

# Lecture 6

- No such things as  $\psi(x, p)$  at the same time

## Fourier principle in music and QM

Breakthrough in 1867

$\omega$  &  $t$  are Fourier conjugates w/ conjug. coeff of 1

$\Delta\omega\Delta t = 1/2$ :  $\psi(\omega, t)$  is ill-defined

$$\Rightarrow \psi(t) \xrightleftharpoons[\text{inverse Fourier transform}]{\text{Fourier}} \psi(\omega) \sim \int_{-\infty}^{\infty} dt \psi(t) e^{i\omega t}$$

uses concept of filtering  
integral  $> 0$  when  $\psi(t)$  has a frequency  $\omega$

$$\hat{\omega} \psi(t) = i \frac{d}{dt} \psi(t) \iff \omega \psi(\omega)$$

in the time domain  $\hat{\omega}$  is a differential operator

Note the symmetry

$$t \psi(t) \iff -i \frac{d}{d\omega} \psi(\omega) = \hat{t} \psi(\omega)$$

time operator is a derivative

can be used to simplify differential equations

## Quantum Mechanics

Heisenberg breakthrough (1925): postulate 1

postulate 1:  $x$  &  $p$  are conjugates w/ c.c of  $\hbar$

$$\Rightarrow \frac{1}{\hbar} \Delta x \Delta p = 1/2 \text{ or } \Delta x \Delta p = \hbar/2$$

$$\psi(p) \iff \psi(x) \sim \int_{-\infty}^{\infty} dp \psi(p) e^{i/\hbar x \cdot p}$$

$$\hat{x} \psi(p) = i\hbar \frac{d}{dp} \psi(p) \iff x \cdot \psi(x)$$

$$p \cdot \psi(p) \iff -i\hbar \frac{\partial}{\partial x} \psi(x) = \hat{p} \psi(x)$$

↑  
Momentum operator

$$\hat{p} \equiv -i\hbar \frac{d}{dx}$$

Remember!

Note:  $\hbar \ll 1$ :  $\hbar \approx 1.05 \times 10^{-34} \text{ m} \cdot \text{kg} \cdot \frac{\text{m}}{\text{s}}$   
 $\underbrace{\text{J} \cdot \text{s}}_{\text{energy} \cdot \text{time}}$

$\Delta x \neq \Delta p$  are very small, hard to detect

Must make a choice

$\psi(x)$  or  $\psi(p)$   
 ↑  
 chemists  
 (think in terms of structure)

↑  
 physicist  
 (think in current)

Postulate 5: Equation of motion

QM:  $E = H = \frac{p^2}{2m} + V(x)$   
 kinetic potential

QM:  $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$   
 $\hat{x} = x$   
 $\hat{p} = -i\hbar \frac{d}{dx}$   
 plugging

$$\Rightarrow \hat{p}^2 = (-i\hbar \frac{d}{dx}) (-i\hbar \frac{d}{dx}) = -\hbar^2 \frac{d^2}{dx^2}$$

plug into  $\hat{H}$

$$\Rightarrow \hat{H} = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

energy operator in QM

In CM,  $xp = px$  (x and p "commute")

$$\hat{x}\hat{p}\psi = x(-i\hbar\frac{\partial}{\partial x})\psi = -i\hbar x\frac{\partial}{\partial x}\psi$$

$$\hat{p}\hat{x}\psi = (-i\hbar\frac{\partial}{\partial x})x\psi = -i\hbar\psi - i\hbar x\frac{\partial}{\partial x}\psi$$

$$(\hat{x}\hat{p}\psi - \hat{p}\hat{x}\psi) = +i\hbar\psi \Rightarrow \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar$$

in QM

do not commute

can't simultaneously  
measure  $x$  and  $p$