$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi \qquad \psi = \psi(x,t)$$

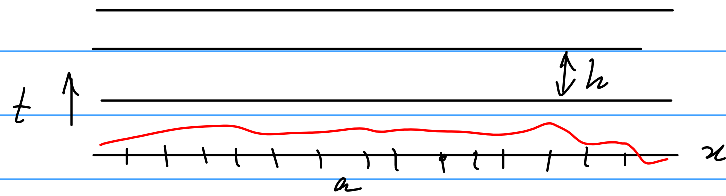
$$\hat{H} = \frac{p^2}{2m} + V(x) \qquad \hat{p}^2 = -\hbar^2 \nabla^2$$

$$i\hbar \frac{\psi(x,t+h) - \psi(x,t)}{h} = \hat{H}\psi = \frac{-\hbar^2}{2m}\left(\frac{\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)}{a^2}\right)$$

$$+ V(x)\,\psi(x,t).$$

Explicit method.

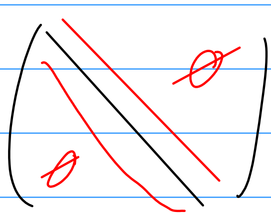
$$i\hbar \frac{\psi(t+h)-\psi(t)}{h} = \hat{H}\psi(t)$$



Implicit method.

$$i\hbar \frac{\psi(t+h)-\psi(t)}{h} = \hat{H}\psi(t+h) \rightarrow \left(\frac{i\hbar}{h} - \hat{H}\right)\psi(t+h) = \hat{H}\psi(t).$$

Requires inversion of $\left(\frac{i\hbar}{h} - \hat{H}\right)$



Sparse scipy.sparse.

Recursive way: C.G. Conjugate Gradient.

$$i\hbar \frac{\psi(t+h)-\psi(t)}{h} = \frac{\hat{H}\psi(t) + \hat{H}\psi(t+h)}{2}$$

more accurate
stable

Crank-Nicholson. A 7.2. (Thijssen).

$$i\hbar\,\partial_t \psi = \hat{H}\psi \qquad \text{Soln}: \ \psi(t) = \hat{\mathcal{U}}(t)\,\psi(0)$$

$$\hat{\mathcal{U}}(t) = e^{-it\hat{H}/\hbar} = e^{-it\left(\frac{\hat{p}^2}{2m} + V(x)\right)/\hbar}$$

$$\cancel{= e^{-it\hat{p}^2/2m\hbar}\, e^{-itV(x)/\hbar}}$$

$$e^{-it\hat{H}/\hbar} = \prod_j e^{-i\Delta t\,\hat{H}/\hbar}. \qquad \Delta t \text{ small.}$$

$$e^{-i\Delta t\left(\frac{\hat{p}^2}{2m} + V(x)\right)/\hbar} \simeq e^{-i\Delta t\,\hat{p}^2/2m\hbar}\, e^{-i\Delta t\,V(x)/\hbar}\, e^{\sim\Delta t^2}$$

Lie Suzuki Trotter.

$$\int dx_j\, dp_j \prod_j |p_{j+1}\rangle\langle p_{j+1}|\, e^{-i\Delta t\,\hat{p}^2/2m\hbar}|p_j\rangle\underbrace{\langle p_j|x_j\rangle}\langle x_j|\, e^{-i\Delta t\,V(\hat{x})/2m\hbar}|x_{j-1}\rangle\langle x_{j-1}|$$

$$\mathbb{1} = \sum_j |\phi_j\rangle\langle\phi_j|.$$

In our case $\quad \int |x\rangle\langle x|\, dx = \mathbb{1} = \int |p\rangle\langle p|\, dp.$

$$\int dx_j\, dp_j \quad e^{-i\Delta t\,p_j^2/2m\hbar}\, \frac{e^{ip_jx_j/\hbar}}{\sqrt{2\pi\hbar}}\, e^{-i\Delta t\,V(x_j)/\hbar}$$

$$\int \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\, e^{-i\Delta t\,V(x)/\hbar}\, \psi(x, t=0)\, dx$$

Fourier transf.

$$\int \frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}}\, e^{-\Delta t\,p^2/2m\hbar}\, \psi'(p)\, dp$$

Inverse Fourier.

$$FFT^{-1} \times e^{-\Delta t\,p^2/2m\hbar}\, FFT\; e^{-\Delta t\,V/\hbar} \times \psi(x, t=0)$$

$$\psi(x, t=h)$$