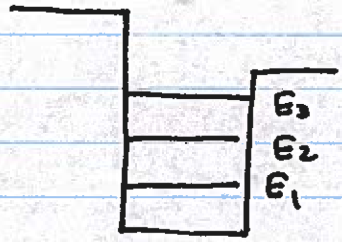
Time evolution of quantum states

Discrete spectrum



The shrodinger eqn has ~~only~~ solutions for specific values of energies $E_1, E_2 \ldots E_N$ (N may be ∞)

Stationary states

$$\hat{H}|n\rangle = E_n|n\rangle \qquad \psi_n = \langle x|n\rangle \Rightarrow \hat{H}\psi_n = E_n\psi_n$$

Time evolution of stationary states

$$|n\rangle \longrightarrow e^{-i\hat{H}t/\hbar}|n\rangle = e^{-iE_nt/\hbar}|n\rangle$$

or

$$\psi_n(x) \longrightarrow \psi_n(x,t) = e^{-iE_nt/\hbar}\psi_n(x)$$

Any other bound state can be presented as a <u>superposition</u> of stationary states

$$|\alpha\rangle = \sum_n c_n|n\rangle \quad \text{or} \quad \underset{\langle x|\alpha\rangle}{\psi_\alpha(x)} = \sum_n c_n\langle x|n\rangle = \sum_n c_n\psi_n(x)$$

Time evolution $e^{-i\hat{H}t/\hbar}|\alpha\rangle = \sum_n c_n e^{-i\hat{H}t/\hbar}|n\rangle =$

$$= \sum_n c_n e^{-iE_nt/\hbar}|n\rangle$$

or

$$\psi_\alpha(x,t) = \sum_n e^{-iE_nt}c_n\cdot\psi_n(x)$$

Average energy: in a state $|\alpha\rangle$ $\langle E\rangle = \langle\alpha|\hat{H}|\alpha\rangle =$

$$= \langle\alpha|\hat{H}\sum c_n\psi_n(t)\rangle = \langle\alpha|\sum c_nE_n\psi_n(t)\rangle$$

$$= \sum c_nE_n\langle\alpha|\psi_n(t)\rangle = \sum|c_n|^2E_n \quad \text{time independent}$$

Operators that commute with Hamiltonian (i.e. have the same eigenbasis) also have time-independent average value.

In general $\langle \hat{A}(t) \rangle = \langle \alpha(t) | \hat{A} | \alpha(t) \rangle$

Average position: at $t=0$ $\langle x \rangle = \int_{-\infty}^{+\infty} \psi_\alpha^*(x)\, x\, \psi_\alpha(x)\, dx$

$$\langle x(t) \rangle = \int_{-\infty}^{+\infty} \psi_\alpha^*(x,t)\, x\, \psi_\alpha(x,t)\, dx \qquad = \sum_{n,m} c_m^* c_n \int_{-\infty}^{+\infty} \psi_m^*(x)\, x\, \psi_n^*(x)$$

$$\psi_\alpha(x,t) = \sum_n c_n e^{-iE_n t/\hbar} \psi_n(x)$$

$$\psi_\alpha^*(x,t) = \sum_m c_m^* e^{+iE_m t/\hbar} \psi_m^*(x)$$

$$\langle x(t) \rangle = \sum_{n,m} c_m^* c_n \underbrace{\left[\int_{-\infty}^{+\infty} \psi_m^*(x)\, x\, \psi_n(x)\, dx \right] e^{i(E_m - E_n)t/\hbar}}$$

unless these terms $= 0$ for $n \neq m$ there will be time dependence in the average value of x

$$\langle p(t) \rangle = \sum_{n,m} c_m^* c_n \left[\int_{-\infty}^{+\infty} \psi_m^*(x) (-i\hbar) \frac{\partial \psi_n}{\partial x}\, dx \right] e^{i(E_m - E_n)t/\hbar}$$

Time evolution of GWP

Easy in momentum representation

$$\varphi(p) \longrightarrow e^{-i\hat{H}t/\hbar}\,\varphi(p) = e^{-i\hat{H}t/\hbar}\langle p | gwp\rangle =$$

$$= e^{-ip^2t/2m\hbar}\,\varphi(p)$$

Time evolution adds a p-dependent phase, but does not change the distribut

$$|\varphi(p,t)|^2 = |e^{-ip^2t/2m\hbar}|^2\,|\varphi(p)|^2 = |\varphi(p)|^2$$

To find the time dependence in the position representation, we need to change basis

$$\psi(x) = \langle x | gwp\rangle = \langle x | \hat{\mathbb{1}} | gwp\rangle \qquad \hat{\mathbb{1}} = \int_{-\infty}^{+\infty} |p'\rangle\langle p'|\,dp'$$

$$\psi(x) = \int_{-\infty}^{+\infty} \langle x|p\rangle\langle p|gwp\rangle\,dp = \sqrt{\frac{a}{\hbar\sqrt{\pi}}}\int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi\hbar}}\,e^{ipx/\hbar}\,e^{-p^2a^2/2\hbar}\,dp$$

$$= \sqrt{\frac{a}{\hbar\sqrt{\pi}}}\cdot\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} e^{-\left(\frac{a}{\sqrt{2}\hbar}p - \frac{\sqrt{2}xi}{a}\right)^2 - \frac{x^2}{2a^2}}\,dp =$$

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

$$\psi(x,t) = \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi\hbar}}\,e^{ipx/\hbar}\cdot\sqrt{\frac{a}{\sqrt{\pi}\,\hbar}}\,e^{-p^2a^2/2\hbar}\,e^{-ip^2t/2m}\,dp$$

$$= \frac{1}{\sqrt{2\pi\hbar}}\sqrt{\frac{a}{\sqrt{\pi}\,\hbar}}\int_{-\infty}^{+\infty} e^{-\left[\frac{a^2}{2\hbar}+\frac{it}{2m}\right]p^2 + ipx/\hbar}\,dp =$$

$$= \frac{1}{\sqrt{\sqrt{\pi}\left(a + \frac{i\hbar t}{ma}\right)}}\,e^{-x^2/2a^2(1+i\hbar t/ma^2)}$$

Continuous spectrum : the Schrodinger equation has solutions for any value of energies

Free - moving particle $\hat{H} = \frac{\hat{p}^2}{2m}$ $\quad \hat{H}|p\rangle = \frac{p^2}{2m}|p\rangle$

$|p\rangle$ are eigen states for $E = p^2/2m$

$$|p\rangle \xrightarrow{t} \cancel{\frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}} \; e^{-i(p^2/2m\hbar)t} \; |p\rangle$$

$$\varphi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \; e^{-ip^2 t/2m\hbar}$$

This describes a plane wave $\rightarrow$ completely delocalized

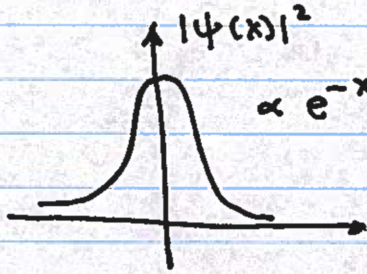
More realistic situation : Gaussian wavepacket $|gwp\rangle$

<u>t=0</u>

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

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

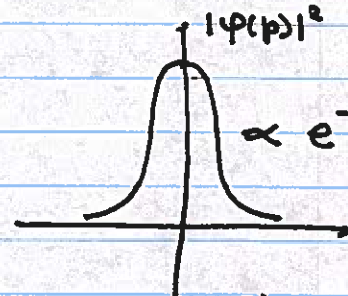
$|\psi(x)|^2$



$\propto e^{-x^2/a^2}$

$\Longleftrightarrow$

$|\varphi(p)|^2$



$\propto e^{-p^2 a^2/\hbar^2}$

$\Delta x \propto a$ $\qquad \Delta p \propto \hbar/a$

$$\Delta x \cdot \Delta p \propto \hbar$$

We have some information about particle's position and momentum
More precisely: $\langle x \rangle = \frac{1}{\sqrt{\pi}\,a} \int_{-\infty}^{+\infty} x \cdot e^{-x^2/a^2} dx = 0$

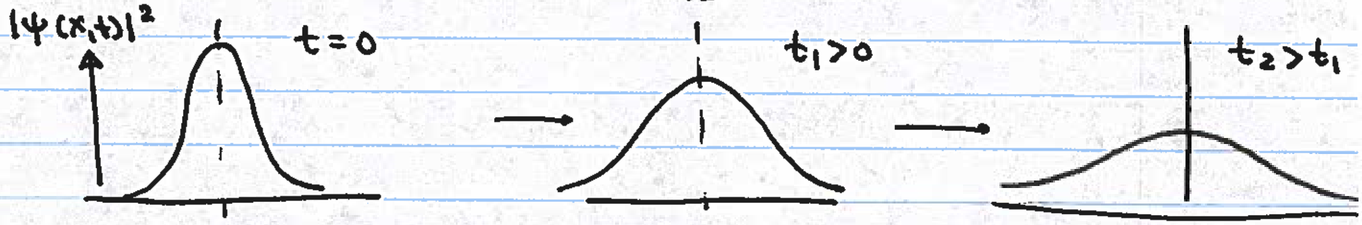
$$\langle x^2 \rangle = \frac{1}{\sqrt{\pi}\,a} \int_{-\infty}^{+\infty} x^2 e^{-x^2/a^2} dx = \frac{a^2}{2} \qquad \Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \frac{a}{\sqrt{2}}$$

Probability density

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

If we calculate the width of the particle distribution as a function of time

$$\Delta x(t) = \sqrt{\langle x^2 \rangle} = \frac{a}{\sqrt{2}} \sqrt{1 + \hbar^2 t^2/(ma^2)^2}$$



The wave packet spreads in space as time passes by, while its distribution in momentum space remains unchanged

What if the wave packet is moving?

$$\varphi_{p_0}(p) = \sqrt{\frac{a}{\sqrt{\pi}\,\hbar}}\; e^{-(p-p_0)^2 a^2/2\hbar^2}$$

$$\langle p \rangle = \int_{-\infty}^{+\infty} p\,|\varphi(p)|^2\, dp = p_0$$

$$\psi_{p_0}(x) = \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi\hbar}}\, e^{ipx/\hbar} \sqrt{\frac{a}{\sqrt{\pi}\,\hbar}}\; e^{-(p-p_0)^2 a^2/2\hbar^2}\, dp$$

$$= e^{ip_0 x/\hbar} \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi\hbar}}\, e^{i(p-p_0)x/\hbar} \sqrt{\frac{a}{\sqrt{\pi}\,\hbar}}\; e^{-(p-p_0)^2 a^2/2\hbar^2}\, d(p-p_0)$$

$$= e^{ip_0 x/\hbar}\, \frac{1}{\sqrt{\sqrt{\pi}\,a}}\, e^{-x^2/2a^2}$$

The overall motion adds a phase, put doesn't affect the probability distribution.