WEEK 2 EXACT DIAGONALIZATION

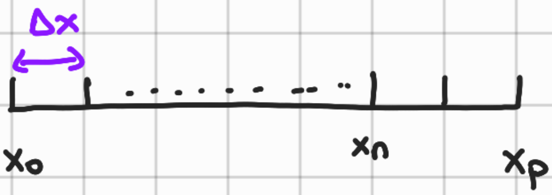
1. ONE-BODY QUANTUM PROBLEM

$$\hat{H} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \hat{V}(x)$$

$$-\frac{1}{2}\frac{\partial^2}{\partial x^2}\Psi(x) + \hat{V}(x)\Psi(x) = E\Psi(x)$$

unknown

Discretize Space



$\Psi(x) \quad \forall x \in [x_0, x_p]$

$x_n = x_0 + n\Delta x$

$n \in [0, p]$

$\Psi(x_n) \equiv \Psi_n$

Discretize Hamiltonian

$$\langle x | \hat{V} | x' \rangle = V(x)\,\delta(x-x')$$

$$V(x) \longrightarrow V_n \equiv V(x_n)$$

Finite Difference

second derivative

$$f(x+\Delta_x) = f(x) + \Delta_x f'(x) + \frac{\Delta_x^2}{2} f^2(x) + O(\Delta_x^3)$$

$$f(x-\Delta_x) = f(x) - \Delta_x f'(x) + \frac{\Delta_x^2}{2} f^2(x) + O(\Delta_x^3)$$

Central Difference

$$f(x+\Delta_x) + f(x-\Delta_x) = 2f(x) + \Delta_x^2 f''(x) + O(\Delta_x^4)$$

$$f''(x) = \frac{1}{\Delta_x^2}\left[f(x+\Delta_x) - 2f(x) + f(x-\Delta_x) \right] + O(\Delta_x^2)$$

$$\frac{\partial^2}{\partial x^2}\psi(x_n) \simeq \frac{1}{\Delta_x^2}\left[\psi_{n+1} - 2\psi_n + \psi_{n-1} \right]$$

Hamiltonian as a Matrix:

TRIDIAGONAL MATRIX

$$\hat{H}_{\Delta_x} \doteq \begin{pmatrix} V_0 + \frac{1}{\Delta_x^2} & & & & 0 \\ & \ddots & & & \\ 0, & -\frac{1}{2\Delta_x^2}, & V_n + \frac{1}{\Delta_x^2}, & -\frac{1}{2\Delta_x^2}, & 0 \\ 0 \ldots, 0 & & -\frac{1}{2\Delta_x^2}, V_{n+1} + \frac{1}{\Delta_x^2}, & -\frac{1}{2\Delta_x^2}, & 0 \\ & & & \ddots & \\ 0 & & & & V_p + \frac{1}{\Delta_x^2} \end{pmatrix} \begin{pmatrix} \psi_0 \\ \vdots \\ \psi_n \\ \vdots \\ \psi_p \end{pmatrix} = \begin{pmatrix} -\frac{1}{2\Delta_x^2}(\psi_{n+1} - 2\psi_n + \psi_{n-1}) + V_n \psi_n \end{pmatrix}$$

$(p+1) \times (p+1)$ matrix

$$\Psi_{-1} = \Psi_{p+1} = 0 \rightsquigarrow \text{Boundary Condition}$$

Find Eigenvalues:

$$\hat{H}_{\Delta x} \vec{\Psi} = E \vec{\Psi} \longrightarrow \text{Solve this with any linear algebra solver}$$

Computational Cost $\sim O(p)$

Higher Dimensions

1. Reduce to 1D Problem

$$V(\vec{r}) = V_1(x) + V_2(y) + V_3(z)$$

$$\text{e.g. } V(\vec{r}) = \frac{1}{2}\left[x^2 + y^2 + z^2\right]$$

$$\Psi(\vec{r}) = \Psi_x(x)\, \Psi_y(y)\, \Psi_z(z)$$

2. Using Symmetries

$$V(\vec{r}) = V(|\vec{r}|) \longrightarrow \text{Spherical Symmetry}$$

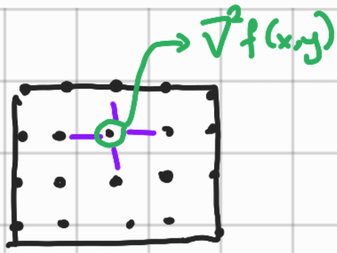
$$\Psi(\vec{r}) = \frac{U(r)}{r} Y_{\ell m}(\vartheta, \varphi)$$

Bound States

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial r^2} + \frac{\ell(\ell+1)}{2r^2} + V(r)\right] U(r) = E\, U(r) \quad (r_p \gg 1,\ E<0)$$

$$r \in [0, \infty),\quad U(r \to \infty) = 0,\quad U(r_p) \simeq 0$$

Finite-Difference



$$\nabla^2\Psi(x_n,y_n) = \frac{\partial^2}{\partial x^2}\Psi + \frac{\partial^2}{\partial y^2}\Psi$$

$x_n \in [x_0, x_p]$

$y_n \in [y_0, y_p]$

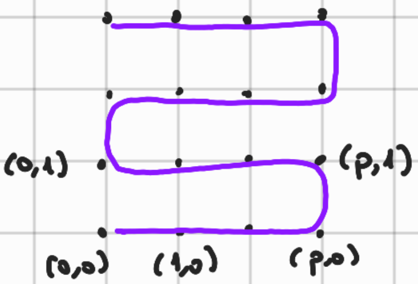
$$= \frac{1}{\Delta_x^2}\left[\Psi(x_{n+1},y_n) - 2\Psi(x_n,y_n) + \Psi(x_{n-1},y_n)\right]$$

$$+ \frac{1}{\Delta_x^2}\left[\Psi(x_n,y_{n+1}) - 2\Psi(x_n,y_n) + \Psi(x_n,y_{n-1})\right]$$

$(p+1) \times (p+1)$

spatial points

MAP $(x_n,y_n) \longrightarrow i$



$(0,0) \to 0$

$(1,0) \to 1$

$\vdots$

$(p,0) \to p$

$(p,1) \to p+1$

$$\hat{H}^{2D}_{\Delta x} =$$

Time-Dependent Case

$$i\frac{\partial}{\partial t}\Psi(x,t) = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t)$$

Initial Conditions : $\Psi(x, t=0)$

Spectral Method

$$|\Psi(t)\rangle = e^{-i\hat{H}t}\,|\Psi(t=0)\rangle$$

$\hat{H}_{\Delta x} \longrightarrow \varepsilon_n$, Eigenvalues

$|\phi_n\rangle$, Eigenstates

$$|\Psi(t)\rangle = \sum_n c_n e^{-i\varepsilon_n t}\,|\phi_n\rangle$$

$$c_n = \langle \Psi(0)|\phi_n\rangle^*$$

Direct Integration

$$t_\ell = t_0 + \ell\Delta_t$$

1st Order Euler

$$\langle x|\Psi(t_{\ell+1})\rangle = \langle x|\Psi(t_\ell)\rangle - i\,\delta_t\langle x|\hat{H}_{\Delta x}|\Psi(t_\ell)\rangle + O(\delta_t^2)$$

$$\Psi_n^{\ell+1} = \Psi_n^{\ell} - i\,\delta_t\left(\hat{H}_{\Delta x}\vec{\Psi}^{\ell}\right)_n + O(\delta_t^2)$$

Complexity $\rightarrow$ $O(p \times N_t)$ $\rightarrow$ time steps

$$\hat{U}(\Delta_t) = \exp\left[-i \hat{H} \Delta_t\right]$$

$$\hat{N}_{EULER}(\Delta_t) = \hat{I} - i \Delta_t \hat{H}$$ $\rightarrow$ Non. Unitary

$$(1 - i \Delta_t \hat{H})(1 - i \Delta_t \hat{H})^{\dagger} = \hat{I} + \Delta_t^2 \hat{H}^2 \neq \hat{I}$$

Unitary Scheme

$$e^{-i \hat{H} \Delta_t} = \left(e^{+i \hat{H} \Delta_t/2}\right)^{-1} e^{-i \hat{H} \Delta_t/2}$$

$\downarrow$ Linear Approximation

$$\hat{U}_{\Delta t} = \left(\hat{I} + i \frac{\Delta_t}{2} \hat{H}\right)^{-1} \left(I - i \frac{\Delta_t}{2} \hat{H}\right)$$

$$\hat{U}_{\Delta t} \hat{U}_{\Delta t}^{\dagger} = \hat{I}$$

Implicit Scheme

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

$$\left(I + i\frac{\Delta t}{2}\hat{H}_{\Delta x}\right)|\psi^{l+1}\rangle = \left(I - i\frac{\Delta t}{2}\hat{H}_{\Delta x}\right)|\psi^{l}\rangle$$

$$\hat{A}\,\underbrace{\vec{\psi}^{\,l+1}}_{\text{unknown}} = \vec{b}^{\,l}$$

Linear System $\longrightarrow$ Line Time $\longrightarrow O(?\times N_t)$