PYL101: EM Waves & Quantum Mechanics

Quantum Mechanics - Lecture 5

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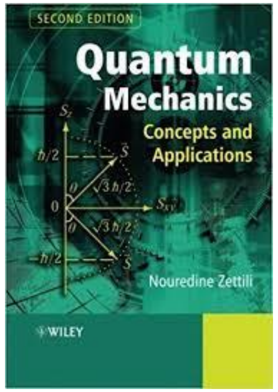
- **Schedule: Monday & Thursday (8:00 – 9:30, Slot A)**
- **TAs:**

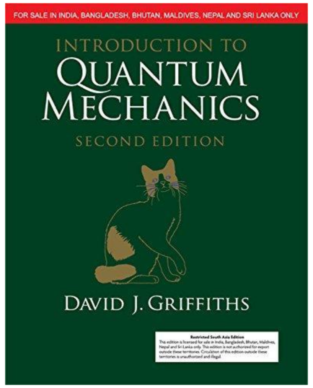
  Radhika T P (phz198033@physics.iitd.ac.in)

  Manoj Singh (phz198494@physics.iitd.ac.in)

- **Tutorials: From January 25th, Monday-Friday, 03:00PM-04:00PM**

Reference Books





I will cover the following topics:

Module 8: Quantum Mechanical Operators: observables and operators, linear operators, eigenvalues and eigen vectors of operators, Hermitian operators, product of operators, expectation values and uncertainty relations,

Module 9: Time-Independent Schrodinger Equation: stationary states, free particle solution, bound states

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Module 10: One Dimensional Problems: 1-D infinite potential well, 1-D finite potential well, and quantum mechanical tunneling and alpha-decay.

(will be covered by Prof. Saswata Bhattacharya)

A quick revision of what you have done so far

Birth of Quantum Mechanics

The "Classical Physics" fails miserably to explain

- the dynamics of the particles moving with very high speeds (comparable to the speed of light)
- the structure and dynamics of particles/systems at microscopic level. For example, the structure of atoms and molecules, and interaction with light.

1. The Particle-like Behaviour of Waves

- Black-body radiation (1900)
- Photoelectric effect (1905)
- Compton effect (1923)

2. The Wave-like Behaviour of Particles

- de Broglie hypothesis (1923)
- Electron diffraction (Davisson-Germer experiment) (1927)
- Wave particle duali

3. The Puzzling Stability of the Atom

- What is the origin of atomic spectra?

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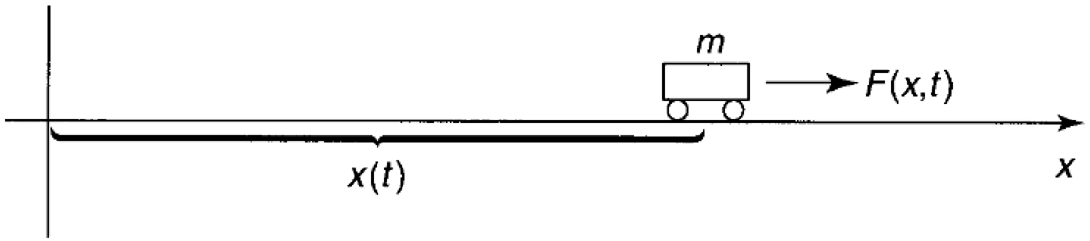
Wave-Particle Duality: Complementarity

Wave Function in Quantum Mechanics



Classical Mechanics:

We can determine all these properties by solving the Newton's equation with appropriate boundary conditions.

$$m\frac{d^2x}{dt^2} = F(x,t)$$

Given: mass, force acting on the mass

Wants to know: position, velocity, momentum and kinetic energy at certain time t

Quantum Mechanics:

"a microscopic particle"

In principle, we can determine all these properties if we know the wave function $\Psi(x,t)$ of the particle. And, the wave function can be obtained by solving the equation

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

BC: at t = 0, what is $\Psi(x,0)$?

time dependent Schrodinger equation

A quick revision of what you have done so far

- Ψ is a continuous function.
- It represents the amplitude of the matter wave associates with particle.
- It contains the information about the probability that one would measure, but cannot give pre-determined results.

$$\int_a^b |\Psi(x,t)|^2\, dx = \text{Probability of finding the particle between } a \text{ and } b \text{ at time } t$$

where, $|\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t)$, and $\Psi(x,t)$ represents the probability amplitude. Statistical Interpretation (Born, 1926)

- A wave function describing a particle at position *x* and time *t* can be represented by

$$\Psi(x,t) \qquad Or \qquad < x,t|\Psi > \quad or \quad |\Psi >$$

(Ordinary representation) (Dirac representation)

- For every *ket* vector there is a corresponding dual vector, called the "*bra*" vector, which belongs a dual vector space. That is,

$$|\Psi > \longleftrightarrow < \Psi| \quad \text{(one-to-one correspondence)}$$

New story begins
from here . . . .

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

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

old wave function

new wave function

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- If we can write Φ in terms Ψ such that $\Phi(x,t) = a\,\Psi(x,t)$ then

$$\hat{A}\,\Psi(x,t) = a\,\Psi(x,t), \quad \text{(the eigenvalue equation)} \quad \text{Eq.(1)}$$

$\Psi(x,t)$ is called an eigenfunction of $\widehat{\mathrm{A}}$ and a (a real number for physical systems) is the corresponding eigenvalue.

- If we cannot write Φ in terms of Ψ, $\Phi(x,t) = a\,\Psi'(x,t)$ then

$$\hat{A}\,\Psi(x,t) = a\,\Psi'(x,t), \quad \text{(Not an eigenvalue equation)}$$

$\Psi(x,t)$ is NOT an eigenfunction of $\widehat{\mathrm{A}}$.

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Physical interpretation of eigenvalue equation:

Case I: Consider that the particle is in the state $\Psi(x,t)$:

Using the eigenvalue equation, we can write

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\,\left(\hat{A}\,\Psi(x,t)\right)\,dx = \int_{-\infty}^{\infty} \Psi^*(x,t)\,a\,\Psi(x,t)\,dx = a\int_{-\infty}^{\infty} \Psi^*(x,t)\,\Psi(x,t)\,dx = a$$

→ "if you do a measurement of the observable A, and if the particle in state Ψ then measured value will be the eigenvalue of the operator $\widehat{\mathrm{A}}$"

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The expectation value of the observable A in the state $\Psi(x,t)$. It can be denoted as $\langle A\rangle_\Psi$ or $\langle A\rangle$ or $\langle \Psi|\hat{A}|\Psi\rangle$.

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Case II: Consider that the particle is in any general state $\Phi(x,t)$:

Using the eigenvalue equation, we can write

$$\int_{-\infty}^{\infty} \Phi^*(x,t)\left(\hat{A}\,\Psi(x,t)\right) dx = \int_{-\infty}^{\infty} \Phi^*(x,t)\; a\, \Psi(x,t)\, dx = a \int_{-\infty}^{\infty} \Phi^*(x,t)\, \Psi(x,t)\, dx$$

→ if the particle is in the general state Φ then the measured value will be "*a*" with probability $|\Phi^*\Psi|^2$.

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the matrix element of the observable *A* with respect to states Φ and Ψ.
We denote it as $<\Phi\ |\hat{A}|\Psi>$

Example of Operators

Physical quantity	Operator	Operation
Position ($\vec{r}$)	$\hat{r}$	$r\,\Psi(r,t)$
Linear momentum ($\vec{p}$)	$\frac{\hbar}{i}\vec{\nabla}$	$\frac{\hbar}{i}\vec{\nabla}\Psi(r,t)$
Angular momentum ($\vec{L}$)	$\vec{r}\times\frac{\hbar}{i}\vec{\nabla}$	$\overrightarrow{(r\times\frac{\hbar}{i}\vec{\nabla})}\Psi(r,t)$
Kinetic energy (T)	$-\frac{\hbar^2}{2m}\vec{\nabla}^2$	$\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2\right)\Psi(r,t)$
Potential energy (V)	$V(\vec{r})$	$V(\vec{r})\Psi(r,t)$
Total energy (E)	$-\frac{\hbar^2}{2m}\vec{\nabla}^2+V(\vec{r})$	$\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2\right)\Psi(r,t)+V(\vec{r})\Psi(r,t)$

… we will do more on this later….

Linear Operators

An operator $\hat{A}$ is said to be linear if it obeys the distributive law. That is, for wave functions Ψ_1 and Ψ_2 , and complex numbers α and β, it satisfies the relation

$$\hat{A}\,(\alpha\Psi_1 + \beta\Psi_2) = \alpha\left(\hat{A}\,\Psi_1\right) + \beta\left(\hat{A}\,\Psi_2\right)$$

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Hermitian Operators

An operator $\hat{A}$ is said to be Hermitian if for any two wave functions Ψ_1 and Ψ_2 , it satisfies the relation

$$\int_{-\infty}^{\infty} \Psi_1^*(\hat{A}\,\Psi_2)\,dx = \int_{-\infty}^{\infty} (A\Psi_1\ )^*\Psi_2\,dx$$

OR

An operator $\hat{A}$ is said to be Hermitian if it is equal to its adjoint $A^\dagger$. That is

$$\hat{A} = \hat{A}^\dagger \ \Rightarrow < \Psi_1|A|\Psi_2 > = < \Psi_2|A|\Psi_1 >^*$$

"→ any operator corresponding to a physical observable is a Hermition operator"

"→ all quantum mechanical operators which represent physical observables are Hermitian"

Important Properties of Hermitian operators:

- The eigenvalues of the Hermitian operators are real.
- The eigenvectors corresponding to two different eigenvalues of a Hermitian operator are orthogonal to each other.

Homework problem 1

Projection operator

If $|\Psi>$ is a normalized wave function, then the projection operator is defined as

$$\hat{P} = |\Psi><\Psi| \quad \text{(ket-bra) (also called the outer product)}$$

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- Lets consider $\hat{P}$ acting on a different state $|\Phi>$

$$\hat{P}|\Phi> = (|\Psi><\Psi|)\,|\Phi> = \;|\Psi>(<\Psi|\Phi>) = (<\Psi|\Phi>)\,|\Psi>$$

→ it projects the state $|\Phi>$ onto the state $|\Psi>$ with probability $|<\Psi|\Phi>|^2$

- It is Hermitian: $\hat{P}^{\dagger} = \hat{P}$
- It is idempotent $\hat{P}^2 = \hat{P}$

Homework problem 2

Product of operators

The product of two operators generally do not obey the commutative relation. That is

$$\hat{A}\,\hat{B} \neq \hat{B}\,\hat{A}$$

→ "the order of the application is important". The operators $\hat{A}$ and $\hat{B}$ are called the non − commutating operators.

From above relation we can write: $\hat{A}\,\hat{B} - \hat{B}\,\hat{A} \neq 0 \Rightarrow [\hat{A},\hat{B}] \neq 0$

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→ "$\hat{A}$ and $\hat{\text{B}}$ can have the same eigen functions".

Example: $[\hat{x}, \hat{p}_y] = \hat{x}\,\hat{p}\,_y - \hat{p}_y\hat{x} = 0$

Example Problem 1:

Consider a state $|\psi\rangle = \frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{1}{\sqrt{5}}|\phi_2\rangle + \frac{1}{\sqrt{10}}|\phi_3\rangle$ which is given in terms of three orthonormal eigenstates $|\phi_1\rangle$, $|\phi_2\rangle$ and $|\phi_3\rangle$ of an operator $\hat{B}$ such that $\hat{B}|\phi_n\rangle = n^2|\phi_n\rangle$. Find the expectation value of $\hat{B}$ for the state $|\psi\rangle$.

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Solution: If ψ is not normalized, the expectation value is $< \hat{A} > = \frac{<\psi|A|\psi>}{<\psi|\psi>}$

$$\begin{aligned} \langle\psi \mid \psi\rangle &= \left(\frac{1}{\sqrt{2}}\langle\phi_1 \mid + \frac{1}{\sqrt{5}}\langle\phi_2 \mid + \frac{1}{\sqrt{10}}\langle\phi_3 \mid\right)\left(\frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{1}{\sqrt{5}}|\phi_2\rangle + \frac{1}{\sqrt{10}}|\phi_3\rangle\right) \\ &= \frac{8}{10} \end{aligned}$$

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&= \frac{8}{10}
\end{aligned}$$

$$\begin{aligned}
\langle\psi \mid \hat{B} \mid \psi\rangle &= \left(\frac{1}{\sqrt{2}}\langle\phi_1 \mid + \frac{1}{\sqrt{5}}\langle\phi_2 \mid + \frac{1}{\sqrt{10}}\langle\phi_3 \mid\right)\hat{B}\left(\frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{1}{\sqrt{5}}|\phi_2\rangle + \frac{1}{\sqrt{10}}|\phi_3\rangle\right) \\
&= \frac{1}{2} + \frac{2^2}{5} + \frac{3^2}{10} \\
&= \frac{22}{10}.
\end{aligned}$$

Hence, the expectation value of $\hat{B}$ is given by

$$\langle \hat{B} \rangle = \frac{\langle \psi \mid \hat{B} \mid \psi \rangle}{\langle \psi \mid \psi \rangle} = \frac{22/10}{8/10} = \frac{11}{4}.$$

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Example Problem 2: Prove the commutation relations (a) $[\hat{x}, \hat{p}_x] = i\hbar$ (b) $[\hat{x}, \hat{p}_y] = 0$

Solution: (a) Let us assume $\psi(x)$ represent the wave function of the system. Then we can write

$$[\hat{x}, \hat{p}_x]\psi(x) = (\hat{x}\,\hat{p}_x - \hat{p}_x\,\hat{x})\psi(x) = x\left(-i\hbar\frac{d}{dx}\right)\psi(x) - \left(-i\hbar\frac{d}{dx}\right)x\psi(x)$$

$$= -i\hbar\, x\frac{d\psi(x)}{dx} + i\hbar\psi(x) + i\hbar\, x\frac{d\psi(x)}{dx}$$

$$= i\hbar\,\psi(x)$$

This implies that $[\hat{x}, \hat{p}_x] = i\hbar$

Solution: (b) Using the wavefuction $\psi(x)$ we can write

$$[\hat{x}, \hat{p}_y]\psi(x) = (\hat{x}\,\hat{p}_y - \hat{p}_y\,\hat{x})\psi(x) = x\left(-i\hbar\frac{d}{dy}\right)\psi(x) - \left(-i\hbar\frac{d}{dy}\right)x\psi(x)$$

$$= -i\hbar\, x\frac{d\psi(x)}{dy} + 0 + i\hbar\, x\frac{d\psi(x)}{dy}$$

$$= 0$$

This implies that $[\hat{x}, \hat{p}_y] = 0$