Gaussian Wavepacket for Free Particle Potential ($V=0$).

At $t=0$, construct $\Psi(x,0) = A e^{-ax^2} = \langle x | \Psi_0 \rangle$

Normalize $\int_{-\infty}^{\infty} dx \, |\Psi(x,0)|^2 = 1 \Rightarrow A = \left(\frac{2a}{\pi}\right)^{1/4}$

How does $|\Psi_0\rangle$ evolve in time?

Expand $|\Psi_0\rangle$ in energy eigenstates, but for free particles the energy eigenstates are also eigenstates of $\hat{p}$, $\hat{k} = \frac{\hat{p}}{\hbar}$: $\langle x|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$

$\langle k|k'\rangle = \delta(k-k')$

For energy eigenstates, the time evolution is simple:

multiply by $e^{\frac{-iEt}{\hbar}}$, $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$

Expand $|\Psi_0\rangle$ in momentum basis $\leftrightarrow$ take Fourier transform

$\langle k|\Psi_0\rangle = \tilde{\Psi}_0(k) = c(k) = (2\pi a)^{-1/4} \cdot e^{\frac{-k^2}{4a}}$

also a gaussian, the function that is its own Fourier transform.

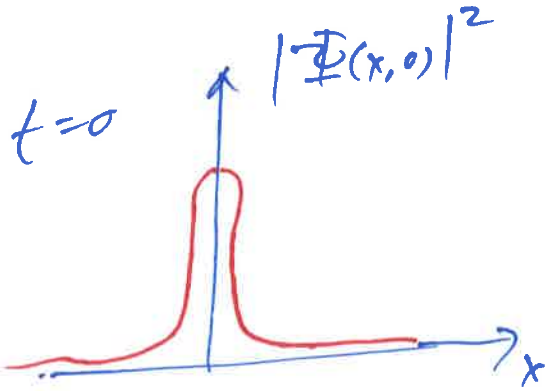
Put in the time dependence: $e^{-i\frac{\hbar k^2 t}{2m}}$

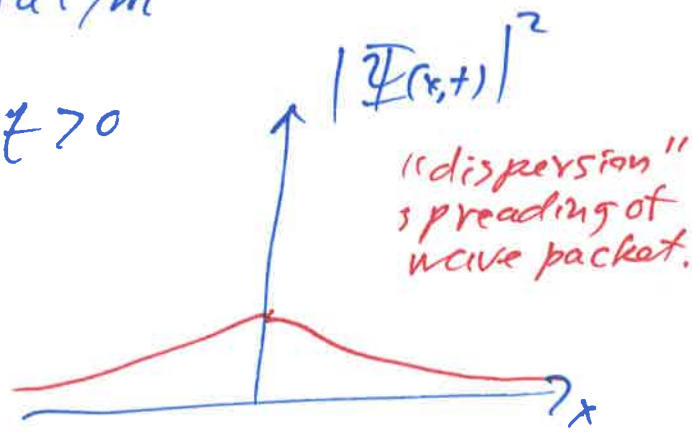
Now take the inverse Fourier transform.

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{k=-\infty}^{+\infty} dk\, e^{ikx}\, \tilde{\Psi}(k,t)$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk\, e^{ikx} (2\pi a)^{-1/4} e^{\frac{-k^2}{4a}} \cdot e^{-i\frac{\hbar k^2 t}{2m}}$$

$$= \left(\frac{2a}{\pi}\right)^{1/4} \frac{\exp\left[\dfrac{-ax^2}{(1+2i\hbar a t/m)}\right]}{\sqrt{1+2i\hbar a t/m}}$$





At time t $\quad \sigma_p = \Delta p = \hbar\sqrt{a}\,, \quad \sigma_x = \Delta x = \dfrac{1}{2\sqrt{\dfrac{a}{1+\left(\frac{2\hbar a t}{m}\right)^2}}}$

$\underline{t=0}$ $\quad \sigma_x \sigma_p = \frac{\hbar}{2}$ $\qquad \underline{t>0}$ $\quad \sigma_x \sigma_p > \frac{\hbar}{2}$

phase velocity $v_\varphi = \frac{\omega}{k} = \frac{\left(\frac{\hbar k^2}{2m}\right)}{k} = \frac{\hbar k}{2m} = \frac{p}{2m} = \frac{v_{class}}{2}$

group velocity $v_g = \frac{d\omega}{dk} = \frac{d}{dk}\left(\frac{\hbar k^2}{2m}\right) = \frac{\hbar k}{m} = \frac{p}{m} = v_{class}$

$v_g = 2 v_\varphi$ for free particle.

Gaussian Integrals

$$I = \int_{-\infty}^{+\infty} e^{-x^2}\,dx$$

← number not a function of x

$f(x)$	$f'(x)$
3	0
x	1
x^n	$n x^{n-1}$
$\sin(x)$	$\cos(x)$
⋮	⋮

e^{-x^2} never occurs

$$I^2 = \left(\int_{-\infty}^{+\infty} e^{-x^2}\,dx\right)\left(\int_{-\infty}^{+\infty} e^{-y^2}\,dy\right)$$

Reinterpret x and y as Cartesian coordinates

$$I^2 = \int_{x}^{+\infty}\int_{y}^{-\infty} e^{-(x^2+y^2)}\,dx\,dy$$

Switch to Polar Coordinates

from Jacobian

$$I^2 = \int_{r=0}^{\infty}\int_{\varphi=0}^{2\pi} e^{-r^2}\,r\,dr\,d\theta = \underbrace{\int_{\varphi=0}^{2\pi} d\varphi}_{2\pi} \cdot \underbrace{\int_{r=0}^{\infty} r e^{-r^2}\,dr}_{1/2}$$

$$I^2 = (2\pi)\left[-\frac{1}{2}e^{-r^2}\right]_0^\infty = (2\pi)\left[0-\left(-\frac{1}{2}\right)\right] = \pi$$

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

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change variables $x \to \sqrt{a}\,z$, $dx = \sqrt{a}\,dz$

$$\sqrt{\pi} = \int_{z=-\infty}^{+\infty} e^{-az^2}\,dz\,\sqrt{a} \Longrightarrow \int_{-\infty}^{+\infty} e^{-ax^2}\,dx = \sqrt{\frac{\pi}{a}}$$

$\uparrow \frac{d}{da}$ both sides

$$\int_{-\infty}^{+\infty} (-x^2)e^{-ax^2}\,dx = \sqrt{\pi}\,\frac{d}{da}\left(a^{-1/2}\right) = \sqrt{\pi}\left(-\frac{1}{2}\right)a^{-3/2}$$

$$\int_{-\infty}^{+\infty} x^2 e^{-ax^2}\,dx = \frac{1}{2}\left(\frac{\pi}{a^3}\right)^{1/2}$$ rather, rinse, repeat

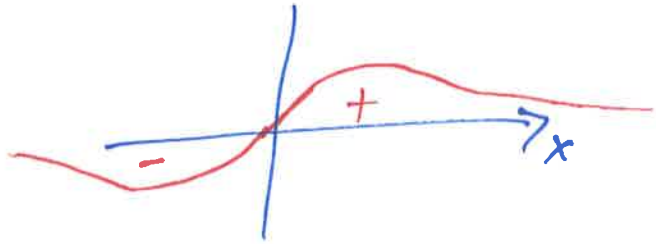
$\vdots$

$$\int_{-\infty}^{+\infty} x^{2n} e^{-ax^2}\,dx = ?$$ for $n = 0, 1, 2 \ldots$

even powers of x

odd powers of x

$$\int_{-\infty}^{+\infty} x^{2n+1} e^{-x^2} dx = 0$$



$$\int_{x=0}^{\infty} x e^{-ax^2} dx = \frac{1}{2a}$$ $\left(\frac{d}{da}\right)^n$ both sides

$$\int_{x=0}^{\infty} x^3 e^{-ax^2} dx = \frac{1}{2a^2} , \int_{x=0}^{\infty} x^5 e^{-ax^2} dx = \frac{1}{a^3}$$

$$[\hat{x}, \hat{p}] = i\hbar \hat{1}$$ canonical commutation relation

$$\sigma_x \sigma_p = \Delta x \Delta p \geq \frac{\hbar}{2}$$ generalizes

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Ehrenfest's Theorem - Expectation values of quantum operators obey classical laws.

$$\langle \hat{p} \rangle = \langle \psi | \hat{p} | \psi \rangle = m \frac{d}{dt} \langle \hat{x} \rangle$$

Classically $p = m\frac{dx}{dt}$, $\frac{dp}{dt} = F = -\frac{dV}{dx}$

$$\frac{d}{dt} \langle p \rangle = \left\langle -\frac{dV(\hat{x})}{dx} \right\rangle$$

Generalized Ehrenfest Theorem

$$\frac{d}{dt}\langle \hat{A}\rangle_{\Psi} = \frac{d}{dt}\langle \Psi|\hat{A}|\Psi\rangle$$

$$= \left\langle \frac{\partial\Psi}{\partial t}\middle|\hat{A}\middle|\Psi\right\rangle + \left\langle \Psi\middle|\frac{\partial \hat{A}}{\partial t}\middle|\Psi\right\rangle + \left\langle \Psi\middle|\hat{A}\middle|\frac{\partial\Psi}{\partial t}\right\rangle$$

$$\text{S.E.} \Rightarrow \quad i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle$$

$$\frac{d}{dt}\langle \hat{A}\rangle_{\Psi} = -\frac{1}{i\hbar}\underbrace{\langle \hat{H}\Psi|\hat{A}|\Psi\rangle}_{\langle \Psi|\hat{H}\hat{A}|\Psi\rangle} + \left\langle\frac{\partial \hat{A}}{\partial t}\right\rangle_{\Psi} + \frac{1}{i\hbar}\langle \Psi|\hat{A}|\hat{H}\Psi\rangle$$

$$\frac{d}{dt}\langle \hat{A}\rangle_{\Psi} = \frac{i}{\hbar}\langle \Psi|[\hat{H},\hat{A}]|\Psi\rangle + \left\langle\frac{\partial \hat{A}}{\partial t}\right\rangle_{\Psi}$$

$$\boxed{\frac{d}{dt}\langle \hat{A}\rangle_{\Psi} = \frac{i}{\hbar}\langle [\hat{H},\hat{A}]\rangle_{\Psi} + \left\langle\frac{\partial \hat{A}}{\partial t}\right\rangle_{\Psi}}$$

Schwarz Inequality

Consider two kets $|\varphi_1\rangle$ and $|\varphi_2\rangle$ not necessarily orthogonal, nor normalized, but neither is the zero ket : $\langle zero|zero\rangle = \emptyset$

Define $|\psi\rangle = |\varphi_1\rangle + \lambda|\varphi_2\rangle$

$$\langle\psi|\psi\rangle = \langle\varphi_1|\varphi_1\rangle + \lambda\langle\varphi_1|\varphi_2\rangle + \lambda^*\langle\varphi_2|\varphi_1\rangle + \lambda\lambda^*\langle\varphi_2|\varphi_2\rangle \geq 0$$