AEP 4380 HW 7
Time Dependent Schrödinger Equation

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The time dependent Schrödinger equation for the wavefunction ψ of a particle of mass m moving in a potential energy $V(x,t)$ is:

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

In this homework I calculated the time dependent propogation of an electron wavepacket through a potential barrier. I performed the calculation in a region of $L = 500$ Angstroms. I started with an initial (complex valued) Gaussian wave function (for an electron) of:

$$\psi(x, t=0) = exp\left[-\left(\frac{x-0.3L}{s}\right)^2 + ixk_0\right]$$

with a width of $s = 10$ Angstroms and average wavenumber $k_0 = 1$ Angstroms^{-1}. The potential energy \$V(x) models a one dimensional crystal surface with periodic peaks to mimic atomic layers in the crystal:

$$V(x) = V_1\left[0.75 - \cos\left(\frac{x-x_0}{\omega_x}\right)\right] \quad \text{for} \quad x > x_0$$

$$= 0 \quad \text{otherwise}$$

where $V_1 = 2.0$ eV, $x_0 = 0.5L$, and $\omega_x = 5$ Angstroms.

I used the Crank-Nicolson method for my calculations. The Crank-Nicolson method is a finite difference method that can be used to solve partial differential equations. It is stable and accurate to $\mathcal{O}(\Delta t^2)$ globally.

A finite difference form of the Schrödinger equation for use in the Crank-Nicolson method is:

$$\psi(x-\Delta x, t+\Delta t) + \left[\frac{2m\omega i}{\hbar} - 2 - \frac{2m\Delta x^2}{\hbar^2}V(x)\right]\psi(x, t+\Delta t) + \psi(x+\Delta x, t+\Delta t)$$

where $\omega = 2\Delta x^2/\Delta t$, Δx is the sampling size in space and Δt is the sampling size in time. For this problem the Crank-Nicolson equation has the form:

$$a_j\psi(x_{j-1}, t_{n+1}) + b_j\psi(x_j, t_{n+1}) + c_j(\psi(x_{j+1}, t_{n+1}) = d_j$$

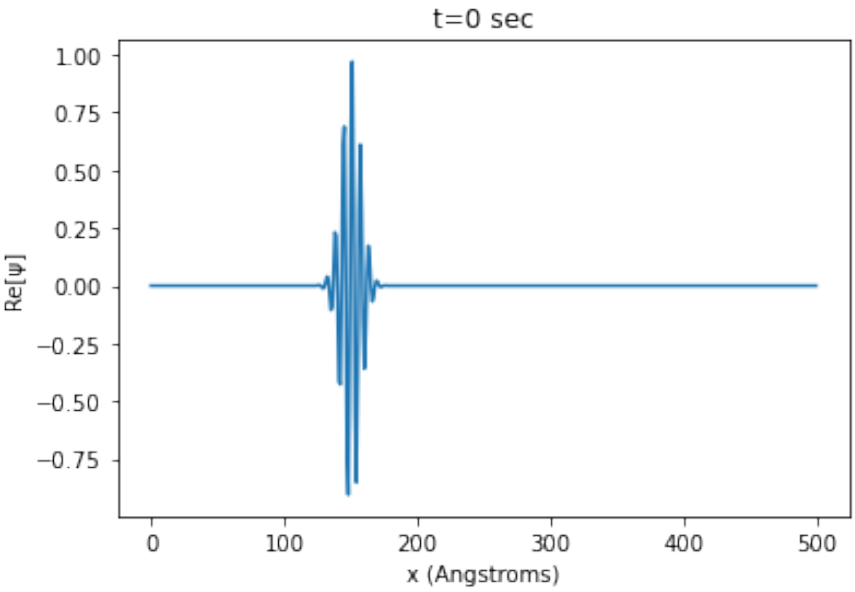
which can be written as a tri-diagonal matrix equation. As shown in the equation above, the Crank-Nicolson involves solving a set of simultaneous equations. $\psi_i = \psi(x_i, t_{n+1})$ are the unknowns to be found. The two endpoints ψ_{-1} and ψ_{N_x} are fixed at 0.

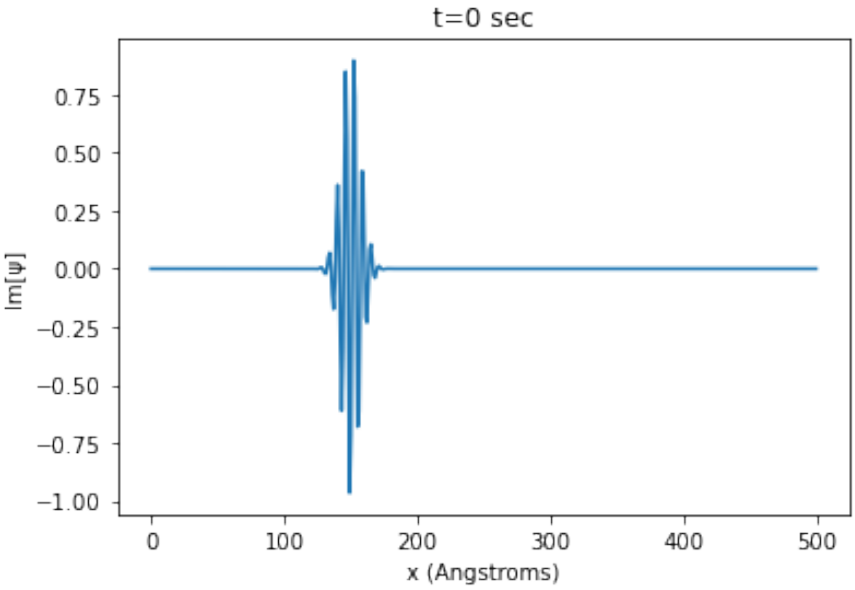
[5]:
```
from pylab import *
```

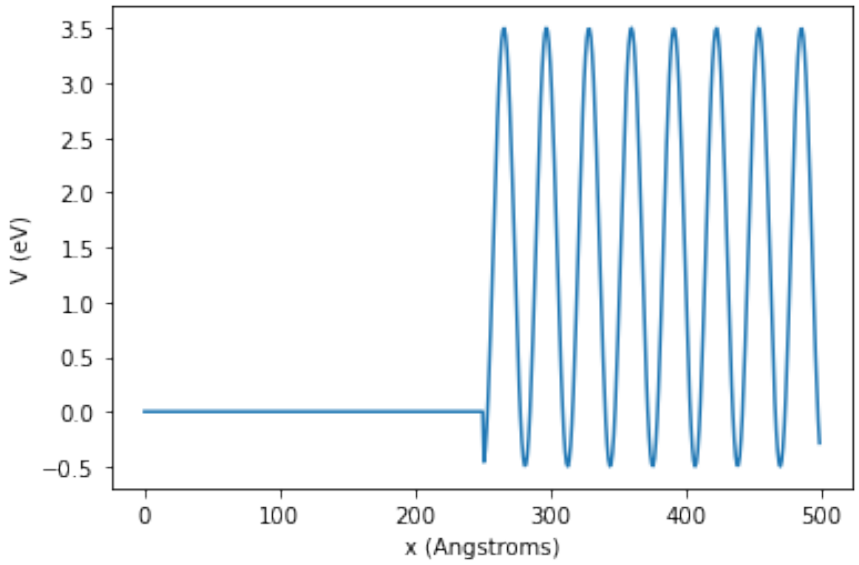
[2]:
```
psi_re0 = loadtxt("hw07-psi-re0.dat", 'float')
psi_im0 = loadtxt("hw07-psi-im0.dat", 'float')
psi_sq0 = loadtxt("hw07-psi-sq0.dat", 'float')
v = loadtxt("hw07-v.dat", 'float')
x = loadtxt("hw07-x.dat", 'float')

psi_sq05 = loadtxt("hw07-psi-sq05.dat", 'float')
psi_sq10 = loadtxt("hw07-psi-sq10.dat", 'float')
psi_sq15 = loadtxt("hw07-psi-sq15.dat", 'float')
psi_sq20 = loadtxt("hw07-psi-sq20.dat", 'float')
psi_sq25 = loadtxt("hw07-psi-sq25.dat", 'float')
```

First I plotted the potential, the real and imaginary parts of ψ, and $|\psi|^2$ at $t = 0$:

[3]:
```
plot(x,psi_re0)
xlabel("x (Angstroms)")
ylabel("Re[\u03C8]")
title("t=0 sec")
savefig("x-vs-psi0re.eps")
show()

plot(x,psi_im0)
xlabel("x (Angstroms)")
ylabel("Im[\u03C8]")
title("t=0 sec")
savefig("x-vs-psi0im.eps")
show()

plot(x,v)
xlabel("x (Angstroms)")
ylabel("V (eV)")
savefig("x-vs-V.eps")
show()
```


t=0 sec
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
Re[ψ]
0
100
200
300
400
500
x (Angstroms)

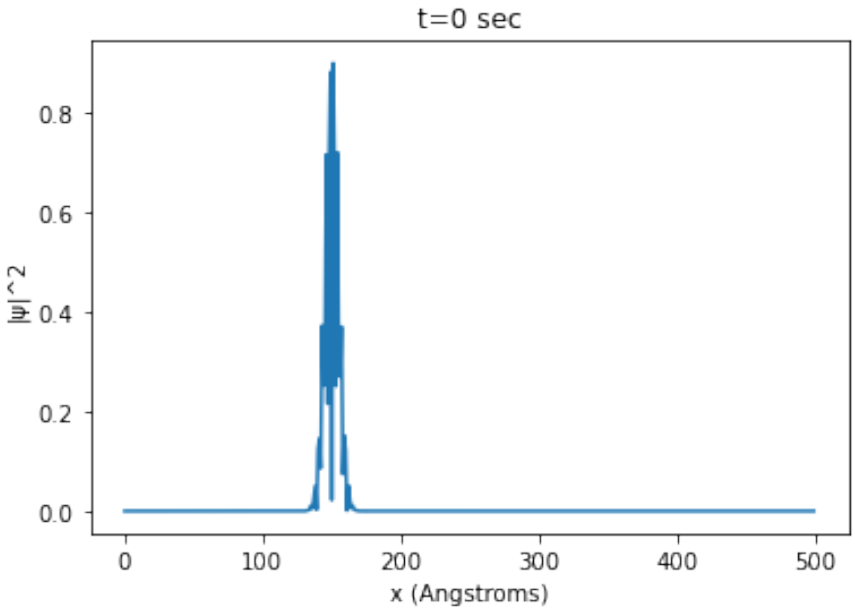

t=0 sec
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Im[ψ]
0
100
200
300
400
500
x (Angstroms)

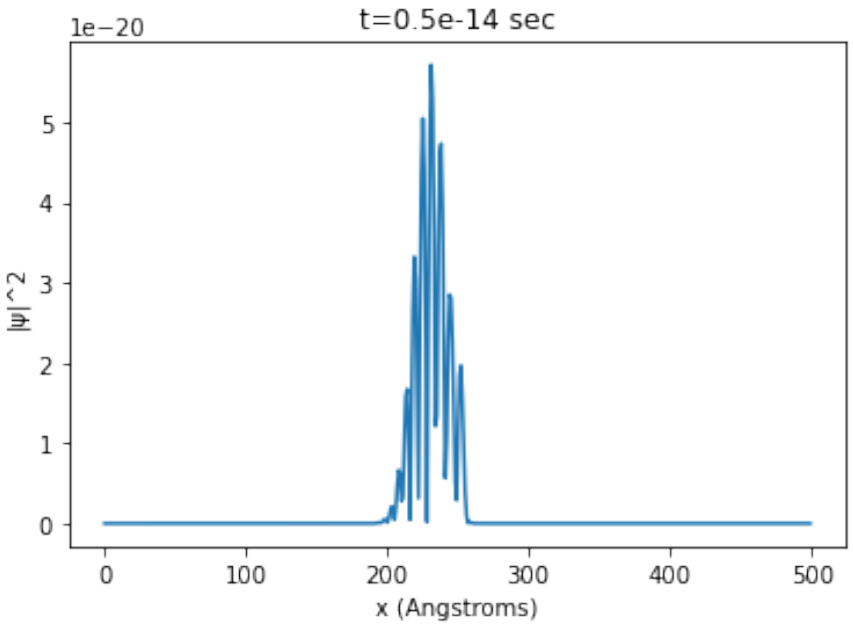


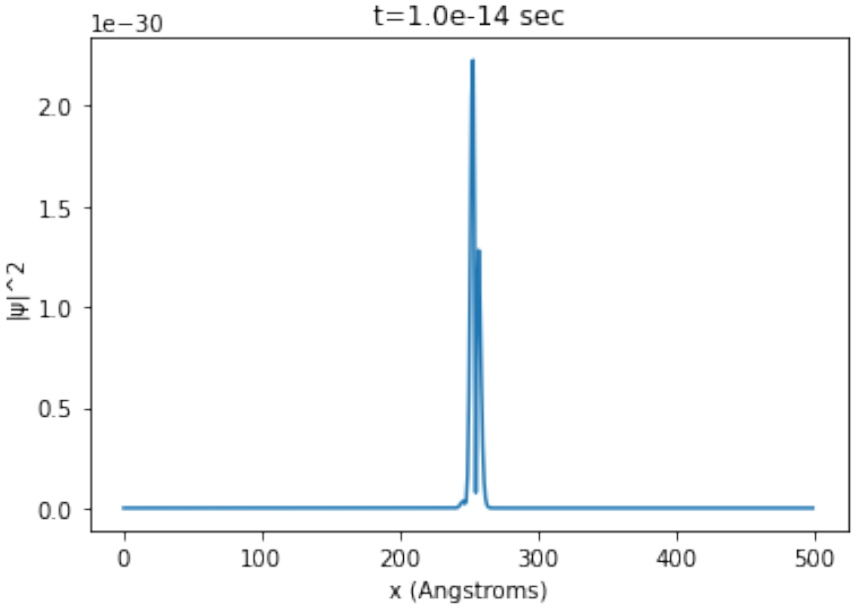
Next I solved for the propogation of the wave packet as a function of time using the Crank-Nicolson meethod. I plotted $|\psi|^2$ at times $t = 0.5 \times 10^{-14}$, $t = 1.0 \times 10^{-14}$, $t = 1.5 \times 10^{-14}$, $t = 2.0 \times 10^{-14}$, $t = 2.5 \times 10^{-14}$ seconds.

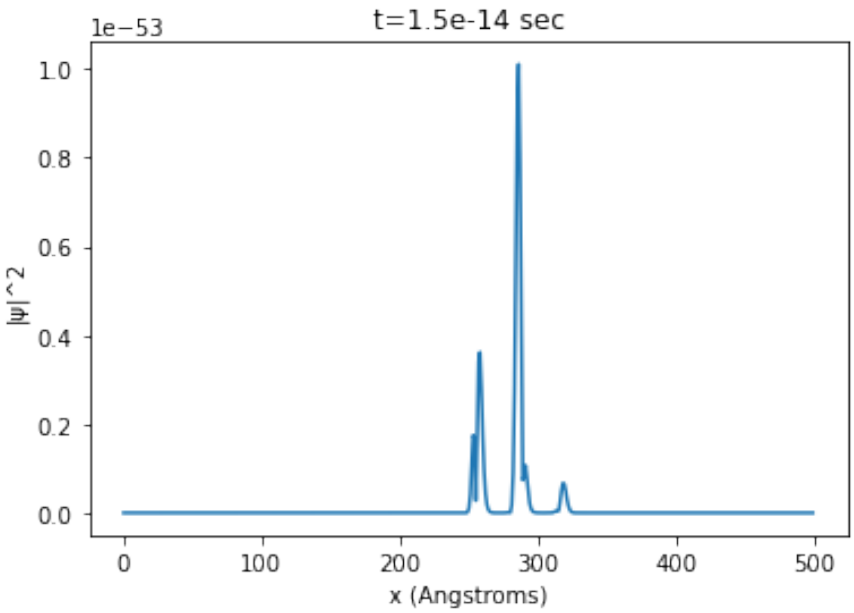
[4]:
```
plot(x,psi_sq0)
xlabel("x (Angstroms)")
ylabel("|\u03C8|^2")
title("t=0 sec")
savefig("x-vs-psi0sq.eps")
show()

plot(x,psi_sq05)
xlabel("x (Angstroms)")
ylabel("|\u03C8|^2")
title("t=0.5e-14 sec")
savefig("x-vs-psi05sq.eps")
show()

plot(x,psi_sq10)
xlabel("x (Angstroms)")
ylabel("|\u03C8|^2")
title("t=1.0e-14 sec")
savefig("x-vs-psi10sq.eps")
show()

plot(x,psi_sq15)
xlabel("x (Angstroms)")
ylabel("|\u03C8|^2")
```

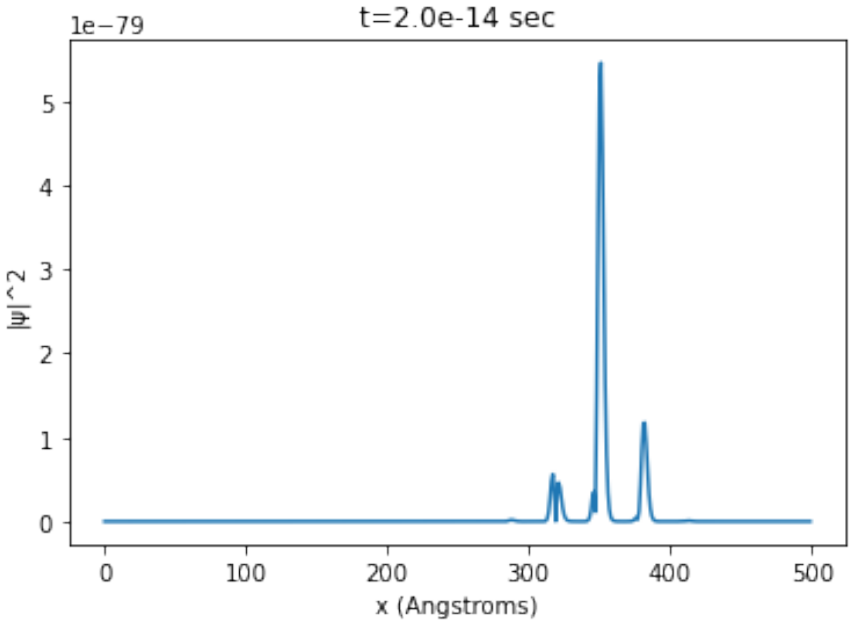
```
title("t=1.5e-14 sec")
savefig("x-vs-psi15sq.eps")
show()

plot(x,psi_sq20)
xlabel("x (Angstroms)")
ylabel("|\u03C8|^2")
title("t=2.0e-14 sec")
savefig("x-vs-psi20sq.eps")
show()

plot(x,psi_sq25)
xlabel("x (Angstroms)")
ylabel("|\u03C8|^2")
title("t=2.5e-14 sec")
savefig("x-vs-psi25sq.eps")
show()
```

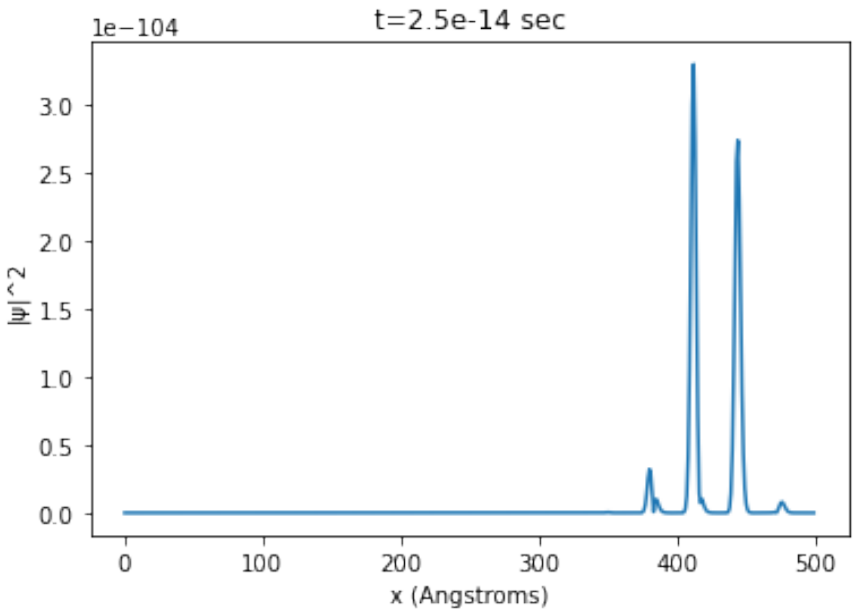



t=0.5e-14 sec
1e−20
5
4
3
2
1
0
|ψ|^2
0
100
200
300
400
500
x (Angstroms)


t=1.0e-14 sec
1e−30
2.0
1.5
1.0
0.5
0.0
|ψ|^2
0
100
200
300
400
500
x (Angstroms)


t=1.5e-14 sec
1e−53
1.0
0.8
0.6
0.4
0.2
0.0
|ψ|^2
0
100
200
300
400
500
x (Angstroms)


t=2.0e-14 sec
1e−79
5
4
3
2
1
0
|ψ|^2
0
100
200
300
400
500
x (Angstroms)


t=2.5e-14 sec
1e−104
3.0
2.5
2.0
1.5
1.0
0.5
0.0
|ψ|^2
0
100
200
300
400
500
x (Angstroms)