Imaginary time propagation

by code

1. Key idea: to apply decay operator on any given wavefunction again and again such that all excited state are suppressed exponentially faster and we are left with ground state.

2. Harmonic oscillator potential

$$V(x) = \frac{1}{2} m \omega^2 x^2$$

we choose $m = 1$ and $\omega = 1$

3. Schrödinger equation

$$\left(\frac{-\hbar^2}{2m} \nabla_x^2 + V(x) \right) \psi(x) = E \psi(x)$$

4. Setup grid X_min, X_max, dx

X_min: left boundary point

X_max: right boundary point

dx: step size.

5.

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \dots$$

$$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + \dots$$

add both equation

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + \frac{2h^4}{4!} f''''(x) + \dots$$

$$\frac{f(x+h) + f(x-h) - 2f(x)}{h^2} = f''(x) + \underbrace{\frac{2h^2}{4!} f''''(x) + \dots}_{\text{neglect when } h \to 0}$$

$$f''(x) \approx \frac{f(x+h) + f(x-h) - 2f(x)}{h^2}$$

(6) Discretization for calculating derivatives.

$$-\frac{\hbar^2}{2m} \nabla_x^2 \psi(x) = -\frac{1}{2} \frac{d^2}{dx^2} \psi(x)$$

$$\approx -\frac{1}{2} \left(\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{(dx)^2} \right)$$

$$\approx 0.5 \left(\frac{2\psi(x) - \psi(x+h) - \psi(x-h)}{(dx)^2} \right)$$

$\underbrace{\cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot}_{N}$ $\longrightarrow$ grid point

$$-\frac{\hbar^2}{2m} \nabla_x^2 \psi(x_i) \approx \underbrace{\frac{0.5}{dx^2} \left(2\psi(x_i) - \psi(x_i+h) - \psi(x_i-h) \right)}_{\longrightarrow \text{ This will be done}}$$

won't be done ∵ extra step

$$T_{ji} \approx \psi(x_j) \left(-\frac{\hbar^2}{2m} \nabla_x^2 \right) \psi(x_i)$$

Visualization of grid when $\langle \psi_j \hat{O} \psi_i \rangle = O_{ji}$

$$N-1 \left\{ \left[\begin{matrix} \square & \cdots & \square \\ \vdots & & \\ \vdots & & \\ \square & \cdots & \square \end{matrix} \right] \right\} N$$

diagonal $\rightarrow$ N points

off-diagonal $\rightarrow$ N-1 points

$$T_{ii} \approx \frac{0.5}{dx^2} (2\delta_{ii}) \nearrow i \ (0 \text{ to } N-1)$$

off-diagonal

extra step

$$T_{i(i-1)} \approx \frac{0.5}{dx^2}(-1) \quad \rightarrow i-1 \ (-1 \text{ to } N-2)$$

$(0 \text{ to } N-2)$ possible

$$T_{i(i+1)} \approx \frac{0.5}{dx^2}(-1) \quad \rightarrow i+1 \ (1 \text{ to } N+1)$$

$(1 \text{ to } N)$ possible

— $V(x_i) * \psi(x_i)$

— $H\psi = \frac{-\hbar^2}{2m} \nabla_x^2 \psi(x_i) + V(x_i) * \psi(x_i)$

— $\frac{d\psi}{dt} = H\psi$

$$\psi_{new} - \psi_{last} = dt * H\psi$$

$$\psi_{new}(x_i) = \psi_{last}(x_i) + dt * H\psi(x_i)$$

— $$\psi_{new}(x_i) = \frac{\psi_{new}(x_i)}{\sqrt{\sum_i (\psi_{new}(x_i))^2 dx}}$$

— after n steps store $\psi_{new}(x_i)$

- One more time make $H\Psi(x_i)$ using $\Psi_{new}(x_i)$

- $$\left(\sum_i \Psi_{new}(x_i)\, H\Psi_{new}(x_i)\right) * dx = \underline{E_0}$$

  ↳ store this