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# A path-integration calculation method based on the real-space finite-difference scheme

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**Abstract**

We propose a new path-integration calculation method to treat the time evolution of a wavefunction within the framework of the real-space finite-difference formalism, and also develop an effective scheme to compute the scattering wavefunction for an incident electron with arbitrary energy, in which an impulse wavefunction is adopted as an initial state of the time evolution. In this method, once the time evolution of the initial impulse wavefunction is calculated, all of the solutions in the scattering problem can be derived by means of Fourier analysis of the time-evolved wavefunction, which leads to a reduction of the calculation time. In order to test the applicability of our newly developed simulation procedures, we implemented simulations for the one-dimensional scattering problem. Each simulation showed the usefulness of the present scheme by yielding the steady scattering states in agreement with exact ones.

## 1. Introduction

Many studies on numerical calculation schemes for solving the time-dependent Schrödinger or Kohn–Sham equations have been reported [1–5]. The prime objectives of these numerical calculations of electron dynamics are mainly for the design of nanoscale electronic devices, because the kinetics of electrons in the nanostructures are ballistic so that many interesting but unexpected quantum effects appear in the electromagnetic properties of the devices, for example the quantization or oscillation of electronic conduction through nanoscale wires or structures. In future applications of these numerical calculations to electronic devices, more accurate and extensive simulations will be required.

In this study we propose a time- and cost-saving numerical calculation scheme to obtain steady scattering eigenstates which directly connect with computing the electron conductivity and designing nanoscale devices. We derive an expression for the time evolution of the

  

wavefunction by starting with the Feynman path-integration representation and using the real-space finite-difference formulation [6]. This formalism has been developed so as to yield an overbridging boundary-matching (OBM) method that has been successfully applied to simulation of the electron conductivity [7–11]. In the obtained formula, we discriminate a part of the integrand which can be calculated in advance, which ensures a drastic diminution of the calculation time and costs for the calculation of the time evolution.

We also present an ingenious method to calculate the eigenstates at arbitrary assigned incident energy in the scattering problem, in which an impulse wavefunction is adopted as an initial state of the time evolution. In this method, once the time evolution of the initial impulse wavefunction is calculated all of the eigenstates of scattering problems can be derived by means of Fourier analysis of the wavefunctions, which means a tremendous reduction of the calculation time.

Finally, in order to test the applicability of the newly developed simulation procedures, we implemented simulations for the one-dimensional scattering problem. Each simulation showed the usefulness of the present scheme by reproducing the steady scattering states which agree with exact ones.

Below, in section 2, we provide detailed formulations within the real-space finite-difference scheme, and propose a new method to calculate the steady scattering states by using an impulse as an initial wavefunction as well as Fourier analysis. In section 3 we test our newly proposed method by applying it to the one-dimensional scattering problem. A summary of our findings is given in section 4.

## 2. Theoretical formulation

### *2.1. Real-space finite-difference formalism for the time-dependent Schrödinger equation*

In this section we discuss a representation of the time evolution of the wavefunction $\psi(x,t)$ based on the real-space finite-difference approach. To avoid unnecessary complexity, we restrict ourselves in this paper to the one-dimensional problem. It is known that the solution of the time-dependent Schrödinger equation,

$$\mathrm{i}\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t), \tag{1}$$

is described by the following integration including the Feynman propagator $K$ [12]:

$$\psi(x,t) = \int_{-\infty}^{\infty} K(x,t;x',t_0)\psi(x',t_0)\,\mathrm{d}x', \tag{2}$$

where $\psi(x,t_0)$ is the wavefunction at an initial time $t_0$, $H = -\frac{1}{2}\nabla^2 + V(x,t)$ is the Hamiltonian and $V(x,t)$ is the potential. According to the Feynman path-integral theory, the time evolution of the wavefunction $\psi(x,t)$ during a small time interval $\Delta t$ is expressed as [12]

$$\psi(x,t+\Delta t) = \sqrt{\frac{1}{2\pi\mathrm{i}\Delta t}}\int_{-\infty}^{\infty}\mathrm{d}x'\mathrm{e}^{\mathrm{i}\frac{(x-x')^2}{2\Delta t}}\mathrm{e}^{-\mathrm{i}\Delta t V(\frac{x+x'}{2})}\psi(x',t). \tag{3}$$

Here, the potential $V$ is assumed to be time independent for simplicity. In equation (3) we encounter some disadvantage that the integrand oscillates with respect to the value of $(x-x')$ so that the numerical value of the integration converges very slowly. In order to avoid this problem we will apply the real-space finite-difference formalism.

Since it is expected that only the neighbourhood of $x$ is significant in the integration over $x'$ in equation (3) [12], the integral variable $x'$ is transformed to $\eta$ as $x' = x + \eta$, and then the

Taylor expansion of $\psi(x+\eta,t)$ and $V(x+\frac{\eta}{2})$ around $x$ is carried out to obtain

$$\begin{aligned}\psi(x,t+\Delta t) &= \sqrt{\frac{1}{2\pi \mathrm{i}\Delta t}}\int_{-\infty}^{\infty} \mathrm{d}\eta\, \mathrm{e}^{\mathrm{i}\frac{\eta^2}{2\Delta t}}\left[1+\eta\frac{\partial}{\partial x}+\frac{1}{2}\eta^2\frac{\partial^2}{\partial x^2}+\cdots\right]\psi(x,t)\\ &\quad\times \mathrm{e}^{-\mathrm{i}\Delta t V(x)}\left[1-\mathrm{i}\Delta t\left(\frac{\eta}{2}\frac{\partial}{\partial x}+\frac{1}{2}\left(\frac{\eta^2}{2}\right)\frac{\partial^2}{\partial x^2}+\cdots\right)V(x)\right]\\ &= \mathrm{e}^{-\mathrm{i}\Delta t V(x)}\left[1+\frac{\mathrm{i}\Delta t}{2}\frac{\partial^2}{\partial x^2}\right]\psi(x,t)+\mathrm{O}((\Delta t)^2). \end{aligned} \tag{4}$$

Here, the integration over $\eta$ has been performed analytically.

Now we move on to the real-space finite-difference scheme. Consider that the space is divided uniformly with the grid spacing $\Delta x$. Then, the wavefunction is expressed in the form of the discrete Fourier transform

$$\psi(x_\ell,t)=\int_{-\frac{\pi}{\Delta x}}^{\frac{\pi}{\Delta x}} \mathrm{d}k\, C(k,t)\mathrm{e}^{\mathrm{i}kx_\ell}, \tag{5}$$

where $x_\ell=\Delta x\times\ell$, $\ell=-\infty,\ldots,-1,0,1,\ldots,\infty$, and

$$C(k,t)=\frac{\Delta x}{2\pi}\sum_{\ell=-\infty}^{\infty}\psi(x_\ell,t)\mathrm{e}^{-\mathrm{i}kx_\ell}. \tag{6}$$

In the real-space finite-difference formulation, the second derivative of $\psi(x_\ell,t)$ with respect to the $x$ coordinate is given by [13]

$$\frac{\partial^2}{\partial x^2}\psi(x_\ell,t)=\sum_{n=-N}^{N}c_n\psi(x_\ell+n\Delta x)+\mathrm{O}((\Delta x)^{2N+2}). \tag{7}$$

Adopting $N=1$, $c_n=-\frac{2}{(\Delta x)^2}$ and $c_{n\pm1}=\frac{1}{(\Delta x)^2}$, which correspond to the central difference formula, the second derivative of the wavefunction can be approximated as [13]

$$\begin{aligned}\frac{\partial^2}{\partial x^2}\psi(x_\ell,t) &\approx \frac{\psi(x_\ell-\Delta x,t)-2\psi(x_\ell,t)+\psi(x_\ell+\Delta x,t)}{(\Delta x)^2}\\ &= \int_{-\frac{\pi}{\Delta x}}^{\frac{\pi}{\Delta x}}\mathrm{d}k\, C(k,t)\frac{1}{(\Delta x)^2}\left[\mathrm{e}^{\mathrm{i}k(x_\ell-\Delta x)}-2\mathrm{e}^{\mathrm{i}kx_\ell}+\mathrm{e}^{\mathrm{i}k(x_\ell+\Delta x)}\right]\\ &= \int_{-\frac{\pi}{\Delta x}}^{\frac{\pi}{\Delta x}}\mathrm{d}k\, C(k,t)\frac{-2}{(\Delta x)^2}\mathrm{e}^{\mathrm{i}kx_\ell}\left[1-\cos(k\Delta x)\right]. \end{aligned} \tag{8}$$

Consequently, inserting equations (5), (6) and (8) into equation (4), we have the following representation:

$$\begin{aligned}\psi(x_\ell,t+\Delta t) &\approx \mathrm{e}^{-\mathrm{i}\Delta t V(x)}\int_{-\frac{\pi}{\Delta x}}^{\frac{\pi}{\Delta x}}\mathrm{d}k\, C(k,t)\left[1-\frac{\mathrm{i}\Delta t}{(\Delta x)^2}[1-\cos(k\Delta x)]\right]\mathrm{e}^{\mathrm{i}kx_\ell}\\ &\approx \sum_{\ell'}U(x_\ell,t+\Delta t;x_{\ell'},t)\psi(x_{\ell'},t), \end{aligned} \tag{9}$$

where

$$U(x_\ell,t+\Delta t;x_{\ell'},t)=\mathrm{e}^{-\mathrm{i}\Delta t V(x_\ell)}P(\ell-\ell'), \tag{10}$$

$$P(\ell-\ell')=\frac{\Delta x}{2\pi}\int_{-\frac{\pi}{\Delta x}}^{\frac{\pi}{\Delta x}}\mathrm{d}k\,\mathrm{e}^{\mathrm{i}k(x_\ell-x_{\ell'})}\mathrm{e}^{-\mathrm{i}\frac{\Delta t}{(\Delta x)^2}[1-\cos(k\Delta x)]}. \tag{11}$$

The function $P(\ell-\ell')$ attenuates rapidly with $\ell-\ell'$; for example, when $\Delta x=0.5$ au, $\Delta t=0.2$ au and $\ell-\ell'=10$, the absolute value of $P(\ell-\ell')$ is less than $1.0\times10^{-8}$. It implies

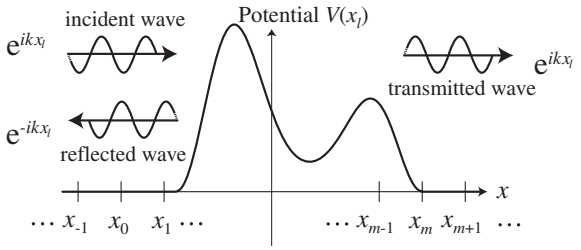


**Figure 1.** Schematic representation of a one-dimensional system with a transition region composed of the potential with barrier height $V(x_\ell)$. In this model, the incident wave comes from the left side and is scattered by the potential.

that a small number of grid points $\ell'$ near $\ell$ is sufficient for the summation in equation (9) depending on the required accuracy. In addition, $P(\ell - \ell')$ does not depend on the potential and the wavefunction so that the numerical value of $P(\ell - \ell')$ can be calculated in advance. These facts clearly ensure a drastic reduction of the calculation time and cost. Here, we note that $U(x_\ell, t; x_{\ell'}, t_0)$ corresponds to the propagator, that is, $\langle x_\ell | e^{-i\widehat{H}(t-t_0)} | x_{\ell'} \rangle$, and $\widehat{H}$ is the matrix representation of the Hamiltonian in the real-space finite-difference form.

### *2.2. A method to treat scattering states with an impulse response*

We present an ingenious method to compute the scattering wave function $\varphi(x; E)$ for an electron with incident energy $E$, in which an impulse wavefunction $\psi(x, t_0)$ is adopted as an initial state of the time evolution.

Defining $E^+ = E + i\epsilon$, with $\epsilon$ being a positive infinitesimal, we have

$$\int_{t_0}^{\infty} e^{i(E+i\epsilon)(t-t_0)} U(x_\ell, t; x_{\ell'}, t_0)\, dt = \langle x_\ell | \int_{t_0}^{\infty} e^{[i(E-\widehat{H})-\epsilon](t-t_0)}\, dt\, | x_{\ell'} \rangle$$
$$= i \left[ \frac{1}{E + i\epsilon - \widehat{H}} \right]_{\ell,\ell'}. \tag{12}$$

On the other hand, by the definition of the retarded Green's function,

$$G^r(x_\ell, x_{\ell'}; E) = \lim_{\epsilon \to 0^+} \left[ \frac{1}{E + i\epsilon - \widehat{H}} \right]_{\ell,\ell'}. \tag{13}$$

We thus find the relationship between Green's function and the propagator to be

$$iG^r(x_\ell, x_{\ell'}; E) = \int_{t_0}^{\infty} e^{iE(t-t_0)} U(x_\ell, t; x_{\ell'}, t_0)\, dt. \tag{14}$$

Consider the one-dimensional scattering problem as shown in figure 1, in which the incident wavefunction $\varphi_L^{\text{in}}(x_\ell, E) = e^{ikx_\ell}$ ($\ell \leqslant 0, k > 0$) comes from the left side and propagates to the right side. Under the real-space finite-difference formalism, the whole scattering wavefunction $\varphi_L(x_\ell; E)$ corresponding to this incident wavefunction $\varphi_L^{\text{in}}(x_\ell, E)$ is given by [6]

$$\varphi_L(x_\ell; E) = \frac{i}{\Delta x} v_g(E) G^r(x_\ell, x_{\ell'}; E) e^{ikx_{\ell'}}, \qquad (\ell' \leqslant 0 \leqslant \ell), \tag{15}$$

where $v_g(E) \equiv \frac{dE}{dk} = \frac{\sin(k\Delta x)}{\Delta x}$ is the group velocity of the incident wavefunction, and the wavenumber $k = \frac{1}{\Delta x} \cos^{-1}(1 - (\Delta x)^2 E)$. By inserting equation (14) into (15), the scattering wavefunction is written as

$$\varphi_L(x_\ell; E) = \frac{1}{\Delta x} v_g(E) \int_{t_0}^{\infty} dt\, e^{iE(t-t_0)} U(x_\ell, t; x_{\ell'}, t_0) e^{ikx_{\ell'}}. \tag{16}$$

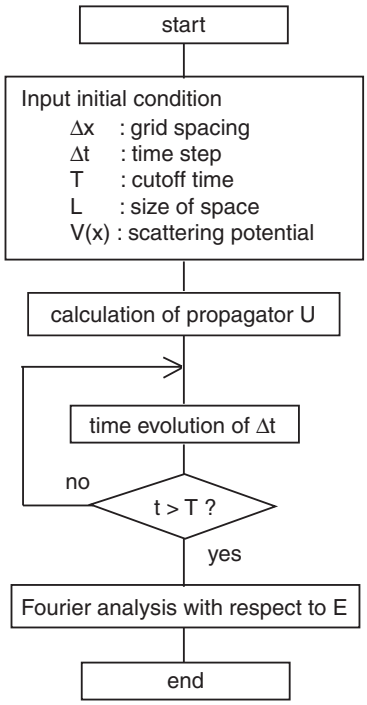


**Figure 2.** Flow diagram of the procedure for numerical calculations.

To make the argument concrete, let us choose $\ell' = 0$. Then equation (16) reads as

$$\varphi_L(x_\ell; E) = \frac{1}{\Delta x} v_g(E) e^{ikx_0} \int_{t_0}^{\infty} dt\ e^{iE(t-t_0)} U(x_\ell, t; x_0, t_0). \tag{17}$$

Now, we install an impulse function as an initial wavefunction $\psi(x_\ell, t_0)$,

$$\psi(x_\ell, t_0) = \begin{cases} 1 & \text{for } \ell = 0 \\ 0 & \text{for } \ell \neq 0. \end{cases} \tag{18}$$

The time-evolved $\psi(x_\ell, t_0)$ is given by

$$\begin{aligned} \psi(x_\ell, t) &= \sum_{\bar{\ell}} U(x_\ell, t; x_{\bar{\ell}}, t_0) \psi(x_{\bar{\ell}}, t_0) \\ &= U(x_\ell, t; x_0, t_0). \end{aligned} \tag{19}$$

Employing equations (17) and (19), we obtain the following final representation for the steady scattering states $\varphi_L(x_\ell; E)$, which is defined only in the right side of the initial impulse:

$$\varphi_L(x_\ell; E) = \gamma(E) \lim_{T\to\infty} \int_{t_0}^{T} dt\ e^{iE(t-t_0)} \psi(x_\ell, t) \qquad (0 \leqslant \ell) \tag{20}$$

with $\gamma(E)$ being $\frac{1}{\Delta x} v_g(E) e^{ikx_0}$. Here, $T$ is the cut-off parameter of time integration.

A flow diagram of the procedure for numerical calculation of the above formulation is shown in figure 2. Once the time-evolved form $\psi(x_\ell, t)$ of the initial impulse wavefunction is calculated, all of the eigenstates of the scattering problem $\varphi_L(x_\ell; E)$ can be derived by means of the Fourier analysis of $\psi(x_\ell, t)$. This calculation treatment explicitly gives rise to the reduction of the calculation time.

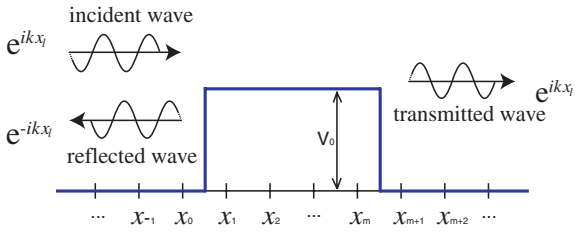


**Figure 3.** Schematic depiction of the configured one-dimensional system in which a constant potential barrier is assigned for the examination of the proposed calculation procedure.

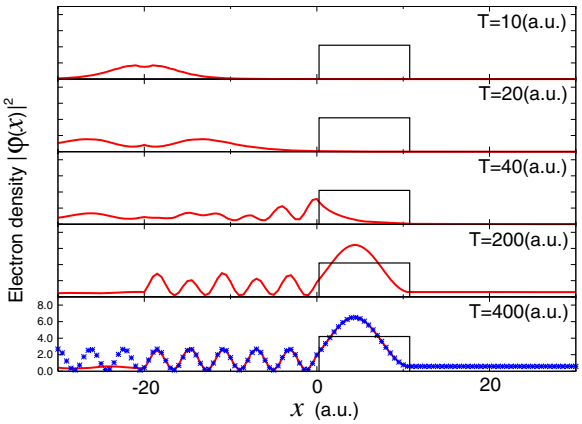


**Figure 4.** Convergence of the electron-charge densities for the case of assigned incident energy $E = 0.33$ au derived by Fourier analysis of the time-evolved wavefunction. The exact solution is also shown by '$\times$' in comparison with the calculated result at $T = 400$ au.

## 3. Application to the one-dimensional scattering problem

In order to examine the accuracy of the above-mentioned scheme, we apply it to the one-dimensional scattering problem. Solving the scattering problem with an arbitrary potential barrier is an important issue, because its solution yields to a knowledge of electron conduction through a nanoscale structure and leads to effective design of nanoscale electronic devices.

Figure 3 illustrates a schematic depiction of the test model of the one-dimensional problem including a constant barrier potential $V_0$. In the present examination, we assigned the parameters for calculations as follows: grid spacing $\Delta x = 0.5$ au, time step $\Delta t = 0.2$ au, the barrier height of the constant potential $V = 0.3$ au and the width of the barrier 10.5 au. We configured an initial impulse wave function at a distance of 20 au on the left side of the potential barrier.

Figure 4 describes the calculated charge density of the eigenstates $\varphi_L(x; E)$ at an assigned incident energy $E = 0.33$ au. The calculated state approaches the exact solution depending on the time evolution, and it agrees sufficiently with the exact solution at the time cut-off $T = 400$ au. The resulting eigenstates are independent of the position of the initial impulse, on the condition that the initial impulse wave function is set at the left side region of the scattering potential. We used equation (20), which is defined only in the right side of the initial impulse, so that the resulting eigenstate has no physical significance in the region of the left side of the initial impulse. In figure 4, the initial impulse was set at $-20$ au, so any discussion or

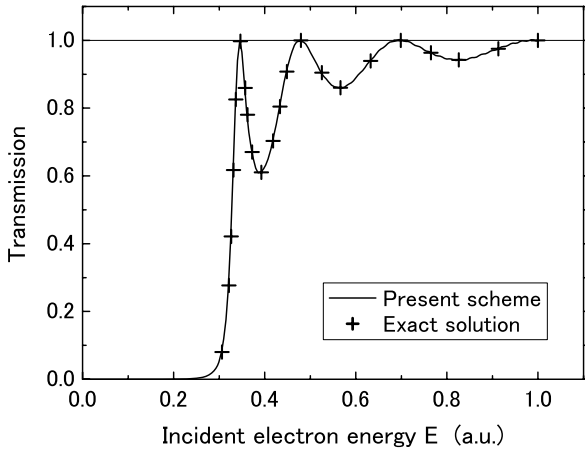


**Figure 5.** Calculated transmission as a function of the incident energy $E$, in comparison with the exact solutions plotted by '+'.

estimation on the coincidence between the obtained numerical value and the exact one in the region of $x \leqslant -20$ has no significance.

In figure 5, we show the calculated transmissions of the electron as a function of the incident energy $E$, and the exact solution given by the real-space finite-difference scheme is also indicated. These obtained results using the newly developed scheme are found to be in good agreement with the exact solutions.

## 4. Conclusions

We have proposed a new path-integration calculation method to treat the time evolution of a wavefunction within the framework of the real-space finite-difference formalism, and have also developed an effective method to compute the scattering wavefunction at an arbitrary assigned incident energy.

In our newly derived formulation for the time evolution no difficulty appears in the calculation when in using the Feynman path-integration representation. In addition, we discriminate part of the integrand that can be calculated in advance, which ensures a drastic diminution of the calculation time and costs.

We have proposed a new method for determining the eigenstates on the scattering problems, in which once the time evolution of an initial impulse wavefunction is calculated all of the eigenstates at arbitrary assigned incident energy $E$ can be derived by means of Fourier analysis of the time-evolved wavefunctions. Also, we propose an effective calculation procedure based upon the theoretical formulation.

Finally, in order to test the accuracy and applicability of the newly developed simulation procedures, we implemented simulations for the one-dimensional scattering problem in which the usefulness of the present scheme was shown in yielding the steady states which agree with exact ones.

On the basis of the present results, we are optimistic about the further development of our proposal. We will apply our procedures to two- and three-dimensional scattering problems with the aim of discussing the conduction or any other electromagnetic properties of nanoscale structures.

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