2D Scattering of Quantum Wave Packets

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Background

- The time dependant Schrödinger equation shows how wave packets evolve in time
- Thus far, we have only been able to analytically calculate reflection/transmission probabilities
- We dealt with only simple potentials

Numerical calculations

- Goldberg et al. show a possible numerical method to solve 1D problems
- 2D is much more interesting than 1D, but easier to visualize than 3D problems

Schrödinger Equation

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

- ψ(x,y,t) is the wave function of the particle
- V(x,y) is an arbitrary potential we can create in space

Numerical Methods

- 2nd Order Centered Finite Difference Method for space derivatives
- Cayley form for unitary time development operator
- Crank-Nicolson method to implicitly step in time

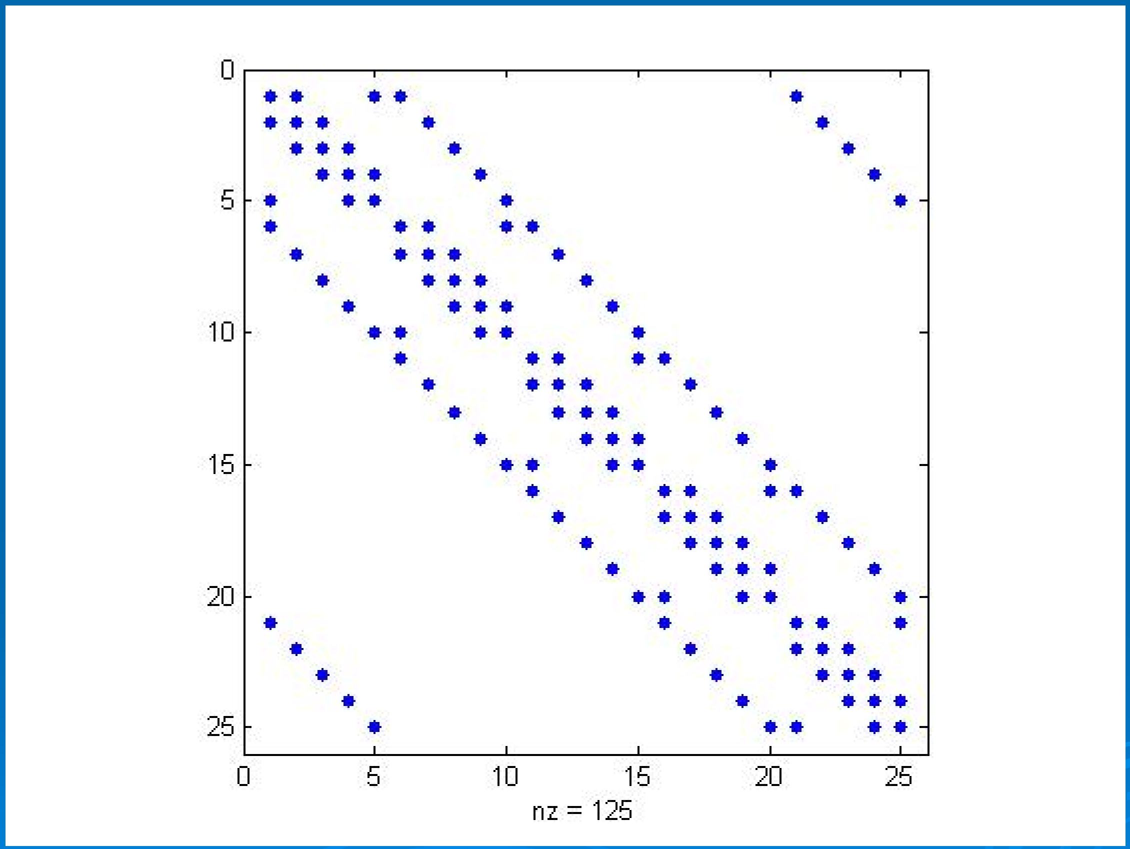
$$\psi_{j+1,k}^{n+1} + \psi_{j,k+1}^{n+1} + \left[i \cdot \frac{2\varepsilon^2}{\delta} - 4 - \varepsilon^2 V_{j,k} \right] \psi_{j,k}^{n+1} + \psi_{j-1,k}^{n+1} + \psi_{j,k-1}^{n+1} =$$

$$-\psi_{j+1,k}^{n} - \psi_{j,k+1}^{n} + \left[i \cdot \frac{2\varepsilon^2}{\delta} + 4 + \varepsilon^2 V_{j,k} \right] \psi_{j,k}^{n} - \psi_{j-1,k}^{n} - \psi_{j,k-1}^{n}$$

Boundary Conditions and Potential

- Periodic boundary conditions
- To study ‘particle in a box’ we can create a potential barrier that is huge on the borders
- Potential need not be constant in height or even a ‘nice’ shape

Periodic Conditions add a few more diagonals to our sparse matrix



Concerns and Future Work

- Final behavior highly dependant on final time used
- Large time steps result in peculiar behavior
- Grid size appears to affect particle energy and thus behavior at potential
- Need to test further to determine why spatial resolution affects behavior
- Try out crazy potentials including wells