

## 5.1: Momentum and Energy Operator

$$\Psi(x,t) = e^{i\hbar kx - i\omega t}$$

$$P = \hbar k$$

$$E = \hbar \omega$$

Non Relativistic particles:

$$E = \frac{p^2}{2m}$$

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

operator

Momentum operator  $\hat{p}$

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

$$\hat{p} \Psi(x,t) = p \Psi(x,t)$$

If this holds, then:

$\Psi(x,t)$  is an eigenstate of  $\hat{p}$

(operator  $A$ ,  $\Psi = A\Psi = \lambda\Psi$ )  
with eigenvalue  $p$

$\Psi(x,t)$  is a state of definite momentum

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

$$\downarrow$$
$$E = \frac{p^2}{2m}$$

$$E\Psi = 0\Psi$$

(invent an '0')

$$\begin{aligned} E\Psi &= \frac{p^2}{2m}\Psi = \frac{p}{2m}(p\Psi) = \frac{p}{2m} \frac{\hbar}{i} \frac{\partial \Psi}{\partial x} \\ &= \frac{\hbar}{2m} \frac{\partial}{\partial x} \left( \frac{\hbar}{i} \frac{\partial \Psi}{\partial x} \right) \end{aligned}$$

## 5.1: Momentum and Energy Operator (continued)

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = E\Psi$$

$$\hat{E} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} = \text{Energy operator}$$

The energy operator times wave function is energy times the wave function.

$$\hat{E}\Psi = E\Psi$$

$\Psi$  is an energy eigenstate

$$\hat{E} = \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} = \frac{1}{2m} \hat{P}^2$$

$$\hat{P}\hat{P} = \frac{\hbar}{i} \frac{\partial}{\partial x} \frac{\hbar}{i} \frac{\partial}{\partial x}$$

Combines to Schrödinger Equation

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

## 5.2: Free Schrödinger Equation

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

$$\text{try } \Psi = e^{ikx - i\omega t}$$

$$i\hbar(-i\omega)\Psi = -\frac{\hbar^2}{2m}(ik)^2\Psi$$

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} \rightarrow E = \frac{p^2}{2m}$$

$$\Psi(x, t) = \int_{-\infty}^{\infty} \Phi(k) e^{ikx - i\omega(k)t} dk$$

This solves the Schrödinger Equation

$$Vg = \left. \frac{d\omega}{dk} \right|_{k_0} = \frac{dE}{dp} = \frac{d}{dp} \left( \frac{p^2}{2m} \right) = \frac{p}{m} = V$$

## 5.2: Free Schrödinger Equation (continued)

Remarks

$\Psi$  can not be real ( $\Psi \notin \mathbb{R}$ )

not a usual wave equation

$$\frac{\partial^2 \Psi}{\partial x^2} - \frac{1}{V^2} \frac{\partial^2 \Psi}{\partial t^2} = 0 \Rightarrow \text{solutions } \in \mathbb{C}$$

## 5.3: General Schrödinger Equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{E} \Psi$$

$$\hat{E} = \frac{\hat{p}^2}{2m}$$

Potential:  $V(x, t)$

$E = \text{Kinetic} + \text{Potential}$

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

↑ Hamiltonian  $\hat{H}$

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

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

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

Introduce an operator  $\hat{x}$ , which acting on functions of  $x$

multiples them by  $x$

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

Operators:

$$\hat{p}$$

$$\hat{x}$$

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

$$\hat{x}\hat{p}\Psi - \hat{p}\hat{x}\Psi = 0?$$

## 5.3: General Schrödinger Equation (continued)

$$AB\phi \equiv A(B\phi)$$

$$\hat{x}\hat{p}\phi - \hat{p}\hat{x}\phi = \hat{x}(\hat{p}\phi(x,t)) - \hat{p}(\hat{x}\phi(x,t))$$

$$= \hat{x}\left(\frac{i}{\hbar} \frac{\partial}{\partial x} \phi(x,t)\right) - \hat{p}(x\phi(x,t))$$

$$= \frac{i}{\hbar} x \frac{\partial}{\partial x} \phi(x,t) - \frac{i}{\hbar} \frac{\partial}{\partial x} (x\phi) = -\frac{i}{\hbar} \phi = i\hbar \phi$$

$$(\hat{A} + \hat{B})\phi = \hat{A}\phi + \hat{B}\phi$$

$$(\hat{x}\hat{p} - \hat{p}\hat{x})\phi = i\hbar\phi$$

$\hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar$  Equality between operators

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

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

## 5.4: Commutators, Matrices and 3-D Schrödinger

Operators

Wave functions

Eigenstates

Matrices

Vectors

Eigenvectors

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\vec{\sigma} = \frac{\pi}{2} \sigma$$

$$\sigma_1 \sigma_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$

$$\sigma_2 \sigma_1 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$$

$$[\sigma_1, \sigma_2] = \sigma_1 \sigma_2 - \sigma_2 \sigma_1 = 2 \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = 2i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_3$$

$$[\sigma_1, \sigma_2] = 2i \sigma_3$$

## 5.4: Commutators, Matrices, and 3-D Schrödinger (continued)

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x} \rightarrow p_1 = \frac{\hbar}{i} \frac{\partial}{\partial x_1}$$

$$\hat{p}_y = \frac{\hbar}{i} \frac{\partial}{\partial y} \rightarrow p_2 = \frac{\hbar}{i} \frac{\partial}{\partial x_2}$$

$$\hat{p}_z = \frac{\hbar}{i} \frac{\partial}{\partial z} \rightarrow p_3 = \frac{\hbar}{i} \frac{\partial}{\partial x_3}$$

$$e^{i\vec{k} \cdot \vec{x} - i\omega t} \quad \hat{\vec{p}} = \hbar \vec{k}$$

$$p_k = \frac{\hbar}{i} \frac{\partial}{\partial x_k} \quad k=1,2,3$$

$$\hat{\vec{p}} = \frac{\hbar}{i} \vec{\nabla}$$

$$\begin{aligned} \hat{\vec{p}} e^{i\vec{k} \cdot \vec{x} - i\omega t} &= \frac{\hbar}{i} \vec{\nabla} e^{i\vec{k} \cdot \vec{x} - i\omega t} \\ &= \frac{\hbar}{i} |\vec{k}| e^{i\vec{k} \cdot \vec{x}} \\ &= \hbar \vec{k} \Psi \end{aligned}$$

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

$$\hat{p}^2 = \hat{p} \cdot \hat{p} = \frac{\hbar}{i} \vec{\nabla} \cdot \frac{\hbar}{i} \vec{\nabla} = -\hbar^2 \vec{\nabla}^2$$

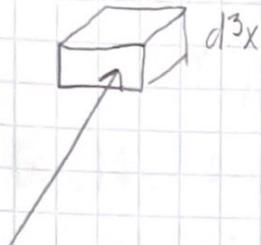
$$i\hbar \frac{\partial}{\partial t} = \left( \frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{x}, t) \right) \Psi(\vec{x}, t)$$

$$[\hat{x}_i, \hat{p}_j] = i\hbar \delta_{ij}$$

$$\delta_{ij} = \begin{cases} 1, & i=j \\ 0, & i \neq j \end{cases}$$

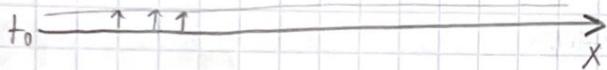
## 5.5: Interpretation of the Wavefunction

$\Psi(x, t)$  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  $t$ .



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

single particle:  $\int_{\text{all}} |\Psi(\vec{x}, t)|^2 d^3x = 1$



## 6.1: Normalizable Wavefunctions

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

$$\int |\Psi(x, t)|^2 dx$$

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1 \quad \text{Holds for } t=t_0$$

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

In order to guarantee this will hold:

$$\lim_{x \rightarrow \pm\infty} \Psi(x, t) = 0$$

$$\lim_{x \rightarrow \pm\infty} \frac{\partial \Psi}{\partial x} \text{ is bounded}$$

## 6.1: Normalizable Wavefunctions (continued)

$$\Psi(x,t)$$

$$\int |\Psi|^2 dx = N \neq 1$$

$\Psi$  is normalizable meaning it can be normalized  
Use instead  $\Psi'$ :

$$\Psi' = \frac{\Psi}{\sqrt{N}}$$

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

## 6.2: Hermiticity of the Hamiltonian

$$\text{If } \int \Psi^*(x, t_0) \Psi(x, t_0) dx = 1 \text{ at } t=t_0$$

then it must hold for later times for  $t > t_0$

Define:  $\rho(x, t) = \text{probability density} = \Psi^*(x, t) \Psi(x, t)$

$$N(t) = \int \rho(x, t) dx$$

$$N(t_0) = 1$$

Will Schrödinger Equation guarantee  $\frac{dN}{dt} = 0$ ?

$$\frac{dN}{dt} = \int \frac{\partial}{\partial t} \rho(x, t) dx$$

$$= \int \left( \left( \frac{\partial \Psi^*}{\partial t} \right) \Psi + \Psi^* \left( \frac{\partial \Psi}{\partial t} \right) \right) dx$$

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

## 6.2: Hermiticity of the Hamiltonian (continued)

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

$$i\hbar \left( \frac{\partial \psi}{\partial t} \right)^* = (\hat{H} \psi)^*$$

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

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

$$\frac{dN}{dt} = \int \frac{1}{\hbar} \left[ (\hat{H} \psi)^* \psi - \psi^* (\hat{H} \psi) \right] dx$$

For this to be zero:

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

True if  $\hat{H}$  is a hermitian operator

The hermitian operator  $\hat{H}$  satisfies that:

$$\int (\hat{H} \psi_1)^* \psi_2 dx = \int \psi_1^* \hat{H} \psi_2 dx$$

In general, given an operator  $T$ , one defines its hermitian conjugate  $T^+$  as follows:

$$\int \psi_1^* T \psi_2 dx \rightarrow \int (T^+ \psi_1)^* \psi_2 dx$$

$T$  is hermitian if  $T^+ = T$

### 6.3: Probability Current

$$\frac{dN}{dt} = \int_{\text{V}} (\hat{H}\psi)^* \psi - \psi^* \hat{H} \psi \, dx$$

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

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

$$\frac{\partial P}{\partial t} = -\frac{i\hbar}{2m} \left( \frac{\partial^2 \psi^*}{\partial x^2} \psi - \psi^* \frac{\partial^2 \psi}{\partial x^2} \right)$$

$$\frac{\partial P}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial}{\partial x} \left( \frac{\partial \psi^*}{\partial x} \psi - \psi^* \frac{\partial \psi}{\partial x} \right) = -\frac{2}{\hbar} \left( \frac{1}{2im} \left( \psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) \right)$$

$$z - z^* = 2i \operatorname{Im}(z)$$

$$\frac{\partial P}{\partial t} = -\frac{2}{\hbar} \underbrace{\left( \frac{1}{m} \operatorname{Im}(\psi^* \frac{\partial \psi}{\partial x}) \right)}_{J(x, t)}$$

$$J(x, t) = \frac{1}{m} \operatorname{Im} \left( \psi^* \frac{\partial \psi}{\partial x} \right)$$

$$\frac{\partial J}{\partial t} = -\frac{\partial J}{\partial x} \rightarrow \frac{\partial P}{\partial t} + \frac{\partial J}{\partial x} = 0$$

Current  
Conservation

$$[\psi] = \frac{1}{\sqrt{L}}$$

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

$$[\psi^* \frac{\partial \psi}{\partial x}] = \frac{1}{L^2}$$

$$[\frac{\hbar}{L}] = \frac{ML^2}{T}$$

$$[\frac{\hbar}{M}] = \frac{L^2}{T}$$

$$[J] = \frac{L^2}{T} = \frac{1}{T}$$

## 6.4: Three Dimensional Current

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

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

$[J] = \frac{1}{L^2} \cdot \frac{1}{T}$  probability per unit area and unit time

$$\frac{dN}{dt} = \int_{-\infty}^{\infty} \frac{\partial \rho}{\partial t} dx = - \int_{-\infty}^{\infty} \frac{\partial J}{\partial x} dx = - [J(x=\alpha, t) - J(x=-\alpha, t)]$$

$$J = \frac{\hbar}{2im} (\underbrace{\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}}_{\rightarrow 0})$$

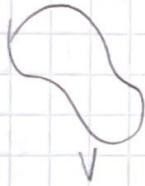
$$\frac{dN}{dt} = 0$$

Consistency

Two ideas

- 1) existence of a current for probability
- 2)  $\hat{A}$  is a hermitian operator

	EM	QM
$\rho$	charge density	probability density
$Q$	charge in Volume	probability to find particle in volume
$J$	current density	probability current density



$$Q_V(t) = \int_V \rho(x, t) d^3x$$

$$\frac{dQ}{dt}(t) = \int_V \frac{\partial \rho}{\partial t} d^3x = - \int_V \nabla \cdot \vec{J} d^3x$$

### 6.4: Three Dimensional Current (continued)

$$\frac{dQ}{dt}(t) = - \int_S \vec{J} \cdot d\vec{\sigma} \quad (\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0)$$

a

b

$$P_{ab} = \int_a^b \rho(x, t) dx$$

$$\frac{dP_{ab}}{dt} = \int_a^b \frac{\partial \rho}{\partial t} dx = - \int_a^b \frac{\partial J}{\partial x} dx = -(J(x=b, t) - J(x=a, t))$$

$$\frac{dP_{ab}}{dt} = -J(b, t) + J(a, t)$$

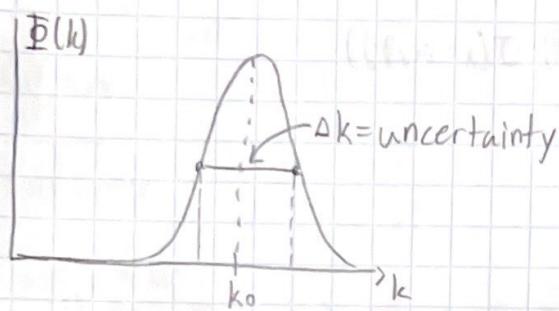
## 7.1: Wavepackets and Fourier

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

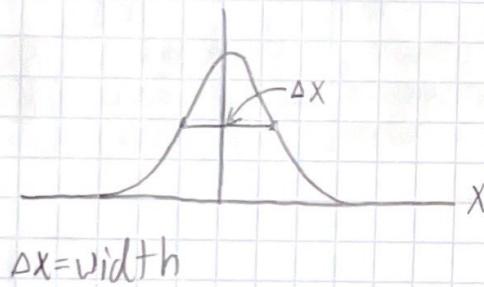
Fourier

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

Reverse Fourier



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



## 7.2: Reality Condition

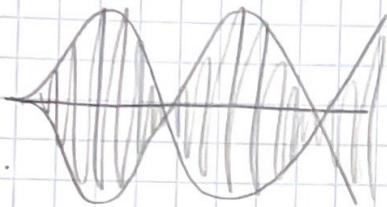
Is  $\Psi(x, 0)$  real?

$$\begin{aligned} (\Psi(x, 0))^* &= \frac{1}{\sqrt{2\pi}} \int (\bar{\Psi}(k))^* e^{-ikx} dk \\ &\downarrow \\ &k \rightarrow -k \\ &\downarrow \\ &= \frac{1}{\sqrt{2\pi}} \int \bar{\Psi}^*(k) e^{ikx} dk \end{aligned}$$

$$\stackrel{?}{=} \frac{1}{\sqrt{2\pi}} \int \bar{\Psi}(k) e^{ikx} dk = \Psi(x, 0)$$

Reality requires  $\frac{1}{\sqrt{2\pi}} \int (\bar{\Psi}(k) - \bar{\Psi}^*(-k)) e^{ikx} dk = 0$

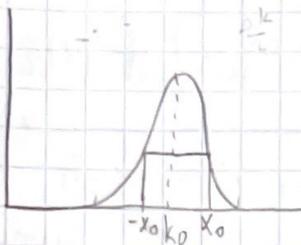
$(\bar{\Psi}(-k))^* = \bar{\Psi}(k)$  is condition for reality



## 2.3: Widths and Uncertainty

$$k = k_0 + \tilde{k}$$

$$\Psi(x, 0) = \frac{1}{\sqrt{2\pi}} e^{ik_0 x} \int \Phi(k + \tilde{k}) e^{i\tilde{k}x} d\tilde{k}$$



Relevant region of integration for  $\tilde{k}$  is from  $[-\frac{\Delta k}{2}, \frac{\Delta k}{2}]$

For any  $x$  different from zero, the phase in the integral will range over  $[-\frac{\Delta k}{2}x, \frac{\Delta k}{2}x]$

Total phase excursion is  $\Delta k \cdot x$

If  $\Delta k \cdot x \ll 1$ , then get contribution

If  $\Delta k \cdot x \gg 1$ , then the contribution goes to 0

$\Psi(x, 0)$  is sizable in an interval  $x \in (-x_0, x_0)$  for  $\Delta k \cdot x_0$  roughly value of 1

$$\Delta k \cdot x_0 \approx 1$$

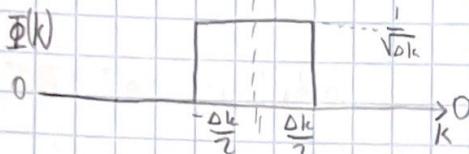
$$\Delta x = 2x_0$$

$$\Delta k \Delta x \approx 1$$

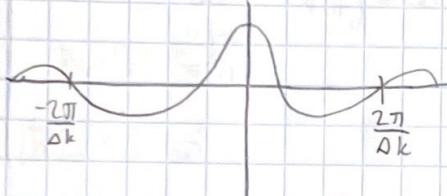
### 7.3: Widths and Uncertainty. (continued)

Since  $P = \hbar k_1$ ,  $\Delta p = \hbar \Delta k \Rightarrow \Delta p \Delta x \approx \hbar$

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$



$$\begin{aligned}\Psi(x, 0) &= \frac{1}{\sqrt{2\pi}} \int_{-\frac{\Delta k}{2}}^{\frac{\Delta k}{2}} \frac{1}{\sqrt{\Delta k}} e^{ikx} dx \\ &= \frac{1}{\sqrt{2\pi \Delta k}} \left[ \frac{e^{ikx}}{ix} \right]_{-\frac{\Delta k}{2}}^{\frac{\Delta k}{2}} \\ &= \frac{\Delta k}{2\pi} \frac{\sin(\frac{\Delta k x}{2})}{(\frac{\Delta k x}{2})}\end{aligned}$$



$$\Delta x = \frac{2\pi}{\Delta k}$$

$$\Delta x \Delta k \approx 2\pi$$

## 7.4: Shape Changes in a Wave

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int \Phi(k) e^{ikx} e^{-iw(k)t} dk$$

$$w(k) = w(k_0) + (k - k_0) \frac{dw}{dk} \Big|_{k_0} + \frac{1}{2}(k - k_0)^2 \frac{d^2w}{dk^2} \Big|_{k_0} + \dots$$

$$\frac{dw}{dt} = \frac{dE}{dt} = \frac{P}{m} = \frac{\hbar k}{m}$$

$$\frac{d^2w}{dk^2} = \frac{\hbar}{m}$$

$$\frac{d^3w}{dk^3} = 0$$

$$e^{-iw(k)t} = e^{-i\frac{1}{2}(k - k_0)^2 \frac{\hbar}{m} t}$$

$$(k - k_0)^2 \frac{\hbar}{m} t \ll 1$$

$$(\Delta k)^2 \frac{\hbar^2}{m} \ll 1$$

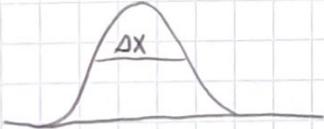
$$\frac{(\Delta p)^2}{\hbar m} \ll 1$$

$$|\hbar| \ll \frac{\hbar m (\Delta x)^2}{\hbar^2}$$

$$\Delta x \Delta p \approx \hbar$$

$$\frac{\Delta p |\hbar|}{m} \leq \frac{\hbar}{\Delta p}$$

$$\frac{\Delta p}{m} |\hbar| \ll \Delta x$$



## 7.4: Shape Changes in a Wave (continued)

$\Delta x = 10^{-10} \text{ m}$  for an electron, how long does it remain localized

$$t \approx \frac{m}{\hbar} (\Delta x)^2 = \frac{mc^2}{\hbar c} \cdot \frac{(\Delta x)^2}{c} = 10^{-16} \text{ sec}$$

## 7.5: Time Evolution

Suppose you know  $\Psi(x, 0) =$

1) calculate  $\Phi(k)$

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

2) With this rewrite

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

3)

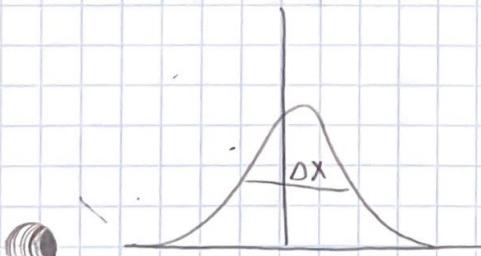
$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int \Phi(k) e^{ikx - i\hbar\omega(k)t} dk$$

$$\hbar\omega(k) = \frac{\hbar^2 k^2}{2m}$$

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

4) Do the k integral

$$\Psi_a(x, 0) = \frac{e^{-\frac{x^2}{4a^2}}}{(2\pi)^{\frac{1}{4}} \sqrt{a}}$$



$$\Delta x \approx a$$

$$T = \frac{2ma^2}{\hbar}$$

## 8.1: Fourier Transforms and Delta Functions

Uncovering Momentum Space

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int \Phi(k) e^{ikx} dk$$

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

$\Phi(k)$  has the same information as  $\Psi(x)$

$\Phi(k)$  is the weight of the planewaves in the superposition

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int e^{ikx} dk \frac{1}{\sqrt{2\pi}} \int \Psi(x') e^{-ikx'} dx'$$

$$\Psi(x) = \int_{-\infty}^{\infty} \Psi(x') dx' \underbrace{\frac{1}{2\pi} \int e^{ik(x-x')} dk}_{\delta(x'-x)}$$

Delta function

$$k \rightarrow -k$$

$$\frac{1}{2\pi} \int e^{ik(x'-x)} dk$$

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

$$\text{prop} \begin{cases} \delta(-x) = \delta(x) \\ \delta(ax) = \frac{1}{|a|} \delta(x) \end{cases}$$

## 8.2: Parseval Identity

$$\begin{aligned} & \int \underline{\Psi^*(x)} \underline{\Psi(x)} dx \\ & \quad \downarrow \quad \downarrow \\ & = \int dx \frac{1}{\sqrt{2\pi}} \int \underline{\Phi^*(k)} e^{-ikx} dk \frac{1}{\sqrt{2\pi}} \int \underline{\Phi(k')} e^{ik'x} dk' \\ & = \int \underline{\Phi^*(k)} \int \underline{\Phi(k')} dk' \underbrace{\frac{1}{2\pi} \int e^{i(k'-k)x} dx}_{\delta(k'-k)} \\ & = \int \underline{\Phi^*(k)} \underline{\Phi(k)} dk \end{aligned}$$

Parseval's Theorem:

$$\int |\Psi(x)|^2 dx = \int |\Phi(k)|^2 dk$$

Go to momentum language:

$$p = \hbar k$$

$$\frac{dp}{\hbar} = dk$$

$$\Phi(k) = \tilde{\Phi}(p)$$

## 8.2: Parseval Identity (continued)

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int \tilde{\Phi}(p) e^{\frac{ipx}{\hbar}} \frac{dp}{\hbar}$$

$$\tilde{\Phi}(p) = \frac{1}{\sqrt{2\pi}} \int \Psi(x) e^{-\frac{ipx}{\hbar}} dx$$

$$\text{Let } \tilde{\Phi}(p) \rightarrow \Phi(p)\sqrt{\hbar}$$

$$\left. \begin{aligned} \Psi(x) &= \frac{1}{\sqrt{2\pi\hbar}} \int \Phi(p) e^{\frac{ipx}{\hbar}} dp \\ \Phi(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int \Psi(x) e^{-\frac{ipx}{\hbar}} dx \end{aligned} \right\} \text{Fourier in momentum}$$

Parseval:

$$\int |\Psi(x)|^2 dx = \int |\Phi(p)|^2 dp$$

## 8.3: Three Dimensional Fourier

$|\Phi(\vec{p})|^2 dp$  = probability to find particle with momentum  
in the range  $[p, p+dp]$

$$\Psi(\vec{x}) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int \Phi(\vec{p}) e^{\frac{i\vec{p}\cdot\vec{x}}{\hbar}} d^3\vec{p}$$

$$\Phi(\vec{p}) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int \Psi(\vec{x}) e^{-\frac{i\vec{p}\cdot\vec{x}}{\hbar}} d^3\vec{x}$$

3-D case

### 8.3: Three Dimensional Fourier

$$S^3(\vec{x} - \vec{x}') = \frac{1}{(2\pi)^3} \int e^{ik(\vec{x} - \vec{x}')} d^3 k \quad \left. \right\} \text{3-D Delta}$$

$$\int |\psi(\vec{x})|^2 d^3 \vec{x} = \int |\Psi(\vec{p})|^2 d^3 \vec{p} \quad \left. \right\} \text{3-D Parseval}$$

### 8.4: Expectation Values of Operators

Random variable ( $Q$ ) which can take values in the set  $\{Q_1, \dots, Q_n\}$  with probabilities  $\{p_1, \dots, p_n\}$

$$\langle Q \rangle \equiv \sum_{i=1}^n Q_i p_i$$

In a quantum system  $\int \psi^*(x, t) \psi(x, t) dx$  is the probability that the particle is in  $(x, x+dx)$

$$\langle \hat{x} \rangle \equiv \int x \psi^*(x, t) \psi(x, t) dx$$

↑  
expectation value of position

May depend on time

$|\Psi(p)|^2 dp$  is probability to find the particle with momentum in the range  $(p, p+dp)$

$$\langle p \rangle \equiv \int p |\Psi(p)|^2 dp$$

$$\equiv \int p \underbrace{\Psi^*(p)}_{x'} \underbrace{\Psi(p)}_x dp$$

$$= \int_{-\infty}^{\infty} p dp = \int \frac{dx'}{\sqrt{2\pi\hbar}} e^{\frac{ipx'}{\hbar}} \psi^*(x')$$

## 8.4: Expectation Values of Operators (continued)

$$\int \frac{dx}{\sqrt{2\pi\hbar}} e^{-\frac{ipx}{\hbar}} \psi(x)$$

$$= \frac{1}{2\pi\hbar} \int \psi^*(x') dx' \int \psi(x) dx \int_{-\infty}^{\infty} p e^{\frac{ipx'}{\hbar}} e^{-\frac{ipx}{\hbar}} dp$$

$$\int \left(-\frac{\hbar}{i} \frac{\partial}{\partial x}\right) e^{\frac{ipx'}{\hbar}} e^{-\frac{ipx}{\hbar}} dp$$

$$= \int \psi^*(x') dx' \int \psi(x) \left(-\frac{\hbar}{i} \frac{\partial}{\partial x}\right) dx \underbrace{\frac{1}{2\pi\hbar} \int e^{ip(x'-x)/\hbar} dp}_{\delta(x'-x)}$$

Integrate  
by parts

$$\int \psi^*(x') dx' \int \frac{\hbar}{i} \frac{\partial \psi}{\partial x} \delta(x-x') dx$$

$$= \int \frac{\hbar}{i} \frac{\partial \psi}{\partial x} dx \int \psi^*(x') \delta(x-x') dx'$$

$$\langle p \rangle \equiv \int p |\Psi(p)|^2 dp$$

$$= \int \frac{\hbar}{i} \frac{\partial \psi}{\partial x} \psi^*(x) dx -$$

$$= \int \psi^*(x) \frac{\hbar}{i} \frac{\partial \psi}{\partial x} dx$$

$$\langle p \rangle \equiv \int p |\hat{\psi}(p, t)|^2 dp = \int \psi^*(x) \hat{p} \psi(x) dx$$

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x} = \text{momentum operator}$$

## 8.4: Expectation Values of Operators (continued)

In general, for an operator  $\hat{Q}$ :

$$\langle \hat{Q} \rangle = \int \psi^*(x, t) (\hat{Q} \psi(x, t)) dx$$

↑  
Time dependent

kinetic operator

$$\hat{T} = \frac{\hat{P}^2}{2m} \quad \langle T \rangle = ?$$

$$\langle \hat{T} \rangle = \int \psi^*(x, t) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) \right) dx$$

$$\langle \hat{T} \rangle = \int \frac{p^2}{2m} |\Phi(p)|^2 dp$$

$$= \int \Phi^*(p) \frac{p^2}{2m} \Phi(p) dp$$

$$= \int \frac{\hbar^2}{2m} \left| \frac{\partial \psi}{\partial x} \right|^2 dx$$

## 6.5: Time Dependence

$$\begin{aligned}\frac{d}{dt} \langle \hat{Q} \rangle &= \frac{d}{dt} \int \psi^*(x, t) Q \psi(x, t) dx \\ &= \int \frac{\partial \psi^*}{\partial t} Q \psi(x, t) + \psi^* Q \frac{\partial \psi}{\partial t} dx \\ &= \int \frac{i}{\hbar} (\hat{H} \psi)^* Q \psi(x, t) - \frac{i}{\hbar} \psi^* Q \hat{H} \psi(x, t) dx\end{aligned}$$

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi$$

$$\begin{aligned}i\hbar \frac{d}{dt} \langle \hat{Q} \rangle &= \int \psi^* Q \hat{H} \psi - (\hat{H} \psi)^* Q \psi dx \\ &= \int \psi^* Q \hat{H} \psi - \psi^* \hat{H} Q \psi dx\end{aligned}$$

$$i\hbar \frac{d}{dt} \langle \hat{Q} \rangle = \int \psi^* (Q \hat{H} - \hat{H} Q) \psi(x, t) dx$$

$$\downarrow$$
$$i\hbar \frac{d}{dt} \langle \hat{Q} \rangle = \langle [Q, H] \rangle$$

$$\hat{H} = \frac{\hat{p}^2}{2m}$$