UNIVERSITY OF AGRICULTURE, ABEOKUTA

DEPARTMENT OF PHYSICS

PHS 411…Quantum Mechanics (3 units)

Module	Short-Description	Duration
1	Postulates of Quantum Mechanics	3 lectures
2	Commutator relations in Quantum Mechanics	2 lectures
3	Function spaces and Hermitian Operators	3 lectures
4	Harmonic Oscillator	3 lectures
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		11 lectures

References:

1. E. Merzbacher , Quantum Mechanics
2. L.I.Schiff ; Quantum Mechanics
3. R. Shankar ; Principles of Quantum Mechanics
4. A. Ghatak and S.Lokanathan ;Quantum Mechanics

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Module 1 …. Postulates of Quantum Mechanics
(3 Lectures)

1.1 Basic postulates of Quantum Mechanics

There are 4 basic postulates of Quantum Mechanics summarized as follows**:**

(1) Observables and operators
(2) Measurement in Quantum Mechanics
(3) The state function and expectation values
(4) Time development of the state function

Tutorial 1

1. The state $\psi(x)$ of a system of electrons of mass m in 1-D is given by

$\psi(\mathrm{x}) = \mathrm{Ae}^{-2\pi\mathrm{x}^2}$.

(a) Normalize to determine the value of A.
(b) What is the normalized state function?
(c) Calculate the average energy of the electrons in this normalized state.

2. The **Dirac delta** function $\delta(x-a)$ may be accurately expressed as an eigenfunction of $\hat{x}$ in the coordinate representation.

(a) State any **three** properties of $\delta(x-a)$.
(b) If a system is in a state $\psi(x) = \delta(x+2)$, what does the measurement of x give?
(c) Evaluate the following: (i) $\int dx \delta(x-2)$ (ii) $\int dx (x-4)\delta(x+3)$

(iii) $\int dx (\log_{10} x)\delta(x-0.01)$ (iv) $\int dx (e^{x+2})\delta(x+2)$

(v) $\int_0^\infty dx [\cos(3x) + 2e^{ix}](\delta(x-\pi) + \delta(x))$

3. (a) Given that the identity operator $\hat{I}$ is a 2-D unit matrix; that is, $\hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Construct its inverse $\hat{I}^{-1}$ provided it exists.

Module 2 …. Commutator Relations in Quantum Mechanics
(2 Lectures)

2.1 Definition : The commutator between 2 operators A and B is :

$[A, B]$ such that :

$$[A, B] = AB - BA \tag{2.1}$$

2.2 Property : If $[A, B] = -[B, A]$ **,** the 2 operators A and B are said to commute with each other. i.e. A and B are ***compatible***.

Thus $AB = BA$ (2.2)

i.e. $[A, B] = 0$ (2.3)

If $[A, B] \neq 0$ (2.4)

$\Rightarrow$ A and B are ***not compatible***

Tutorial 2

(1) Prove that for the operators A,B and C, the following identities are valid :

(i) $[A + B, C] = [A, C] + [B, C]$ (ii) $[A, BC] = [A, B]C + B[A, C]$

(iii) $[A, B + C] = [A, B] + [A, C]$ (iv) $[AB, C] = A[B, C] + [A, C]B$

(2) One of the most important ***commutators*** in physics is that between the coordinate, $\hat{x}$, and the momentum, $\hat{p}$.

(i) Show that $[\hat{x}, \hat{p}] = i\hbar$

Hence,or otherwise,deduce that

(ii) $[\hat{x}^2, \hat{p}] = 2i\hbar\hat{x}$; (iii) $[\hat{x}, \hat{p}^2] = 2i\hbar\hat{p}$; (iv) $[\hat{H}, \hat{x}] = \frac{-i\hbar}{m}\hat{p}$;

(v) If g is an arbitrary function of x, show that $[\hat{p}, g] = -i\hbar\frac{dg}{dx}$

Module 3 …. Function Spaces and Hermitian operators
(3 Lectures)

3.1 Solution of a Particle-in-a-box problem : Consider a point mass m constrained to move on an infinitely thin,frictionless wire which is strung tightly between two impenetrable walls a distance L apart. This simply is a one-dimensional box to be solved as follows:

3.11 Potential: $v(x) = \infty .....(x \le 0, x \ge L)$ (3.11)

$$v(x) = 0........(0 < x < L) \quad (3.12)$$

3.12 Hamiltonian: $\hat{H}_1 = \dfrac{\hat{p}^2}{2m} + \infty .....(x \le 0, x \ge L)$ (3.13)

$$\hat{H}_2 = \frac{\hat{p}^2}{2m}........(0 < x < L) \quad (3.14)$$

The ***eigenvalues*** can be shown to be : $E_n = n^2 E_1$ (3.15)

Where $E_1 = \dfrac{\hbar^2 \pi^2}{2mL^2}$ (3.16)

Also, the ***eigenstates*** can be shown to be : $\phi_n = \sqrt{\dfrac{2}{L}} \sin\left(\dfrac{n\pi x}{L}\right)$ (3.17)

3.2 Dirac Notation : gives a monogram to the integral of the product of two state functions, $\psi(x)$ and $\phi(x)$:

i.e. $\langle \psi | \phi \rangle = \int_{-\infty}^{\infty} \psi^*(x)\phi(x)dx$ (3.21)

N.B.(1) $\langle \psi | \equiv$ 'bra vector' ; $| \phi \rangle \equiv$ 'ket vector'

(2) *Rules:* If a is any complex number and the functions ψ and ϕ are such that $\int_{-\infty}^{\infty} \psi^* \phi dx < \infty$ (3.22)

the following rules hold:

(i) $\langle \psi | a\phi \rangle = a\langle \psi | \phi \rangle$

(ii) $\langle a\psi | \phi \rangle = a^* \langle \psi | \phi \rangle$

(iii) $\langle \psi | \phi \rangle^* = \langle \phi | \psi \rangle$

(iv) $\langle \phi + \psi | = \langle \psi | + \langle \phi |$

(v) $\int_{-\infty}^{\infty} (\psi_1 + \psi_2)^* (\phi_1 + \phi_2) dx = \langle \psi_1 | \phi_1 \rangle + \langle \psi_1 | \phi_2 \rangle + \langle \psi_2 | \phi_1 \rangle + \langle \psi_2 | \phi_2 \rangle$

(3.23)

3.3 Hermitian Operator : is an operator that is equal to its adjoint
i.e. a self-adjoint operator.

3.31: Properties of Hermitian operators : There are 2 important properties:

1st : The eigenvalues of o hermitian operator ***real .***

2nd : The eigenfunctions of a Hermitian operator are ***orthogonal***.

Tutorial 3

1. **Spin Matrices** are special matrices that occur in Quantum mechanics.

In 2-D, they are namely : $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Show that each of the matrices is **Hermitian**.

2. Show that the linear momentum operator is **Hermitian**.

3. The eigenstate of a particle may be represented by each of the following kets :

(i) $|\psi_1\rangle = \begin{pmatrix} i \\ -1 \\ 1 \end{pmatrix}$; (ii) $|\psi_2\rangle = \begin{pmatrix} 1 \\ -i \\ -1 \end{pmatrix}$; (iii) $|\psi_3\rangle = \begin{pmatrix} 1 \\ -1 \\ i \end{pmatrix}$

Calculate (a) $\langle\psi_1|\psi_1\rangle$; (b) $\langle\psi_1|\psi_2\rangle$; (c) $\langle\psi_2|\psi_3\rangle$; (d) $|\psi_1\rangle\langle\psi_1|$;
(e) $|\psi_1\rangle\langle\psi_2|$; (f) $|\psi_2\rangle\langle\psi_3|$ **(18 marks)**

Module 4 …. Harmonic Oscillator (3 Lectures)

Introduction : A brief review of the classical Harmonic Oscillation
Operators : *(1) Annihilation* operator $\hat{a}$ is defined as :

$$\hat{a} = \frac{\beta}{\sqrt{2}}\left(\hat{x} + i\frac{\hat{p}}{m\omega}\right), \qquad (4.21)$$

***(2)* creation** operator $\hat{a}^+$ is defined as:

$$\hat{a}^+ = \frac{\beta}{\sqrt{2}}\left(\hat{x} - i\frac{\hat{p}}{m\omega}\right) \qquad (4.22)$$

where $\beta^2 = \frac{m\omega}{\hbar}$ (4.23)

Dimensionless transformation : If the non-dimensional displacement ζ is defined as : $\zeta^2 \equiv \beta^2 x^2 \equiv \frac{m\omega}{\hbar}x^2$, (4.31)

It can be shown that $\hat{a}$ in equation (4.21) transforms as :

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\zeta + \frac{\partial}{\partial\zeta}\right) \qquad (4.32)$$

Also, $\hat{a}^+$ in equation (4.22) transforms as:

$$\hat{a}^+ = \frac{1}{\sqrt{2}}\left(\zeta - \frac{\partial}{\partial\zeta}\right) \qquad (4.33)$$

Hamiltonian for the Harmonic Oscillator :

The Hamiltonian $\hat{H}$ of the 1-D harmonic oscillator is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \qquad (4.41)$$

It can be shown that equation (4.41) is expressible as

$$\hat{H} = \hbar\omega(\hat{a}\hat{a}^+ - 1/2) \quad ; \qquad (4.42)$$

Eigenvalues : An algebraic solution of the 1-D harmonic oscillator shows the energy eigenvalues as:

$$E_n = \hbar\omega_0\left(n + \frac{1}{2}\right) \qquad (4.51)$$

Where $(n = 0,1,2,...)$

Eigenfunctions ϕ_n are given by:

$$\phi_n = A_n H_n(\zeta) e^{-\frac{\zeta^2}{2}} \qquad (4.61)$$

Where the Hermite Polynomials $H_n(\zeta)$ are given by:

$$H_n(\zeta) = \left(\zeta - \frac{\partial}{\partial \zeta}\right)^n \qquad (4.62)$$

and the normalization constant $A_n = (2^n n! \sqrt{\pi})^{-\frac{1}{2}}$ (4.63)

Tutorial 4

1. **Annihilation** and **creation** operators $\hat{a}$ and $\hat{a}^+$ are defined in the Harmonic Oscillator problem respectively as : $\hat{a} = \frac{\beta}{\sqrt{2}}\left(\hat{x} + i\frac{\hat{p}}{m\omega}\right)$, $\hat{a}^+ = \frac{\beta}{\sqrt{2}}\left(\hat{x} - i\frac{\hat{p}}{m\omega}\right)$

where $\beta^2 = \frac{m\omega}{\hbar}$ and other symbols have their usual meanings.

. If the non-dimensional displacement ζ is defined as : $\zeta^2 \equiv \beta^2 x^2 \equiv \frac{m\omega}{\hbar} x^2$,

show that $\hat{a}$ and $\hat{a}^+$ transform as:

(i) $\hat{a} = \frac{1}{\sqrt{2}}\left(\zeta + \frac{\partial}{\partial \zeta}\right)$, (ii) $\hat{a}^+ = \frac{1}{\sqrt{2}}\left(\zeta - \frac{\partial}{\partial \zeta}\right)$, (iii) $\hat{a}^+\hat{a} = \frac{1}{2}\left(\zeta^2 - \frac{\partial^2}{\partial \zeta^2} - 1\right)$

2. Given that $[\hat{x}, \hat{p}] = i\hbar$,show that $[\hat{a}, \hat{a}^+] = 1$

(a) Show that the Hamiltonian $\hat{H}$ of the 1-D harmonic oscillator given by $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$ is expressible as $\hat{H} = \hbar\omega(\hat{a}\hat{a}^+ - 1/2)$; **(6 marks)**

(b) Hence, deduce that the ground state energy :

$E_0 = \frac{1}{2}\hbar\omega$.

3. The n^{th} eigenstate of the simple harmonic oscillator (SHO) Hamiltonian is given by $\psi_n(\xi) = A_n H_n(\xi) e^{-\xi^2/2}$ where the normalization constant $A_n = (2^n n! \sqrt{\pi})^{-\frac{1}{2}}$ and Hermite polynomials are given by : $H_n(\xi) = (\xi - \frac{\partial}{\partial \xi})^n$

(a) Deduce expressions for the first three eigenstates(n=0,1,2)

(b) Sketch carefully on the same page these eigenstates(i.e. $\psi_0(\xi)$, $\psi_1(\xi)$, and $\psi_2(\xi)$)