Absorbing boundary conditions for the finite-difference time-domain calculation of the one-dimensional Schrödinger equation

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The absorbing boundary conditions for the finite-difference calculation of the time-dependent one-dimensional Schrödinger equation are presented. These are the local boundary conditions that approximate the one-way wave equation of a wave function. The conditions minimize undesirable reflections at the artificial boundaries of the area of computation, thus enabling us to limit the computation area efficiently. The calculations of the transmission coefficient of multibarrier tunneling show the validity of the method.

INTRODUCTION

The solutions of a time-dependent Schrödinger equation have been studied in order to provide insight into the dynamics of quantum-mechanical systems.[1] These time-domain calculations also seem to be useful in estimating the responses of various quantum-effect devices[2] now becoming possible by the recent progress in fine process technologies. In a one-dimensional case, the following equation is set to the starting point of the discussion:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial^2 x}+U(x)\right]\Psi(x,t)\ , \tag{1}$$

where $U(x)$ is the potential given as a function of x, m^* is effective mass of the particle, and $\hbar=h/2\pi$ in which h is Planck's constant. Temporal evolution of the wave function $\Psi(x,t)$ can be integrated from the initial values $\Psi(x,0)$ step by step in time by using the finite difference expression of Eq. (1) given as

$$\begin{aligned}i\hbar\frac{\Psi(x,t+\Delta t)-\Psi(x,t-\Delta t)}{2\Delta t}&\\ =-\frac{\hbar^2}{2m^*}\frac{\Psi(x+\Delta x,t)-2\Psi(x,t)+\Psi(x-\Delta x,t)}{\Delta x^2}&\\ +U(x)\Psi(x,t)\ ,&\end{aligned} \tag{2}$$

where Δx and Δt are discretization length in space and time, respectively. In such a calculation, the problem of the numerical stability and the preservation of normalization of the wave function are often raised. It may be helpful to notice that expression (2) is derived from the equation of the time-increment operator:

$$\Psi(x,t+\Delta t)=e^{-2i\Delta tH/\hbar}\Psi(x,t-\Delta t)$$

by substituting

$$e^{-2i\Delta tH/\hbar}\cong\frac{1-i\Delta tH/\hbar}{1+i\Delta tH/\hbar}\ ,$$

$$\frac{\Psi(x,t+\Delta t)+\Psi(x,t-\Delta t)}{2}\cong\Psi(x,t)\ ,$$

and

$$H\cong-\frac{\hbar^2}{2m^*}\frac{\Psi(x+\Delta x,t)-2\Psi(x,t)+\Psi(x-\Delta x,t)}{\Delta x^2}+U(x)\Psi(x,t)\ .$$

The above approximation of $e^{-2i\Delta tH/h}$ preserves the unitarity of the operator, so that Eq. (2) ensures the constancy of normalization of the wave function as time goes on. Also noticed is that Eq. (2) has an explicit form that differs from that presented in Ref. 1. For more details concerning this problem, the reader is referred to Ref. 1. The other problem is the subject of this Brief Report. In practical calculations, because of the finite capacity of memories, the area of computation must be limited to appropriate size. In many cases, one hopes to set the absorbing boundary conditions at the end of the computation area so that the undesirable spurious reflections at the boundaries affect the solution in the long time period. Here, we concentrate on the details of the absorbing boundary conditions and the scattering (reflection-transmission) problem is considered.

ABSORBING BOUNDARY CONDITIONS

Let us consider the computation area of $x=[0,N\Delta x]$, where N is a positive integer. Then, using Eq. (2), the values Ψ_n^l, $n=1,2,\ldots,N-1$, can be calculated from Ψ_n^{l-1} and Ψ_n^{l-2}. (Different expressions that allow calculating Ψ_n^l only from Ψ_n^{l-1} are presented in Ref. 1.) Here, we denoted the wave-function values $\Psi(n\Delta x,l\Delta t)$ as Ψ_n^l. If one takes a boundary condition such as $\Psi_0^l=\Psi_N^l=0$ for all l, perfect reflections occur as if the infinite potential walls exist at the boundaries. In order to obtain the formulas for the absorbing boundary conditions, we first consider the special solutions of Eq. (1):

$$\Psi(x,t)=e^{-i(\omega t-kx)}\ . \tag{3}$$

These are the states of the definite energy E and satisfy the dispersion relation

$$\hbar^2k^2=2m^*(\hbar\omega-U)\ , \tag{4}$$

which is obtained by substituting $E=\hbar\omega$ and $p=\hbar k$ into $p^2=2m^*(E-U)$, where p is the momentum of the parti-

cle. Solving (4) in terms of $\hbar k$, we get

$$\hbar k = \pm[2m^*(\hbar\omega - U)]^{1/2} . \tag{5}$$

In this equation, plus and minus signs means the right-going and left-going waves, respectively. Thus, the absorbing boundary conditions should be designed to satisfy the dispersion relation given by the plus-signed Eq. (5) at the boundary $x = N\Delta t$ and the minus-signed Eq. (5) at the boundary $x = 0$. These are the one-way wave equations[3] for the wave function. This dispersion relationship is illustrated in Fig. 1 in the case of the right-going wave. Unfortunately, function (5) is not rational and cannot be converted into a partial differential equation. Therefore we approximate this relation to

$$\hbar k = \pm\frac{(2m^*\alpha_2)^{1/2} - (2m^*\alpha_1)^{1/2}}{\alpha_2 - \alpha_1}(\hbar\omega - U) \pm \frac{\alpha_2(2m^*\alpha_1)^{1/2} - \alpha_1(2m^*\alpha_2)^{1/2}}{\alpha_2 - \alpha_1} . \tag{6}$$

Equation (6) is a straight line in Fig. 1, crosses Eq. (5) at $\hbar\omega - U = \alpha_1$ and α_2. The plus and minus signs in (5) correspond to the right-going and left-going waves, respectively. The correspondence of $\partial/\partial t \Longleftrightarrow -i\omega$ and $\partial/\partial x \Longleftrightarrow ik$ leads us to rewrite Eq. (6) into a partial differential equation of

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[-i\hbar\frac{1}{g_1}\frac{\partial}{\partial x} + U - \frac{g_2}{g_1}\right]\Psi(x,t) , \tag{7}$$

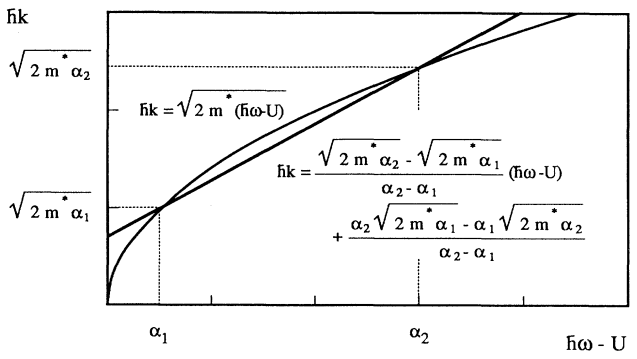

FIG. 1. The dispersion relation and its first-order approximation for the right-going wave.

where

$$g_1 = \pm\frac{(2m^*\alpha_2)^{1/2} - (2m^*\alpha_1)^{1/2}}{\alpha_2 - \alpha_1}$$

and

$$g_2 = \pm\frac{\alpha_2(2m^*\alpha_1)^{1/2} - \alpha_1(2m^*\alpha_2)^{1/2}}{\alpha_2 - \alpha_1} . \tag{8}$$

Then, the finite-difference expression of Eq. (7) is

$$i\hbar\frac{\Psi(x+\Delta x,t+\Delta t)+\Psi(x,t+\Delta t)-\Psi(x+\Delta x,t)-\Psi(x,t)}{2\Delta t} = -i\hbar\frac{1}{g_1}\frac{\Psi(x+\Delta x,t+\Delta t)+\Psi(x+\Delta x,t)-\Psi(x,t+\Delta t)-\Psi(x,t)}{2\Delta x} + \left[U - \frac{g_2}{g_1}\right]\frac{\Psi(x+\Delta x,t+\Delta t)+\Psi(x+\Delta x,t)+\Psi(x,t+\Delta t)+\Psi(x,t)}{4} . \tag{9}$$

Thus, we obtain the calculation formula at $x = 0$ as

$$\Psi_0^l = \frac{-C_1(\Psi_1^l - \Psi_1^{l-1} - \Psi_0^{l-1}) + C_2(\Psi_1^l + \Psi_1^{l-1} - \Psi_0^{l-1}) + C_3(\Psi_1^l + \Psi_1^{l-1} + \Psi_0^{l-1})}{C_1 + C_2 - C_3} \tag{10}$$

and at $x = N\Delta x$ as

$$\Psi_N^l = \frac{-C_1(\Psi_{N-1}^l - \Psi_N^{l-1} - \Psi_{N-1}^{l-1}) + C_2(\Psi_N^{l-1} - \Psi_{N-1}^l - \Psi_{N-1}^{l-1}) + C_3(\Psi_N^{l-1} + \Psi_{N-1}^l + \Psi_{N-1}^{l-1})}{C_1 - C_2 - C_3} , \tag{11}$$

where $C_1 = i\hbar/2\Delta t$, $C_2 = -i\hbar/2\Delta x g_1$, and $C_3 = (U - g_2/g_1)/4$, taking minus signs in Eqs. (8) for g_1 and g_2 of (10) and plus signs for (11).

NUMERICAL RESULTS

Figure 2 shows the calculated temporal evolution of wave packet propagating toward the boundary of the computation area. In this calculation, $U(x) = 0$, $\Delta x = 5$ Å, and $\Delta t = 0.01$ fs. A Gaussian wave packet given by Eq. (12) is supposed for the initial wave function $\Psi(x,0)$:

$$\Psi(x,0) = \exp\left[-\frac{(x - x_0)^2}{2\sigma^2} + ik_0 x\right] . \tag{12}$$

In this case, $\sigma = 20\Delta x = 100$ Å and k_0 is taken as $k_0 = (2m^*E_0)^{1/2}/\hbar$, where $E_0 = 0.5$ eV. It is clearly demonstrated that the wave packet is absorbed at the end of the computation area $x = 200\Delta x$ in which Eq. (11) is applied. No reflection is recognized from the figure. Figure 3 presents a typical energy dependence of the reflection coefficient at the absorbing boundary. The

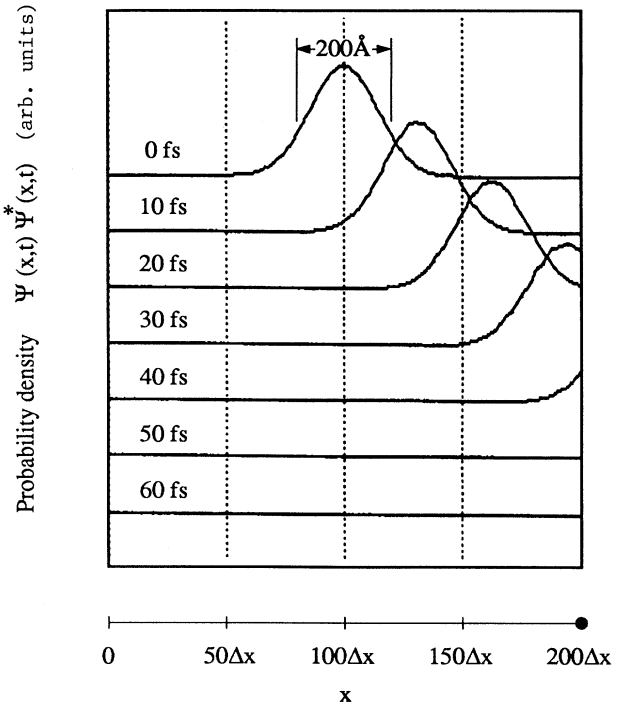

FIG. 2. The temporal evolution of the Gaussian wave packet. The absorbing boundary condition ($\alpha_1=0.7$ eV, $\alpha_2=0.9$ eV) is applied at the boundary $x=200\Delta x$. The wave packet has a mean energy of about 0.5 eV and a dispersion of about 0.1 eV in energy space.

reflection characteristics depend upon not only the parameters α_1 and α_2 but also the discretizing length Δx and Δt. However, less than -40 dB (1% error) is easily achieved over a wide range of energy.

To test the validity in practical applications, the

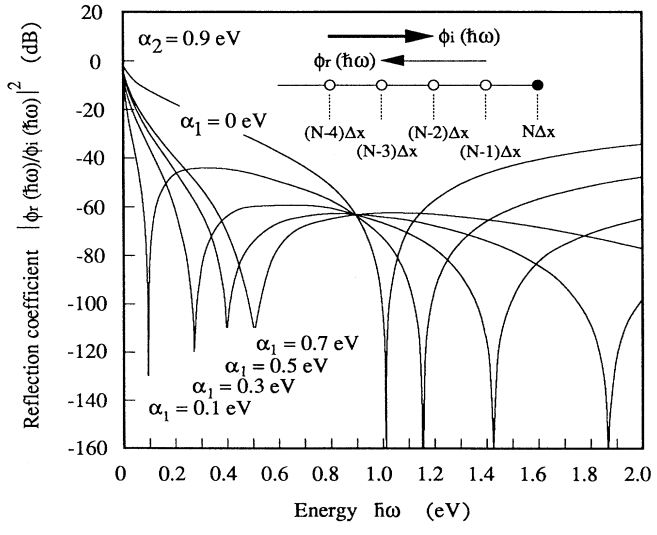

FIG. 3. The typical reflection (reflection coefficient vs energy) characteristics of the absorbing boundary conditions. α_1 is taken as a parameter. $\alpha_2=0.9$ eV, $U=0$ eV, $\Delta x=5$ Å, and $\Delta t=0.01$ fs.

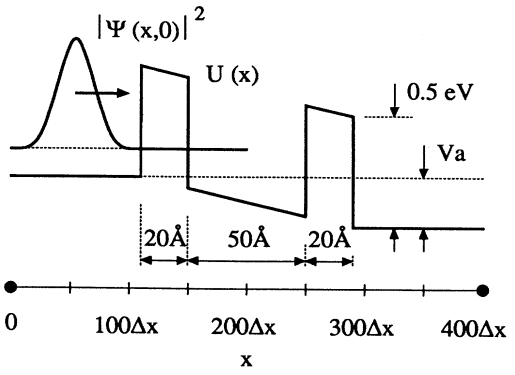

FIG. 4. The calculated multibarrier structure and analysis conditions. The computation area is $[0,400\Delta x]$. $\Delta x=0.5$ Å and $\Delta t=10^{-19}$ s. The absorbing boundary condition is adopted at the points $x=0$ and $400\Delta x$. The initial wave function $\Psi(x,0)$ is described by Eq. (12) in which σ is equal to $20\Delta x=10$ Å, $k_0=[(2m^*)0.5\text{ eV}]^{1/2}/\hbar$.

transmission coefficients of multibarrier tunneling are calculated in the following way. Figure 4 shows the potential profile of the calculated multibarrier structure. The profile used for the initial wave function $|\Psi(x,0)|^2$ is also illustrated. $\Psi(x,0)$ is defined by Eq. (12), in which the parameters σ and k_0 (>0) are determined so as to have a broadened spectrum in the interested area of energy space. The temporal evolution of the wave function in this system is calculated by the previously described finite-difference time-domain scheme. If the right-going wave is perfectly absorbed at the boundary $x=400\Delta x$ and the left-going wave reflected by the multibarrier is perfectly absorbed at the boundary $x=0$, the transmission coefficient $T(\hbar\omega)T^*(\hbar\omega)$ is calculated by

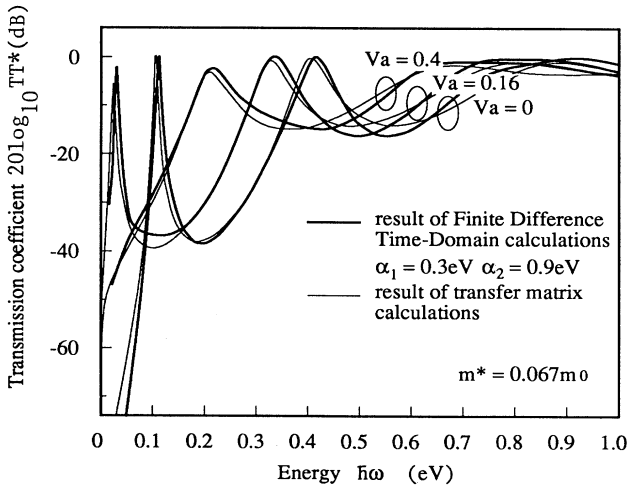

FIG. 5. The comparison of the transmission coefficients of multibarrier tunneling obtained from the finite-difference time-domain calculation and the transfer-matrix calculation.

$$T(\hbar\omega)T^*(\hbar\omega)=\frac{|\phi_{x=400\Delta x}(\hbar\omega)|^2 k_{x=400\Delta x}}{|\phi_{\text{initial}}(\hbar\omega)|^2 k_{\text{initial}}}\ , \qquad (13)$$

where $|\phi_{x=400\Delta x}(\hbar\omega)|$ is an amplitude of the transmitted wave component in the energy space obtained by the Fourier transform of $\Psi(400\Delta x,t)$. $|\phi_{\text{initial}}(\hbar\omega)|$ is that of the component $k\geq 0$ involved in the initial wave function $\Psi(x,0)$. $\hbar k_{\text{initial}}=(2m^*\hbar\omega)^{1/2}$ and $\hbar k_{x=400\Delta x}=[2m^*(\hbar\omega+eV_a)]^{1/2}$. The calculation was performed with the discretization length of $\Delta x=0.5$ Å and $\Delta t=10^{-19}$ s. The results are plotted in Fig. 5. For comparison, the transfer-matrix calculation[4] of the same structure is carried out. Excellent agreement is obtained between both results as shown in Fig. 5.

SUMMARY

The absorbing boundary conditions are derived for the finite-difference time-domain calculation of a one-dimensional Schrödinger equation. Using these conditions, the undesirable reflection of the impinging wave packet can be strongly reduced at the boundary of the computation area. This makes it possible to solve the scattering problem by time-domain calculations as demonstrated. Extensions to the two-dimensional problem are now being planned.[5]

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