PHYS 410 HW8

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Schrodinger equation

$$i\frac{\partial\Psi}{\partial t} = -\frac{\partial^2\Psi}{\partial x^2} + \Psi V$$

$$\Psi(t,x)$$

Discretizing

$$i\frac{\Psi_j^{n+1} - \Psi_j^n}{\Delta t} = -\frac{\Psi_{j+1}^{n+1} - 2\Psi_j^{n+1} + \Psi_{j+1}^{n+1}}{\Delta x^2} + \Psi_j^{n+1}V_j$$

Where $\Psi_j^n = \Psi(n\Delta t, j\Delta x)$

Rearranging and writing in matrix form

$$\begin{pmatrix} \Psi_1^n \\ \Psi_2^n \\ \vdots \\ \Psi_j^n \\ \vdots \end{pmatrix} = \begin{pmatrix} 1+2is+i\Delta tV_1 & -is & 0 & \cdots & 0 & \cdots \\ -is & 1+2is+i\Delta tV_2 & -is & 0 & \cdots & 0 \\ 0 & -is & \ddots & \cdots & 0 & \cdots \\ \vdots & \cdots & -is & 1+2is+i\Delta tV_j & -is & \cdots \\ 0 & \cdots & \cdots & \cdots & -is & \ddots \end{pmatrix} \begin{pmatrix} \Psi_1^{n+1} \\ \Psi_2^{n+1} \\ \vdots \\ \Psi_j^{n+1} \\ \vdots \end{pmatrix}$$

Will use this equation to find the nest time step by taking the inverse of the matrix

$$\begin{pmatrix} \Psi_1^{n+1} \\ \Psi_2^{n+1} \\ \vdots \\ \Psi_j^{n+1} \\ \vdots \end{pmatrix} = \begin{pmatrix} 1+2is+i\Delta tV_1 & -is & 0 & \cdots & 0 & \cdots \\ -is & 1+2is+i\Delta tV_2 & -is & 0 & \cdots & 0 \\ 0 & -is & \ddots & \cdots & 0 & \cdots \\ \vdots & \cdots & -is & 1+2is+i\Delta tV_j & -is & \cdots \\ 0 & \cdots & \cdots & \cdots & -is & \ddots \end{pmatrix}^{-1} \begin{pmatrix} \Psi_1^n \\ \Psi_2^n \\ \vdots \\ \Psi_j^n \\ \vdots \end{pmatrix}$$

Where $s = \frac{\Delta t}{\Delta x^2}$,To have numerical stability $\frac{\Delta t}{\Delta x^2} \ll 1$

The range of t is chosen to show all important behavior (reflection ,transmission, spreading)

The code of both part 1 and part 2 are the same just set V to 0 in part 1 and to the given potential in part 2

In part 2 the wave function before x=9.9 is consider reflected and after x=10.1 is consider transmitted

A videos of both parts are attached

Code

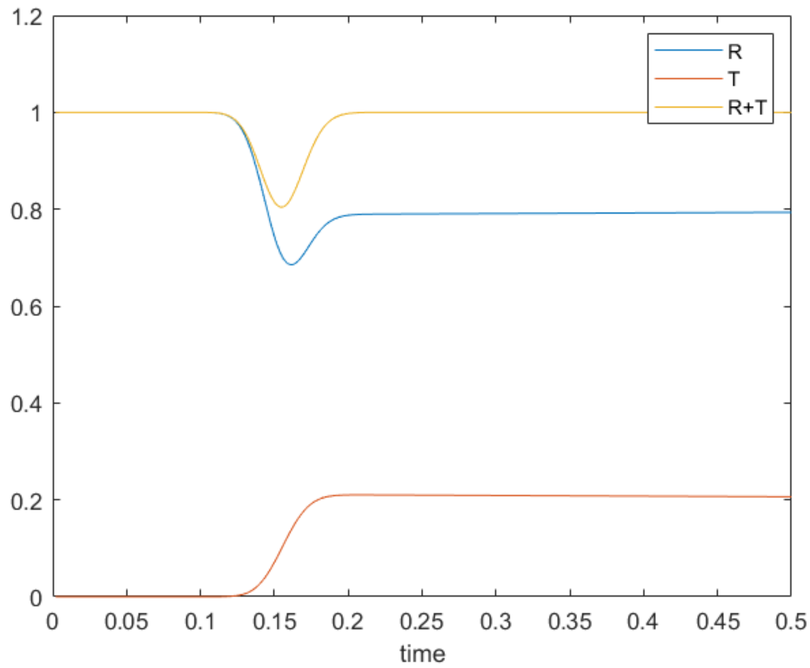
```
dx = 0.015;
dt = 0.000004;
s  = dt/(dx^2);
x = 0:dx:20;
n =length(x);
t = 0:dt:0.5;
psi = exp(20*1i*x-(x-4).^2).';
 A = sum(abs(psi).^2)*dx;
 psi = psi/sqrt(A);
 V=400*(heaviside(x-9.9)-heaviside(x-10.1));
 V=diag(V);% in part 1 V=0;
U_1 = diag((1+2i*s)*ones([1,n]));
U_1 = U_1 + 1i*dt*V;
for j=1:n-1
    U_1(j,j+1)= -1i*s;
    U_1(j+1,j)= -1i*s;
end
U=inv(U_1);
p = [psi];
k=0;
for j=1:length(t)
   psi=U*psi;
   A = sum(abs(psi).^2)*dx;
 psi = psi/sqrt(A);
   k=k+1;
   if(k==500)
       p=[p,psi];
       k=0;
   end
end

for j=1:size(p,2)-1
  tv(j)=t(500*j);
  R(j)=sum(abs(p(1:660,j)).^2)*dx;
  T(j)=sum(abs(p(675:1334,j)).^2)*dx;
 plot(x,abs(p(:,j)).^2);ylim([0 0.85])
 title("|\psi|^2")
 pause(0.01)
end
figure
plot(tv,R,tv,T,tv,T+R)
legend("R","T","R+T")
xlabel("time")
```

Results

R and T do not always add to 1 because there is part of the wave function inside the barrier

Plot of R and T vs time



The transmission coefficient found numerically $T = 0.208$

Comparing with plane wave approximation

If we use the plane wave approximation with $p = 20$ then $E = 400$

$$T^{-1} = \lim_{E \to 400} 1 + \frac{400^2}{4E(400 - E)} \sinh^2(0.2\sqrt{400 - E}) = 5$$

$$T = 0.20$$

Which is very close to the value found numerically