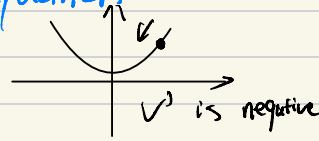


An overview of Quantum mechanics

Linearity and nonlinear theories. Schrödinger's equation

For motion in 1D:

$$V(x); x(t) \longrightarrow m \frac{d^2 x(t)}{dt^2} = -V'(x(t))$$



QM is linear!

Ψ wavefunction (depends on time) $\rightarrow$ Nonlinear $\rightarrow$ complicated to solve!

$$i\hbar \frac{d\Psi}{dt} = \hat{H} \Psi$$

$\hat{H}$ Hamiltonian $\rightarrow$ linear operator.

So, it's linear $\rightarrow L\Psi = 0 \leftarrow SE$

$$L\Psi \equiv i\hbar \frac{d\Psi}{dt} - \hat{H}\Psi$$

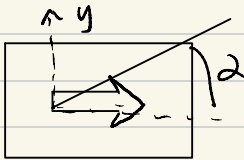
$$\Psi \in \mathcal{F}$$

Necessity of complex numbers

$$i = \sqrt{-1} \rightarrow \boxed{z} = a + ib \in \mathbb{C}, a, b \in \mathbb{R}$$

$$|z|^2 = \sqrt{a^2 + b^2} = z z^* \rightarrow \text{complex number}$$

Determinism



$$\vec{E}_\alpha = E_0 \cos \alpha \hat{x} + E_0 \sin \alpha \hat{y}$$

$$\text{After polarizer } \vec{E}_\alpha = E_0 \cos \alpha \hat{x}$$

Polarizer. fraction of energy through $(\cos \alpha)^2$

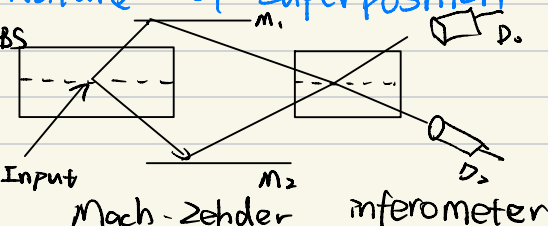
photons either go through or not can only predict probabilities

$|\text{photon}; x\rangle, |\text{photon}; y\rangle \rightarrow$ photon polarized along y , a vector

So, according to linearity, do superposition.

$$|\text{photon}; \alpha\rangle = \cos \alpha |\text{photon}; x\rangle + \sin \alpha |\text{photon}; y\rangle$$

Nature of Superposition



Superposition of state $|A\rangle$, and $|B\rangle$

Assume measure some property on $|A\rangle \rightarrow$ get "a"
on $|B\rangle \rightarrow$ get "b"

Q/N state $\alpha|A\rangle + \beta|B\rangle = ? \rightarrow$ Not intermediate state = e.g. $\frac{a+b}{2} \times$
or $a+b \times$

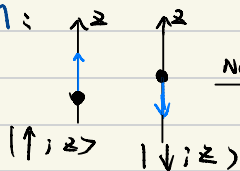
prob(a) $\sim |\alpha|^2$ If get "a", state becomes $|A\rangle$

prob(b) $\sim |\beta|^2$ If get "b", state becomes $|B\rangle$

Physical Assumption: Superposition of a state to itself does not change the state

$$|A\rangle \cong \alpha|A\rangle \cong -|A\rangle \cong i|A\rangle$$

Spin:



New quantum state
by superposition

$$|\psi\rangle = |\uparrow; z\rangle + |\downarrow; z\rangle$$

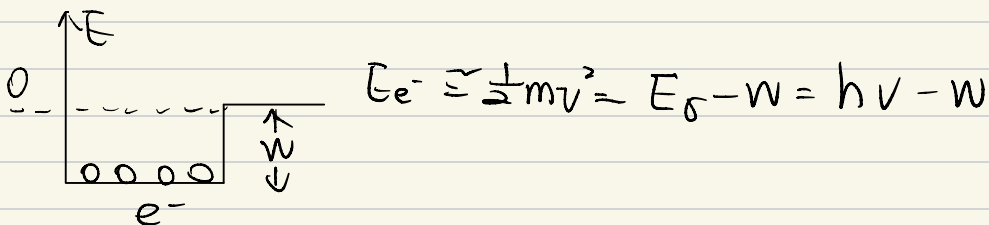
find 50% $|\uparrow; z\rangle$

find 50% $|\downarrow; z\rangle$

Entanglement

The photoelectric effect

1. polished metal irradiated may emit electrons $\rightarrow$ "photo electron"
2. There is a threshold frequency ν_0 , only $\nu > \nu_0$.
 ν_0 depend on the metal and configuration of atoms on surface
3. Magnitude of the current is proportional to the light intensity
4. Energy of photo electrons is independent of intensity of light



Units of h and Compton wavelength of particles

Unit of h : $[h] = \frac{[E]}{[\nu]} = \frac{M \frac{L^2}{T^2}}{\frac{1}{T}} = M \frac{L^2}{T} = L \cdot M \frac{L}{T} = [r] [p] = [L]$
 angular momentum

If I have a particle in, it's associated with length

m) $\frac{h}{p} \rightarrow \frac{h}{mc} \equiv$ Compton wavelength of a particle

$\rightarrow$ Different from De Broglie wavelength.
 $\rightarrow$ use true moment instead of mc

Compton scattering

photon scattering on electrons that are "virtually" free

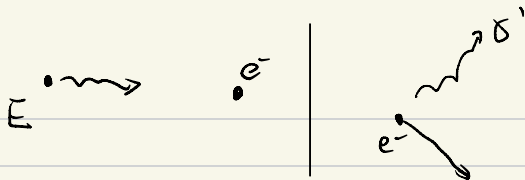
$$E^2 - p^2 c^2 = m^2 c^4$$

$$E = \frac{mc^2}{\sqrt{1 - \frac{v^2}{c^2}}}$$

$$p = \frac{m\vec{v}}{\sqrt{1 - \frac{v^2}{c^2}}}$$

for a photon, $m_r = 0$

$$\therefore E_r = p_r c \rightarrow p_r = \frac{E_r}{c} = \frac{h\nu_r}{c} = \frac{h}{\lambda_r}$$



photon loses energy

$$\lambda_f = \lambda_i + \frac{h}{m_e c} (1 - \cos \theta)$$

de Broglie's proposal

Particle $\longleftrightarrow$ wave
 E, p "v"

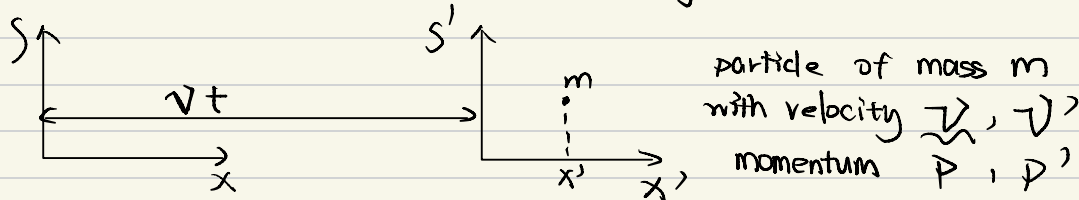
for a particle with momentum p , we associate with a plane wave of $\lambda = \frac{h}{p}$ (de Broglie wavelength)

$\Psi(\vec{x}, t) \in \mathbb{C}$ $\xleftarrow{\text{wave function (SE)}}$ measurable? meaning?

de Broglie wavelength in different frames

$$p = \frac{h}{\lambda} = \frac{h}{2\pi} \frac{2\pi}{\lambda} = \hbar k \quad \text{wave number} \quad \gamma', \omega = 2\pi \nu$$

Frame S , frame S' moves with velocity $+V$ in the x -dimension.



$$x' = x - Vt \quad ; \quad t' = t$$

$$\frac{dx'}{dt'} = \frac{dx}{dt} - V \Rightarrow u' = u - V$$

$$\therefore p' = p - mV$$

$$\lambda' = \frac{h}{p'} = \frac{h}{p - mV} \neq \frac{h}{p} = \lambda \quad \text{de Broglie doesn't agree!}$$

Galilean transformation of ordinary waves.

$$\phi = \text{phase} = kx - \omega t \quad \xrightarrow{\text{angular frequency } \frac{2\pi\nu}{\lambda}}$$

$$\begin{aligned}\phi &= k(x - vt) = \frac{2\pi}{\lambda}(x - vt) \\ &= \underbrace{\frac{2\pi x}{\lambda}}_k - \underbrace{\frac{2\pi vt}{\lambda}}_{\omega}\end{aligned}$$

c. $\phi' = \phi$ when frame to the same point and same time

$$\begin{aligned}\phi' = \phi &= \frac{2\pi}{\lambda}(x - vt) = \frac{2\pi}{\lambda}(x' + vt' - vt) \\ &= \underbrace{\frac{2\pi}{\lambda}}_{k'} x' - \underbrace{\frac{2\pi}{\lambda} v \left(1 - \frac{v}{v}\right)}_{\omega'} t'\end{aligned}$$

$$c. k' = k \Rightarrow \lambda' = \lambda \quad ! \text{ for ordinary wave.}$$

which means:

ψ can not be directly measurable.

Not Galilean invariant

$$\psi(x, t) \neq \psi'(x', t')$$

The frequency of a matter wave

$$p = \hbar k, \quad \boxed{E = \hbar \omega} \rightarrow \omega = \frac{E}{\hbar}$$

$$\text{wave phase: } \phi = kx - \omega t, \quad v_{\text{phase}} = \frac{\omega}{k} = \frac{E}{p} = \frac{\frac{1}{2}mv^2}{\frac{1}{2}mv} = \frac{1}{2}v$$

phase wave velocity of a particle is not equal to particle's velocity

$$v_{\text{group}} = \left. \frac{d\omega}{dk} \right|_k = \frac{dE}{dp} = \frac{d\left(\frac{p^2}{2m}\right)}{dp} = \frac{p}{m} = v !!$$

Special relativity

$$\left(\frac{E}{c}, \vec{p}\right) = \hbar \cdot \left(\frac{\omega}{c}, \vec{k}\right)$$

4-vector

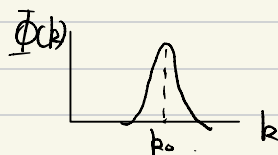
↓
position and time

Group velocity and stationary phase approximation

Group velocity is a wave of a packet constructed by superposition of waves.

$$\Psi(x,t) = \int dk \Phi(k) e^{i(kx - \omega(k)t)}$$

$\Phi(k)$



principle of stationary phase.

Since only for $k=k_0$, the integral has a chance to be non-zero.

$$\varphi(k) = kx - \omega t \rightarrow \left. \frac{d\varphi(k)}{dk} \right|_{k_0} = x - \left. \frac{d\omega(k)}{dk} \right|_{k_0} t = 0, \quad x = \left. \frac{d\omega(k)}{dk} \right|_{k_0} t$$

Motion of a wave packet

$$\Psi(x,t) = \int dk \Phi(k) e^{i(kx - \omega(k)t)}, \quad \Psi(x,t=0) = \int dk \Phi(k) e^{ikx}$$

$$\text{Taylor series } \omega(k) = \omega(k_0) + (k-k_0) \left. \frac{d\omega}{dk} \right|_{k_0} + \mathcal{O}(k-k_0)^2$$

$$\begin{aligned} \therefore \Psi(x,t) &= \int dk \Phi(k) e^{ikx} \cdot e^{-i\omega(k_0)t} \cdot e^{-i(k-k_0) \left. \frac{d\omega}{dk} \right|_{k_0} t} \cdot e^{i k_0 \left. \frac{d\omega}{dk} \right|_{k_0} t} \cdot e^{\text{negligible}} \\ &= e^{-i\omega(k_0)t} \cdot e^{i k_0 \left. \frac{d\omega}{dk} \right|_{k_0} t} \int dk \Phi(k) e^{ik(x - \left. \frac{d\omega}{dk} \right|_{k_0} t)} \end{aligned}$$

Due to imaginary number, hard to see bump (real number)

→ we use absolute value.

$$|\Psi(x,t)| = |\Psi(x - \left. \frac{d\omega}{dk} \right|_{k_0} t, 0)|$$

The wave for a free particle.

particle E, P, $E = \hbar\omega$, $P = \hbar k$, $\omega = 2\pi V \Rightarrow$ angular frequency,

Momentum operator, Schrödinger equation, and interpretation of the wavefunction.

Momentum operator, energy operator, and a differential equation

The matter wave: $\psi(x,t) = e^{ikx - i\omega t}$, $p = \hbar k$, non-relativistic particle
 $E = \hbar\omega$ $E = \frac{p^2}{2m}$

Momentum operator.

$$\frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x,t) = \hbar k \psi(x,t) = p \psi(x,t)$$

↪ operator $\rightarrow \hat{p} \equiv \frac{\hbar}{i} \frac{\partial}{\partial x} \rightarrow \hat{p} \psi(x,t) = p \psi(x,t)$

If this holds, $\psi(x,t)$ is an eigenstate (eigenvector)

Energy operator

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = i\hbar (-i\omega) \psi = \hbar\omega \psi = E \psi(x,t)$$

↪ $\hat{E} \psi = E \psi \rightarrow$ right but not implicate too much info.

Recall that $E = \frac{p^2}{2m} \rightarrow \hat{E} \psi = \frac{p^2}{2m} \psi = \frac{p}{2m} \hat{p} \psi = \frac{p}{2m} \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x,t)$

" p is a number, $\hat{E} \psi = \frac{1}{2m} \frac{\hbar}{i} \frac{\partial}{\partial x} p \psi(x,t) = \frac{1}{2m} \frac{\hbar}{i} \frac{\partial}{\partial x} \hat{p} \psi$

$$\therefore \hat{E} \psi = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t)$$

$$\therefore \hat{E} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} = \frac{1}{2m} \hat{p}^2$$

Free Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$$

Remarks =

* ψ cannot be wave

* Not a usual wave equation type: $\frac{\partial^2 \phi}{\partial x^2} - \frac{1}{v^2} \frac{\partial^2 \phi}{\partial t^2} = 0$.

The general Schrödinger equation. x, p commutator.
 Now, we had $i\hbar \frac{\partial \psi}{\partial t} = \hat{E} \psi$, $\hat{E} = \frac{p^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi$

for classic physics, $E = KIN + POT$

Assume potential to be $V(x, t)$

$$\hat{H} = \hat{E} = \frac{p^2}{2m} + V(x, t)$$

→ Hamiltonian $\hat{H}$

$V(x, t)$ should be treated as an operator.

$$\begin{aligned} i\hbar \frac{\partial \psi}{\partial t} &= \hat{H} \psi \\ i\hbar \frac{\partial \psi(x, t)}{\partial t} &= \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) \right) \psi \end{aligned}$$

→ full schordinger equation.

Introduce an operator $\hat{x}$, which acting on function of x , multiply them by x

$$\hat{x} f(x) \equiv x f(x)$$

Commutator of $\hat{x}, \hat{p}$

$$\text{Ops. } \hat{p}, \hat{x}, \hat{H} = \frac{p^2}{2m} + V(\hat{x}, t)$$

$$\hat{x} \hat{p} \phi - \hat{p} \hat{x} \phi = 0 ?? \rightarrow \text{proof} \Rightarrow$$

$$\begin{aligned} \hat{x}(\hat{p}\phi) - \hat{p}(\hat{x}\phi) &= \hat{x}p\phi - \hat{p}(x\phi) = x p\phi - \frac{\hbar}{i} \frac{\partial}{\partial x} (x\phi) \\ &= x p\phi - \frac{\hbar}{i} \phi - p x\phi = -\frac{\hbar}{i} \phi = i\hbar \phi \end{aligned}$$

$$\therefore \hat{x} \hat{p} - \hat{p} \hat{x} = i\hbar \quad (\text{equality between ops.})$$

Commutators, matrices and 3-dimensional Schrödinger equation

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}, \text{ commutation of } \hat{A} \text{ and } \hat{B}$$

$$[\hat{x}, \hat{p}] = i\hbar$$

3D physics

$$p_x = \frac{\hbar}{i} \frac{\partial}{\partial x}$$
$$p_y = \frac{\hbar}{i} \frac{\partial}{\partial y}$$
$$p_z = \frac{\hbar}{i} \frac{\partial}{\partial z}$$

extend to i dimension $\rightarrow$

$$p_i = \frac{\hbar}{i} \frac{\partial}{\partial x_i}, \quad i = 1, 2, 3, \dots$$

$$\text{So, } \hat{p} = \frac{\hbar}{i} \nabla$$

$$\hat{H} = \frac{(\hat{p})^2}{2m} + V(x, t), \quad (\hat{p})^2 = \hat{p} \cdot \hat{p} = \frac{\hbar}{i} \nabla \cdot \frac{\hbar}{i} \nabla = -\hbar^2 \nabla^2$$

$\downarrow$
Laplacian

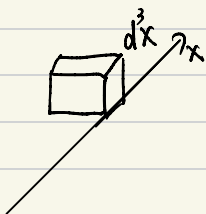
$$\therefore i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\bar{x}, t) \right) \Psi(\bar{x}, t)$$

For commutation rule:

$$[\hat{x}_i, \hat{p}_j] = i\hbar \delta_{ij}, \quad \delta_{ij} = \begin{cases} 1, & \text{if } i=j \\ 0, & \text{if } i \neq j \end{cases}$$

Interpretation of the wave function

$\Psi(x, t)$ does not tell how much of the particle is at x at time t , but rather what is the probability to find it at x at time t .



$$dP(x, t) = |\Psi(\bar{x}, t)|^2 d^3x$$

within the cube

$$\text{and } \int_{\text{all space}} d^3x |\Psi(x, t)|^2 = 1$$

Probability density and current. Hermitian conjugation.

Normalizable wavefunctions and question of time evolution.

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x,t) \right) \Psi(x,t)$$

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$$

In order to guarantee Ψ can conceivably hold

$$\lim_{x \rightarrow \pm\infty} \Psi(x,t) = 0, \quad \lim_{x \rightarrow \pm\infty} \frac{\partial \Psi}{\partial x} \text{ is bounded!}$$

Normalize / Normalizable.

$$\text{for a wavefunction } \Psi(x,t) \longrightarrow \int |\Psi|^2 dx = N (\neq 1) < \infty$$

$$\text{using instead: } \Psi' = \frac{\Psi}{\sqrt{N}}$$

Ψ is normalizable.

$$\int |\Psi'|^2 dx = \int \left| \frac{\Psi}{\sqrt{N}} \right|^2 dx = \frac{1}{N} \int |\Psi|^2 dx = 1$$

Is probability conserved? Hermiticity of Hamiltonian

Recall that $\int \Psi^*(x,t_0) \Psi(x,t_0) dx = 1$ at $t=t_0$, then it must hold for $t > t_0$

$$\therefore P(x,t) = \Psi^*(x,t) \Psi(x,t); \quad N(t) = \int P(x,t) dx$$

when $N(t_0) = 1$, will SE guarantee that $\frac{\partial N}{\partial t} = 0$?

$$\frac{dN}{dt} = \frac{d}{dt} \int P(x,t) dx = \int dx \left[\frac{\partial \Psi^*}{\partial t} \Psi + \Psi^* \frac{\partial \Psi}{\partial t} \right]$$

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi \longrightarrow \frac{\partial \Psi}{\partial t} = -\frac{i}{\hbar} \hat{H} \Psi$$

$$-i\hbar \frac{\partial \Psi^*}{\partial t} = (\hat{H} \Psi)^* \longrightarrow \frac{\partial \Psi^*}{\partial t} = \frac{i}{\hbar} (\hat{H} \Psi)^*$$

$$\therefore \frac{dN}{dt} = \int dx \frac{i}{\hbar} [\hat{H} \Psi^* \Psi - \Psi^* \hat{H} \Psi]$$

$$\text{For this to be zero, it needs } \int (\hat{H} \Psi)^* \Psi dx = \int \Psi^* \hat{H} \Psi dx$$

A Hermitian $\hat{H}$ should satisfy:

$$\int (\hat{H} \Psi_1)^* \Psi_2 dx = \int \Psi_1^* \hat{H} \Psi_2 dx$$

true if $\hat{H}$ is a Hermitian operator

In general, given an operator T , one define to Hermitian conjugate $T^\dagger$

$$\int \psi_1^* T \psi_2 = \int (T \psi_1)^* \psi_2, \quad T \text{ is Hermitian: if } T^\dagger = T$$

Probability current and current conservation

$$\frac{dN}{dt} = \int \frac{\partial \rho(x,t)}{\partial t} dx = \frac{\partial [\psi^*(x,t) \cdot \psi(x,t)]}{\partial t}$$

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= \frac{i}{\hbar} \left[-\frac{\hbar^2}{2m} \frac{\partial^2 \psi^*}{\partial x^2} \psi + V(x,t) \psi^* \psi + \frac{\hbar^2}{2m} \psi^* \frac{\partial^2 \psi}{\partial x^2} - \psi^* V(x,t) \psi \right] \\ &= -\frac{i\hbar}{2m} \left(\frac{\partial^2 \psi^*}{\partial x^2} \psi - \psi^* \frac{\partial^2 \psi}{\partial x^2} \right) = \left(-\frac{i\hbar}{2m} \right) \frac{\partial}{\partial x} \left(\frac{\partial \psi^*}{\partial x} \psi - \psi^* \frac{\partial \psi}{\partial x} \right) \\ &= -\frac{\partial}{\partial x} \left[\frac{\hbar}{2im} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) \right] = 2i \operatorname{Im} \left(\psi^* \frac{\partial \psi}{\partial x} \right) \end{aligned}$$

$$\text{So, } \frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x} \left[\frac{\hbar}{m} \operatorname{Im} \left(\psi^* \frac{\partial \psi}{\partial x} \right) \right]$$

$J(x,t) \rightarrow$ current density

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0$$

current conservation

Three dimensional current and conservation

$$\text{Unit } [\psi] = \frac{1}{\sqrt{L}} \quad , \quad \left[\psi^* \frac{\partial \psi}{\partial x} \right] = \frac{1}{L^2} \quad , \quad [\hbar] = \frac{ML^2}{T} \quad , \quad \left[\frac{\hbar}{m} \right] = \frac{L^2}{T}$$

$$\int |\psi|^2 dx = 1$$

$$[J] = \frac{L^2}{T} \cdot \frac{1}{L^2} = \frac{1}{T} \rightarrow \text{probability per time.}$$

3 Dim case:

$$\vec{J}(x,t) = -\frac{\hbar}{m} \operatorname{Im} \left(\psi^* \nabla \psi \right)$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0$$

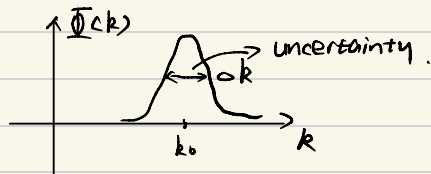
Wavepackets and uncertainty. Time evolution and shape change time evolutions.

Wavepackets and Fourier representation

Assume $t=0$, $\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int \Phi(k) e^{ikx} dk$

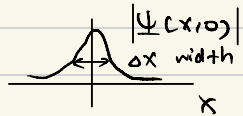
if we know $\psi(x,0)$, the $\Phi(k)$ is calculable.

$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int \psi(x,0) e^{-ikx} dx$$



$|\psi(x,0)|$ peaks at $x=0$

as $\frac{\partial \psi(x,0)}{\partial x} = 0$ when $k=0$.



Is $\psi(x,0)$ real?

$$(\psi(x,0))^* = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (\Phi(k))^* e^{-ikx} dk, \text{ change } k \rightarrow -k$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi^*(-k) e^{ikx} dk \stackrel{?}{=} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k) e^{ikx} dk = \psi(x,0)$$

Reality condition

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (\Phi(k) - \Phi^*(-k)) e^{ikx} dk = 0$$

$$(\Phi(-k))^* = \Phi(k) \longrightarrow \Phi(k) \text{ is not real}$$

width and uncertainties.

Uncovering momentum space. Expectation values and their time dependence.

Fourier transforms and delta functions

Ignore time : $\psi(x) = \frac{1}{\sqrt{2\pi}} \int \Phi(k) e^{ikx} dk$
 $\Phi(k) = \frac{1}{\sqrt{2\pi}} \int \psi(x) e^{-ikx} dx$ → $\Phi(k)$ has same information as $\psi(x)$
↓ weight of the plane waves in the superposition.

$$\begin{aligned} \psi(x) &= \frac{1}{\sqrt{2\pi}} \int dk e^{ikx} \frac{1}{\sqrt{2\pi}} \int \psi(x') e^{-ikx'} dx' \\ &= \int_{-\infty}^{\infty} dx' \psi(x') \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ik(x-x')} \xrightarrow{k \rightarrow -k} \frac{1}{2\pi} \int dk e^{ik(x'-x)} \end{aligned}$$

$$\therefore \boxed{\delta(x-x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ik(x-x')}} \longrightarrow \begin{cases} \delta(x) = \delta(x) \\ \delta(ax) = \frac{1}{|a|} \delta(x) \end{cases}$$