Separation of Variables

$$i\hbar\, \partial_T \Psi(x,T) = -\frac{\hbar^2}{2m}\partial_{xx}\Psi(x,T) + V(x)\Psi(x,T)$$

$$g(x,T) = \Psi(x,T) = f(x)\, g(T)$$

$$i\hbar\, f(x)\, \partial_T g(T) = -\frac{\hbar^2}{2m} g(T)\,\partial_{xx} f(x) + V(x) f(x) g(T)$$

$$i\hbar \frac{1}{g(T)}\partial_T g(T) = -\frac{\hbar^2}{2m}\frac{1}{f(x)}\partial_{xx} f(x) + V(x) = E$$

$$i\hbar \frac{1}{g(T)}\partial_T g(T) = -\lambda^2 \qquad E = \lambda^2$$

eq 1 $\rightarrow$ $$\frac{dg(T)}{dT} = -\lambda^2 \frac{1}{i\hbar}\, g(T)$$

$$+\hbar^2 \frac{1}{2m}\frac{1}{f(x)}\partial_{xx} f(x) +- V(x) = +\lambda^2$$

eq 2 $\rightarrow$ $$\frac{d^2 f(x)}{dx^2} = \lambda^2\, 2m \frac{1}{\hbar^2} f(x) + \cancel{V(x)}\, 2m\frac{1}{\hbar^2} f(x)$$

$V(x) = 0$ for square well

- from eq 1

$$g(T) = A\, e^{-\lambda^2 \frac{1}{i\hbar} T}$$

- from eq 2

$$\hat{H} f(x) = f(x)\,\lambda^2$$

- Try $f(x) = \sin\left(\frac{2\pi n x}{L}\right)$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\sin\left(\frac{2\pi n x}{L}\right) = E\sin\left(\frac{2\pi n x}{L}\right)$$

$$= \frac{\hbar^2}{2m}\left(\frac{2\pi n}{L}\right)^2 \sin\left(\frac{2\pi n x}{L}\right)$$

$$E = 2\hbar^2\pi^2 n^2 / mL^2$$

Computational Formula

$$\underbrace{\frac{\hbar^2}{2m}}_{A} \frac{d^2 f(x)}{dx^2} = E f(x)$$

$$\frac{d^2 f(x)}{dx^2} = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

$$x_1) \; A\left(f(x_2) - 2f(x_1) + \overset{0 \text{ by bound}}{\cancel{f(x_0)}}\right) / h^2 = E f(x_1)$$

$$x_2) \; A\left(f(x_3) - 2f(x_2) + f(x_1)\right) / h^2 = E f(x_2)$$

$$x_n) \; A\left(\overset{0 \text{ by bounds}}{\cancel{f(x_{n+1})}} - 2f(x_n) + f(x_{n-1})\right) / h^2 = E f(x_n)$$

$$\overleftrightarrow{A} x = E x$$

$$\frac{\hbar^2}{2m} \frac{1}{h^2} \begin{bmatrix} -2 & 1 & 0 & 0 & \cdots \\ 1 & -2 & 1 & 0 & \cdots \\ 0 & 1 & -2 & 1 & \cdots \\ & & \vdots & & \end{bmatrix} \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \end{bmatrix} = E \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \end{bmatrix}$$

Choosing N

$$Nh = L = 10^{-10}$$

$$h = 10^{-10}/N$$

$$\frac{\hbar^2}{2mh^2} = \frac{(1.05457182 \times 10^{-34})^2}{2(9.10938356 \times 10^{-31})h^2} = c$$

- when $N = 1000$

$$c = 6.104264 \times 10^{-13}$$

$K = 10^{10}$ ← mult to avoid error

$$cK = 6.104264 \times 10^{-3}$$

Time step

$$e^{+E\frac{i}{\hbar}T} = \cos(E\tfrac{1}{\hbar}T) + i\sin(E\tfrac{1}{\hbar}T)$$

- only real part so use

$$\cos(E\tfrac{1}{\hbar}T)$$

eigenvalues

$$1/\hbar = 9.482522 \times 10^{33}$$

Part C computational Formula

V_0 = constant within the well

$$\frac{d^2 f(x)}{dx^2} = \lambda^2 \, 2m \frac{1}{\hbar^2} f(x) + V_0 \, 2m \frac{1}{\hbar^2} f(x)$$

$$\underbrace{\frac{\hbar^2}{2m}}_{A} \frac{d^2 f(x)}{dx^2} - V_0 f(x) = E f(x)$$

$$A \begin{bmatrix} -2 & 1 & 0 & \cdots \\ 1 & -2 & 1 & \cdots \end{bmatrix} f(x) - \begin{bmatrix} V_0 & 0 & 0 & \cdots \\ 0 & V_0 & 0 & \cdots \end{bmatrix} f(x) = E f(x)$$

$$A \begin{bmatrix} -2-V_0 & 1 & 0 & 0 & \cdots \\ 1 & -2-V_0 & 1 & 0 & \cdots \\ 0 & 1 & -2-V_0 & 1 & \cdots \end{bmatrix} \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \end{bmatrix} = E \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \end{bmatrix}$$

- set V_0 = large mult of $\frac{\hbar^2}{2mL^2}$

$$\frac{\hbar^2}{2mL^2} = 6.104264 \times 10^{-59}$$

- multiplying by 10^{55} to get: $6.104264 \times 10^{-4} = V_0$