Solving the time-dependent Schrödinger equation: Suppression of reflection from the grid boundary with a filtered split-operator approach

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We present the split-operator approach, with an additional filtering step, for solving the time-dependent Schrödinger equation that significantly suppresses the backreflection of waves from the grid boundaries. [S1063-651X(98)01712-7]

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Currently the split-operator technique [1] is the most popular method for solving the time-dependent Schrödinger equation. It is very efficient if the system being studied does not involve any free (unbound) states. It, as well as any other numerical methods, does not have a satisfactory way of handling unbound states because of its finite-size grid. Reflection from the grid boundary back into the interior is always a problem. There are two ways to handle this problem. The first way is to use a grid large enough such that the reflected waves will not reach the region of interest before the simulation is done. This is clearly not a good solution because in certain cases, such as in long interaction processes, the grid would have to be so big that it is impractical to implement. The second way, which is used often, is to put an absorbing potential at the grid boundary to absorb the wave packet. Unfortunately, the absorption is not always 100%. As an example, we show in Fig. 1 the evolution of a wave packet that starts out at the center of a static potential. The static potential only has one bound state, so the wave packet is a superposition of the lone bound state and continuum states. Details of the problem and the calculation will be described later, but in Fig. 1 we see the unbound part of the wave packet starts to move out of the static trapping potential and to the right. There is an absorbing potential at both ends of the grid. As the wave packet hits the right absorbing potential, reflection is generated. The reflected wave then travels back toward and through the trapping potential. This artificial reflection will contaminate any simulation result involving transition between the bound state and the continuum. An example of a bound to continuum transition situation is IR excitation and dissociation of molecular bonds. In general, the amount of reflection depends on the absorbing potential as well as the velocity of the wave packet when it approaches the absorbing potential. Tailoring the absorbing potential can always be done, but prior knowledge of the wave packet's velocity is not always possible. In this paper we describe a modification to the split-operator technique that suppresses reflection generated by the absorbing potential.

We begin with a recap of the split-operator technique. The system we want to simulate is the time-dependent Schrödinger equation,

$$i\hbar \frac{\partial\psi(x,t)}{\partial t} = \left[\frac{p^2}{2m} + V(x,t)\right]\psi(x,t) = H(x,t)\psi(x,t). \quad (1)$$

From now on we will assume $\hbar = 1$ and everything else is dimensionless. For a time step small enough so that the potential can be taken as constant, Eq. (1) can be integrated to give

$$\psi(x,t+\Delta t) = \exp[-iH(x,t)\Delta t]\psi(x,t). \quad (2)$$

Given the initial wave function, Eq. (2) is the recipe for getting the wave function at all subsequent time. The split-operator technique approximates the right hand side of Eq. (2) with

$$\begin{aligned}\exp[-iH(x,t)\Delta t] \approx \exp[-iV(x,t)\Delta t/2] \\ \times \exp[-ip^2\Delta t/2m] \\ \times \exp[-iV(x,t)\Delta t/2]. \quad (3)\end{aligned}$$

The error in using Eq. (3) is $O(\Delta t^3)$. The operation of the first and last exponential in Eq. (3) on the wave function is just straightforward multiplication. The middle exponential can be performed using fast Fourier transform (FFT) as in the original formulation of the split-operator technique [1] or done entirely in real space [2]. We have used the FFT approach to generate the result shown in Fig. 1. For that case, the trapping potential has the form

$$V_{\mathrm{trap}}(x) = \frac{[(2s+1)^2 - 1]}{8mW^2} \frac{1}{\cosh^2(x/W)}. \quad (4)$$

The number of bound states for this potential [3] is $n+1$ where n is the largest integer smaller than the parameter s. We chose $s = 0.1$, so there is only one bound state. The width parameter W is taken to be 0.2. The absorbing potential is a Gaussian

$$V_{\mathrm{abs}}(x) = -i\,\frac{10}{dt}\exp[-(x-x_c)^2/(8\Delta x)^2], \quad (5)$$

where $dt = 0.01$ is the time step, $\Delta x = 0.02$ is the spatial resolution, and x_c is the center is the absorbing potential. We chose the center to be a distance of 0.8 from either end of the grid. The length of the grid is 20.48 (1024 points on the grid). The initial wave function is

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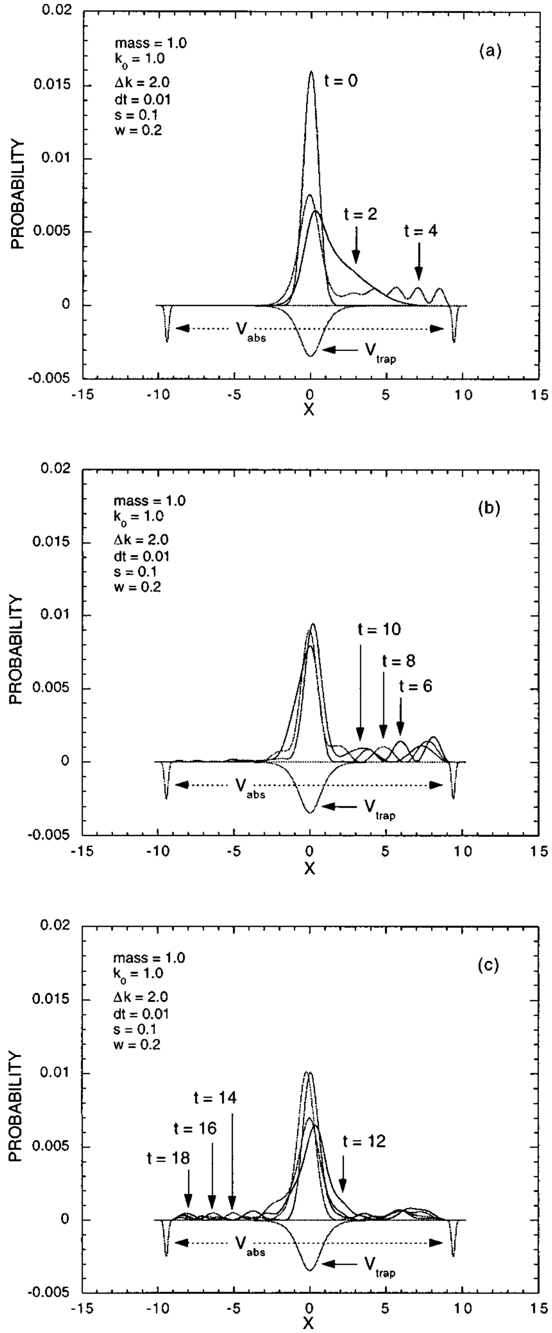

FIG. 1. Plot of the the wave function, with no filtering, at various times. The depiction of the trapping and absorbing potential are for visual purposes only, and their strengths are not to scale. Note that all quantities are dimensionless.

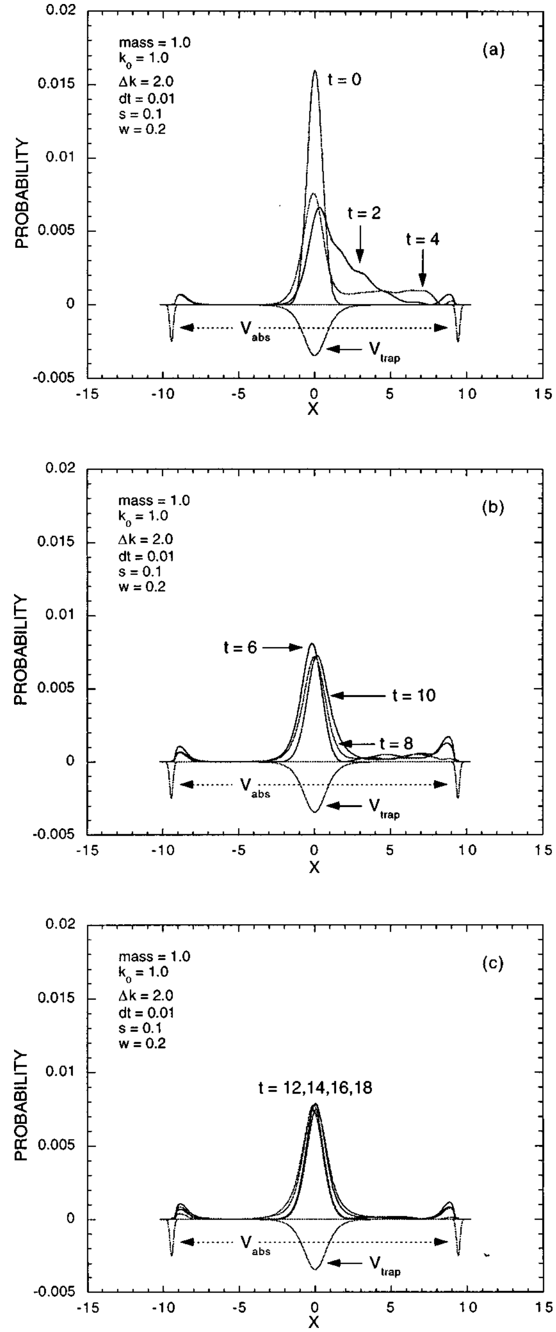

FIG. 2. Plot of the wave function, with filtering, at various times.

$$\psi(x,0)=\frac{1}{N}\exp[ik_0(x-x_0)-(x-x_0)^2\Delta k^2/4], \qquad (6)$$

where N is a normalization factor, $k_0=1.0$, $x_0=0$, and $\Delta k=2.0$. The mass m is taken to be 1.0. Given this initial wave function and the potential, we use the split-operator technique to produce the result shown in Fig. 1.

The idea for reducing reflection from the absorbing potential is based upon the fact that these reflected waves originate near the absorbing potential. So if we can filter them out as they are being generated then they will not reach the interior region of the grid. To do this we split the wave function into a right and a left traveling part

$$\psi(x)=\int_0^\infty dk\ \psi(k)e^{ikx}+\int_{-\infty}^0 dk\ \psi(k)e^{ikx}$$
$$=\psi_+(x)+\psi_-(x). \qquad (7)$$

After each time step we perform a filtering operation as follows. For the absorbing potential on the left (right) end of the grid, we subtract from the wave function the + (−) part of the wave function,

$$\psi_{\rm filter}(x)=\psi(x)-\psi_-(x), \quad \text{near the right boundary}, \qquad (8a)$$

$$\psi_{\text{filter}}(x) = \psi(x) - \psi_{+}(x), \quad \text{near the left boundary.} \tag{8b}$$

The region where the subtraction is carried out is limited to a small distance near the absorbing potential. This is to prevent spurious alteration to the bound state of the problem. In other words, the region where the subtraction is performed should be far enough away such that there is no probability of finding a bound state there. In this paper we use a distance of 2.0 from the center of the absorbing potential for the subtraction region. In summary the absorbing potential will absorb, with some reflection, any wave traveling away from the interior of the grid, and the filtering operation will remove the reflected waves traveling toward the interior of the grid. The absorbing potential ensures that the wave function is zero at the boundary, so that we can get an accurate Fourier transform.

The result of this filtering operation on the same system corresponding to Fig. 1 is shown in Fig. 2. Notice the lack of the rippling that indicates reflected waves, particularly to the left of the trapping potential. In panel (c) we see the bound state sloshing back and forth in the well. In the subtraction region near the absorbing potentials, we have an enhancement of the wave function which we currently do not understand. In this region the probability just grows to some value and decays but does not seem to leak into the interior of the grid. The lack of leakage is not surprising since by construction this region can only move toward and not away from the absorbing potential. This artificial enhancement in the filtering region does not always occur as we will show in the next example of a free wave packet. To really see how much the filtering operation removes the reflected waves, we study the propagation of a free wave packet. In Fig. 3 we show the propagation of the free wave packet with $m=5.0$ and $k_0=5.0$ on a grid of length 10.24 (512 grid points). If the simulation was done on an infinite grid, the probability of

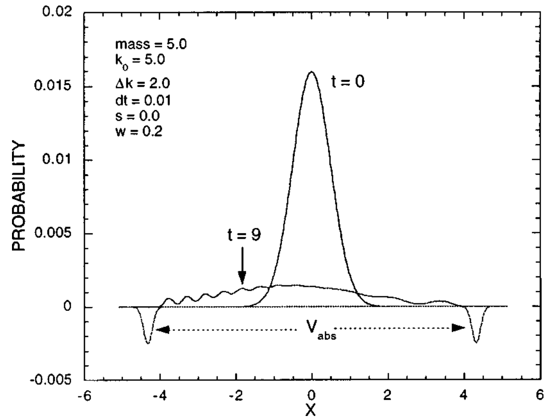

FIG. 3. Plot of the wave function at $t=0$ and at $t=9$ in absence of the trapping potential. The solid line corresponds to no filtering. The result with filtering at $t=9$ is indistinguishable from zero at this scale.

finding the particle in the region $-4<x<4$ will be zero after $t=9.0$ because the particle will have moved out of this region. Without the filtering, there is a significant part of the wave packet left in the grid at $t=9.0$ because of reflection. With filtering, the result is indistinguishable from 0 on the plot. We integrate over the grid to find the total probability in the filtered case, and it is less than 2×10^{-3}.

In conclusion, we have described a filtering step for the split-operator approach that can enhance the suppression of reflection from grid boundaries. This is of great utility for simulation involving continuum states.

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