Scientific Computing, Final Project

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Introduction

In this final project assignment, we are solving the time dependent Schrodinger equation for the problem of a Gaussian wavepacket travelling in free space, with some potential artifacts. The 1d Schrodinger equation,

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi,$$

is discretized for us in the problem with the unitary operator,

$$\psi^{n+1} = \frac{(1 + iH\Delta t/2)}{(1 - iH\Delta t/2)}\psi^n, \tag{1}$$

derived from the time evolution operator, split into two, and expanded in small δt. While unitary (which is great), this scheme will require the inverting of the matrix that is in the denominator of the above expression. To make this easier on us, we can define,

$$(1 + iH\Delta t/2)\chi^n = \psi^n,$$

which, when plugged into equation 1, yeilds the simple expression:

$$\psi^{n+1} = \chi^n - \psi^n.$$

Fortunately for us, the professor has provided an explicit form pf the relation between χ and ψ with the expression, that we can implement in a discretized space, indexed by j:

$$\chi^n_{j+1} + \left(-2 + \frac{4im\epsilon^2}{\hbar\Delta t} - \frac{2m\epsilon^2 V_j}{\hbar^2}\right)\chi^n_j + \chi^n_{j-1} = \frac{8im\epsilon^2}{\Delta t}\phi^n_j, \tag{2}$$

in which m is the mass of the particle(=1), ϵ is the grid spacing, and V_j is the potential at a grid point j.
So the key in the problems of this homework is to implement the above scheme in a range from -1 to 1, and see what happens.

Some general aspects of my program are as follows:

- Each gridpoint between -1.01 and 1.01 is indexed so that the end points on each end are forced to be 0. The grid spacing is a=0.01.
- Equation 2 is of the form Aχ = fψ, where f is some factor. Recognizing from the form of 2 that A is tridiagonal, I use the congugate gradient method to solve for χ at every iteration,

setting fψ = b. This works quickly and efficiently. From there I can use the relation between ψ^n and ψ^{n+1} to get the next values to plug in for b. At each iteration step, I take the initial guess for χ to be 0.

- In order to make things more efficient, I build A out of a few sparse matricies, which in Matlab, means that only non-zero elements are stored in memory. The basic form of A is:

$$A_{j,k} = \begin{pmatrix} P_j & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ 1 & P_j & 1 & 0 & \cdots & \cdots & \vdots \\ 0 & 1 & P_j & 1 & 0 & \cdots & \vdots \\ \vdots & & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & & \ddots & \ddots & \ddots & \vdots \\ \vdots & \cdots & & & 1 & P_j & 1 \\ 0 & \cdots & & & & 1 & P_j \end{pmatrix}$$

and,

$$P_j = -2 + \frac{4im\epsilon^2}{\Delta t} - 2m\epsilon^2 V_j$$

- While some plots have been reproduced below to demonstrate the result of the calculation, running the code in Matlab will result in a nice movie playing out.

Problem 1: Gaussian Wavepackets

Code parameters

Variable	Value	Description
a	0.01	Grid spacing
tau	0.01	Δt
time	200	number of forward iterations
k	100	k_0
sigma	0.05	σ

In the first problem we start out with a wavepacket of the form:

$$\psi(x) = \exp(-ik_0x)\exp(-(x-x_0)^2/2\sigma^2).$$

In this wavepacket, σ and k_0 determine the energy of the packet as it propagates through free space. Using the algorithm above, the wave packet is allowed to evolve for 200 timesteps, and we clearly see the packet move in the positive x-direction, and the FWHM increases, widening the packet. After 200 seconds, the process is reversed and the wavepacket evolves backwards in time, and, because our operator in equation 1 is unitary, the final iteration takes us exactly back to the starting point (difference in peak position is on the order of 10^{-12}), as seen in Figure. 1.
Finally we can see that when the packet hits a wall, it bounces off and interferes with itself during the process (Fig. 2).

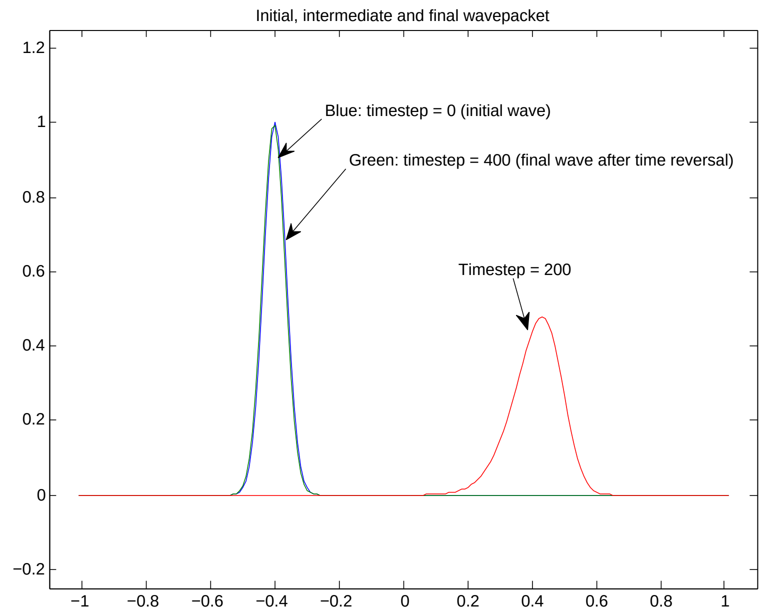


Figure 1: Evolution of the gaussian wavepacket travelling to the right.

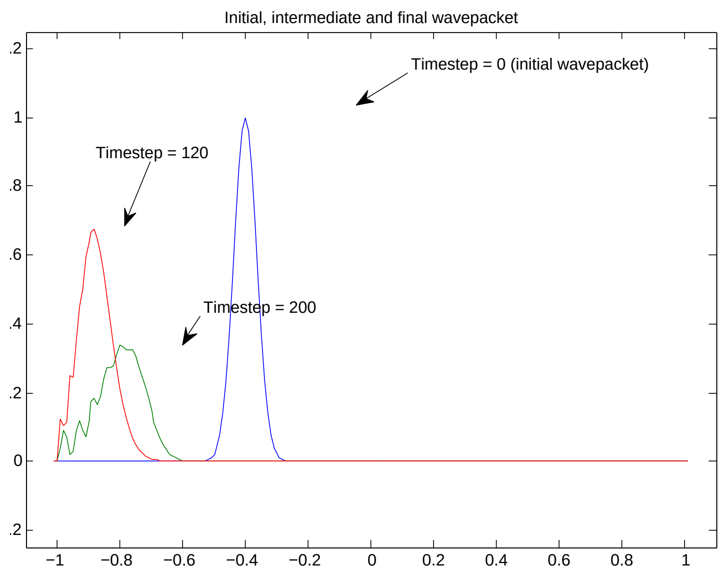


Figure 2: Evolution of the gaussian wavepacket travelling to the left.

Problem 2: Gaussian Wavepackets: A step potential

Variable	Value	Description
a	0.001	Grid spacing
tau	0.005	Δt
time	400	number of forward iterations
k	varies	k_0
sigma	varies	σ

For this question, we are asked to send the wavepacket at a step potential with varying initial conditions. First, we would like to make sure that we understand what is going on analytically here. It is not difficult to solve the problem of a plane wave hitting a potential step, and we generally find that the reflection and transmission coefficients are given by

$$\sqrt{R} = \frac{k_1 - k_2}{k_1 + k_2},$$

$$\sqrt{T} = \frac{2\sqrt{k_1 k_2}}{k_1 + k_2},$$

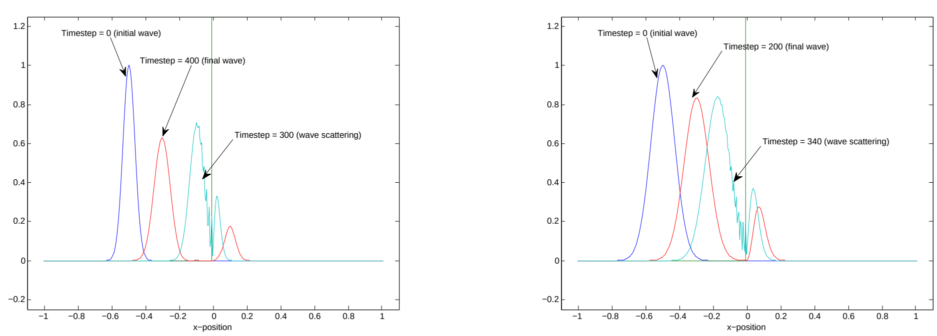
Where,

$$k_1 = \sqrt{2mE/\hbar^2}, k_2 = \sqrt{2m(E - V_0)/\hbar^2}.$$

Now, since we are actually sending in a gaussian wavepacket rather than a plane wave, we don't expect to have the same equations, but the general feature is that R and T should vary with k_1^2 . Energy of the incoming gaussian pulse. This can simply be found by taking $<\psi|H|\psi>$, where $H = p^2/2m$. The result is,

$$<H>= \frac{1}{2m}(k_0^2 + 1/2\sigma)$$

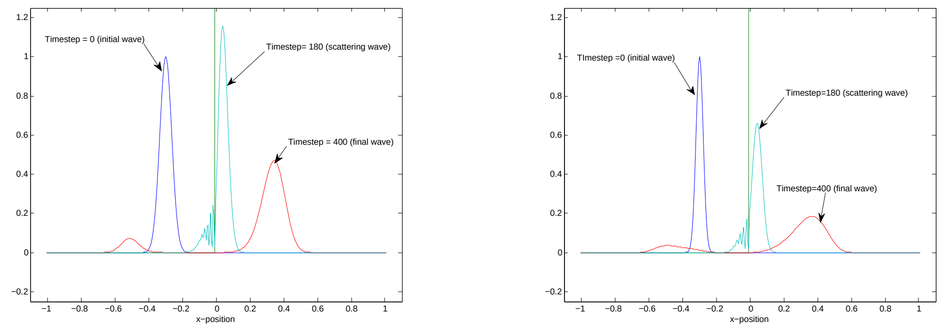
Below, we show some combinations of V, k_0, and σ.



(a) $k_0 = 400$, $\sigma = 0.05$. R=0.84, T=0.16. (b) $k_0 = 400$, $\sigma = 0.1$. R=0.87, T=0.13.

Figure 3: Scattering off a Potential step of +140.

The Reflection and Transmission coefficients are calculated from the data by numerically integrating the final ψ for before and after the potential step, and dividing by the total integral. The value of



(a) $k_0 = 200$, $\sigma = 0.05$. R=0.11, T=0.89. (b) $k_0 = 200$, $\sigma = 0.16$. R=0.84, T=0.13.

Figure 4: Scattering off a Potential step of +30.

V is scaled so the value that is listed here is not quite the actual size.

Problem 3: Gaussian Wavepackets: A resonance potential

Variable	Value	Description
a	0.01	Grid spacing
tau	0.01	Δt
time	310	number of forward iterations
k	108	k_0
sigma	0.07	σ
V	16	Well depth and barrier height

The last problem asks us to send the wavepacket at a resonance potential like that in Figure 5. Adjusting the parameters as above, we are able to reproduce a double transmission from an initial gaussian wave packet. This is shown in Fig. 6.

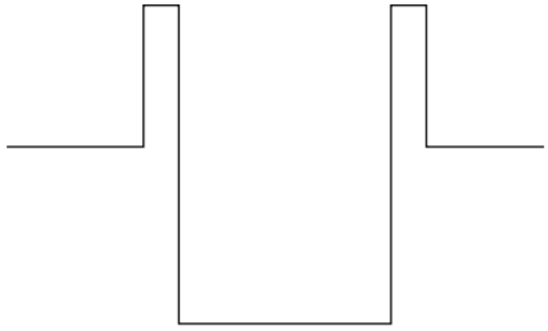


Figure 5: Form of the potential in problem 3.

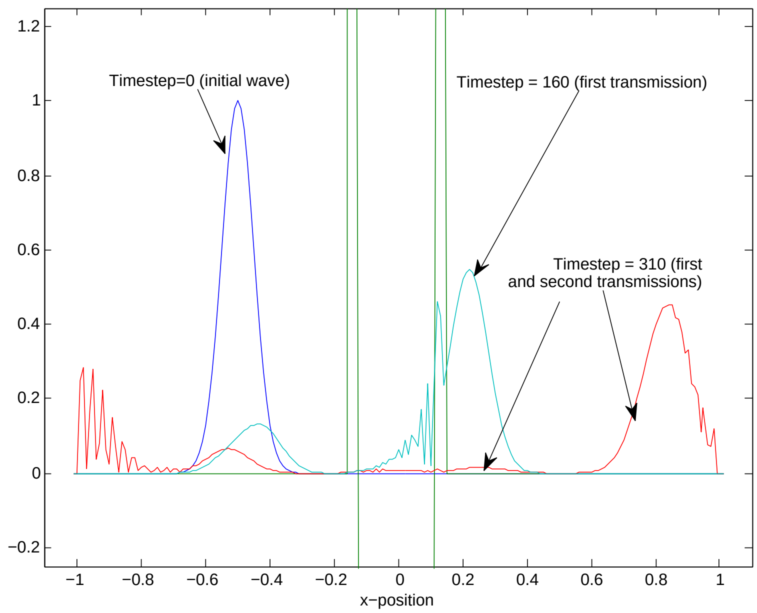


Figure 6: Scattering off of a resonance potential. At t=160 and t= 310, the initial and delayed tranmissions are visible.