Time dependent Schrödinger Eqn.

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$

$$H = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$ for 1 dimension

unitary condition $\int_{-\infty}^{+\infty} |\psi|^2 \, dx = 1$

boundary conditions $\psi(x \to \infty, t) = 0$

Crank-Nicholson

$$\psi^{n+1} = \left(I + \frac{i}{2}\Delta t H\right)^{-1}\left(I - \frac{i}{2}\Delta t H\right)\psi^{n}$$

holds our $\frac{\partial^2}{\partial x^2}$

Psuedo Code

Let N be number of spatial grid points
Let $\psi(x)$ be the complex wave function for $x = 1, \dots, N$

Let m be the mass
Let V(x) be the potential

Step 1 set up parameters & grid, potential
Step 2 set up the wavefunction and boundary cond.

$\psi = e^{ikx} e^{-(x-x_0)^2/2\sigma^2}$

$\psi = 0$ @ ∞

Step 3 Set up Hamiltonian operator matrix
Create Crank-Nicholson matrix

Step 4 Get plotting set up

Step 5 LOOP + SOLVE ψ^{n+1}
for iter = 1; max_iter
$\psi = dCN\ \psi$

plot
sanity checks

Step 6 Plot results & do checks

$\int_{-\infty}^{+\infty} |\psi|^2 \, dx = 1$

!

· H? Matrix with a lot of work to do

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$$

$$\frac{\partial^2}{\partial x^2}(\ ) = \frac{(\ )_{j-1} - 2(\ )_j + (\ )_{j-1}}{\Delta x^2}$$

$$H = \frac{-\hbar^2}{2m\Delta x^2}\left[(\ )_{j-1} - 2(\ )_j + (\ )_{j+1}\right] + V$$

but how do we code that?

i_img = $\sqrt{-1}$

$$c = \frac{\hbar^2}{2m\Delta x^2}$$

$H(i,i) = 2c + V(i)$

$H(i,j-1) = -c$ all at same time

$H(i,j+1) = c$

Now our Crank - Nicholson

$$\psi_j^{n+1} = \left(I + \frac{i\_img}{2}\frac{\Delta t}{\hbar}H\right)^{-1}\left(I - \frac{i\_img}{2}\frac{\Delta t}{\hbar}H\right)\psi_j^n$$

∴ dCN= inv(eye(N) + $\frac{i\_img}{2}$ dt H)

(eye(N) − $\frac{i\_img}{2}$ dt H)