Introduction to ψ and Wave Packets

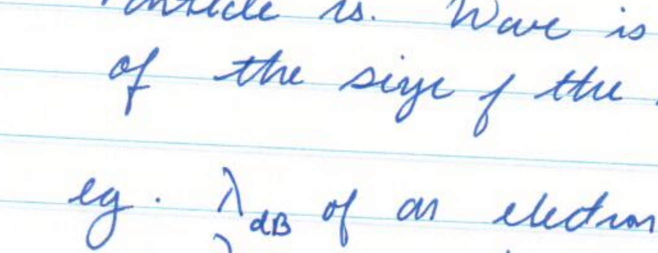
Lectures 3, 4, 5 Week 2 137A

- The physical world can be more accurately described using a wave description.

Particle vs. Wave is a question of the size of the system vs λ.

eg. λ_{dB} of an electron $\sim$ nm, atom $\sim 1 Å$!
λ_{dB} of a human $\sim 10^{-36}$ m, human ~ 1 m!

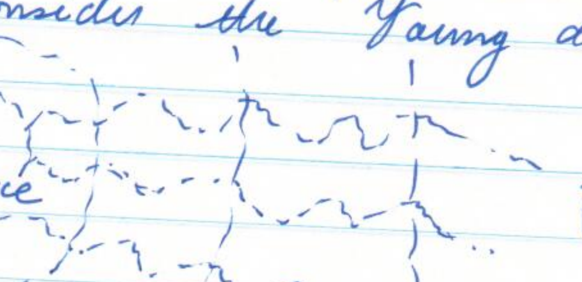
- Wave can interfere and be superposed. Consider the Young double slit experiment:



$$\vec{E} = \vec{E}_0 e^{i(\vec{k}\cdot\vec{r} - \omega t + \varphi)}$$

$|k| = \frac{2\pi}{\lambda}$ direction of wave, spatial freq.

starts to look like a "plane" wave



$\vec{E}$ from each slit
$\vec{E}_1, \vec{E}_2$

$$\vec{E}_{tot} = \vec{E}_{01} e^{i\delta_1} + \vec{E}_{02} e^{i\delta_2}$$

Note $e^{i\overbrace{(\vec{k}\cdot\vec{r} - \omega t + \varphi)}}$ phase δ

Power or intensity is detected (2)

$$I \sim |E|^2 = \vec{E} \cdot \vec{E}^* = E_{01}^2 + E_{02}^2 + \vec{E}_{01} \cdot \vec{E}_{02} \left(e^{i(\delta_2 - \delta_1)} + e^{-i(\delta_2 - \delta_1)} \right)$$

$$= E_{01}^2 + E_{02}^2 + 2 \vec{E}_{01} \cdot \vec{E}_{02} \cos(\delta_2 - \delta_1)$$

* Note: (1) Must add amplitudes not intensities!!

(2) Observable pattern only depends on phase difference and not absolute phase.

* The Quantum Wavefunction

Ψ → is a wave amplitude

→ not physical! Can't picture it as something wiggling

→ cannot observe it!

→ but... contains all the information about the system

So..... how do you use ψ?

<u>Max Born</u> (1926) $\cdot\ |\psi|^2$ probability density to find system at $\vec{r}, t$

- think of a large # of identical systems each with one particle

- repeated measurement generates Probability

- $P(\vec{r},t) = |\psi(\vec{r},t)|^2$ Probability density

- To find particle within a ball $d\vec{r}$ about $\vec{r}$ at time t is

$$P(\vec{r},t)\underbrace{d\vec{r}}_{\text{volume element}} = |\psi(\vec{r},t)|^2 d\vec{r}$$

eg. $dx\,dy\,dz$

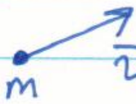
<u>Wave superposition</u>

If ψ_1, ψ_2 are two allowed states,

then $\psi = c_1\psi_1 + c_2\psi_2$ is also allowed.

c_1, c_2 are complex #'s

Wavefunction for a particle with definite momentum

Classical physics  has energy E

$\longrightarrow$ Need to encode some information in a wave.

* 

$E = hf = \hbar\omega \qquad \hbar = h/2\pi$

$p = h/\lambda = \hbar k \qquad k = 2\pi/\lambda$

Consider a particle moving in the $\hat{x}$ direction

$\bullet\!\longrightarrow$

$\vec{P} = p_x \hat{x}$ $\Rightarrow$ associate with a wave traveling in the same direction with wave number k

$$\psi(x,t) = A e^{i(kx - \omega(k)t)}$$

can also write $\psi(x,t) = A e^{i(p_x x - E(p_x)t)/\hbar}$

* To extract information from ψ, use operators (in this case derivatives)

$$\underbrace{-i\hbar\frac{\partial}{\partial x}}_{\text{Operator}}\psi = \underbrace{P_x}_{\text{measurable quantity}}\psi$$

$$i\hbar\frac{\partial}{\partial t}\psi = E\psi$$

3D

$$\psi(\vec{r},t) = Ae^{i(\vec{k}\cdot\vec{r}-\omega(k)t)}$$

$$= Ae^{i(\vec{p}\cdot\vec{r}-E(p)t)/\hbar}$$

$\vec{p} = \hbar\vec{k}$ (momentum is a vector)

$$k = |\vec{k}| = \frac{|\vec{p}|}{\hbar} = \frac{2\pi}{\lambda}$$

Operator relations still hold!

$$i\hbar\frac{\partial}{\partial t}\psi = E\psi$$

$$-i\hbar\vec{\nabla}\psi = \vec{p}\psi$$

gradient

eg. $\frac{\partial}{\partial x}\hat{x} + \frac{\partial}{\partial y}\hat{y} + \frac{\partial}{\partial z}\hat{z}$

Probability and Normalization

Since P is a probability density, when integrated ~~overall~~ over all space, it should equal 1.

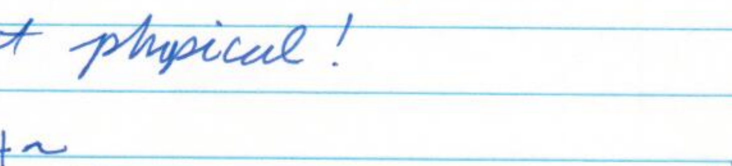
$$\int_{\substack{\text{all}\\ \text{space}}} |\psi(\vec{r},t)|^2 d\vec{r} = 1$$

However, we have a problem for a plane wave.

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = |A|^2 \int_{-\infty}^{\infty} dx \rightarrow \text{diverges.}$$

→ This is because a plane wave has amplitude everywhere in space

→ not physical!

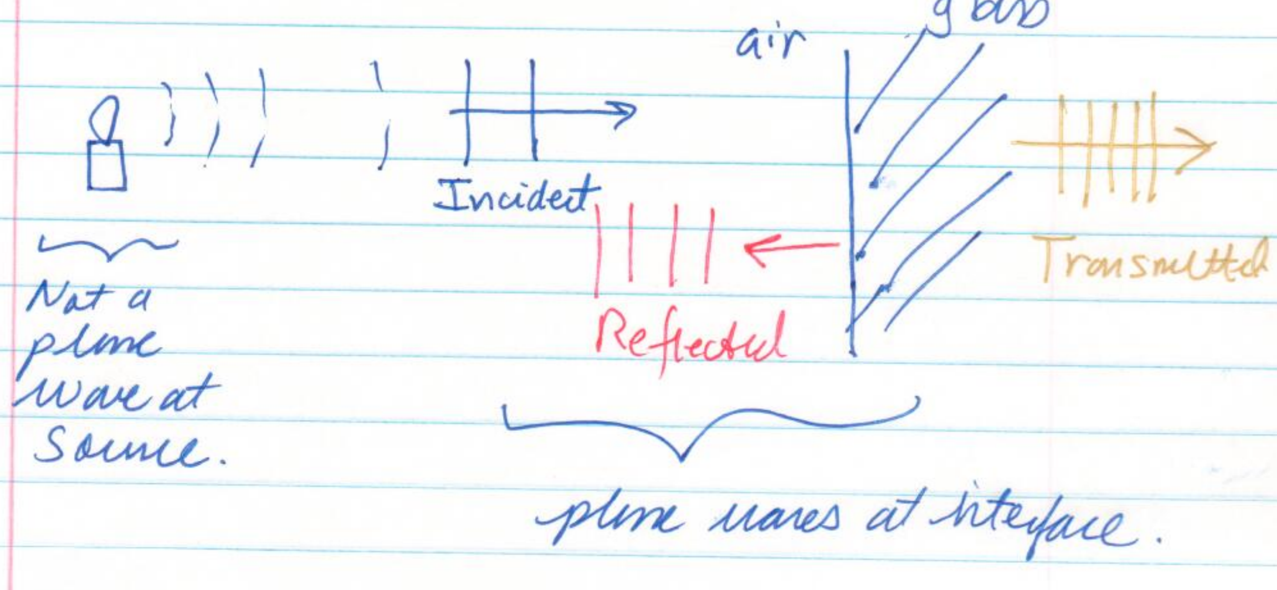
Approx: $\psi \sim$ 

Realistic ψ 

Probability is here

Nonetheless, plane waves are very ⑦
useful in calculations <u>since</u> we
may only care about ψ in a particular
region in space.

Eg. A scattering problem.



- Since $|\psi|^2$ is <u>not</u> square integrable,

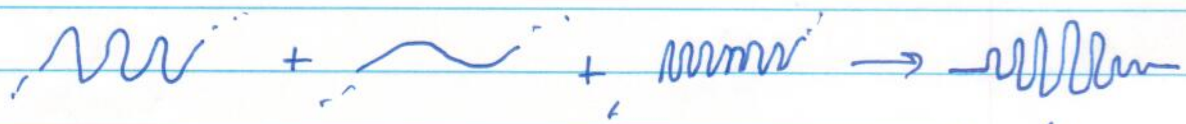
we can use ratios of ψ at different
places instead of normalizing it.

Lecture 3, 4, 5 (1)

Wavepacket

Recall that a sum of different allowed ψ will still be allowed.

If we add different plane waves, we can obtain a wavepacket:



Eg. 1D:

simple example $E = p_x^2/2m$

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{i[p_x x - E(p_x) t]/\hbar} \underbrace{\phi(p_x)}_{\text{weighting function for different } p_x} dp_x$$

This looks very much like a Fourier transform... That's because it is one!!

Review of discrete and continuous Fourier sums and integrals:

<u>Discrete:</u> Consider $f(x)$ in the interval $x \in [-\pi, \pi]$

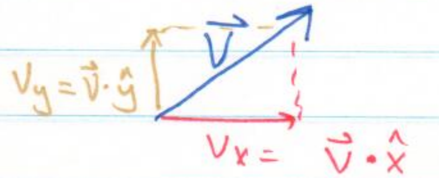
$$f(x + 2\pi) = f(x)$$

$$f(x) = \frac{1}{2} A_0 + \sum_{n=1}^{\infty} \left[A_n \cos(nx) + B_n \sin(nx) \right]$$

Series will converge provided $f(x)$, $f'(x)$ are piecewise continuous on $(-\pi, \pi)$

To find A_n, B_n, multiply by $\cos(mx)$, $\sin(mx)$

<u>cf:</u> Taking the dot product of a vector along the different basis vectors



$\downarrow$

then use

$$\cos(nx)\cos(mx) = \frac{1}{2}\cos((m+n)x) + \frac{1}{2}\cos((m-n)x)$$

$$A_m = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(mx)\,dx \qquad m = 0, 1, \ldots$$

Similarly $B_m = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(mx)\,dx$

Can also combine into exponential form (3)

$$f(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} C_n e^{inx}$$

To find C_n, use Kronecker delta

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i(n-m)x} dx = \delta_{mn}$$

$$\delta_{mn} = 1 \quad m=n$$
$$= 0 \quad m \neq n$$

multiply by $\frac{1}{\sqrt{2\pi}} e^{-imx}$ and integrate

$$C_m = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} f(x) e^{-imx} dx$$

Can consider continuum limit,

Fourier integrals

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx} dk$$

Fourier transform of $f(x)$

$$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$

Dirac Delta Function

Substitute form for $g(k)$ into expression for $f(x)$

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty} f(x')\,e^{-ikx'}\,dx'\right]e^{ikx}\,dk$$

$$= \int_{-\infty}^{\infty} f(x')\,\delta(x-x')\,dx'$$

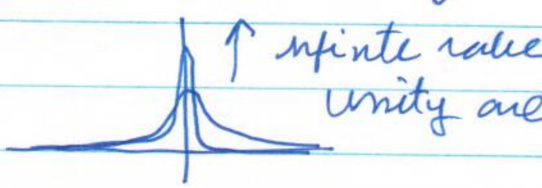
define $\delta(x-x') = \dfrac{1}{2\pi}\displaystyle\int_{-\infty}^{\infty} e^{ik(x-x')}\,dk$

Since $f(x)$ is arbitrary, $\delta(x-x')=0$ if $x = x'$

and $\int \delta$ = unity

$\rightarrow$ No such function exists!

limiting case of a sharply peaked function.



Armed with the basis of Fourier sums & integrals: (5)

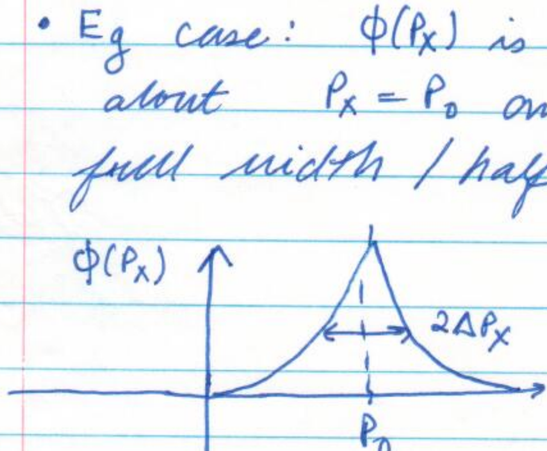
Recall:

1D Wave packet $\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{i[P_x x - E(P_x)t]/\hbar} \phi(P_x)\, dP_x$

$\phi(P_x)$: amplitude of a plane wave with momentum P_x

can be complex

- Eg case: $\phi(P_x)$ is real and sharply peaked about $P_x = P_0$ and falls to 0 with a full width / half max of $2\Delta P_x$.



Let $\beta(P_x) = P_x X - E(P_x)t$

Thus: $\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{i\beta(P_x)/\hbar} \phi(P_x)\, dP_x$

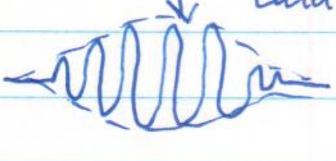
$|\psi(x,t)|$ is largest when $\beta(P_x)$ is nearly constant in the vicinity of P_0.

- Outside of P_0, $\phi(P_x) \to 0$
- If $\beta(P_x)$ varies, $e^{i\beta/\hbar}$ rapidly oscillates and integrates to 0.

Look for a stationary phase condition:

$$\left[\frac{d\beta(P_x)}{dP_x}\right]_{P_x=P_0} = 0$$

determines center of wave packet



If $\beta(P_x) = P_x X - E(P_x)t$

$\longrightarrow$ this implies $X - \dfrac{dE(P_x)}{dP_x}t = 0$

$$\frac{X}{t} \equiv \underbrace{V_g}_{\text{group velocity}} = \left.\frac{dE(P_x)}{dP_x}\right|_{P_x=P_0}$$

speed at which packet moves

also $V_g = \left.\dfrac{\partial\omega(k)}{dk}\right|_{k=k_0}$ since $E=\hbar\omega$, $p=\hbar k$

* This is in general different than the phase velocity: the speed of each individual plane wave

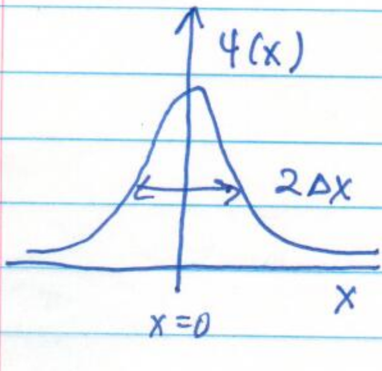
Use identity again,

$$= \frac{\pi^{-1/4}}{\sqrt{\hbar}} (\Delta p_x)^{1/2} \underbrace{e^{i p_0 x/\hbar}}_{\text{phase factor}} \underbrace{e^{-(\Delta p_x)^2 x^2/2\hbar^2}}_{\text{gaussian again!}}$$

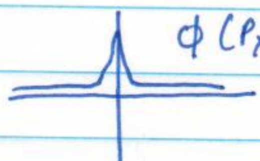
- This Gaussian is centered about $x = 0$

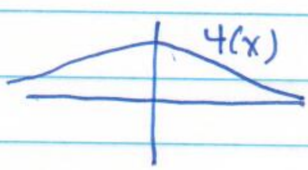
$|\psi|^2$ falls to $1/e$ of the maximum

at $x = \pm \Delta x$ $\quad \Delta x = \dfrac{\hbar}{\Delta p_x}$!!

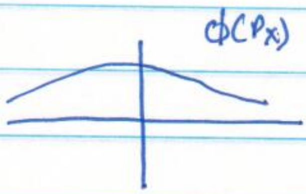


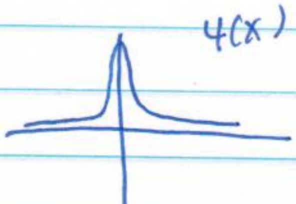
Thus: localizing one quantity, delocalizes the other.





Such that





$\Delta x \Delta p_x = \hbar$

$\Rightarrow$ on the way to the Heisenberg uncertainty principle!