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Subject: Physics

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Paper No. : Quantum Mechanics-I

Module : Postulates of Quantum Mechanics and Representations of Vectors, bases and Unitary Operators

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Description of Module	
Subject Name	Physics
Paper Name	Quantum Mechanics-I
Module Name/Title	Postulates of Quantum Mechanics and Representations of Vectors, bases and Unitary Operators
Module Id	08

Contents of this Unit

Learning Outcomes

After studying this module, you shall be able to …

- Learn the state of a physical system in terms of the state vector in Hilbert space
- Know how a Hermitian operator acting on a state vector gives us the information of a physically observable quantity in terms of various eigenvalues
- Learn the definition of expectation values of the corresponding operator in the state
- Know the properties of quantum mechanical operators and of canonically conjugate operators
- Know tha time evolution of a quantum mechanica state vector
- Learn some important properties of representations, basis of ket and bra state vectors and unitary matrices

1. Introduction

Having developed the properties of vectors and operators in Hilbert space ---an underlying mathematical framework of quantum mechanics, we now present the basic postulates, using Dirac notation, in a form appropriate to the Hilbert –space formalism of quantum mechanics. The next section is devoted to studying the mathematical properties of representations of the ket and bra vectors and operators and unitary transformations from one basis to another.

2.Postulates of Quantum Mechanics

2.1 State Vectors and Observables of a Physical System

Postulate I :

Each state of a physical system is represented by a vector ket, say, $|a\rangle$, referred to as a state vector in a Hilbert space. The vector $|a\rangle$ or any scalar multiple of it corresponds to the same physical state. For convenience, it is required that $|a\rangle$ be normalized so that the vector representing the state is determined upto a constant factor.

To the above postulate is added the **principle of linear superposition,** according to which if $|a_1\rangle$ *and* $|a_2\rangle$ represent the possible state vectors then a linear combination,

$$|a\rangle = \alpha|a_1\rangle + \beta|a_2\rangle \tag{8.1}$$

is also a possible state vector, where α and β are arbitrary complex numbers. Conversely, any state may be considered as a linear superposition of two or more states. In fact, we assume that there exists an orthonormal complete set of state vectors for any state space.

You may recall that in classical mechanics, the dynamical state of a system is specified by dynamical variables such as coordinates and momenta of the particles in the system at a given instant. From this information, not only the value of any other dynamical variable such as energy can be obtained but even the state of the system at any other time can be deduced by means of the equations of motion. In quantum mechanics, however, the definition of the state of the system is significantly different from that of the classical case. Here to get information on the dynamical variables of the system, we introduce the following postulate.

Postulate II :

For every dynamical observable A (like energy, momentum etc.) of the system, there exists a Hermitian operator $\hat{A}$ in the Hilbert space. As stated above, any state vector can be expressed in terms of a complete set of basis vectors. These basis vectors are the eigen vectors of the Hermitian operator. The only measurable values of a physical observable are the various eigenvalues of the corresponding operator. Thus, each of the eigen values α_k (assumed, for the time being, to be discrete) of the operator has associated with it a vector, represented by $|a_k\rangle$, in the Hilbert space. Let it be an eigen vector of operator $\hat{A}$ so that

$$\hat{A}|a_k\rangle = a_k|a_k\rangle \qquad (8.2)$$

The hermitian character of the operator ensures that the eigenvalues are real. Eigen vectors corresponding to different eigen values are orthogonal

i.e., $$\langle a_i|a_j\rangle = 0, \qquad for \quad i \neq j \qquad (8.3a)$$

and also normalized, i.e., $$\langle a_k|a_k\rangle = 1. \qquad (8.3b)$$

2.2 Measurement Postulates : Expectation Values and Probabilities

Postulate III :

If we measure the variable A in the state of the system specified by the eigen-vector $|a_k\rangle$ of the operator $\hat{A}$, we shall have the precise measurement in terms of the eigen value, α_k .

If the measurement is made on large number of identical systems, each characterized by a state represented by a normalized ket $|\psi\rangle$, then the average value (expectation value) of the operator $\hat{A}$ is defined by

$$\langle \hat{A}\rangle_{av} = \langle\psi|\hat{A}|\psi\rangle \qquad (8.4)$$

In case, $|\psi\rangle$ is an eigen vector of $\hat{A}$, say, $|\psi\rangle \equiv |a_k\rangle$, where

$$\hat{A}\,|a_k\rangle = \alpha_k\,|a_k\rangle, \qquad (8.5)$$

Then $$\langle \hat{A}\rangle = \alpha_k, \qquad (8.6)$$

which is in agreement with the statement given earlier. If $|\psi\rangle$ is not an eigenvector of $\hat{A}$, then $|\psi\rangle$ can be expanded in terms of the eigenvectors { $|a_k\rangle$ } of $\hat{A}$, which form a complete orthonormal set of Hermitian operator. We then have

$$|\psi\rangle = \sum_k |a_k\rangle\langle a_k|\psi\rangle \tag{8.7}$$

$$so \;\; that \;\; \langle\psi|\hat{A}|\psi\rangle = \sum_{k.l} \langle\psi\|a_k\rangle\langle a_k|\hat{A}|a_l\rangle\langle a_l\|\psi\rangle \tag{8.8}$$

$$= \sum_{k.l} \langle\psi|a_k\rangle\delta_{kl}a_k\langle a_l|\psi\rangle = \sum_k \langle\psi|a_k\rangle\langle a_k|\psi\rangle\alpha_k \tag{8.9}$$

Note that in Eq. 8.8), we have twice made use of the closure relation. We thus express

the average value of $\hat{A}$ as $\langle\psi|\hat{A}|\psi\rangle = \sum_k |\langle\psi|a_k\rangle|^2 \alpha_k$ (8.10)

Equation (8.10) is to be interpreted as giving us the result of a large number of measurements under identical conditions or, equivalently, the result of a measurement on a large number of identical systems, each measurement yielding one or the other eigenvalue of $\hat{A}$. As one cannot, in general, predict which eigenstate will be obtained, we postulate that the probability of finding the state $|a_k\rangle$ is $P(|a_k\rangle) = |\langle a_k|\psi\rangle|^2$. (8.11)

Thus, $\langle a_k|\psi\rangle$ may be regarded as the probability amplitude for the system to be found in $|a_k\rangle$. Indeed the concept of probability amplitude is based on the premise that $|\psi\rangle$, as expressed by Eq.(8.7), represents the state of the physical system. The justification for this premise has its origin in experiments on interference and diffraction phenomena discussed in the first module.

2.3 Quantum Mechanical Operators

Postulate IV:

Let there be a dynamical variable, as for instance a Hamiltonian, in classical mechanics, which is a function of canonically conjugate variables. The corresponding quantum mechanical operator of the system is obtained from the dynamical variable in classical mechanics by replacing the canonically conjugate variables by the corresponding quantum mechanical operators.

Consider the example of a linear (one-dimensional) harmonic oscillator in classical mechanics, where its Hamiltonian (in Cartesian co-ordinates) is given by

$$H \equiv H(x,p) = \frac{p_x^2}{2m} + \frac{1}{2}Kx^2 , \qquad (8.12)$$

where m is the mass of the oscillator and K is a spring constant. Here the Hamiltonian is a function of the position co-ordinate ,x, and the momentum, p_x , which are the canonical variables.

According to the postulate, the quantum mechanical operator corresponding to H is obtained as

$$\hat{H} \equiv \hat{H}(\hat{x}, \hat{p}_x) = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}K\hat{x}^2 , \qquad (8.13)$$

where $\hat{x}$ *and* $\hat{p}_x$ are Hermitian operators corresponding to x a nd p_x respectively.

It is important to keep in mind that quantum mechanical operators of the conjugate variables need not commute; therefore proper order of the variables has to be preserved.

To make the point clear, let us consider, for example, the orbital angular momentum ; $\vec{L} = \vec{r} \times \vec{p}$, where its x-component is given by

$$L_x = yp_z - zp_y, \qquad cyclic, \qquad (8.14)$$

So that

$$L_x^2 = y\,p_z y p_z + zp_y zp_y - yp_z zp_y - zp_y yp_z \qquad (a)$$

$$= y^2 p_z^2 + z^2 p_y^2 - 2yp_y zp_z \qquad (b) \qquad (8.15)$$

Classically, both the expressions (a) and (b) of Eq.(8.15) are equivalent. However, when the canonical variables are replaced by the operators, the corresponding expressions would not give the same result for the operator $\hat{L}_x^2$. The correct expression is obtained by replacing the variables by corresponding operators in the equation given by Eq.(8.15a). Only those operators which commute can be permuted.

Another point to note is that a dynamical variable C which is the product two other dynamical variables , say, A and B, i.e., C=A B, then the Hermitian operator corresponding to C is not $\hat{A}\,\hat{B}$, because if these operators do not commute, i.e.,$\hat{A}\,\hat{B} \neq \hat{B}\,\hat{A}$, the product $\hat{A}\,\hat{B}$ would then be not Hermitian. It is a simple exercise to check that a proper combination is given by $\hat{C} = \frac{1}{2}\,(\hat{A}\,\hat{B} + \hat{B}\,\hat{A})$, which is Hermitian.

Postulate V:

Any pair of canonically conjugate operators satisfies the Heisenberg commutation rules:

$$[\hat{q}_i, \hat{q}_j] = 0; \qquad (a)$$
$$[\hat{p}_i, \hat{p}_j] = 0; \qquad (b)$$
$$[\hat{q}_i, \hat{p}_k] = i\hbar\,\hat{I}\delta_{ik} \qquad (c) \qquad (8.15)$$

where the operator $\hat{q}_i$ represents the generalized coordinate corresponding to q_i and similarly the operator $\hat{p}_i$ is the operator corresponding the generalized momentum p_i canonically conjugate to q_i . Thus, if q_i represent the Cartesian coordinates, the p_i are the components of linear momentum. If, on the othere hand, q_i represent the angle, p_i then are the components of angular momentum and so on.

In this abstract formalism, the commutation relation, like

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

between a position variable and its canonically conjugate momentum may be regarded as a fundamental postulate and is not to be derived . This quantum condition forms the basis of quantum mechanics.

As another example, consider the case of orbital angular momentum. Thus substitution of the operators $\hat{y}, \hat{p}_y, \hat{x}, \hat{p}_x$ etc. in place of the corresponding variables appearing in Eq.(8.14), we find that the components, $\hat{L}_x, \hat{L}_y$ and $\hat{L}_z$ of angular momentum operators satisfy the following commutation relations:

$$[\hat{L}_x, \hat{L}_y] = i\hbar\,\hat{L}_z \quad \text{, (similar relations in cyclic order)} \qquad (8.16)$$

We shall see in the subsequent modules how these commutation relations determine the quantal properties of the physical variables corresponding to angular momentum operators.

2.4 Time evolution of state vector

Postulate VI:

You must be already familiar with time-independent treatment of the Schrodinger equation from the elementary course on quantum mechanics.

Here we postulate that time evolution of the state vector, $|\psi(t)\rangle$, is governed by the Schrodinger equation:

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle, \qquad (8.17)$$

where $\hat{H}(t)$ is the Hamiltonian operator associated with the total energy of the system.

3. Representations, Bases and Unitary Operators

Having learnt the properties of orthonormality, completeness and projection operator of ket and bra vectors, we turn over to learn some general properties of representation.Consider an N-dimensional vector space where any vector can be expanded in terms of the orthonormal basis $[|u_i\rangle]_N$. Thus if $|X\rangle$ *and* $|Y\rangle$ are arbitrary vectors, we write

$$|X\rangle = \sum_{i=1}^{N} x_i |u_i\rangle \qquad (8.18a)$$

$$|Y\rangle = \sum_{i=1}^{N} y_i |u_i\rangle \qquad (8.18b)$$

If there is another vector $|Z\rangle$ such that

$$|Z\rangle = \alpha|X\rangle + \beta|Y\rangle \qquad (8.18c)$$

$$\text{and} \quad |Z\rangle = \sum_{i=1}^{N} z_i |u_i\rangle,$$

$$\text{then} \quad z_i = \alpha x_i + \beta y_i \qquad (8.19)$$

$$\text{Also} \quad \langle X|Y\rangle = \sum_{i=1}^{N} x_i^* y_i \qquad (8.20)$$

Note the relations, Eqs (8.19) and (8.20). These relations suggest that in place of of the abstract vectors $|X\rangle, |Y\rangle, \ldots$, we can even deal with their expansion coefficients (or the components).

[x] $\equiv [x_1, x_2, \ldots\ldots, x_N]$, $[y] \equiv [y_1, y_2, \ldots\ldots, y_N]$, *etc.* These expansion coefficients are called **the representatives of the vectors**. Corresponding to every relationship between vectors, there exists a relationship between representatives. Thus corresponding to Eq.(8.18c) representing a relationship for vectors, we have the Eq.(8.19) expressing the relationship which translates as

$$[z] = \alpha\,[x] + \beta\,[y] \qquad (8.21a)$$

Or $$[z_1, z_2, \ldots, z_N] = [\alpha x_1 + \beta y_1, \alpha x_2 + \beta y_2, \ldots, \alpha x_N + \beta y_N] \qquad (8.21b)$$

The representatives, unlike the vectors, depend on the basis chosen. However, with respect to given basis, the representative [x] corresponding to the vector $|X\rangle$ is unique, which is here represented by [x] in the representation defined by the basis $[|u_i\rangle]_N$.

The basis vectors are represented by

$$[u_1], [u_2], \ldots, [u_N] \,,$$

where

$$[u_1] \equiv [1, 0, 0, \ldots, 0],$$

$$[u_2] \equiv [0, 1, 0, 0, \ldots, 0],$$

$$\vdots \qquad (8.22)$$

$$[u_N] \equiv [0, 0, 0, \ldots, 1]$$

From the above equations, it is clear that one could also express the representative [x] of vector $|X\rangle$ in the form of a column matrix as

$$[x] \equiv \begin{pmatrix} x_1 \\ x_2 \\ .. \\ .. \\ x_N \end{pmatrix} \qquad (8.23)$$

While the representative of the bra vector $\langle X|$ is represented by the row matrix $x^\dagger$, i.e.,

$$x^\dagger = (x_1^*, x_2^{**}, \; \dots\dots \; .., x_N^*) \qquad (8.24)$$

The scalar product given in Eq.(8.20) is then given by the matrix product, $x^\dagger y$ and the vector addition in Eq.(8.18c) is simply obtained by the matrix addition:

$$z = \alpha\, x + \beta\, y$$

The unit vectors, $|u_i\rangle$ are represented by the column vectors;

$$|u_1\rangle \to u_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ .. \\ .. \\ 0 \end{pmatrix} ; \; |u_2\rangle \to u_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ .. \\ 0 \end{pmatrix} ; \; \dots u_N = \begin{pmatrix} 0 \\ 0 \\ .0 \\ .. \\ .. \\ 1 \end{pmatrix} \qquad (8.24)$$

The orthonormality condition and the completeness condition simply reduce to

$$\langle u_i | u_j \rangle \to u_i^\dagger u_j = \delta_{ij} \,, \qquad (8.25a)$$

and

$$\sum_i |u_i\rangle\langle u_i| = \sum_i u_i u_i^\dagger = I \qquad (8.25b)$$

The operator equation

$$\hat{A}|X\rangle = |Y\rangle \qquad (8.26a)$$

is given by the matrix equation:

$$A\,x = y \quad . \qquad (8.27)$$

Note that both x and y are (Nx1) matrices, A is an (NxN) matrix. We thus see that properties of

the linear operators follow from the properties of the square matrices. This procedure of representing vectors and operators by matrices is referred to as matrix representation. Clearly, in this representation, a Hermitian operator is represented by a Hermitian matrix.

According to the definition of a Hermitian operator, we have

$$\langle X|\hat{A}|Y\rangle^{*} = \langle Y|\hat{A}|X\rangle \, ,$$

which in matrix form is given as

$$(X^{\dagger} A Y)^{\dagger} = Y^{\dagger} A^{\dagger} X \, ,$$

i.e., $Y^{\dagger} A^{\dagger} X = Y^{\dagger} A X$, since $\hat{A}$ is given to be Hermitian, $A^{\dagger} = A$.

3.1 Change of Basis :

From the above study it is clear that the matrices representing vectors and operators depend on the representation of the basis. The question, therefore is: if we have the same set of vectors and operators given in different representations (or basis), how to find the relationship between the matrices representing them. In the following,we shall try to find the solution to this question.

Let $[|u_i\rangle]_N$ *and* $[|u_i'\rangle]_N$ be the two orthonormal bases in Hilbert space. Since both the sets are complete, the vectors of one set can be expanded in terms of the vectors of the other set:

$$|u_i'\rangle = \sum_{j=1}^{N} |u_j\rangle S_{ji}, \quad i = 1 \quad to \quad N \, , \qquad (8.28)$$

where the expansion coefficients S_{jk} can be regarded as the matrix elements of an (NxN) matrix S, which transforms the representation $[|u_i\rangle]_N$ to the representation $[|u_i'\rangle]_N$.

Now, taking the scalar product of the Eq.(8.28) by $|u_j\rangle$, we get

$$S_{ji} = \langle u_j | u'_i \rangle \tag{8.29}$$

In other words, S_{ji} is the component of $|u'_i\rangle$ along $|u_j\rangle$.

Using the orthonormality of the set $[|u'_i\rangle]N$, we have

$$\langle u'_j | u'_i \rangle = \delta_{ji} = \sum_{k=1}^{N} \langle u'_j | u_k \rangle \langle u_k | u'_i \rangle$$
$$= \sum_{k=1}^{N} S^*_{kj} S_{ki} = (S^+ S)_{ji} = \delta_{ji} \tag{8.30}$$

where the closure property of the basis $[|u_k\rangle]N$ has been used. Similarly, from the completeness property of $[|u'_i\rangle]N$, we get:

$$\langle u_j | u_i \rangle = \delta_{ji} = \sum_{k=1}^{N} \langle u_j | u'_k \rangle \langle u'_k | u_i \rangle$$
$$= \sum_{k=1}^{N} S_{jk} S^*_{ik} = (SS^+)_{ji} \tag{8.31}$$

From the two Eqs.(8.30) and (8.31), it follows that

$$S^\dagger S = I = SS^\dagger \tag{8.32}$$

Starting from an orthonormal basis, we find that while Eq.(8.30) represents the orthonormality, Eq.(8.31) represents the completeness of the transformed basis.Thus **we have shown that change of orthonormal basis in a linear vector space is represented by a Unitary matrix**.

To write Eq.(8.28) in terms of the matrix representation, we define a matrix U by

$$U \equiv (u_1, u_2, \dots \dots \dots, u_N) \tag{8.33}$$

where u_k is the column matrix representing the basis vector given by Eq.(8.24), so that U is an (NxN) matrix. From the orthonormality of the basis, we require that

$$U^{+}U = \begin{pmatrix} u_1^{+} \\ u_2^{+} \\ \ldots. \\ \ldots \\ u_N^{+} \end{pmatrix} (u_1 \ \ u_2 \ \ .. \ \ .. \ \ .. u_N) = \begin{pmatrix} u_1^{+}u_1 & u_1^{+}u_2 & \ldots\ldots & u_1^{+}u_N \\ u_2^{+}u_1 & u_2^{+}u_2 & \ldots\ldots & u_2^{+}u_N \\ \ldots. & \ldots. & \ldots. & \ldots.. \\ \ldots & \ldots. & \ldots.. & \ldots.. \\ u_N^{+}u_1 & u_N^{+}u_2 & \ldots. & u_N^{+}u_N \end{pmatrix} = I$$

(8.34)

whereas, from the property of completeness we require that

$$UU^{\dagger} = (\textstyle\sum_{i=1}^{N} u_i \, u_i^{\dagger}) = I \quad , \qquad (8.35)$$

where I is the (NxN) matrix.

Thus U is unitary, showing that an orthonormal basis can be represented by a Unitary matrix..

Now, Eq.(8.28) can be expressed in matrix notation as

$$U' = U\,S \qquad (8.36a)$$

and since both U and S are unitary, we also have

$$U = U'S \qquad (8.36b)$$

and

$$S = U^{\dagger}U' \qquad (8.36c)$$

Also note that linear transformation

$$|Y\rangle = \hat{A}|X\rangle \qquad (8.37)$$

in matrix representation is written as

$$y = A\,x \qquad (8.38)$$

in the representation U ;

and by the equation

$$y' = A'\,x \qquad (8.39)$$

in the U′ representation.

Since ′

$$x = S\,x', \tag{8.40}$$

we have from Eq.(8.38)

$$S\,y' = A\,S\,x'$$

Or

$$y' = (S^{\dagger} A\,S)\,x'$$

On comparing with Eq.(8.39), we get

$$A' = (S^{\dagger} A S \tag{8.41}$$

Eqs.(8.40) and (8.41) **determine respectively the transformation law for the vectors and the operators under change of basis..**

5. Summary

After studying this module, you would be able to

- Learn the state of a physical system in terms of the state vector in Hilbert space
- Know how a Hermitian operator acting on a state vector gives us the information of a physically observable quantity in terms of various eigenvalues
- Learn the definition of expectation values of the corresponding operator in the state
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