

# **PYL101: Electromagnetic waves and Quantum Mechanics**

## **Lecture 3**

Prof. Sunil Kumar (Department of Physics)



# Indeterministic nature of microscopic objects/systems

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

State of the system

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

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = E \psi(\vec{r}, t)$$

$$H\psi(\vec{r}, t) = E\psi(\vec{r}, t)$$

Equation of motion  
(Schrodinger's equation)

Statistical interpretation

$$\begin{aligned} \psi^*(\vec{r}, t) \psi(\vec{r}, t) \\ = \psi(\vec{r}, t) \psi^*(\vec{r}, t) \\ = |\psi(\vec{r}, t)|^2 \end{aligned}$$

Number;  
Intensity;  
Probability  
density

$$\vec{\nabla} \psi(\vec{r}, t) = \frac{\partial}{\partial r} \hat{r} \psi(\vec{r}, t) = i \frac{p}{\hbar} \psi(\vec{r}, t) \hat{r}$$

$$\nabla^2 \psi(\vec{r}, t) = i^2 \frac{p^2}{\hbar^2} \psi(\vec{r}, t)$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}, t) = \frac{p^2}{2m} \psi(\vec{r}, t)$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}, t) = E_T \psi(\vec{r}, t)$$

$$H\psi(\vec{r}, t) = E\psi(\vec{r}, t)$$

Equation of motion  
(Schrodinger's equation)

- If we can write H as the energy operator:  $H = T + V$
- In fact all physical observables are to be written in corresponding operator form

(Will come back to this point later)

# Indeterministic nature of microscopic objects/systems

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

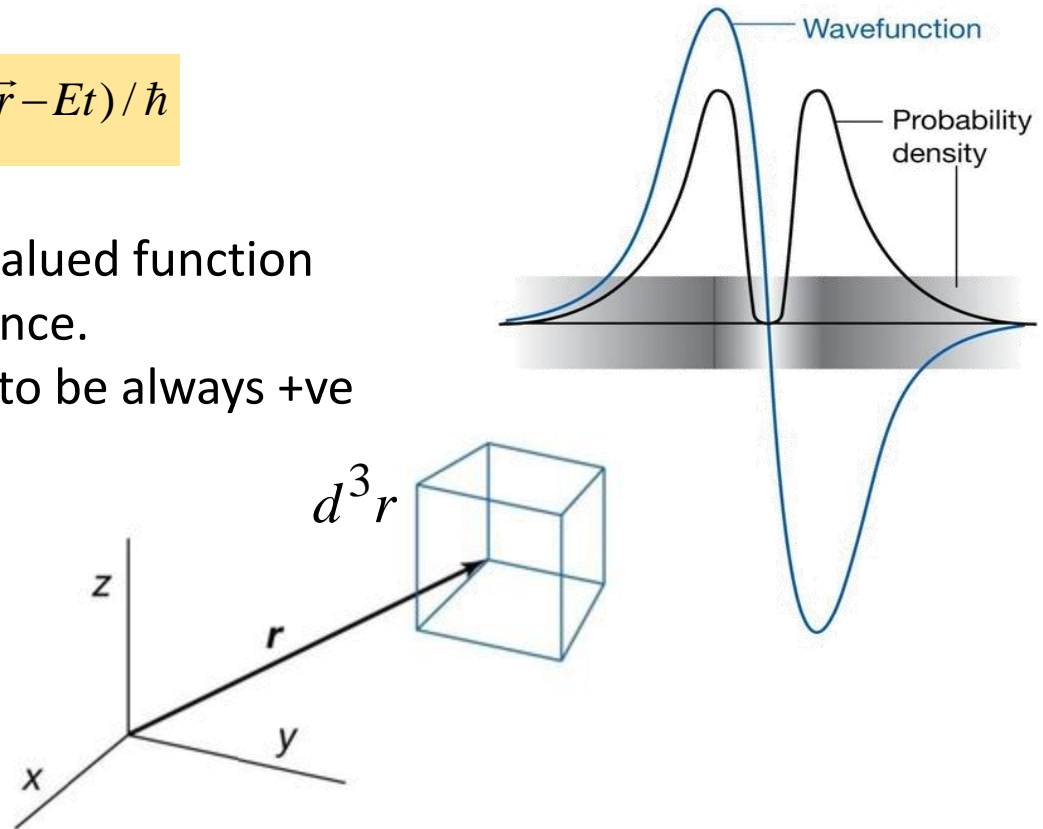
- It's a continuous and complex valued function
- Its sign has no physical significance.
- But the probability density has to be always +ve
- The total probability is 1

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

$$P(t) = \int_{-\infty}^{+\infty} |\psi(\vec{r}, t)|^2 d^3r = 1$$

- Normalization condition

$$\int_{-\infty}^{+\infty} \psi^*(\vec{r}, t) \psi(\vec{r}, t) d^3r = 1$$



Check the dimensions/units of  $\psi$  and  $|\psi|^2$

# Indeterministic nature of microscopic objects/systems

- The system can have multiple states possible, a linear superposition also is one state of the system

$$\psi(\vec{r}, t) = a_1\psi_1(\vec{r}, t) + a_2\psi_2(\vec{r}, t) + \dots \quad a_1, a_2, \text{ etc. are complex numbers}$$

$$P = P_1 + P_2 + \dots$$

Check the conditions on  $a_1, a_2, \text{ etc.}$

- Classical physics is completely deterministic  $\vec{r}(0) \rightarrow \vec{r}(t), \vec{p}(0) \rightarrow \vec{p}(t)$   
... but quantum physics not, i.e., and so on..

Wave function is not localized  $\psi(\vec{r}, t)$

- Heisenberg's uncertainty principle:** It is impossible to devise an experiment that can measure simultaneously two complimentary observables to arbitrary accuracy.

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

$$\Delta r \Delta p_r \geq \frac{\hbar}{2}$$

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

Mind that we can not make a measurement on a quantum system without perturbing it.

Check if the uncertainties at macroscopic level make any sense to you

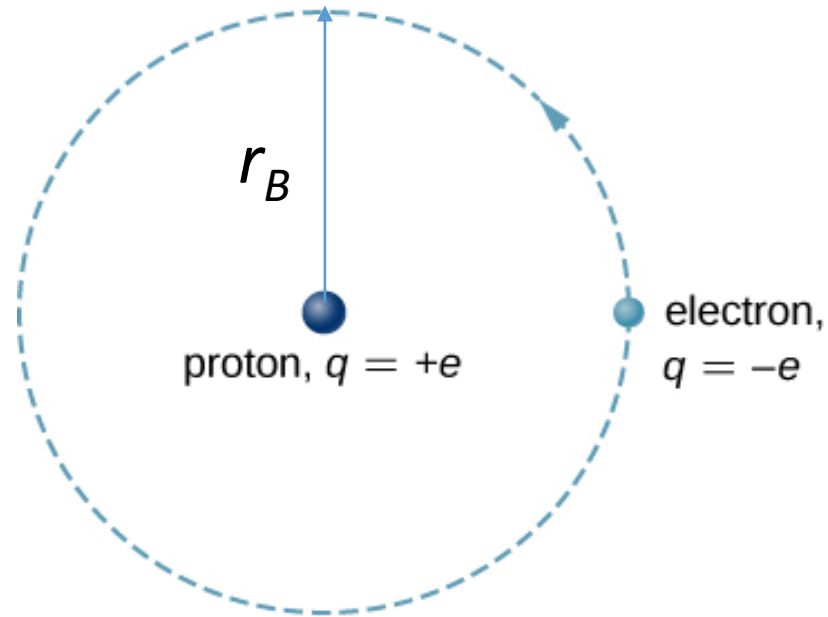
# Indeterministic nature of microscopic objects/systems

- **Example:**

Bohr's atomic radius in ground state and it's energy can be estimated.

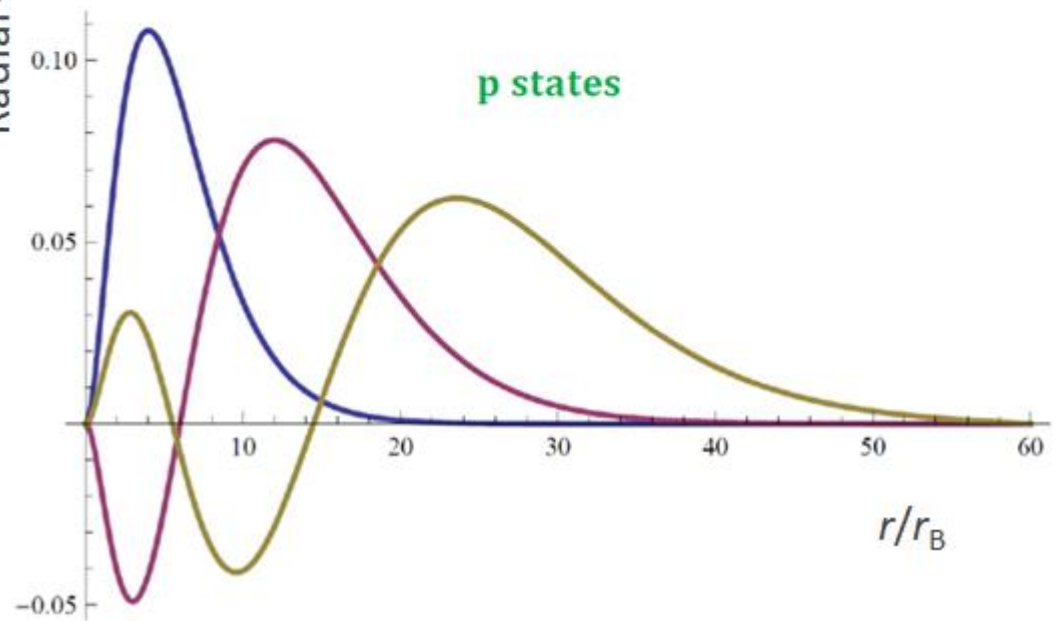
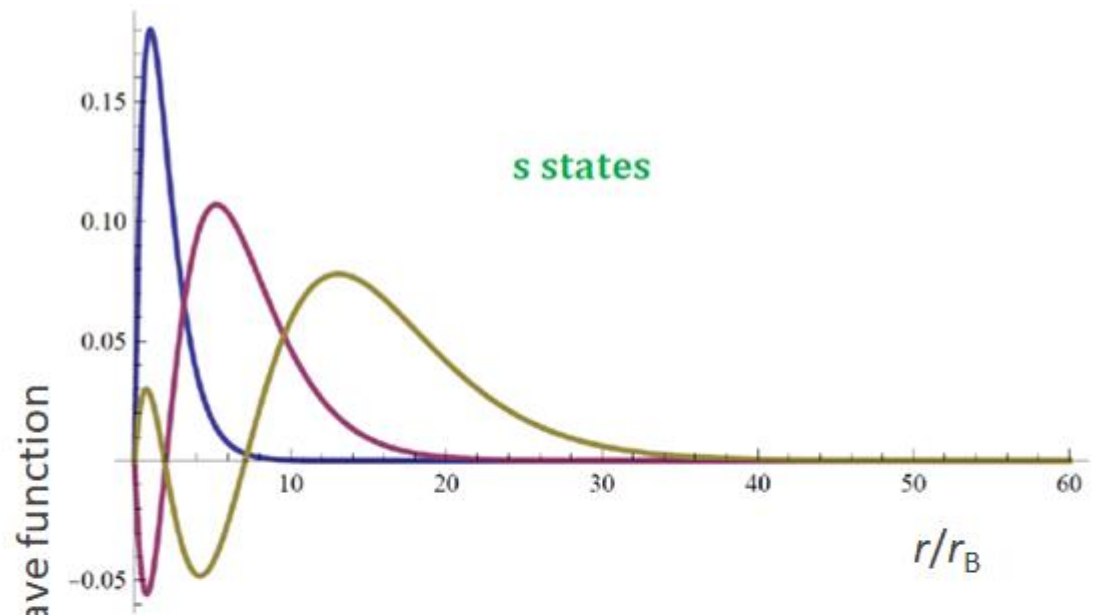
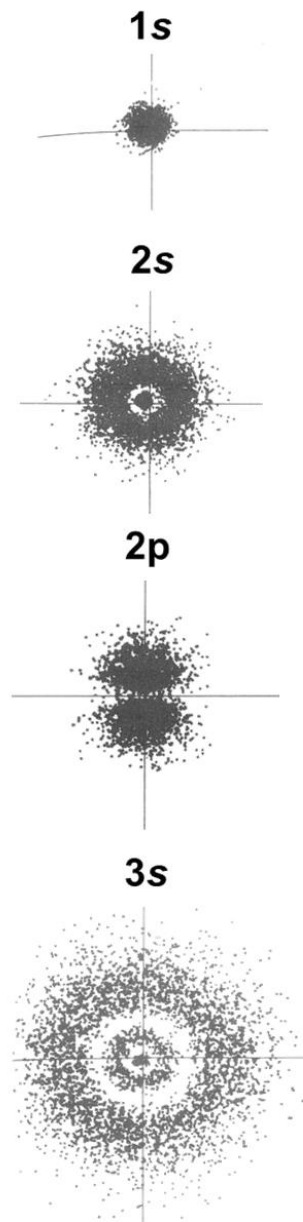
Note: large  $\Delta p$  means large  $p$  on an average. Same for all observables.

$$\text{Take } r_B \geq \Delta r = \frac{\hbar}{2\Delta p}$$
$$p \geq \Delta p = \frac{\hbar}{2r_B}$$



$$E = -13.6 \text{ eV}$$

$$r_B = 0.53 \times 10^{-10} \text{ m}$$
$$= 0.053 \text{ nm}$$



# Rules and properties of the wave function

- To satisfy the observations
- Particle is real and it exists there in some region of the space
- $\psi$  is a complex valued function
- State of the system is found by solving the Schrodinger's equation

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = H\psi(\vec{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}, t) + V(\vec{r}, t)\psi(\vec{r}, t)$$

$$\psi(\vec{r}, t) = \psi(\vec{r})e^{-iEt/\hbar}$$

Under certain conditions, the complete wave function  
= time-dependent part\*stationary solution

- Solutions for time-independent potentials are called stationary states, i.e., when the **probability density is stationary** (independent of time)

$$|\psi(\vec{r}, t)|^2 = |\psi(\vec{r})|^2$$

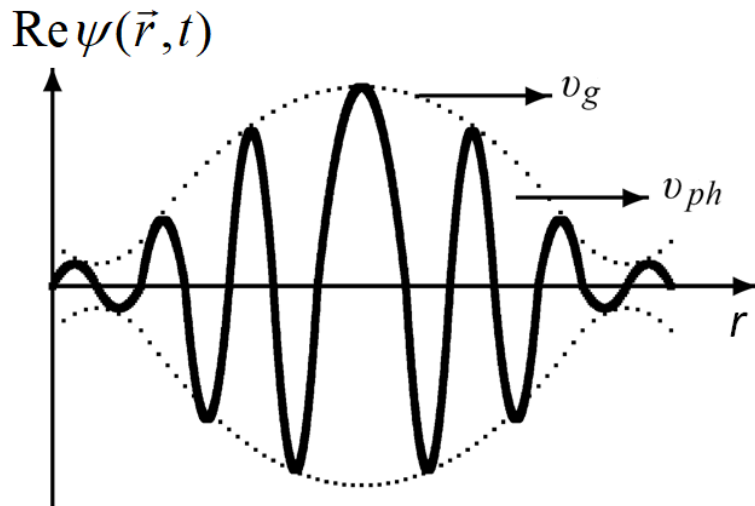
# Rules and properties of the wave function

- Since quantum particles are both particles and waves, to describe it through Schrodinger's equation, it is best to consider it in terms of a wave packet

otherwise  $\psi(\vec{r}, t) = Ae^{i(\vec{k} \cdot \vec{r} - \omega t)} = Ae^{i(\vec{p} \cdot \vec{r} - Et) / \hbar}$  is infinitely extended

- Therefore, wave functions are made to vanish everywhere except in the neighborhood of the particles.

**Localized wave functions**



Can be constructed by superposing many waves of nearby wavelengths in the same region of space

$$\psi(\vec{r}, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(\vec{k}) e^{i(\vec{k} \cdot \vec{r} - \omega t)} dk$$

**We leave this discussion about wave packets at this point for now.**



# Rules and properties of the wave function

**TDSE** 
$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}, t) + V(\vec{r}, t) \psi(\vec{r}, t)$$

**Stationary states**  $\psi(\vec{r}, t)$  are the solutions of

**TISE** 
$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \psi(\vec{r}, t) = E \psi(\vec{r}, t)$$
 when  $|\psi(\vec{r}, t)|^2 = |\psi(\vec{r}, 0)|^2$

$V(\vec{r}, t) = V(\vec{r}, 0) = V(\vec{r})$

**Operators and expectation values:**

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \psi(\vec{r}, t) = E \psi(\vec{r}, t)$$

H operator

$$H \psi(\vec{r}) = E \psi(\vec{r})$$

$$H = T + V$$

“Eigen value equation, eigen states, eigen values; E is a constant that represents the energy of the particle in state

$$\psi(\vec{r}) \text{ or } \frac{a}{b} \psi(\vec{r})$$

# Rules and properties of the wave function

## Operators and expectation values:

- An operator is a mathematical object that maps one quantum mechanical wave function to another

$$A\psi(\vec{r}) = \phi(\vec{r})$$

In most cases,  $\phi(\vec{r})$  is also a solution

$$A\psi(\vec{r}) = a\psi(\vec{r})$$

**Eigen value equation**

**"a" is the expectation value of operator "A" in the state  $\psi(\vec{r})$**

$$\int_{-\infty}^{+\infty} \psi^*(\vec{r}) \{ A\psi(\vec{r}) \} d^3r = a$$

If we do a measurement of observable 'A' on a system in it's state  $\psi(\vec{r})$  then the outcome is 'a', the eigen value of 'A'

**Stationary states**

Like probability density, expectation values are stationary, i.e., their time derivative is zero

# Rules and properties of the wave function

## Operators and expectation values:

- If the system is in some general state  $\phi(\vec{r})$  then the measurement of observable  $A$  for the system's state  $\psi(\vec{r})$ ,

$$\int_{-\infty}^{+\infty} \phi^*(\vec{r}) \{ A\psi(\vec{r}) \} d^3r = a \int_{-\infty}^{+\infty} \phi^*(\vec{r}) \psi(\vec{r}) d^3r$$

provides value ' $a$ ' with probability



- The expectation value of an observable is the average of repeated measurements on an ensemble of identically prepared systems.
- But .... It is NOT the average of the repeated measurements done on the same system.
- If  $A\psi(\vec{r}) = a\phi(\vec{r})$  This is not an eigen value equation,  $\psi(\vec{r})$  is not eigen function.

## Operators and expectation values:

- All dynamical observables (not  $t$ ) such as  $r$ ,  $p$ ,  $E$ ,  $T$ ,  $V$  have operators

Observable	Corresponding operator
$\vec{r}$	$\hat{\vec{R}}$
$\vec{p}$	$\hat{\vec{P}} = -i\hbar \vec{\nabla}$
$T = \frac{p^2}{2m}$	$\hat{T} = -\frac{\hbar^2}{2m} \nabla^2$
$E = \frac{p^2}{2m} + V(\vec{r}, t)$	$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \hat{V}(\hat{\vec{R}}, t)$
$\vec{L} = \vec{r} \times \vec{p}$	$\hat{\vec{L}} = -i\hbar \hat{\vec{R}} \times \vec{\nabla}$