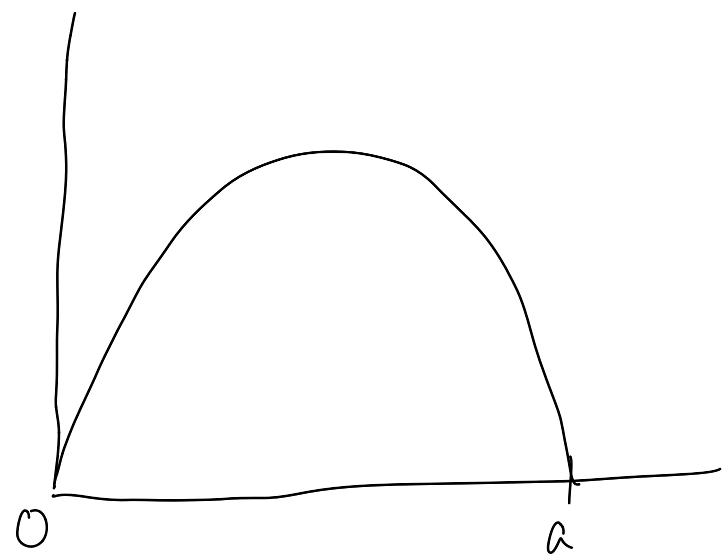
$$C_m = \sqrt{\frac{2}{a}} \int_0^a \Psi_0(x) \sin\left(\frac{m\pi}{a}x\right) dx$$

$$\Psi(x,t) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi}{a}x\right) e^{-\frac{i}{\hbar} E_n t}$$

Example:

$\Psi_0(x,0)$



$\Psi_0(x,0) \propto x(a-x)$

$\Psi_0(x,0) = Ax(a-x)$

What is A?

$$\int_{-\infty}^{\infty} A^2 \Psi_0^2 \, dx = 1$$

$$A^2 \int_0^a x^2(a-x^2) \, dx = A^2 \frac{a^5}{30}$$

$$A = \sqrt{\frac{30}{a^5}}$$

$$\Psi_0 = \sqrt{\frac{30}{a^5}} \, x(a-x)$$

Now just find c_n

$$c_m = \sqrt{\frac{2}{a}} \int_0^a \Psi_0(x) \sin\left(\frac{m\pi}{a} x\right) dx$$

$$c_n = \sqrt{\frac{2}{a}} \sqrt{\frac{30}{a^5}} \int_0^a x(a-x) \sin\left(\frac{n\pi}{a} x\right) dx$$

$$= \frac{2\sqrt{15}}{a^3}\left[\int_0^a ax\sin\left(\frac{n\pi}{a}x\right)dx - \int_0^a x^2\sin\left(\frac{n\pi}{a}x\right)dx\right]$$

$$\int x\sin\left(\frac{n\pi}{a}x\right)dx =$$

$$\int u\,dv = uv - \int v\,du$$

$$u = x$$
$$dv = \sin\left(\frac{n\pi}{a}x\right)$$

$$\int_0^a x\sin\left(\frac{n\pi}{a}x\right)dx = -\frac{a}{n\pi}x\cos\left(\frac{n\pi}{a}x\right)\Big|_0^a - \frac{a}{n\pi}\int_0^a \cos\left(\frac{n\pi}{a}x\right)dx$$

$$\int_0^a x^2\sin\left(\frac{n\pi}{a}x\right)dx = \frac{-a}{n\pi}x^2\cos\left(\frac{n\pi}{a}x\right)\Big|_0^a - \frac{2a}{n\pi}\int_0^a x\cos\left(\frac{n\pi}{a}x\right)dx$$

$$C_n = \frac{4\sqrt{15}}{\pi^3 n^3}\left[1 - \cos(n\pi)\right]$$

$$C_n = \begin{cases} 0, & n \text{ is even} \\ \dfrac{8\sqrt{15}}{\pi^3 n^3}, & n \text{ odd} \end{cases}$$

$$\Psi(x,t) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi}{a}x\right) e^{-\frac{i}{\hbar}E_n t}$$

$$\Psi(x,t) = \sqrt{\frac{2}{a}}\, \frac{8\sqrt{15}}{\pi^3} \sum_{n=1,3,5,\ldots}^{\infty} \frac{1}{n^3} \sin\left(\frac{n\pi}{a}x\right) e^{-iE_n t}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

$$\Psi(x,t) = \sqrt{\frac{2}{a}}\, \frac{8\sqrt{15}}{\pi^3} \sum_{n=1,3,5,\ldots}^{\infty} \frac{1}{n^3} \sin\left(\frac{n\pi}{a}x\right) e^{-\frac{i n^2\pi^2\hbar}{2ma^2}}$$

Solve computationally

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi + V\Psi$$

Normalize:

$$x_0 = \sqrt{\frac{m}{\hbar t_0}}$$

$$(\hbar = 1, m = 1)$$

$$V_0 = \frac{\hbar}{t_0}$$

$$\frac{\partial \Psi}{\partial t} = \frac{i}{2} \frac{\partial^2}{\partial x^2} \Psi - iV\Psi$$

Digitize everything!

$$x_j = x_0 + j\Delta x$$

$$t_n = t_0 + n\Delta t$$

$$\psi(x_j, t_n) = \psi_j^n$$

Finite difference derivative

$$\frac{\partial^2}{\partial x^2}\psi = \frac{\psi_{j+1}^n + \psi_{j-1}^n - 2\psi_j^n}{\Delta x^2}$$

$$\frac{\partial \psi_j^n}{\partial t} = \frac{i}{2\Delta x^2}\left(\psi_{j+1}^n + \psi_{j-1}^n - 2\psi_j^n\right) - iV_j^n \psi_j^n$$

$$= \frac{i}{2\Delta x^2}\psi_{j-1}^n - i\left(\frac{1}{\Delta x^2} + V_j^n\right)\psi_j^n + \frac{i}{2\Delta x^2}\psi_{j+1}^n$$

$$V_j^n = V_j$$

$$= \frac{i}{2\Delta x^2}\psi_{j-1}^n - i\left(\frac{1}{\Delta x^2} + V_j\right)\psi_j^n + \frac{i}{2\Delta x^2}\psi_{j+1}^n$$

$$\vec{\Psi}^n = \begin{pmatrix} \Psi_0^n \\ \Psi_1^n \\ \Psi_2^n \\ \vdots \\ \Psi_j^n \\ \vdots \end{pmatrix}$$

$$\frac{\partial \vec{\Psi}^n}{\partial t} = \begin{pmatrix} -i\left(\frac{1}{\Delta x^2}+V_0\right) & \frac{i}{2\Delta x^2} & 0 & 0 \\ \frac{i}{2\Delta x^2} & -i\left(\frac{1}{\Delta x^2}+V_1\right) & \frac{i}{2\Delta x^2} & 0 \\ 0 & \frac{i}{2\Delta x^2} & -i\left(\frac{1}{\Delta x^2}+V_2\right) & \frac{i}{2\Delta x^2} \\ 0 & 0 & \frac{i}{2\Delta x^2} & -i\left(\frac{1}{\Delta x^2}+V_3\right) \end{pmatrix} \begin{pmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{pmatrix}$$

$$
= \begin{array}{c} 0 \\ 1 \\ 2 \\ j \end{array}
\begin{pmatrix}
-i\left(\frac{1}{\Delta x^2}+V_0\right)\psi_0 + \frac{i}{2\Delta x^2}\psi_1 \\
\frac{i}{2\Delta x^2}\psi_0 - i\left(\frac{1}{\Delta x^2}+V_1\right)\psi_1 + \frac{i}{2\Delta x^2}\psi_2 \\
\frac{i}{2\Delta x^2}\psi_1 - i\left(\frac{1}{\Delta x^2}+V_2\right)\psi_2 + \frac{i}{2\Delta x^2}\psi_3 \\
\frac{i}{2\Delta x^2}\psi_{j-1} - i\left(\frac{1}{\Delta x^2}+V_j\right)\psi_j + \frac{i}{2\Delta x^2}\psi_{j+1}
\end{pmatrix}
$$

✓

$$
\hat{H} = \begin{pmatrix}
-i\left(\frac{1}{\Delta x^2}+V_0\right) & \frac{i}{2\Delta x^2} & 0 & 0 \\
\frac{i}{2\Delta x^2} & -i\left(1/\Delta x^2+V_1\right) & \frac{i}{2\Delta x^2} & 0 \\
0 & \frac{i}{2\Delta x^2} & -i\left(\frac{1}{\Delta x^2}+V_2\right) & \frac{i}{2\Delta x^2} \\
 & & & \ddots
\end{pmatrix}
$$

$\hat{H}$: Along diagonal

$$-i\left(\frac{1}{\Delta x^2} + V_j\right)$$

Above & ~~Be~~low
diagonal

$$\frac{i}{2\Delta x^2}$$

$$\frac{\partial \vec{\Psi}^n}{\partial t} = \hat{H}\vec{\Psi}^n$$

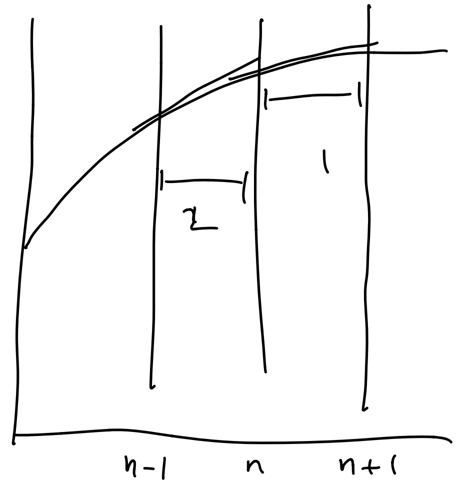
What is $\frac{\partial \vec{\Psi}^n}{\partial t}$?

Either:

$$\underset{(1)}{\frac{\vec{\Psi}^{n+1} - \vec{\Psi}^n}{\Delta t}} \quad \text{OR} \quad \underset{(2)}{\frac{\vec{\Psi}^n - \vec{\Psi}^{n-1}}{\Delta t}}$$

(1):

$$\frac{\vec{\Psi}^{n+1} - \vec{\Psi}^{n}}{\Delta t} = \hat{H}\vec{\Psi}^{n}$$



$$\vec{\Psi}^{n+1} = \vec{\Psi}^{n} + \Delta t \hat{H}\vec{\Psi}^{n}$$

$$\vec{\Psi}^{n+1} = \left(\hat{I} + \Delta t \hat{H}\right)\vec{\Psi}^{n}$$

(2)

$$\frac{\vec{\Psi}^{n} - \vec{\Psi}^{n-1}}{\Delta t} = \hat{H}\vec{\Psi}^{n}$$

$$\vec{\Psi}^{n} - \Delta t \hat{H}\vec{\Psi}^{n} = \vec{\Psi}^{n-1}$$

$$\left(\hat{I} - \Delta t \hat{H}\right)\vec{\Psi}^{n} = \vec{\Psi}^{n-1}$$

$$\left(\hat{I} - \Delta t \hat{H}\right)\vec{\Psi}^{n+1} = \vec{\Psi}^{n}$$

$$(3) = \frac{1}{2}\left[(1) + (2)\right]$$

$$\vec{\Psi}^{n+1} = \left(\hat{I} + \Delta t \hat{H}\right)\vec{\Psi}^{n}$$

$$+$$

$$\left(\hat{I} - \Delta t \hat{H}\right)\vec{\Psi}^{n+1} = \vec{\Psi}^{n}$$

$$\vec{\Psi}^{n+1} + \left(\hat{I} - \Delta t \hat{H}\right)\vec{\Psi}^{n+1} = \left(\hat{I} + \Delta t \hat{H}\right)\vec{\Psi}^{n} + \vec{\Psi}^{n}$$

$$\left(2\hat{I} - \Delta t \hat{H}\right)\vec{\Psi}^{n+1} = \left(2\hat{I} + \Delta t \hat{H}\right)\vec{\Psi}^{n}$$

$$\div \ 2$$

$$\left(\hat{I} - \frac{\Delta t \hat{H}}{2}\right)\vec{\Psi}^{n+1} = \left(\hat{I} + \frac{\Delta t \hat{H}}{2}\right)\vec{\Psi}^{n}$$

$$\hat{A}\,\vec{\Psi}^{n+1} = \hat{B}\,\vec{\Psi}^{n}$$

$$\vec{\Psi}^{n+1} = \left(\hat{A}^{-1} \cdot \hat{B}\right)\vec{\Psi}^{n}$$

If we know V everywhere,

we know $\hat{H}$ & therefore $\hat{A}$ & $\hat{B}$

just do $C = A^{-1}B$ once

then

$$\vec{\Psi}^{n+1} = C\,\vec{\Psi}^{n}$$

Start with

$$\vec{\Psi}^{0}$$

then

$$\vec{\Psi}^{1} = C\,\vec{\Psi}^{0}$$

$$\vec{\Psi}^{2} = C\,\vec{\Psi}^{1}$$

etc ....