Solving the Time Dependent Schrödinger Equation using the Crank-Nicolson Method

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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 program 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:

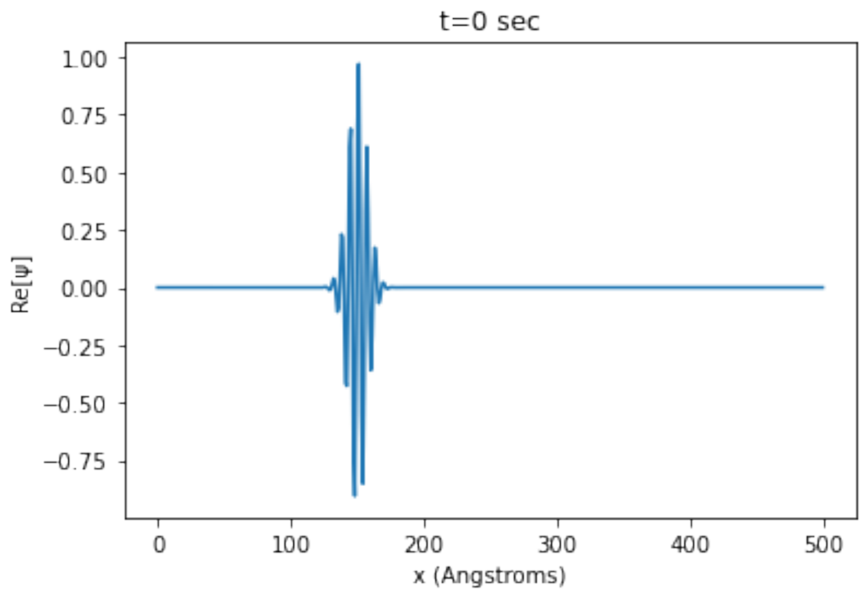
$$\psi(x-\Delta x, t+\Delta t) + \left[\frac{2m\omega i}{\hbar} - 2 - \frac{2m\Delta x^2}{\hbar^2}V(x)\right]\psi(x,t+\Delta t) + \psi(x+\Delta x, t+\Delta t)$$

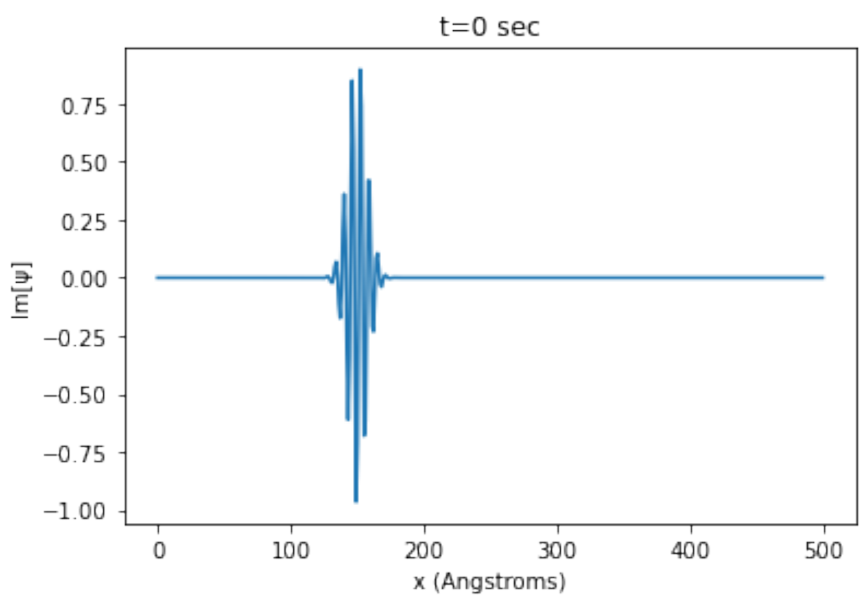
where $\omega = 2\Delta x^2/\Delta t$, Δx is the sampling size in space and Δt is the sampling size in time. For this problem the Crank-Nicolson equation has the form:

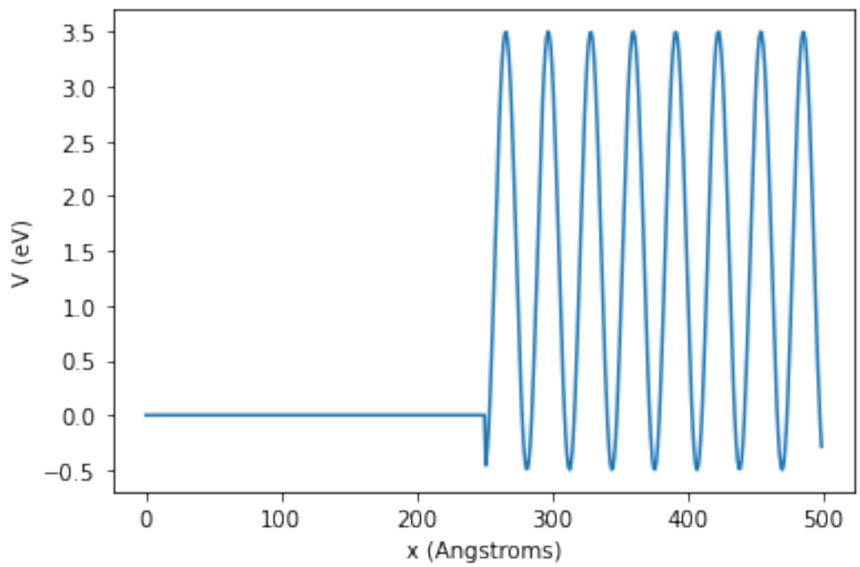
$$a_j\psi(x_{j-1}, t_{n+1}) + b_j\psi(x_j, t_{n+1}) + c_j(\psi(x_{j+1}, t_{n+1}) = d_j$$

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.

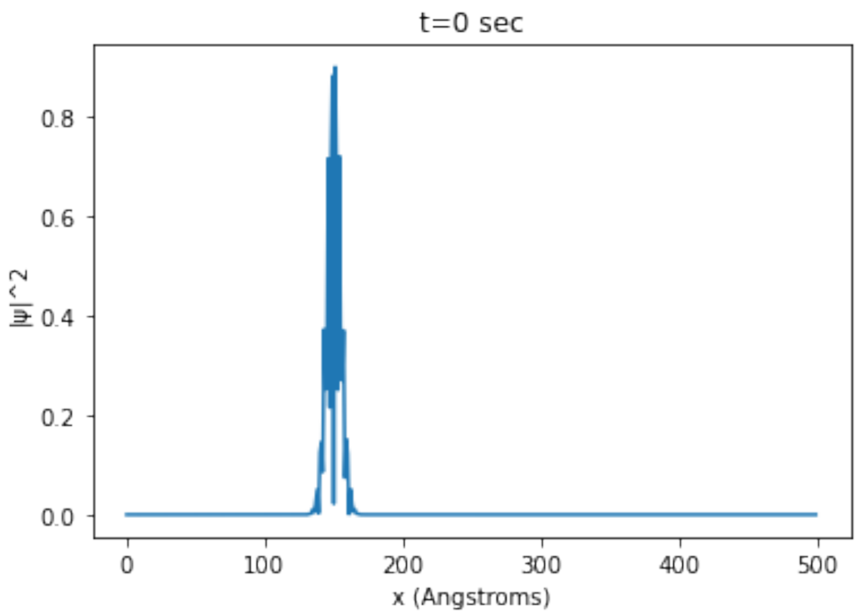
Her are plots of the potential, the real and imaginary parts of ψ, and $|\psi|^2$ at $t = 0$:

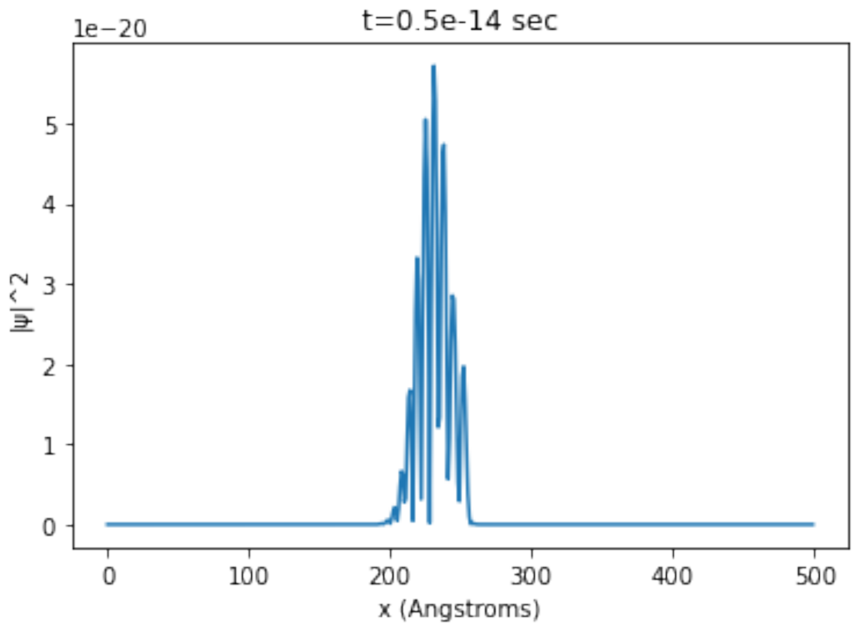


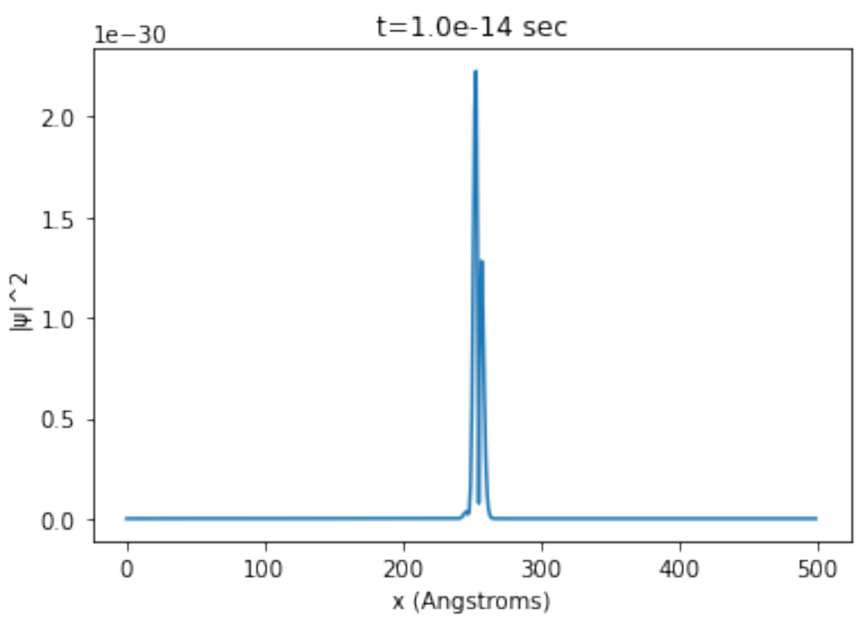


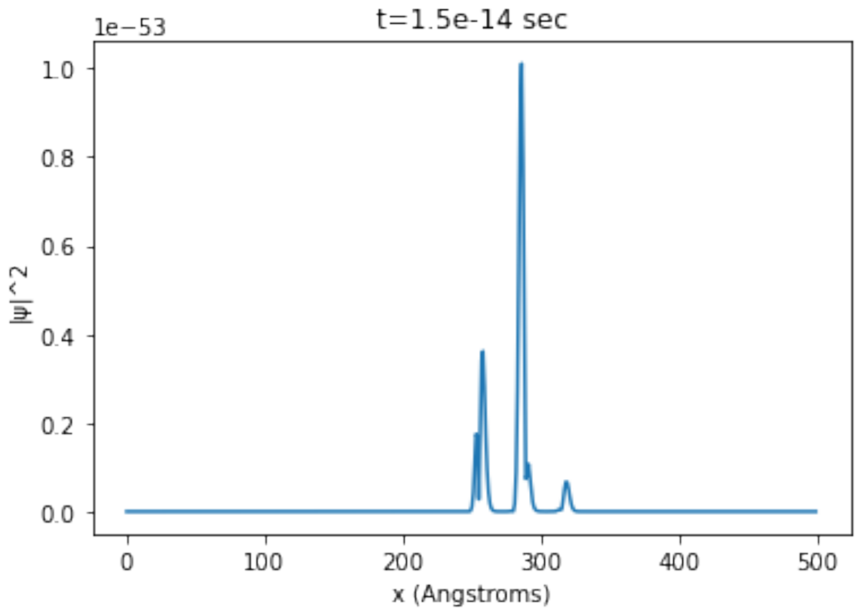


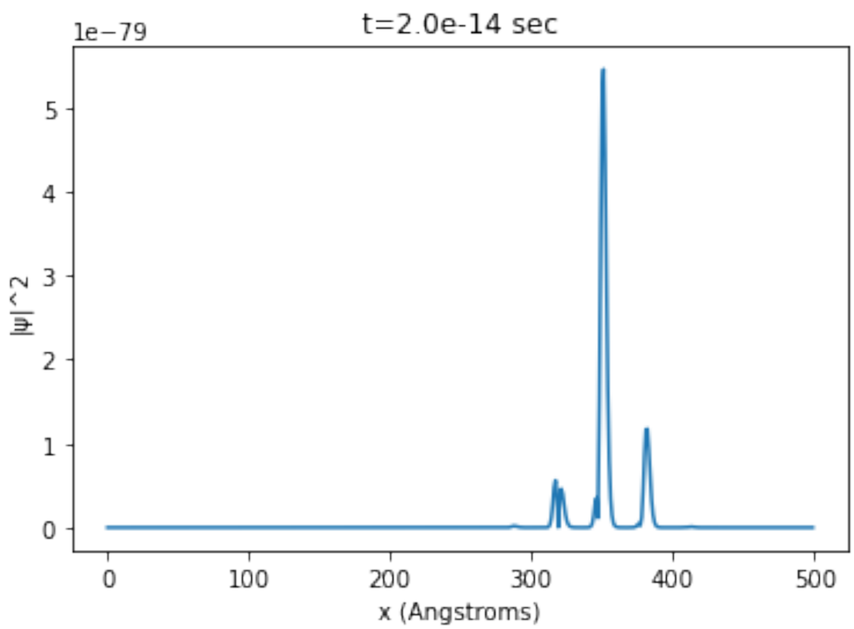
Solving for the propogation of the wave packet as a function of time using the Crank-Nicolson method produced the following plots for $|\psi|^2$ at times $t = 0.5 \times 10^{-14}$, $t = 1.0 \times 10^{-14}$, $t = 1.5 \times 10^{-14}$, $t = 2.0 \times 10^{-14}$, $t = 2.5 \times 10^{-14}$ seconds:

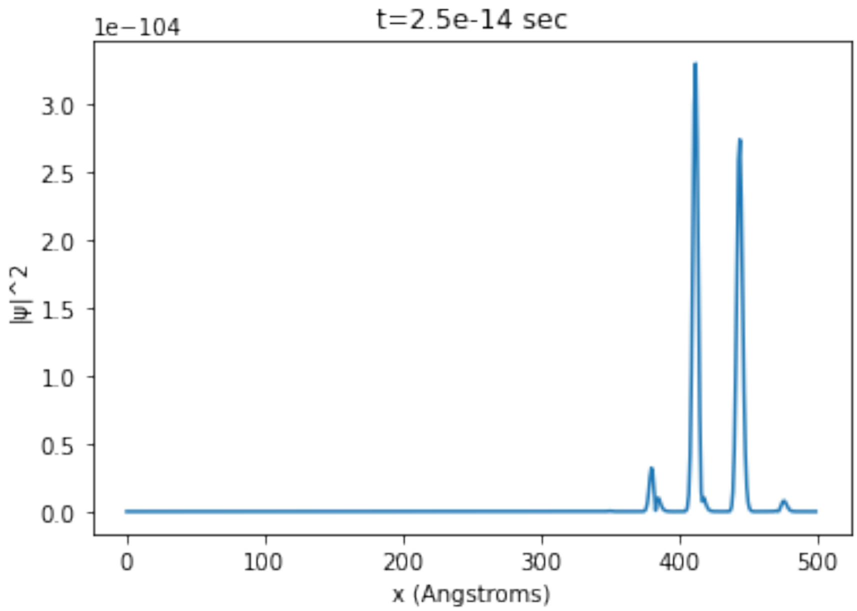



t=0.5e-14 sec
1e−20
|ψ|^2
x (Angstroms)
0
100
200
300
400
500
0
1
2
3
4
5


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


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)