Summary of previous Lecture

$$\langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle$$

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{\frac{ipx}{\hbar}} \qquad \langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{-\frac{ipx}{\hbar}}$$

$$\lambda = \frac{h}{p}$$ $\leftarrow$ de Broglie wavelength

$$\hat{X}|x\rangle = x|x\rangle \qquad \hat{P}_x|p\rangle = p|p\rangle$$

$$\langle x|\psi\rangle = \psi(x) \qquad \langle p|\psi\rangle = \psi(p)$$

position space momentum space

$$\hat{1} = \int |p\rangle\langle p|\, dp$$

$$\psi(x) = \langle x|\psi\rangle = \int \langle x|p\rangle\langle p|\psi\rangle\, dp = \frac{1}{\sqrt{2\pi\hbar}}\int e^{\frac{ipx}{\hbar}}\psi(p)\, dp$$

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ipx}{\hbar}}$$

$$\hat{1} = \int |x\rangle\langle x|\, dx$$

$$\psi(p) = \langle p|\psi\rangle = \int \langle p|x\rangle\langle x|\psi\rangle\, dx = \frac{1}{\sqrt{2\pi\hbar}}\int e^{-\frac{ipx}{\hbar}}\psi(x)\, dx$$

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{-\frac{ipx}{\hbar}}$$

Fourier Transforms

a Little bit of Math: Gaussian Integrals

$$I(\alpha)=\int_{-\infty}^{\infty} e^{-\alpha x^2}\,dx=\sqrt{\frac{\pi}{\alpha}}$$

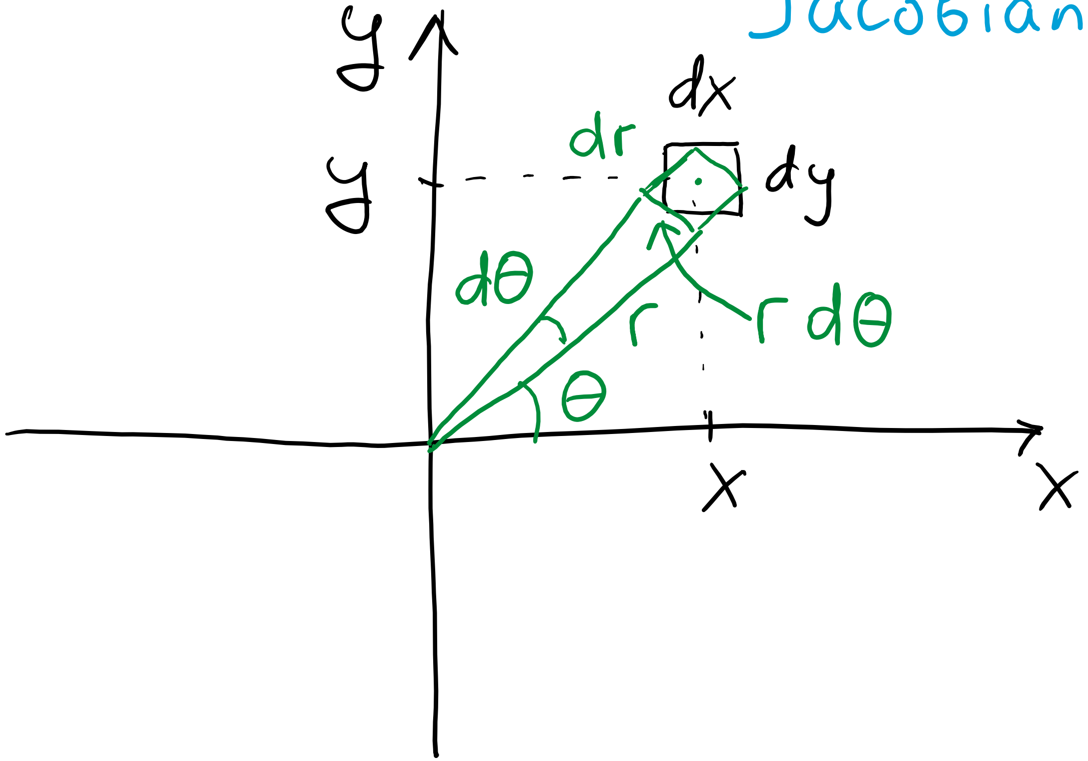
$$I^2(\alpha)=\int_{-\infty}^{\infty} e^{-\alpha x^2}\,dx\int_{-\infty}^{\infty} e^{-\alpha y^2}\,dy=\iint_{-\infty}^{\infty} e^{-\alpha(\overbrace{x^2+y^2}^{r^2})}\underbrace{dx\,dy}_{dr\cdot r\,d\theta}$$

Jacobian

$$I^2(\alpha)=\int_0^{2\pi} d\theta\int_0^{\infty} e^{-\alpha r^2}\,r\,dr=2\pi\cdot\frac{1}{2\alpha}=\frac{\pi}{\alpha}$$

$$\theta\Big|_0^{2\pi}=2\pi$$

$$-\frac{1}{2\alpha}e^{-\alpha r^2}\Big|_0^{\infty}=\frac{1}{2\alpha}$$



$$I(\alpha,\beta)=\int_{-\infty}^{\infty} e^{-\alpha x^2+\beta x}\,dx=\int_{-\infty}^{\infty} e^{-\alpha\left(\underbrace{x^2-\frac{\beta}{\alpha}x+\left(\frac{\beta}{2\alpha}\right)^2}_{\left(x-\frac{\beta}{2\alpha}\right)^2}-\left(\frac{\beta}{2\alpha}\right)^2\right)}dx$$

$$=e^{\frac{\beta^2}{4\alpha^2}}\int_{-\infty}^{\infty} e^{-\alpha\left(x-\frac{\beta}{2\alpha}\right)^2}dx=e^{\frac{\beta^2}{4\alpha^2}}\underbrace{\int_{-\infty}^{\infty} e^{-\alpha x_1^2}dx_1}_{\sqrt{\frac{\pi}{\alpha}}}=e^{\frac{\beta^2}{4\alpha^2}}\sqrt{\frac{\pi}{\alpha}}$$

$$x_1=x-\frac{\beta}{2\alpha}$$

$$\frac{d}{d\alpha}\int_{-\infty}^{\infty} e^{-\alpha x^2}dx=\frac{d}{d\alpha}\sqrt{\frac{\pi}{\alpha}} \Longrightarrow \int_{-\infty}^{\infty} -x^2 e^{-\alpha x^2}dx=-\frac{1}{2}\frac{\sqrt{\pi}}{\alpha^{3/2}}$$

$$\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2}dx=\frac{1}{2}\sqrt{\frac{\pi}{\alpha^3}}$$

Summary:

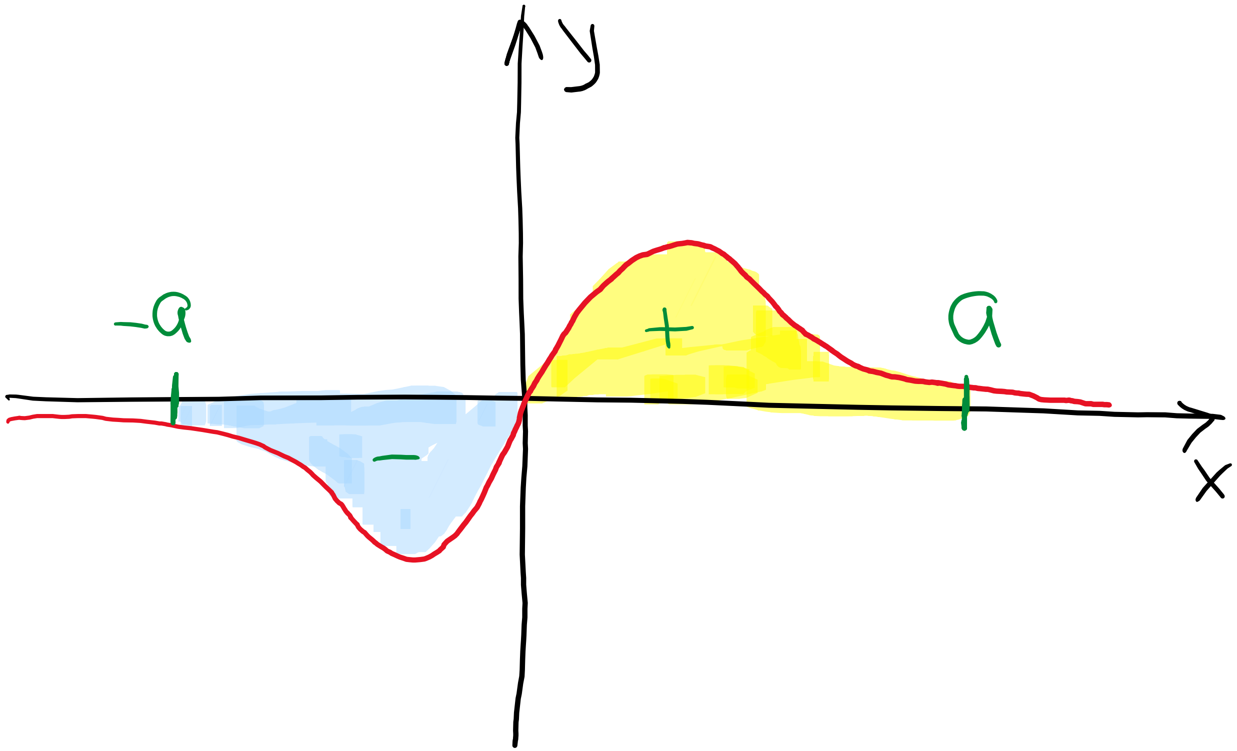
$$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}$$

$$\int_{-\infty}^{\infty} e^{-\alpha x^2 + \beta x} dx = e^{\frac{\beta^2}{4\alpha^2}} \sqrt{\frac{\pi}{\alpha}}$$

$$\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{\alpha^3}}$$

Question: Evaluate Integral

$$\int_{-\infty}^{\infty} e^{-x^2} \cdot \frac{\sin x \cdot \cos^2 x}{(x^2+1)(x^4+2)}\,dx = 0$$



$$\int_{-a}^{a} f(x)\,dx = 0$$

for all odd $f(x)$

Gaussian Wave Packet

1) Why wave packet?

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}} \quad : \quad \left.\begin{array}{l}\Delta p = 0 \\ \Delta x \to \infty\end{array}\right\} \text{not localized}$$

2) Why Gaussian?

<u>Simplicity</u> (Seriously!)

$$\psi(x) = \langle x|\psi\rangle = N e^{-\frac{x^2}{2a^2}}$$

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}$$

$$N = \frac{1}{\sqrt{a\sqrt{\pi}}}$$

$$\alpha = \frac{1}{a^2}$$

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = N^* N \int_{-\infty}^{\infty} e^{-\frac{x^2}{a^2}} dx = |N|^2 \sqrt{\frac{\pi}{1/a^2}} = |N|^2 a\sqrt{\pi} = 1$$

$$\Delta X = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\frac{a^2}{2} - 0} = \frac{a}{\sqrt{2}}$$

$$\psi(x) = \frac{1}{\sqrt{a\sqrt{\pi}}}\, e^{-\frac{x^2}{2a^2}}$$

$$\hat{1} = \int dx\, |x\rangle\langle x|$$

$$\langle x\rangle = \langle\psi|\hat{x}|\psi\rangle = \int dx \langle\psi|\hat{x}|x\rangle\langle x|\psi\rangle = \int dx \langle\psi|x\rangle x \langle x|\psi\rangle$$

$$\langle x\rangle = \int_{-\infty}^{\infty} x|\psi(x)|^2 dx = \frac{1}{a\sqrt{\pi}}\int_{-\infty}^{\infty} x e^{-\frac{x^2}{a^2}} dx = 0$$

odd function integrated in symmetrical limits

$$\langle x^2\rangle = \int_{-\infty}^{\infty} x^2 |\langle x|\psi\rangle|^2 dx = \frac{1}{a\sqrt{\pi}}\int_{-\infty}^{\infty} x^2 e^{-\frac{x^2}{a^2}} dx = \frac{1}{a\sqrt{\pi}} \cdot \frac{1}{2}\sqrt{\frac{\pi}{(1/a^2)^3}} = \frac{a^2}{2}$$

$$\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{\alpha^3}}$$

Momentum Space

$$\psi(p)=\langle p|\psi\rangle=\frac{1}{\sqrt{2\pi\hbar}}\int e^{-\frac{ipx}{\hbar}}\psi(x)=\frac{1}{\sqrt{2\pi\hbar}}\cdot\frac{1}{\sqrt{a\sqrt{\pi}}}\int_{-\infty}^{\infty}e^{-\frac{x^2}{2a^2}-\frac{ip}{\hbar}x}dx=\sqrt{\frac{a}{\hbar\sqrt{\pi}}}\,e^{-\frac{a^2p^2}{2\hbar^2}}$$

$$\psi(x)=\frac{1}{\sqrt{a\sqrt{\pi}}}e^{-\frac{x^2}{2a^2}}$$

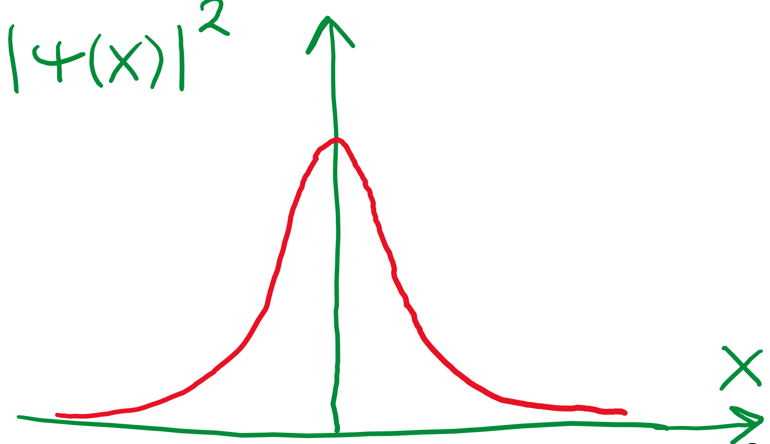
$$\alpha=\frac{1}{2a^2}\qquad \beta=-\frac{ip}{\hbar}$$

$$\int_{-\infty}^{\infty}e^{-\alpha x^2+\beta x}dx=e^{\frac{\beta^2}{4\alpha}}\sqrt{\frac{\pi}{\alpha}}$$

$$\psi(x)=\frac{1}{\sqrt{a\sqrt{\pi}}}e^{-\frac{x^2}{2a^2}}\cdot\underbrace{e^{\frac{ip_0x}{\hbar}}}$$

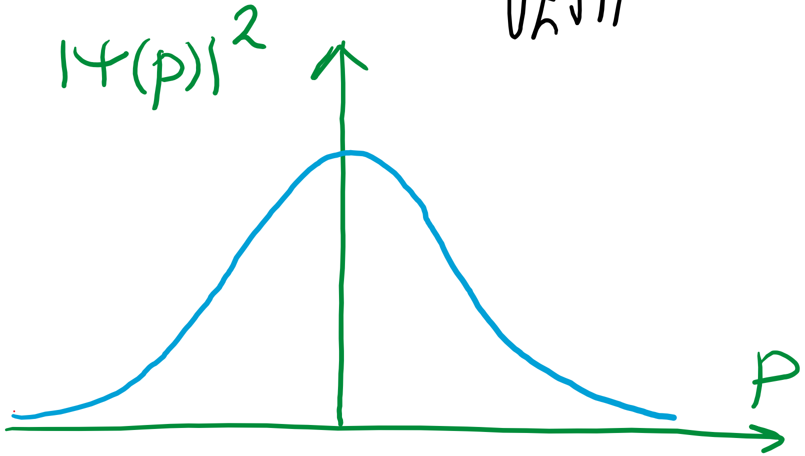
$$\psi(p)=\langle p|\psi\rangle=\frac{1}{\sqrt{2\pi\hbar}}\int e^{-\frac{ipx}{\hbar}}\psi(x)=\frac{1}{\sqrt{2\pi\hbar}}\cdot\frac{1}{\sqrt{a\sqrt{\pi}}}\int_{-\infty}^{\infty}e^{-\frac{x^2}{2a^2}-\frac{i(p-p_0)x}{\hbar}}dx=\sqrt{\frac{a}{\hbar\sqrt{\pi}}}\,e^{-\frac{a^2(p-p_0)^2}{2\hbar^2}}$$

$$\psi(x) = \langle x|\psi\rangle = \frac{1}{\sqrt{a\sqrt{\pi}}}\, e^{-\frac{x^2}{2a^2}}$$

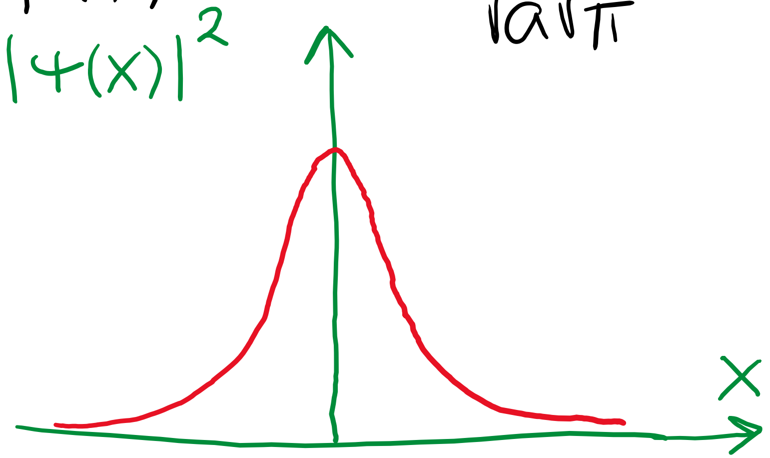


$$\Longleftrightarrow$$

$$\psi(p) = \langle p|\psi\rangle = \sqrt{\frac{a}{\hbar\sqrt{\pi}}}\, e^{-\frac{a^2p^2}{2\hbar^2}}$$

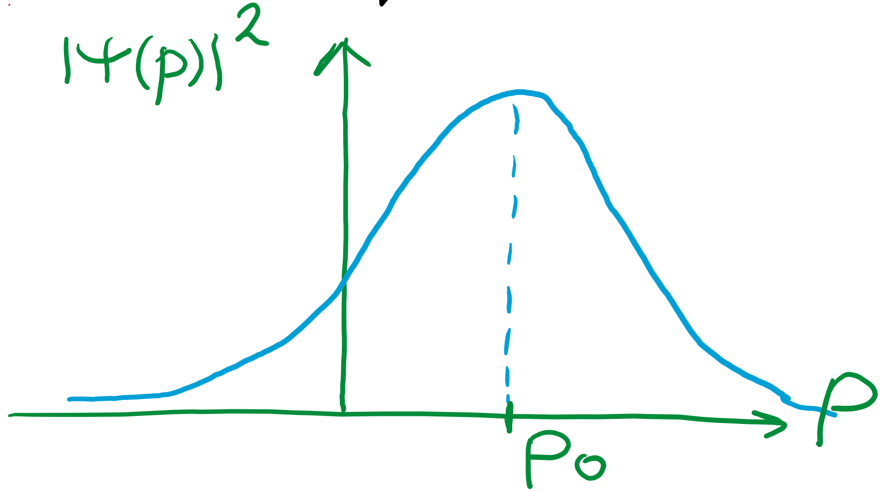


$$\psi(x) = \langle x|\psi\rangle = \frac{1}{\sqrt{a\sqrt{\pi}}}\, e^{-\frac{x^2}{2a^2}} \cdot e^{\frac{ip_0x}{\hbar}}$$



$$\Longleftrightarrow$$

$$\psi(p) = \langle p|\psi\rangle = \sqrt{\frac{a}{\hbar\sqrt{\pi}}}\, e^{-\frac{a^2(p-p_0)^2}{2\hbar^2}}$$



Find Δp:

$$\langle p\rangle = \langle\psi|\hat{p}|\psi\rangle = \int_{-\infty}^{\infty} dp\cdot p\,|\psi(p)|^2 = \frac{a}{\hbar\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-\frac{a^2p^2}{\hbar^2}}\,p\cdot dp = 0$$

$$\alpha = \frac{a^2}{\hbar^2}$$

$$\langle p^2\rangle = \langle\psi|\hat{p}^2|\psi\rangle = \int_{-\infty}^{\infty} dp\cdot p^2|\psi(p)|^2 = \frac{a}{\hbar\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-\frac{a^2p^2}{\hbar^2}}\,p^2\,dp = \frac{\hbar^2}{2a^2}$$

$$\int_{-\infty}^{\infty} x^2 e^{-\alpha x^2}\,dx = \frac{1}{2}\sqrt{\frac{\pi}{\alpha^3}}$$

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \frac{\hbar}{a\sqrt{2}}$$

Recall:

$$\Delta x = \frac{a}{\sqrt{2}}$$

$$\Delta x\,\Delta p = \frac{a}{\sqrt{2}}\cdot\frac{\hbar}{a\sqrt{2}} = \frac{\hbar}{2}$$

Time evolution: Free Space

$$V(x) = \text{const} = 0$$

$$\hat{H} = \frac{\hat{p}_x^2}{2m} \Rightarrow U(t) = e^{-\frac{i\hat{H}t}{\hbar}} = e^{-\frac{i\hat{p}_x^2 t}{2m\hbar}}$$

$$|\psi(t)\rangle = e^{-\frac{i\hat{p}_x^2 t}{2m\hbar}} |\psi(0)\rangle = e^{-\frac{i\hat{p}_x^2 t}{2m\hbar}} \int_{-\infty}^{\infty} dp\, |p\rangle\langle p|\psi(0)\rangle$$

$$\hat{1} = \int dp\, |p\rangle\langle p|$$

$$\sqrt{\frac{a}{\hbar\sqrt{\pi}}}\, e^{-\frac{a^2 p^2}{2\hbar^2}}$$

$$\langle x|\psi(t)\rangle = \int_{-\infty}^{\infty} dp \cdot e^{-\frac{ip^2 t}{2m\hbar}} \langle x|p\rangle\langle p|\psi(0)\rangle$$

$$\frac{1}{\sqrt{2\pi\hbar}}\, e^{\frac{ipx}{\hbar}}$$

$$\langle x|\psi(t)\rangle = \psi(x,t) = \frac{1}{\sqrt{\sqrt{\pi}\left[a + \frac{i\hbar t}{ma}\right]}} e^{-\frac{x^2}{2a^2\left[1+\frac{i\hbar t}{ma^2}\right]}}$$

$$\Delta X = \frac{a}{\sqrt{2}}\sqrt{1 + \frac{\hbar^2 t^2}{m^2 a^4}}$$

Examples:

$$\psi(x,0) = \langle x | \psi(0) \rangle = \frac{1}{\sqrt{a\sqrt{\pi}}} e^{-\frac{x^2}{2a^2}}$$

$$\psi(x,0) = \langle x|\psi(0)\rangle = \frac{1}{\sqrt{\ }} e^{-\frac{x^2}{2a^2}} \cdot e^{\frac{i p_0 x}{\hbar}}$$

3.27. Show that

$$e^{\hat{A}+\hat{B}} \neq e^{\hat{A}} e^{\hat{B}}$$

unless the operators $\hat{A}$ and $\hat{B}$ commute. Problem 7.19 shows what happens if $\hat{A}$ and $\hat{B}$ do not commute but each commutes with their commutator $[\hat{A}, \hat{B}]$.

$$e^{\hat{A}+\hat{B}} = 1 + (\hat{A}+\hat{B}) + \frac{1}{2!}(\hat{A}+\hat{B})(\hat{A}+\hat{B}) + \dots = 1 + \hat{A} + \hat{B} + \frac{1}{2}\left(\hat{A}^2 + \hat{A}\hat{B} + \hat{B}\hat{A} + \hat{B}^2\right) + \dots$$

$$e^{\hat{A}} \cdot e^{\hat{B}} = \left(1 + \hat{A} + \frac{1}{2!}\hat{A}^2 + \dots\right)\left(1 + \hat{B} + \frac{1}{2}\hat{B}^2 + \dots\right) = 1 + \hat{A} + \hat{B} + \frac{1}{2}\left(\hat{A}^2 + 2\hat{A}\hat{B} + \hat{B}^2\right) + \dots$$

We may say that

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} + O([\hat{A},\hat{B}])$$

$$\hat{U}(\Delta t) = e^{-\frac{i\hat{H}\Delta t}{\hbar}} = e^{-\frac{i}{\hbar}\left(\frac{\hat{p}_x^2}{2m} + V(\hat{x})\right)\Delta t} = e^{-\frac{i\hat{p}_x^2\Delta t}{2m\hbar}} \cdot e^{-\frac{iV(\hat{x})}{\hbar}\Delta t} + O([\hat{p}_x^2, \hat{x}]\Delta t^2)$$

$\sim \Delta t^2$

Algorithm:

1) $\psi(x,t) \longrightarrow e^{-\frac{iV(x)}{\hbar}\Delta t}\psi(x,t) = \psi_1(x,t)$

2) $\psi_1(x,t) \xrightarrow{FFT} \psi_1(p,t)$

3) $\psi_1(p,t) \longrightarrow e^{-\frac{ip^2\Delta t}{2m\hbar}}\psi_1(p,t) = \psi_2(p,t)$

4) $\psi_2(p,t) \xrightarrow{FFT} \psi(x, t+\Delta t)$

https://jakevdp.github.io/blog/2012/09/05/quantum-python/