x, y)$ respectively denote the $n$-th eigenenergies and eigenfunctions of $H$. Using the denotations, we have the following time-independent Schrödinger equation:

$$E_n\phi_n(x, y) = H\phi_n(x, y)$$ (2)

Any wave function satisfying Eq. (1) is the linear combination of

$$\phi_n(x, y, t) = \phi_n(x, y) \exp(-i\frac{E_n}{\hbar}t)$$ (3)

We discretize $x$-$y$ plane to get a lattice with $x$ and $y$-directional grid intervals $\Delta x$ and $\Delta y$. The second-order partial differential operators in $H$ are represented on the lattice by

$$\frac{\partial^2 \phi_n(x, y)}{\partial x^2} \bigg|_{(x,y)=(i\Delta x,j\Delta y)} \approx \frac{1}{\Delta x^2} (\phi_n((i+1)\Delta x,j\Delta y) - 2\phi_n(i\Delta x,j\Delta y) + \phi_n((i-1)\Delta x,j\Delta y))$$

$$\frac{\partial^2 \phi_n(x, y)}{\partial y^2} \bigg|_{(x,y)=(i\Delta x,j\Delta y)} \approx \frac{1}{\Delta y^2} (\phi_n(i\Delta x,(j+1)\Delta y) - 2\phi_n(i\Delta x,j\Delta y) + \phi_n(i\Delta x,(j-1)\Delta y))$$ (4)

Then, Eq. (2) is represented with eigenvalues $E_n$, eigenvectors $\phi_n$, and Hamiltonian $H$ in a Matrix form by

$$E_n\phi_n = H\phi_n$$ (5)

The $I$-th element of $\phi_n$ is the value of eigenfunction $\phi_n$ at grid $(i, j)$, that is,

$$\phi_n[I(i, j)] = \phi_n(i\Delta x, j\Delta y)$$ (6)

From Eq. (4), the $(I, J)$ element of $H$ operates on the $I$ and $J$-th elements of $\phi_n$ which are the values of $\phi_n$ at $(i_1, j_1)$ and its adjacent grids $(i_2, j_2)$ as follows:

$$H[I(i_1, j_1), J(i_2, j_2)] = \left\{ V(i_1\Delta x, j_1\Delta y) + \frac{\hbar^2}{2m_e} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) \right\} \delta_{i_1, i_2}\delta_{j_1, j_2}$$

$$-\frac{\hbar^2}{2m_e} \left\{ \frac{1}{\Delta x^2} (\delta_{i_1-1, i_2}\delta_{j_1, j_2} + \delta_{i_1+1, i_2}\delta_{j_1, j_2}) + \frac{1}{\Delta y^2} (\delta_{i_1, i_2}\delta_{j_1-1, j_2} + \delta_{i_1, i_2}\delta_{j_1, j_2+1}) \right\}$$ (7)

where $\delta_{p,q}$ ($p, q$: integers) denotes Kronecker delta.

2.2 Time-dependent discretized Schrödinger equation

As mentioned previously, any time-evolving wave function satisfying Eq. (1) is expressed as a linear combination of eigenfunctions (3). However, if the structure of potential $V(x, y, t)$ is complicated, matrix $H$ is large and its eigenfunctions may not be obtained easily. In this case, we rely on numerical methods. One method of them is the finite difference method (FDM) [14]. Its computational procedure is as follows: In addition to $x$-$y$ plane, time axis is discretized with interval $\Delta t$. Then, the space and time coordinate system is converted into a three-dimensional lattice. Let a discretized wave function,

$$\psi(k\Delta t)[I(i, j)] = \psi(i\Delta x, j\Delta y, k\Delta t),$$ (8)

be the solution, for example, to the following system of difference equations:

$$i\hbar \frac{\psi((k+1)\Delta t) - \psi(k\Delta t)}{\Delta t} = H\psi(k\Delta t)$$ (9)
which is the Euler discretization of the Schrödinger equation (1). The discrete wave function is obtained by the iteration of Eq. (9) for $k$ with an initial condition $\psi(0)[I(i, j)]$ and fixed boundary condition $\psi(t)[I(i_b, j_b)]$, $(i_b, j_b)$: boundary lattice points, for example. The left hand side of Eq. (9) has purely imaginary number $i\hbar$. Therefore, the equation is considered as discretized coupled linear oscillators whose states are expressed by complex variables $\psi(k\Delta t)[I(i, j)]$. Since linear oscillators are structurally unstable, the norm of $\psi(k\Delta t)$ should be normalized at every step of the iteration.

Another method of computing wave functions numerically is the spectral method (SM) [15]. Its computational procedure is as follows: The wave function is given, for example, by the following superposition of sinusoidal waves:

$$\psi(x, y, t) = \sum_{l,m} a_{l,m}(t) \phi_{l,m}(x, y), \quad \phi_{l,m}(x, y) = \exp(i(k_{lx}x + k_{ly}y))$$

(10)

By substituting Eq. (10) into the Schrödinger equation (1), a system of ordinary differential equations in terms of $a_{l,m}(t)$ is obtained. From given boundary conditions, some of $a_{l,m}(t)$ are zeros. Others are computed by integrating numerically the system of the differential equations with initial conditions $a_{l,m}(0)$ satisfying $\psi(x, y, 0) = \sum_{l,m} a_{l,m}(0) \phi_{l,m}(x, y)$. Generally, $\{\phi_{l,m}(x, y)\}$ can not always be eigenfunctions satisfying boundary conditions. Therefore, the wave function in the form of (10) may not necessarily be obtained analytically. The proposed method to be explained in the subsequent sections is a kind of spectral method. Functions $\phi_{l,m}(x, y)$ satisfying boundary conditions are given by continuum approximation of spatially discrete eigenfunctions of Eq. (2). Then, time-varying coefficients $a_{l,m}(t)$ are obtained without integrating the system of the differential equations numerically.

3. Eigenfunctions of symmetric electron-wave stub-filter and their Fourier series expansion

Electron-wave stub-filters containing an electron which should be modeled as a probabilistic particle are quantum potential systems. Figures 1(a) and (b) respectively show the potentials of one and four-stub filters. Propagation of electron wave packets and motion of particle models of electrons in the two filters will be computed in subsections 5.1 and 5.2. The $x$-directional waveguide of each filter is finite in length. As a result, when the potential height is $V_H = \infty$, the eigenenergies of the quantum potential systems take discrete values $E_n$ and eigenfunctions $\phi_n$ are determined for each $E_n$, which enables wave functions $\psi(x, y, t)$ of the systems to be expressed in the form of Eq. (3)

Generally, analog distributed parameter filters based on electro-magnetics possess symmetric structure [16, 17]. By the analogy between electro-magnetic waves and electron waves [2], the potentials of the electron wave filters are symmetric with respect to $y$-axis. The symmetry is reflected to the eigenfunctions. They may be even and odd functions satisfying $\phi_n(-x, y) = \pm \phi_n(x, y)$. Figure 2 shows eigenvectors of the potential system in Fig. 1(a) satisfying $\phi_n[J(-i, j)] = \pm \phi_n[I(i, j)]$. This characteristic of the eigenfunction set decreases complexity to compute their Fourier series expansion because the series consist of either cosine or sine functions of $x$. Otherwise, eigenfunction pairs $\{\phi_n, \phi_{n+1}\}$ may satisfy the relation $\phi_{n+1}(x, y) \approx \phi_n(-x, y)$. Figure 3 exemplifies eigenvectors of the

![Fig. 1. The potentials of electron wave filters.](image-url)
potential system in Fig. 1(b) when all the stubs in the figure are same in length and width and spaced equally. We see that the eigenvectors possess the above property. This property of the eigenfunction set may also decrease complexity to compute their Fourier series expansion because the dominant terms of $\phi_n$ and $\phi_{n+1}$ are same in magnitude.

As will be shown in the next section, the eigenfunctions should be smooth analytical functions in establishing a stochastic ordinary differential equation which governs the behavior of a probabilistic particle model of electrons. We approximate the eigenvalues $\phi_n$ by the following equation:

$$\phi_n = \sum_{k_o} \sum_{l} a_{n,k_o,l} \zeta_{k_o,l} + \sum_{k_e} \sum_{m} b_{n,k_e,m} \eta_{k_e,m}$$

where the elements of vectors $\zeta_{k_o,l}$ and $\eta_{k_e,m}$ are given by

$$\zeta_{k_o,l}(i\Delta x, j\Delta y) = \frac{k_o \pi i \Delta x}{b} \sin \left( \frac{l \pi j \Delta y}{a} \right), \quad k_o: \text{odd integer}$$

$$\eta_{k_e,m}(i\Delta x, j\Delta y) = \frac{k_e \pi i \Delta x}{b} \sin \left( \frac{m \pi j \Delta y}{a} \right), \quad k_e: \text{even integer}$$

Integers $k_o$ and $k_e$ must be odd and even to satisfy the boundary conditions $\phi_n[I(i, j)] = 0$ at $i\Delta x = \pm b/2$ when $V_H = \infty$. When the eigenvectors are even, $b_{n,k_e,m} = 0$. When they are odd, $a_{n,k_o,l} = 0$. This property reduces the computational cost for the Fourier series expansion. By continuation of the eigenvectors, $(i\Delta x, j\Delta y) \to (x, y)$, continuous and smooth eigenfunctions $\phi_n(x, y)$ are obtained. We then approximate wavefunctions, the solutions of the Schrödinger equation (1) by the superposition of the eigenfunctions as follows:
\[ \psi(x, y, t) = \sum_n c_n \phi_n(x, y) \exp(-i E_n \frac{\hbar}{\hbar} t) = \sum_{k_n} \sum_l a_{k_n, l}(t) \zeta_{k_n, l}(x, y) + \sum_{k_e} \sum_m b_{k_e, m}(t) \eta_{k_e, m}(x, y) \] (13)

\[
\zeta_{k_n, l}(x, y) = \cos\left(\frac{k_n \pi x}{b}\right) \sin\left(\frac{l \pi y}{a}\right),
\]

\[
\eta_{k_e, m}(x, y) = \sin\left(\frac{k_e \pi x}{b}\right) \sin\left(\frac{m \pi y}{a}\right)
\] (14)

The coefficients \(a_{k_n, l}(t)\) and \(b_{k_e, m}(t)\) in Eq. (13) are periodic time-varying coefficients given by

\[
a_{k_n, l}(t) = \sum_n c_n a_{n, k_n, l} \exp(-i E_n \frac{\hbar}{\hbar} t),
\]

\[
b_{k_e, m}(t) = \sum_n c_n b_{n, k_e, m} \exp(-i E_n \frac{\hbar}{\hbar} t)
\] (15)

4. Probabilistic particle model: stochastic quantization

A probability that an electron exists in \( [x - dx/2, x + dx/2] \times [y - dy/2, y + dy/2] \) at time \( t \) be given by \(|\psi(x, y, t)|^2 \) \( dx \, dy \). A probability density function \( \rho(x, y, t) \) that a probabilistic particle follows must be

\[
\rho(x, y, t) = |\psi(x, y, t)|^2
\] (16)

for the particle to be a model of the electron. The Fokker-Planck equation (FPE) [18] whose solution is given by Eq. (16) and a nonlinear stochastic ordinary differential equation (NSODE) which governs the motion of the particle are described respectively by

\[
\frac{\partial \rho(x, y, t)}{\partial t} = -\left[ \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right] b \rho(x, y, t) + \nu \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \rho(x, y, t)
\] (17)

and

\[
[dx, dy] = b(x, y, t) dt + \sqrt{\nu} \sqrt{2} [d\Gamma_x(t), d\Gamma_y(t)]
\] (18)

The two independent white Gaussian fluctuations \( \Gamma_x/y(t) \) in Eq. (18) satisfy the following correlation properties:

\[
<d\Gamma_x/y(t)d\Gamma_x/y(t + \tau) > = 2\delta(\tau), \quad <d\Gamma_x(t)d\Gamma_y(t + \tau) > = 0,
\] (19)

The diffusion coefficient and the drift term of FPE (17) and NSODE (18) are respectively given with \( \hbar, m_e \) in the Schrödinger equation and its wave function \( \psi(x, y, t) \) by [8, 13]

\[
\nu = \frac{\hbar}{m_e}
\] (20)

and

\[
b(x, y, t) = \frac{\hbar}{m_e} \left[ \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right] (\Re(\log \psi(x, y, t)) + \Im(\log \psi(x, y, t)))
\] (21)

where \( \Re(z) \) and \( \Im(z) \) respectively are real and imaginary parts of complex value \( z \).

If propagation of wave function \( \psi(x, y, t) \) in \( x \)-direction on the straight line parts with no stub is in a single mode, that is, \( \psi(x, y, t) \) distributes sinusoidally in \( y \)-direction, \( \psi(x, y, t) \) is represented in the following form of variable separation:

\[
\psi(x, y, t) = \sum_{k_n} a_{k_n, l}(t) \zeta_{k_n, l}(x, y) + \sum_{k_e} b_{k_e, l}(t) \eta_{k_e, l}(x, y)
\]

\[
= \left\{ \sum_{k_n} a_{k_n, l}(t) \cos\left(\frac{k_n \pi x}{b}\right) + \sum_{k_e} b_{k_e, l}(t) \sin\left(\frac{k_e \pi x}{b}\right) \right\} \sin\left(\frac{l \pi y}{a}\right)
\]

\[
= \psi(x, t) \psi(y)
\] (22)

Then, drift term \( b \) is given by

\[
b(x, y, t) = \frac{\hbar}{m_e} \left[ \Re\left( \frac{1}{\psi(x, t)} \frac{\partial \psi(x, t)}{\partial x} \right) + \Im\left( \frac{1}{\psi(x, t)} \frac{\partial \psi(x, t)}{\partial x} \right) \right] \frac{1}{\psi(y)} \frac{\partial \psi(y)}{\partial y}
\] (23)

We see that the \( x \) and \( y \)-directional components of \( b(x, y, t) \) are respectively independent of \( y \) and \( x \) coordinates and that the \( y \)-directional component is a simple real function.
The single-stub electron wave filter has the potential structure shown in Fig. 1(a). The dimensions of the filter are normalized as \( \bar{h} = 1 \) and \( m_e = 1 \) in numerical experiments in this section. The electron wave filters are potential systems as have been shown in Fig. 1. They should be long in \( x \)-direction so that the front edges of time-evolved dispersed wave packets do not collide with the potential walls at the left and right ends of the filters. Electron wave packets are initially given by the following Gaussian packet with initial \( x \)-directional momentum \( \hbar k_{x, \text{init}} \).

\[
\psi(x, y, 0) \equiv \psi_{\text{init}}(x, y) = \frac{1}{2\pi\sigma_x\sigma_y} \exp \left( -\frac{(x - x_0)^2}{2\sigma_x^2} - \frac{(y - y_0)^2}{2\sigma_y^2} + ik_{x, \text{init}}x \right) \tag{24}
\]

Time-evolving wave packets are analytically approximated in the form of Eq. (13) with time-varying coefficients (15). Constant coefficients \( c_n \) in Eqs. (13) and (15) are obtained by computing the following inner products between initial packet (24) and eigenfunctions \( \phi_n(x, y) \):

\[
c_n = \int_{-b/2}^{+b/2} \int_0^{a+d} \psi_{\text{init}}(x, y) \phi_n(x, y) dy dx \tag{25}
\]

For the filter with four stubs, \( d \) is the longest stub length.

5.1 One-stub filter

The single-stub electron wave filter has the potential structure shown in Fig. 1(a). The dimensions of the wave filter are \( a = 0.3, b = 13.0, c = 0.9, \) and \( d = 0.26 \). The height of the potential wall is \( V_H = 1000 \) because \( V_H \) must be finite in computing the eigenvectors \( \phi_n \). The discrete space is a lattice with grid intervals \( \Delta x = b/300 \) and \( \Delta y = (a + d)/40 \). Eigenvalues in Eq. (5) were computed and transformed to the Fourier series (11) of 140 terms.

The center and variances of initial Gaussian wave packet given by Eq. (24) are \( (x_0, y_0) = (-3.5, 0.15) \), \( \sigma_x^2 = 1, \sigma_y^2 = (0.06)^2 \). Its initial momentum is \( \hbar k_{x, \text{init}} = 8.0/13.0 \) (transmission/reflection).

The time-evolving wave packets were approximated by the superposition of 31 eigenfunctions. Time-evolution of the wave packets are shown in the form of probability density function \( \psi(x, y, t)^2 \) in Fig. 4. These figures draw \( \psi(x, y, t)^2 \) at time \( t_s = 0, 0.300/0.200, 0.600/0.400, \) and \( 0.900/0.700 \) ((Ta)–(Td)/(Ra)–(Rd)) when the wave packets are transmitted and reflected.

Trajectories of probabilistic particle models of electrons were obtained by integrating numerically NSODE (18), that is, by the following iteration:

\[
[x(t + \Delta t), y(t + \Delta t)] \leftarrow [x(t), y(t)] + b(x(t), y(t), t)\Delta t + \sqrt{\frac{\hbar}{2m_e}} \Delta t \left[ d\Gamma_x(t), d\Gamma_y(t) \right] \tag{26}
\]

The initial points \( (x(0), y(0)) = (x_{\text{init}}, y_{\text{init}}) \) of the trajectories are samples of random vectors following initial distribution (24). Time step is \( \Delta t = 9.5/(800k_{x, \text{init}}) \). Finite-length trajectories are shown in (Ta)–(Td) and (Ra)–(Rd) of Fig. 4 for time intervals from 0 to time \( t_s \) at which \( \psi(x, y, t_s)^2 \) are depicted over them. Their zigzag motion is due to the random fluctuation elements \( d\Gamma_x/y(t) \). The turnings of the zigzag trajectories are the positions obtained by the iteration (26). Each end (red circle) of the trajectories in Fig. 4 is one of the samples which follow distribution \( \psi(x, y, t_s)^2 \) in the figure. Comparing each propagating wave packet and electron trajectory, we see that electron exists where distribution \( \psi(x, y, t)^2 \) is high.

We computed \( 10^3 \) trajectories of the particle models and obtained probability distribution in terms of the locations of the probabilistic particles. The distribution is given by

\[
\rho(x, y, t) = N_{p,ij} \times 10^{-5} \tag{27}
\]

\( N_{p,ij} \) : The number of the particles in \( \Delta S_{ij} \) such that \( (x, y) \in \Delta S_{ij} \).
ΔS_{ij} = [(i - 1/2)\Delta x, (i + 1/2)\Delta x] \times [j\Delta y, (j + 1)\Delta y],
i \in \{-m_x, -m_x - 1, \cdots, m_x - 1, m_x\}, \ j \in \{0, 1, \cdots, m_y - 1, m_y\},
\Delta x = b/(2m_x + 1), \ \Delta y = (a + d)/(m_y + 1)

Figure 5(a) shows the distribution ρ(x, y, t_s) of the particles with initial momentum \(\hbar k_{x,\text{init}} = 8.0\) at time \(t_s = 0.9\). Spatial discretization parameters are set as \(m_x = 12\) and \(m_y = 11\). The distribution
$\rho(x, y, t_s)$ corresponds to the distribution densities $|\psi(x, y, t_s)|^2$ shown in Fig. 4(Td). We evaluated the difference between two probability distributions $\rho(x, y, t_s)$ and $|\psi(x, y, t_s)|^2$. The difference $P_\Delta(i, j)$ is defined as

$$
P_\Delta(i, j) = \int_{j\Delta y}^{(j+1)\Delta y} \int_{(i-1/2)\Delta x}^{(i+1/2)\Delta x} \left\{ \frac{1}{\Delta x \Delta y} \rho(x, y, t_s) - |\psi(x, y, t_s)|^2 \right\} \, dx \, dy
$$

(28)
Fig. 5. Probability distribution $\rho(x, y, t)$ and difference $P_\Delta = \rho(x, y, t) - |\psi(x, y, t)|^2$ for the one-stub filter. $\hbar k_x = 8.0, t_s = 0.9, m_x = 12, m_y = 11$.

Fig. 6. Transfer characteristics of the one-stub filter as a function of momentum $\hbar k_{x,\text{init}}$. Red line: wave packet (Fourier series), blue line: wave packet (FDM), black line: plane wave (MMM), broken red line: NSODE with wavepacket, broken blue line: NSODE with single-mode wave.

Figure 5(b) shows the difference between $\rho(x, y, t_s)$ in Fig. 5(a) and $|\psi(x, y, t_s)|^2$ in Fig. 4(Td). The average distribution difference $P_\Delta$ given by

$$P_\Delta = \frac{1}{(2m_x + 1)(2m_y + 1)} \sum_{i=-m_x}^{m_x} \sum_{j=0}^{m_y} |P_\Delta(i, j)|$$

is $P_\Delta = 8.4 \times 10^{-4}$.

We find from Fig. 4 that electrons are transmitted or reflected in the filter depending on their initial momenta $\hbar k_{x,\text{init}}$. Figure 6 shows probabilities $P_T$ that wave packets, plane waves, and particle models starting at the left part of the filter attain at the right part as a function of their (initial) momenta $\hbar k_x$. For the wave packets, the probabilities were computed as follows: Initial state of the wave packets was given by Eq. (24). Time-evolution of the wave packets were computed by both analytical and numerical methods: The analytical method is to obtain time-evolving wave functions given by Eqs. (13), (14), and (15). The numerical method is to compute time-evolving wave function by FDM. Probabilities $P_T$ were evaluated by the following integral:

$$P_T = \int_0^\infty \int_0^a \int_{c/2}^{b/2} |\psi(x, y, t)|^2 \, dx \, dy \, dt$$

For the probabilistic particle models, the probabilities were computed as follows: The particles started at points $(x_{\text{init}}, y_{\text{init}})$ which are samples of random vectors following Eq. (24) with initial momentum.
The four-stub filter is used in an interval $[1, 10]$. All start points $(x_{\text{init}}, y_{\text{init}})$ were in the left part of the stub-filter, that is $x_{\text{init}} < -c/2$. Motion of the particles was computed by integrating numerically Eq. (18) with two different drift terms. One drift term was obtained by substituting Eq. (13) into Eq. (21). The other drift term was given by Eq. (23) with $\ell = 1$ when the particle was not on the stub, that is, the electron wave propagation was in single-mode in the straight waveguides of the filter. Probabilities $P_T$ were evaluated by counting particles which reached on right area such that $x > c/2$ among 1000 particles. For the plane waves, the probability is the transfer ratio of the filter for plane waves of wave number $\hbar k_x$. The transfer ratio was computed by MMM. Figure 6 shows that the probabilities evaluated in the five different ways have the same tendency against the initial momenta.

In subsection 5.3, we will discuss further the results of these numerical experiments.

5.2 Four-stub filter

The four-stub electron wave filter has the potential structure shown in Fig. 1(b). The dimensions of the wave filter are $a = 0.3$, $b = 14.0$, $c_1 = c_2 = 0.3$, $d_1 = d_2 = 0.23$, and $e_1 = e_2 = 0.3$. The height of the potential wall is $V_H = 1000$. The discretization intervals are $\Delta x = b/300$ and $\Delta y = (a + d)/40$. Eigenvectors in Eq. (5) were computed and transformed to the Fourier series (11) of 175 terms. The center and variances of initial Gaussian wave packet are $(x_0, y_0) = (-4.0, 0.15)$, $\sigma_x^2 = 1$, $\sigma_y^2 = (0.06)^2$. Its initial momentum is $\hbar k_{x,\text{init}} = 13.0$ or 10.0 (transmission/reflectiom). The time-evolving wave packets were approximated by the superposition of 31 eigenfunctions. Probability density function $|\psi(x, y, t)|^2$ is shown on the upper parts in (Ta)–(Td) and (Ra)–(Rd) of Fig. 7. The transmission ratio computed by the proposed method can not be evaluated. For references, transmission ratios of electron waves computed by FDM and MMM are presented. Figures 6 and 9 show similar tendency between the dependences of the probability curves and the transmission ratio computed by FDM on momentum $\hbar k_x$. We see gaps between the transmission ratio computed by MMM and other $P_T$ characteristic curves. This is due to the difference of the inputs of the filters, plane waves or Gaussian wave packets. The transmission ratio curve for the plane waves possessing only a single component is sensitive on the wave number $k_x$ of the component.

In subsection 5.3, we will discuss further the results of these numerical experiments.

5.3 Discussion

5.3.1 On experimental results

The four-stub filter is superior to the one-stub filter in blocking electron of low kinetic energy. When the four-stub filter is used in an interval $[1, 10]$ of momentum $\hbar k_x$, the filter possesses bandpass characteristic while the $P_T$ characteristic of the one-stub filter is moderately varying in the interval.

There is no mathematical method of obtaining exact time-evolving packets that are the solutions of the Schrödinger equation (1) with the potentials shown in Fig. 1. Therefore, the precision of probability curves $P_T$-$\hbar k_x$ obtained by the proposed method can not be evaluated. For references, transmission ratios of electron waves computed by FDM and MMM are presented. Figures 6 and 9 show similar tendency between the dependences of the probability curves and the transmission ratio computed by FDM on momentum $\hbar k_x$. We see gaps between the transmission ratio computed by MMM and other $P_T$ characteristic curves. This is due to the difference of the inputs of the filters, plane waves or Gaussian wave packets. The transmission ratio curve for the plane waves possessing only a single component is sensitive on the wave number $k_x$ of the component.

The $P_T$ characteristics obtained by computing trajectories of the particle models are close to that
obtained by computing wave packets approximated by Fourier series expansion. This is because it is theoretically proven [8] that the trajectories follow statistically the probability density distribution satisfying Eq. (16). The approximation of the Gaussian packet propagation to the single-mode propagation reduces terms organizing $y$-directional component of the drift term of NSODE (18) by 86% and the NSODE can be variable-separated. Nevertheless, we obtained almost the same $P_T$ characteristics.

We tried numerical integration of NSODE (18) whose drift term was computed by partial-
differentiating numerically the wave packets obtained by FDM. However, we encountered a problem that the partial differential coefficients sometimes took apparently imprecise values and the particle models sometimes strayed from the waveguides of the filters. Therefore, the transmission ratio for the particles are not shown in Figs. 6 and 9. For steady plane waves obtained by MMM, drift term (21) of NSODE (18) becomes zero on the straight waveguides without stubs. As a result, the probabilistic particles are just wandering around initial points.
5.3.2 On computational cost and accuracy

Computational cost

Generally, quality of communication systems such as those mentioned in Section 1 is evaluated by calculating bit error rate (BER). In order to estimate BER, computer simulation of the communication is executed and error bits are counted in a decoded bit-sequence of the order of $10^6$ bits. Therefore, we will estimate computational cost for $N_{trj} = 10^6$ sample trajectories of the probabilistic electron model. We adopt the counts of real number multiplications as a measure of the cost.

The proposed method to compute sample trajectories of the probabilistic model of electrons consists of the three processes, computing eigenvectors $\phi_n$ and their approximation with trigonometric functions, expansion of initial wave packet by the approximate eigenvectors, and computing the trajectories by the numerical integration of NSODE (18). Among these processes, most of computation cost is consumed for the numerical integration. In order to obtain trajectories, the drift term (21) of NSODE (18) must be computed at a point where the particle exists. The term is obtained from the wave packet given by Eqs. (13), (14), and (15) and its partial differential coefficients with respect to $x$ and $y$. The number of multiplication necessary to compute the drift term at every iteration (26) for the trajectory computation is $2N_{trj}N_{ef}$, where $N_{trj} (= 140$ or $175)$ and $N_{ef} (= 31)$ respectively denote the number of trigonometric functions to approximate an eigenfunctions and the number of eigenfunctions.
to approximate the initial distribution of the wave packets. Other costs to compute the trajectories are small. Let the number of iteration to compute one trajectory be denoted by $N_{\text{step}}$. Then, the total number of multiplication necessary to compute $N_{\text{trj}}$ trajectories is $2N_{\text{trj}}N_{\text{trj}}N_{\text{ef}}N_{\text{step}} \approx 10^{13}$. If we prepare a table of trigonometric functions, computation cost for spatial and temporal periodic functions in Eqs. (14) and (15) is saved. Polynomials of order $(N_{\text{ord}} =) 15$ approximate the trigonometric functions with error of $10^{-9}$. If we use the polynomials, $N_{\text{ord}} \cdot 2(N_{\text{ev}} + 2N_{\text{trj}})N_{\text{step}}N_{\text{trj}} \approx 10^{13}$ multiplications are necessary additionally.

We estimate cost to compute electron trajectories by using FDM although we have a problem with FDM, as mentioned at the end of 5.3.1. In computing time-evolving wave packet on an electron wave filter by FDM, the filter is spatially discretized into a lattice. In the numerical examples in subsections 5.1 and 5.2, the numbers of lattice points $N_{\text{lts}}$ are approximately $10^4$. Computing sample trajectories of the probabilistic particle model of electrons consists of the following processes: (i) Time-evolution of a wave packet is computed by iterating Eq. (9) in subsection 2.2. (ii) The volume of the packet is normalized every time the iteration is executed. (iii) The partial differential coefficients of the packet with respect to $x$ and $y$ are computed by numerical differentiation at which the probabilistic particle exists. (iv) From the wave packet and its partial differential coefficients, the drift term of the NSODE is obtained and a trajectory of the particle is computed by iterating Eq. (26) in subsection 5.1. In (i), the packet is multiplied by $(\hbar/2m_{e}x^{2})$ and by the potential term $V(x, y, t)$. Then, the total number of real value multiplication is $4N_{\text{lts}}$ at every iteration (26). In (ii), approximately $4N_{\text{lts}}$ real value multiplication is necessary. The number of necessary multiplications to execute (iii) and (iv) is very much smaller than $N_{\text{lts}}$. Then, the total number of multiplication necessary to compute $N_{\text{trj}}$ trajectories is $N_{\text{trj}} \cdot 8N_{\text{lts}}N_{\text{step}} \approx 8 \times 10^{13}$. If $N_{\text{lts}}$ is small, the partial differential coefficients needed to compute the trajectories are low in precision. Therefore, large computational cost reduction equivalent to the $y$-directionally single-mode approximation shown in 5.3.1 seems difficult.

### Computational accuracy

We confirmed that probability distributions of the probabilistic particle models in Figs. 5(a) and 8(a) coincide respectively with those obtained from the wave packets in Figs. 4(Td) and 7(Rd) and saw that average differences between the probability distributions of the particles and those by the wave packets were $8.4 \times 10^{-4}$ and $1.1 \times 10^{-3}$ . It was theoretically proven in [8] and confirmed with preceding numerical examples in [5, 9, 10] that equality (16) holds. The two comparisons shown in Figs. 5(b) and 8(b) also exemplified this equality.

For evaluating the probability distributions shown in Figs. 5 and 8, we computed $10^{5}$ trajectories of the particle models when the initial momentum of the particles on the single-stub filter is $\hbar k_x, \text{init} = 8.0, 13.0$ and the momentum for the four-stub filter is $\hbar k_x, \text{init} = 13.0, 10.0$. Transmission ratios in Figs. 6 and 9 were computed from $10^{5}$ trajectories. Then, 100 transmission ratios for one and four-stub filters are obtained at the two different initial momenta. The average $a_{tr}$ and the standard deviation $\sigma_{tr}$ for four sets of the 100 ratios are shown in Table I. The transmission ratios shown in Figs. 6 and 9 are considered to contain errors of $10 \log(1 + \sigma_{tr}/a_{tr})$ dB shown in Table I.

### 6. Conclusions

This paper has presented a method of computing sample trajectories of electrons modeled as prob-
ability of probabilistic particles on symmetric electron-wave stub-filters. It was difficult to compute probabilistic trajectories of electrons from the wave functions obtained by conventional methods such as FDM and MMM. Numerical experiments conducted by the proposed method have shown that the statistical behavior of the particles is almost equal to that of the wave packets.

The Fourier series expansion of the eigenvectors in Eq. (5) is reduced in computational complexity by taking the symmetry of eigenvectors reflecting the filter structure into account. Computational complexity for the trajectories was decreased by approximating the wave packets propagating on the filters in single-mode variable-separable form which leads to the simplification of the drift term of NSODE (18).

One of our future works is to apply the presented method to performance estimation of physical mesoscopic devices.

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