Time-Dependent Schroedinger Equation in 2-D

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Introduction

- Quantum mechanics
  - Black body radiation
  - Stable electron orbits
- Many fields of physics and chemistry

Quantum mechanics

- Quantization of certain physical quantities
- Wave-particle duality
- Uncertainty principle
- Quantum entanglement

Motive

- What does it look like?

  propagation in free space

  reflection from a potential step

  tunneling through a barrier

Schrodinger equation

- Time independent

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{r})\psi = E\psi$$

- Time dependent

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

Formal solution

$$\psi(\vec{r},t) = e^{-\frac{i}{\hbar}\mathrm{H}t}\psi(\vec{r},0) \qquad \left(e^{-\frac{i}{\hbar}\mathrm{H}t}\right)^{+} = \left(e^{-\frac{i}{\hbar}\mathrm{H}t}\right)^{-1}$$

$$\mathrm{H} \equiv -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) = \mathrm{H}^{+}$$

$$\nabla^2 = \frac{\partial^2}{\partial {x_i}^2} \qquad i = 1,2,3$$

Probability is conserved

$$\int \left|\psi(\vec{r},t)\right|^2 dr = \int \left|\psi(\vec{r},0)\right|^2 dr$$

Approach

- Matrix Approach
- Variational Approach
- Centered Difference Method
- Quantum Monte Carlo
- Spectral Method
- …

Time centered space

- Forward Time Centered Space

  1. It is numerically unstable.

  2. The probability is not conserved.

- Backward Time Centered Space

  It is stable, the probability is not conserved, either.

$$\psi(\vec{r}, t + \Delta t) \approx (1 - i\Delta t H/\hbar)\psi(\vec{r}, t)$$

Symmetric Time Centered Space

$$\psi^{n+1} = \psi^{n} - \frac{i\tau}{2\hbar} H(\psi^{n} + \psi^{n+1})$$

- Cayley form

$$\exp(-i\Delta t H / \hbar) \approx \frac{1 - i\Delta t H / 2\hbar}{1 + i\Delta t H / 2\hbar}$$

$$\psi^{n+1} = (I + \frac{i\tau}{2\hbar} H)^{-1} (I - \frac{i\tau}{2\hbar} H)\psi^{n}$$

Crank-Nicolson Method

In 2 dimensions

$$\psi^{n+1} = (I + \frac{i\tau}{2\hbar}H)^{-1}(I - \frac{i\tau}{2\hbar}H)\psi^{n}$$

$$\mathrm{H} = -\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}) + V \qquad (I + \frac{i\tau}{2\hbar}H)^{-1}(I - \frac{i\tau}{2\hbar}H) = Q^{-1} - I$$

$$Q = \frac{1}{2}(I + \frac{i\tau}{2\hbar}H) \qquad Q\chi = \psi^{n}, \chi = Q^{-1}\psi^{n}$$

For convenience, we take x and y lattices to be the same.

Partial Differential Equations

- Elliptic partial differential equations
- Parabolic partial differential equations
- Hyperbolic partial differential equations

Parabolic partial differential equations

- Initial conditions are specified at some time
- Boundary conditions are specified at the boundaries of the closed region for all time

$$\frac{\partial n(\vec{r},t)}{\partial t} - \nabla \cdot (D(\vec{r})\nabla n(\vec{r},t)) = S(\vec{r},t)$$

Discrete in two dimensions

$$\frac{\partial^2 \psi_{i,j}}{\partial x^2} + \frac{\partial^2 \psi_{i,j}}{\partial y^2} \Rightarrow \frac{\psi_{i+1,j} + \psi_{i-1,j} - 2\psi_{i,j}}{(\Delta x)^2} + \frac{\psi_{i,j+1} + \psi_{i,j-1} - 2\psi_{i,j}}{(\Delta y)^2}$$

- For Dirichlet Boundary conditions

$$\psi(x,0,t) = \psi(0,y,t) = \psi(L_x,y,t) = \psi(x,L_y,t) = 0$$

For example N=3*3

$$M = \begin{pmatrix} -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 \end{pmatrix} \qquad \psi = \begin{pmatrix} \psi_{1,1} \\ \psi_{2,1} \\ \psi_{3,1} \\ \psi_{1,2} \\ \psi_{2,2} \\ \psi_{3,2} \\ \psi_{1,3} \\ \psi_{2,3} \\ \psi_{3,3} \end{pmatrix}$$

$$H_{Dirichlet} = -\frac{\hbar^2}{2mh^2} M + V$$

h= unit lattice of x and y

Process

Trouble

- Create the wave package can move in 2 dimensions
- Algorithm for solving the matrix elements
- Plot the 3D graphics using gnuplot

Goal

- Simulate the movement in different potential
- Observe the phenomena which is forbidden in classical

Continued...