Quantum Mechanics and its Applications to Physical Systems

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By

Sham S. Malik

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Preface

The present monograph is based on lectures delivered at Indian institutions during the period 1992 through 2023, especially the Graduate and Postgraduate courses in quantum mechanics. A well-organized and self-contained text that is backed by a rich collection of fully solved examples illustrates various aspects of non-relativistic quantum mechanics. This book accomplishes a dual objective: firstly, to furnish instructors with a teaching aid that is pedagogically appropriate, and secondly, to aid students in not only comprehending the theoretical foundation but also transforming into proficient practitioners of quantum mechanics.

Quantum mechanics has helped us in understanding various physical phenomena. For example, it tells us why atoms are stable, radioactive nuclei decay, and carbon dioxide is a greenhouse gas. Its theoretical formalism is used to design microscopes, lasers, solar cells, nuclear reactors, and secure methods of sending encrypted information. Scientists around the world are constantly discovering new applications of quantum mechanics.

Historically, Heisenberg matrix mechanics and Schrodinger wave mechanics were the two separate formulations of quantum mechanics that existed in the past. These two ostensibly different approaches were shown to be equivalent. Eventually, Dirac combined both of these methods and proposed a more general formulation based on **kets**, **bras** and operators. The Heisenberg picture is produced when Dirac's formalism is represented in a discrete basis, while Schrodinger wave mechanics is produced when Dirac's formalism is represented in a continuous basis.

Following Dirac's **bra-ket** formalism, the underlying principles of both discrete and continuous quantum systems are discussed, respectively, in chapters **1** and **2**. These systems use a complex vector space whose dimensionality depends on the type of physical system being investigated. Chapter **3** commences with the experimental foundation of quantum mechanics, wherein we examine atomic and subatomic phenomena that confirm the failure of classical physics at the microscopic level and establish the necessity for such a novel approach. Chapter **4** is devoted exclusively to the dynamic development of the state vectors and observables. This chapter specifically establishes the Schrodinger equation for the time-evolution operator. A thorough understanding of angular momentum is essential in almost all branches of science. For instance, angular momentum considerations are crucial in the explanation of bound-state and scattering problems, as well as molecular, atomic, and nuclear spectroscopy. Therefore, chapter **5** presents a methodical approach to the topic of angular momentum in a significant detail. There are very few problems involving either time-independent or time-dependent Hamiltonians that can be solved exactly. We will inevitably need to use some types of approximation techniques. Chapter **6** is devoted to discuss various approximation techniques for obtaining the bound-state solutions. The differentiation between bosons and fermions, as well as the indistinguishability of each of the two particle types, are necessary for the description of many-body systems. Chapter **7** is assigned to a discussion of striking quantum mechanical effects arising from the identity of particles. Chapter **8** focuses on the theory of scattering and, in a broader sense, on collision processes. The significance of this area cannot be overstated. For students who are interested in conducting research in this field, chapter **9** covers a number of research-oriented topics that are highly beneficial. Each chapter includes a number of solved examples to illustrate and reinforce the concepts discussed in the text. Furthermore, several appendices are provided to help students gain a deeper understanding of the subject.

The author would like to express his deepest gratitude to his wife, Vibha Malik, for shouldering the greatest burden while he was working on this text. It must have been difficult to be married to a man who was mentally absent for the better part of almost two years. The author also acknowledges his son Saurabh and daughter-in-law Devanshi, who have been a constant source of motivation. Even from overseas, they were able to offer their support.

Sham S. Malik

Chapter 1

Mathematical formulation for discrete systems

Initially, two different but apparently equivalent formalisms, namely, Heisenberg matrix mechanics and Schrodinger wave mechanics were introduced to explain the quantum phenomena. Later on, both these approaches (i.e., Heisenberg and Schrodinger) were unified together by Dirac's formalism based on complex linear vector space algebra. Within this formalism, the representation using a continuous set of basis vectors yields the Schrodinger picture, whereas the Heisenberg picture emerges from the discrete set of basis vectors.

Even though the theory of complex linear vector spaces existed prior to the beginning of quantum mechanics, the development of these spaces by Dirac with **bra** and **ket** notations has been quite useful for explaining the physical phenomena in the micro-world. The **bra** refers to a conjugate transpose of a vector, whereas the **ket** acts as analogous to an ordinary vector. The inner (or scalar) product in Dirac **bra** and **ket** notations is defined as $\langle . | . \rangle$, where two dots separated by a vertical line refer to the vector elements of a given vector space.

If the vector space is spanned by a set of vectors such that an inner product is defined, this space is known as an inner product space. A complete inner product space refers to a Hilbert space. Here, completeness means all possible sequences of elements within this space have a well-defined limit, i.e., itself an element of this space. The dimensionality of a Hilbert space is decided by the nature of the physical system under consideration. As a result, it may be categorized as either a finite or an infinite dimension space depending on discrete (finite) or continuous (infinite) alternative paths a physical system follows.

Since the wave function, which is represented by a **ket** vector in the Hilbert space, contains all of the information about a quantum state, the Hilbert space plays a crucial role in the explanation of quantum mechanical processes. A detailed understanding of that Hilbert space is discussed below.

1.1 Finite-Dimensional Hilbert Space

The finite-dimensional Hilbert space is defined by the finite-dimensional inner product space, and its topology is the same as that defined for the finite-dimensional complex vector space. Thus, the Hilbert space is a complex linear vector space and is generally represented by the symbol $\mathcal{H}$ throughout the discussion. The finite or infinite dimensional Hilbert spaces are well described by Dirac **ket** and **bra** vectors, therefore, these vectors are discussed in the following subsections.

1.1.1 Dirac ket vector

Let the physical system be in the quantum state u, where u refers to some physical quantity, like spin, isospin and so on. Following Dirac notation, the quantum state is concisely expressed as a **ket** vector $|u\rangle$ in the complex vector space, and $|u\rangle$ is postulated to contain complete information about the physical state. The following are the important characteristics of the **ket** vectors.

(a) The addition of two **ket** vectors always commute with each other and their sum leads to another **ket** vector, i.e.,

$$|u\rangle + |v\rangle = |v\rangle + |u\rangle = |w\rangle. \tag{1.1}$$

(b) The multiplication of a **ket** vector $|u\rangle$ by a complex number α leads to

$$\alpha|u\rangle = |u\rangle\alpha. \tag{1.2}$$

The complex number α can be placed on either the left or right side of the **ket** vector $|u\rangle$.

(c) If two or more **ket** vectors $|u_i\rangle$ with $1 \leq i \leq n$ describe possible states of a physical system, then any linear combination

$$|v\rangle = \sum_{i=1}^{n} \alpha_i |u_i\rangle, \tag{1.3}$$

also describes a possible state of the same physical system. Here, α_i with $1 \leq i \leq n$ are the complex numbers. Equation 1.3 refers to the linear superposition principle.

The coefficient α_i in equation 1.3 may be interpreted as the weight factor of the quantum state $|u_i\rangle$ in the linear superposition quantum state $|v\rangle$. In a particular case, the coefficient α_i=0 implies that the quantum state u_i does not participate in the superposition of the quantum state $|v\rangle$. As a result, the product $0|u_i\rangle$ leads due to an absence of quantum state $|u_i\rangle$ in the sum of equation 1.3 and is named as a null state vector. It is important to emphasize that the null state vector emerging from the product $0|u_i\rangle$ and the ground state of the vector $|0\rangle$ are entirely different. Obviously, the null state does not exist at all, while the ground state of a physical system not only exists but is the most important quantum state of a physical system.

1.1.2 Dirac bra vector and Inner-product

A vector dual to **ket** vector is defined as a **bra** vector. According to Dirac, for every **ket** vector $|u\rangle$ there exists **bra** vector $\langle u|$ in the dual or **bra** vector space. The **ket** vector $|u\rangle$ and the corresponding **bra** vector $\langle u|$ describe the same physical state and the unique correspondence between these vectors is drawn from the following rules.

(a) The addition of two **bra** vectors always commute with each other and their sum leads to another **bra** vector, i.e.,

$$\langle u| + \langle v| = \langle v| + \langle u| = \langle w|. \tag{1.4}$$

(b) The multiplication of a **bra** vector $\langle u|$ by a complex number α leads to

$$\alpha^* \langle u| = \langle u|\alpha^* \tag{1.5}$$

where α^* refers to a complex conjugate of complex numbers α and can be placed on either the left or right side of the **bra** vector $\langle u|$.

(c) If two or more **bra** vectors $\langle u_i|$ with $1 \leq i \leq n$ describe possible states of a physical system, then any linear combination

$$\langle v| = \sum_{i=1}^{n} \alpha_i^* \langle u_i|, \tag{1.6}$$

also describes a possible state of the same physical system. Similar to **ket** vector space, the **bra** vector space as shown in equation 1.6 obeys the linear superposition principle.

The **bra** vector cannot be added to the **ket** vector. The importance of these two types of vectors, namely, the **bra** and **ket**, is quite evident from their inner product and is realized from its shorthand notation **bra(c)ket**. Let $|v\rangle$ be the **ket** vector be clubbed with the **bra** vector $\langle w|$ to form an inner product and is defined as

$$(\langle w|)(|v\rangle) = \langle w|v\rangle. \tag{1.7}$$

The inner product represented by the equation 1.7 is analogous to the scalar product of the usual geometric vectors of the Euclidean vector space, but the main difference is that the product 1.7 may be a complex number rather than a real number. The properties of the inner product are summarized below.

(a) The linearity with respect to any of the inner product component vectors is one of its main characteristics. For example, if $|v\rangle$ is described by a linear superposition of **ket** vectors $|u_i\rangle$ as represented in equation 1.3, then

$$\langle w|v\rangle = \sum_{i=1}^{n} \alpha_i \langle w|u_i\rangle. \tag{1.8}$$

Similarly, if equation 1.6 is true, then

$$\langle v|w\rangle = \sum_{i=1}^{n} \alpha_i^* \langle u_i|w\rangle. \tag{1.9}$$

(b) The inner product obeys

$$\langle v|w\rangle = \langle w|v\rangle^*, \tag{1.10}$$

and it follows from the following discussion. Taking the complex conjugate of equation 1.8 on both sides and using equation 1.9 leads to equation 1.10, i.e.,

$$\langle w|v\rangle^* = \sum_{i=1}^{n} \alpha_i^* \langle w|u_i\rangle^* = \sum_{i=1}^{n} \alpha_i^* \langle u_i|w\rangle = \langle v|w\rangle. \tag{1.11}$$

This implies that $\langle v|w\rangle$ and $\langle w|v\rangle$ and complex conjugate of each other.

(c) The norm is defined as the square root of the inner product of the **ket** and **bra** vectors describing the same state and is represented by the symbol $||.||$, where . represents a quantum state of a physical system. The square of the norm is real and non-negative and is given by

$$||v||^2 = \langle v|v\rangle \geq 0. \tag{1.12}$$

The equality sign in this expression is applicable only if $|v\rangle$ is a null **ket** vector. Generally, the norm, i.e., $\sqrt{\langle v|v\rangle}$ is analogous to the magnitude of vector $\sqrt{\vec{v}.\vec{v}}$ and refers to the concept of the length of a vector in the Euclidean vector spaces.

(d) Further, the norm is used for obtaining normalization of all vectors. Let us consider a **ket** vector $|u\rangle$ and its normalized expression is given by

$$|\bar{u}\rangle = \frac{1}{||u||}|u\rangle,$$

such that $\langle\bar{u}|\bar{u}\rangle$=1.

Ex. 1.1 — If an inner product between the vectors $|u\rangle$ and $|v\rangle$ in the complex vector space $\mathcal{V}$ is defined as $\langle u|v\rangle$ then show that

$$|\langle u|v\rangle| \leq ||u||.||v||, \tag{1.13}$$

for all $|u\rangle$, $|v\rangle\in \mathcal{V}$. This inequality refers to Cauchy-Schwartz inequality.

Answer (Ex. 1.1) — Suppose neither $|u\rangle$ nor $|v\rangle$ is a null state vector and also $|u\rangle$ is not a scalar multiple of $|v\rangle$, then $|u-\alpha v\rangle \neq$0 for any $\alpha\in \mathcal{C}$, i.e., the complex space. The square of the norm $||u-\alpha v||^2$ strictly obeys an inequality

$$0 \leq \langle u-\alpha v|u-\alpha v\rangle$$
$$0 \leq \langle u-\alpha v|u\rangle - \alpha\langle u-\alpha v|v\rangle$$
$$0 \leq \langle u|u\rangle - \alpha^*\langle v|u\rangle - \alpha\langle u|v\rangle + \alpha\alpha^*\langle v|v\rangle,$$

Let the complex number α be expressed as

$$\alpha = a + \iota b,$$

where both a and b are real. Using this expression, the inequality becomes

$$0 \leq \langle u|u\rangle - \Big(a-\iota b\Big)\langle u|v\rangle^* - \Big(a+\iota b\Big)\langle u|v\rangle + \Big(a^2+b^2\Big)\langle v|v\rangle. \tag{1.14}$$

In equation 1.14, both a and b are independent variables and are fixed by the minimum condition of its right-hand side by taking the first derivative with respect to a and b. This gives

$$\frac{d}{da}\Big[||u||^2 - \Big(a-\iota b\Big)\langle u|v\rangle^* - \Big(a+\iota b\Big)\langle u|v\rangle + \Big(a^2+b^2\Big)||v||^2\Big] = 0$$
$$\implies -\langle u|v\rangle^* - \langle u|v\rangle + 2a||v||^2 = 0$$
$$\implies a = \frac{\langle u|v\rangle^* + \langle u|v\rangle}{2||v||^2},$$

and

$$\frac{d}{db}\Big[||u||^2 - \Big(a-\iota b\Big)\langle u|v\rangle^* - \Big(a+\iota b\Big)\langle u|v\rangle + \Big(a^2+b^2\Big)||v||^2\Big] = 0$$
$$\implies \iota\langle u|v\rangle^* - \iota\langle u|v\rangle + 2b||v||^2 = 0$$
$$\implies b = \frac{-\iota\langle u|v\rangle^* + \iota\langle u|v\rangle}{2||v||^2}.$$

Using these expressions for a and b, we have

$$a - \iota b = \frac{\langle u|v\rangle}{||v||^2}$$
$$a + \iota b = \frac{\langle u|v\rangle^*}{||v||^2}$$
$$a^2 + b^2 = \frac{\langle u|v\rangle\langle u|v\rangle^*}{||v||^4},$$

substituting these results into the inequality 1.14:

$$0 \leq ||u||^2 - 2\frac{|\langle u|v\rangle|^2}{||v||^2} + \Big[\frac{|\langle u|v\rangle|}{||v||^2}\Big]^2 ||v||^2$$
$$\implies |\langle u|v\rangle|^2 \leq ||u||^2.||v||^2.$$

Its simplification generates the Cauchy-Schwartz inequality 1.13.

1.1.3 Bases for a given vector space

The bases of a given vector space generally refer to a set of minimal linearly independent vectors that are required to represent all other vectors in that space. A set of vectors $\Big\{|u_i\rangle\Big\}$ with $1\leq i \leq n$ is called linearly independent if

$$\sum_{1=1}^{n} \alpha_i |u_i\rangle = 0, \tag{1.15}$$

with α_i=0 for all i. If let us suppose $\alpha_1 \neq$0 in a set of $\Big\{\alpha_i\Big\}$, then from equation 1.15 we get

$$|u_1\rangle = -\frac{1}{\alpha_1}\sum_{1=2}^{n} \alpha_i |u_i\rangle. \tag{1.16}$$

This implies that the $|u_1\rangle$ is linearly dependent because it depends on the other vectors of a given vector space.

The maximum number of linearly independent vectors that can be traced in the Hilbert space $\mathcal{H}$ are responsible for determining its dimension. Thus, if n is the dimension of $\mathcal{H}$, then any vector in $\mathcal{H}$ can be expressed as a linear combination of n independent vectors. This set of linearly independent vectors in the Hilbert space $\mathcal{H}$ is known as bases.

1.1.4 Orthonormal Basis-vectors

A set of vectors $\Big\{|u_i\rangle\Big\}$ with $1\leq i \leq n$ is called orthonormal if the following two conditions are satisfied.

- All the vectors are mutually orthogonal to each other, i.e., each pair of vectors $|u_i\rangle$ and $|u_j\rangle$ with $i \neq j$ satisfies
$$\langle u_i|u_j\rangle = 0. \tag{1.17}$$
- The square of the norm of each of these vectors is a unit magnitude, i.e., for each i
$$||u_i||^2 = \langle u_i|u_i\rangle = 1. \tag{1.18}$$

Using Kronecker delta function $\delta_{i,j}$ which is defined as

$$\delta_{i,j} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \tag{1.19}$$

both above conditions represented by 1.17 and 1.18 are clubbed into a single expression

$$\langle u_i|u_j\rangle = \delta_{i,j}. \tag{1.20}$$

Ex. 1.2 — Given an independent set of vectors $\{|u_i\rangle\}$ with $1\leq i \leq n$ in the finite dimensional Hilbert space. Construct an orthogonal set of vectors $\{|v_i\rangle\}$ such that the set of vectors $\{|v_i\rangle\}$ acts as bases for the subspace spanned by the vectors $\{|u_i\rangle\}$.

Answer (Ex. 1.2) — Let us fix

$$|v_1\rangle = |u_1\rangle,$$

and define

$$|v_2\rangle = |u_2\rangle + \alpha_{21}|v_1\rangle.$$

The constant α_{21} is obtained by using the orthogonality constraint between the vectors $|v_1\rangle$ and $|v_2\rangle$, i.e.,

$$\langle v_1|v_2\rangle = 0,$$

and it gives

$$\alpha_{21} = -\frac{\langle v_1|u_2\rangle}{\langle v_1|v_1\rangle}.$$

Thus,

$$|v_2\rangle = |u_2\rangle - \frac{\langle v_1|u_2\rangle}{\langle v_1|v_1\rangle}|v_1\rangle.$$

Next,

$$|v_3\rangle = |u_3\rangle + \alpha_{31}|v_1\rangle + \alpha_{32}|v_2\rangle,$$

and the constants α_{31} and α_{32} are extracted by using the following orthogonality constraints:

$$\begin{aligned}
\langle v_1|v_2\rangle &= 0,\\
\langle v_1|v_3\rangle &= 0,\\
\langle v_2|v_3\rangle &= 0.
\end{aligned}$$

Within these constraints, we get

$$\begin{aligned}
\alpha_{31} &= -\frac{\langle v_1|u_3\rangle}{\langle v_1|v_1\rangle},\\
\alpha_{32} &= -\frac{\langle v_2|u_3\rangle}{\langle v_2|v_2\rangle}.
\end{aligned}$$

Thus,

$$|v_3\rangle = |u_3\rangle - \frac{\langle v_1|u_3\rangle}{\langle v_1|v_1\rangle}|v_1\rangle - \frac{\langle v_2|u_3\rangle}{\langle v_2|v_2\rangle}|v_2\rangle.$$

Following these steps, we get

$$|v_n\rangle = |u_n\rangle - \sum_{j=1}^{n-1} \frac{\langle v_j|u_n\rangle}{\langle v_j|v_j\rangle}|v_j\rangle.$$

The newly constructed set of vectors $\{|v_i\rangle\}$ obviously fulfills the characterization of orthogonality, i.e.,

$$\langle v_j|v_{j+1}\rangle = 0,$$

The normalization of the **ket** vector $|v_i\rangle$ is given by

$$|\bar{v_i}\rangle = \frac{1}{||v_i||}|v_i\rangle,$$

and form a complete orthonormal set of basis vectors. Hence, determine the dimensionality of the complex vector space.

1.2 Operators and their characteristics in the Hilbert space

Operators are used to represent physical processes that result from the change of quantum state (generally represented by a **ket** vector) of a system. The evolution of the quantum state with time is determined by the Unitary operator and is one of the class of operators. The experimentally measured physical properties of the quantum system, for example, position, momentum, energy, etc., are also represented by another class of operators, known as Hermitian operators. Such operators are known as observables associated with a given physical system, and each quantum system will have, in general, a different set of observables.

In the Hilbert space of the system, an operator operating from the left side of the **ket** vector leads to another **ket** vector belonging to the same Hilbert space. Let $\hat{\mathcal{A}}$ be an operator operating on a **ket** vector $|u\rangle$ leads to another **ket** vector $|v\rangle$, i.e.,

$$\hat{\mathcal{A}}|u\rangle = |v\rangle, \tag{1.21}$$

where both $|u\rangle$ and $|v\rangle$ belong to the same Hilbert space.

Whereas an operator always operates on the **bra** vector from its right side and generates another **bra** vector, i.e.,

$$\langle u|\hat{\mathcal{A}} = \langle v|. \tag{1.22}$$

Here, both $\langle u|$ and $\langle v|$ belong to the same Hilbert space of the physical system.

1.2.1 Characteristics of Operators

- **Equality** Two operators are said to be equal if their operations on all elements of the Hilbert space are identical. This implies that the operation of two operators $\hat{\mathcal{A}}$ and $\hat{\mathcal{B}}$ on all the state **kets** $\{|u_i\rangle\}$ belonging to the Hilbert space of a quantum system is such that

$$\hat{\mathcal{A}}|u_i\rangle = \hat{\mathcal{B}}|u_i\rangle, \tag{1.23}$$

then

$$\hat{\mathcal{A}} = \hat{\mathcal{B}}. \tag{1.24}$$

- **Identity** and **Zero operators** The identity, i.e., the unit operator is defined as

$$\hat{\mathcal{I}}|u_i\rangle = |u_i\rangle, \tag{1.25}$$

whereas the null, i.e., the zero operator gives

$$\hat{\mathcal{O}}|u_i\rangle = 0, \tag{1.26}$$

The operations of both these operators hold for all the state **kets** $\{|u_i\rangle\}$ belonging to the Hilbert space of a quantum system.

- **Addition**: The addition of two operators, $\hat{\mathcal{A}}$ and $\hat{\mathcal{B}}$ leads to another operator $\hat{\mathcal{C}}$ such that

  $$\hat{\mathcal{C}}|u_i\rangle = \Big(\hat{\mathcal{A}} + \hat{\mathcal{B}}\Big)|u_i\rangle = \hat{\mathcal{A}}|u_i\rangle + \hat{\mathcal{B}}|u_i\rangle, \tag{1.27}$$

  for all the state **kets** $\{|u_i\rangle\}$ belonging to the Hilbert space of a quantum system.

  The additive operators always obey commutative

  $$\hat{\mathcal{A}} + \hat{\mathcal{B}} = \hat{\mathcal{B}} + \hat{\mathcal{A}}, \tag{1.28}$$

  and distributive laws

  $$\Big(\hat{\mathcal{A}} + \hat{\mathcal{B}}\Big) + \hat{\mathcal{C}} = \hat{\mathcal{A}} + \Big(\hat{\mathcal{B}} + \hat{\mathcal{C}}\Big). \tag{1.29}$$

- **Linearity** Except for the time reversal operator, all other operators in the Hilbert space are linear in character. A linear operator is the one which satisfies both the associative and distributive laws, i.e.,

  $$\hat{\mathcal{A}}\Big[\alpha_1|u_1\rangle + \alpha_2|u_2\rangle\Big] = \alpha_1\hat{\mathcal{A}}|u_1\rangle + \alpha_2\hat{\mathcal{A}}|u_2\rangle, \tag{1.30}$$

  where, $|u_i\rangle$ are the state **ket** vectors and α_i are the complex numbers for i=1,2.

  One of the important consequences of linearity is as follows. In the Hilbert space, any state **ket** vector $|u\rangle$ can be expressed as a linear combination of a complete set of bases $\{|e_i\rangle\}, i = 1, 2, ..., n$ associated with this Hilbert space, i.e.,

  $$|u\rangle = \sum_{i=1}^{n} \alpha_i|e_i\rangle. \tag{1.31}$$

  Using the orthonormalization property of bases $\{|e_i\rangle\}, i = 1, 2, ..., n$, i.e,

  $$\langle e_i|e_j\rangle = \delta_{i,j},$$

  the coefficients α_i are obtained as

  $$\alpha_i = \langle e_i|u\rangle. \tag{1.32}$$

  Then applying the linear operator $\hat{\mathcal{A}}$ on the state **ket** vector $|u\rangle$ gives

  $$\hat{\mathcal{A}}|u\rangle = \hat{\mathcal{A}}\sum_{i=1}^{n} \alpha_i|e_i\rangle = \sum_{i=1}^{n} \alpha_i\Big(\hat{\mathcal{A}}|e_i\rangle\Big). \tag{1.33}$$

  The result shown in equation 1.33 implies that the operation of the operator $\hat{\mathcal{A}}$ on each basis state $|e_i\rangle$ of a given Hilbert space is responsible for determining its effect on a general state $|u\rangle$ belonging to the same Hilbert space. That is an operation of the operator $\hat{\mathcal{A}}$ on the base set $\{|e_i\rangle\}$ correlates with its operation on any other state $|u\rangle$ to which that operator was applied.

- **Multiplication of an operator by a complex number** Since the operation of an operator $\hat{\mathcal{A}}$ on a state vector $|u\rangle$ generates a new state vector $|v\rangle$, i.e.,

  $$\hat{\mathcal{A}}|u\rangle = |v\rangle.$$

  Now consider another operator $\hat{\mathcal{C}}$ that is obtained from the multiplication of the operator $\hat{\mathcal{A}}$ by a complex number α, i.e.,

  $$\hat{\mathcal{C}} = \alpha\hat{\mathcal{A}}.$$

  The operation of this operator $\hat{\mathcal{C}}$ on a state vector $|u\rangle$ gives a state vector $|v\rangle$ times α, i.e.,

  $$\hat{\mathcal{C}}|u\rangle = \left(\alpha\hat{\mathcal{A}}\right)|u\rangle = \alpha|v\rangle. \tag{1.34}$$

- **Multiplication of operators** The multiplication of two operators $\hat{\mathcal{A}}$ and $\hat{\mathcal{B}}$ produces a single operator $\hat{\mathcal{C}} = \hat{\mathcal{A}}\hat{\mathcal{B}}$, such that an operation of $\hat{\mathcal{C}}$ on a state vector $|u\rangle$ generates a new state vector $|w\rangle$, i.e.,

  $$\hat{\mathcal{C}}|u\rangle = \hat{\mathcal{A}}\hat{\mathcal{B}}|u\rangle = |w\rangle. \tag{1.35}$$

  Generally, the multiplication of two operators is non-commutative, i.e.,

  $$\hat{\mathcal{A}}\hat{\mathcal{B}} \neq \hat{\mathcal{B}}\hat{\mathcal{A}}. \tag{1.36}$$

  Further, the commutator of two operators $\hat{\mathcal{A}}$ and $\hat{\mathcal{B}}$ is defined as the difference between the product of $\hat{\mathcal{A}}\hat{\mathcal{B}}$ and $\hat{\mathcal{B}}\hat{\mathcal{A}}$, i.e.,

  $$\left[\hat{\mathcal{A}}, \hat{\mathcal{B}}\right] = \hat{\mathcal{A}}\hat{\mathcal{B}} - \hat{\mathcal{B}}\hat{\mathcal{A}}. \tag{1.37}$$

  The commutator plays a fundamental role in quantum mechanics and, physically, it tells us whether or not two observable properties of a quantum system can be determined simultaneously with arbitrary precision according to the Heisenberg uncertainty relation (will be discussed in the subsequent chapters).

- **Outer product acts as an operator** In the Hilbert space, any arbitrary state **ket**, say, $|u\rangle$ is expressed as a linear combination of base set $\{|e_i\rangle, i = 1, 2, ..., n\}$, i.e.,

  $$|u\rangle = \sum_{i=1}^{n} \alpha_i |e_i\rangle. \tag{1.38}$$

  The expansion coefficients, $\alpha_i, i = 1, 2, , n$ are obtained by using the orthonormalization of bases and are given by

  $$\alpha_i = \langle e_i|u\rangle. \tag{1.39}$$

  Substitution of these expansion coefficients $\alpha_i, i = 1, 2, ..., n$ in equation 1.38 gives

  $$|u\rangle = \sum_{i=1}^{n} \langle e_i|u\rangle |e_i\rangle. \tag{1.40}$$

Since $\langle e_i|u\rangle$ is a complex number and is likely to be shifted on the right side of base **ket** $|e_i\rangle$ in equation 1.40. We get

$$|u\rangle = \sum_{i=1}^{n} |e_i\rangle\langle e_i|u\rangle. \tag{1.41}$$

Obviously, the product $|e_i\rangle\langle e_i|$ is neither an inner product nor a complex number. It is defined as an outer product and acts as an operator. Thus, the equality of equation 1.41 leads to an Identity operator

$$\hat{\mathcal{I}} = \sum_{i=1}^{n} |e_i\rangle\langle e_i|. \tag{1.42}$$

Equation 1.42 is known as a completeness or closure relation.

- **Projection operator**: The projection operator is a special case of outer product and is defined as

$$\hat{\mathcal{P}}_{e_i} = |e_i\rangle\langle e_i|. \tag{1.43}$$

Its operation on state **ket** vector $|u\rangle$ gives

$$\hat{\mathcal{P}}_{e_i}|u\rangle = |e_i\rangle\langle e_i|u\rangle = \alpha_i|e_i\rangle. \tag{1.44}$$

Physically, it tells us that the operator $|e_i\rangle\langle e_i|$ selects that portion of state **ket** vector $|u\rangle$ which is parallel to the base **ket** $|e_i\rangle$. In other words, the operator $\hat{\mathcal{P}}_{e_i}$ projects the state **ket** vector $|u\rangle$ onto the direction selected by the base **ket** $|e_i\rangle$.

Also, the sum of projection operators leads to a completeness relation. i.e.,

$$\sum_{i=1}^{n} \hat{\mathcal{P}}_{e_i} = \hat{\mathcal{I}}. \tag{1.45}$$

- **Hermitian adjoint**: From the above discussion, it is quite evident that for each **ket** vector state $|u\rangle$ in the Hilbert space, there exists a corresponding **bra** vector state $\langle u|$, which is generally referred to as the complex conjugate of the **ket** vector state $|u\rangle$. A parallel formalism of operators in the **bra** vector space needs to be addressed.

The **ket** vector obtained from $\hat{\mathcal{A}}|u\rangle$ and the **bra** vector obtained from $\langle u|\hat{\mathcal{A}}$ are, in general, not dual to each other. This implies that we have to introduce another operator $\hat{\mathcal{A}}^\dagger$ whose operation on **bra** vector is dual to that of $\hat{\mathcal{A}}$ operating on a **ket** vector, i.e.,

$$\hat{\mathcal{A}}|u\rangle \xleftrightarrow{\text{DC}} \langle u|\hat{\mathcal{A}}^\dagger. \tag{1.46}$$

Here, the symbol DC on the arrow refers to dual correspondence.

Now the question arises, "How does this Hermitian adjoint operator $\hat{\mathcal{A}}^\dagger$ operate on a **ket** vector?". It can be understood by considering the product $\langle w|\hat{\mathcal{A}}|u\rangle$. Let $\hat{\mathcal{A}}|u\rangle = |v\rangle$, then the product $\langle w|\hat{\mathcal{A}}|u\rangle$ is expressed as

$$\langle w|\hat{\mathcal{A}}|u\rangle = \langle w|\Big(\hat{\mathcal{A}}|u\rangle\Big) = \langle w|v\rangle. \tag{1.47}$$

The complex conjugate of equation 1.47 is represented by

$$\langle w|\hat{\mathcal{A}}|u\rangle^* = \langle w|v\rangle^* = \langle v|w\rangle. \tag{1.48}$$

if $\langle u|\hat{\mathcal{A}}^\dagger = \langle v|$, then

$$\langle w|\hat{\mathcal{A}}|u\rangle^* = \langle v|w\rangle = \Big(\langle u|\hat{\mathcal{A}}^\dagger\Big)|w\rangle = \langle u|\hat{\mathcal{A}}^\dagger|w\rangle. \tag{1.49}$$

1.2.2 Matrix Representation of State Vectors and Operators

Let a finite dimensional Hilbert space be spanned by a complete set of orthonormal base **kets** $\{|e_i\rangle; i = 1, 2, ..., n\}$.

- **ket-vector Representation**: An arbitrary **ket** vector $|u\rangle$ is expressed as

$$|u\rangle = \sum_{i=1}^{n} \alpha_i |e_i\rangle.$$

Using the orthonormalization of bases, we get

$$\langle e_i|u\rangle = \alpha_i, \tag{1.50}$$

with 1$\leq i \leq n$. In matrix formalism, the equation 1.50 is expressed as a column matrix, i.e,

$$\begin{bmatrix} \langle e_1|u\rangle \\ \langle e_2|u\rangle \\ \vdots \\ \langle e_n|u\rangle \end{bmatrix} = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_n \end{bmatrix}$$

Thus, the **ket** vector is represented by a column matrix.

- **bra-vector Representation**: An arbitrary **bra** vector $\langle u|$ is also expressed as

$$\langle u| = \sum_{i=1}^{n} \alpha_i^* \langle e_1|.$$

Using the orthonormalization of bases, we get

$$\langle u|e_i\rangle = \alpha_i^*, \tag{1.51}$$

with 1$\leq i \leq n$. In matrix formalism, the equation 1.51 is expressed as a row matrix, i.e,

$$\begin{bmatrix} \langle e_1|u\rangle^* & \langle e_2|u\rangle^* & \cdots & \langle e_n|u\rangle^* \end{bmatrix} = \begin{bmatrix} \alpha_1^* & \alpha_2^* & \cdots & \alpha_n^* \end{bmatrix}$$

Thus, the **bra** vector is represented by a row matrix.

- **Operator representation**: By definition, an operator $\hat{\mathcal{A}}$ operating on an arbitrary **ket** vector $|u\rangle$ generates a new **ket** vector $|v\rangle$, i.e.,

$$\hat{\mathcal{A}}|u\rangle = |v\rangle. \tag{1.52}$$

Using the identity operator expressed in terms of orthonormal base **kets** $\{|e_i\rangle; i = 1, 2, ..., n\}$

$$\hat{\mathcal{I}} = \sum_{i=1}^{n} |e_i\rangle\langle e_i|,$$

equation 1.52 becomes

$$|v\rangle = \hat{\mathcal{A}}\hat{\mathcal{I}}|u\rangle$$

$$|v\rangle = \hat{\mathcal{A}} \sum_{i=1}^{n} |e_i\rangle\langle e_i|u\rangle = \sum_{i=1}^{n} \left(\hat{\mathcal{A}}|e_i\rangle\right)\langle e_i|u\rangle.$$

Now, taking an inner product with base **ket** vector $|e_j\rangle$ on both sides, we get

$$\langle e_j|v\rangle = \sum_{i=1}^{n} \Big(\langle e_j|\hat{\mathcal{A}}|e_i\rangle\Big)\langle e_i|u\rangle. \tag{1.53}$$

Here, the variable j varies between the limits, $1 \leq j \leq n$ and the resulting expression is equivalent to the matrix multiplication equation $v_j = \sum_{i=1}^{n} A_{ji}u_i$. In shorthand notation, it can explicitly be expressed as

$$\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = \begin{pmatrix} A_{11} & A_{12} & \cdot & A_{1n} \\ A_{21} & A_{22} & \cdot & A_{2n} \\ \vdots & & & \\ A_{n1} & A_{n2} & \cdot & A_{nn} \end{pmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}$$

where the operator $\hat{\mathcal{A}}$ is represented by a $n \times n$ square matrix.

Thus, the elements of matrix representation in state vectors (i.e., **bra**, **ket**) as well as the operator depend implicitly or explicitly on the choice of base set. The values of their components will change with the change in the base set in the Hilbert space.

1.2.3 Hermitian operators and their Characteristics

- **Matrix representation of Hermitian adjoint operator**: Firstly, we would like to establish a relation between the matrix elements of the operators $\hat{\mathcal{A}}^\dagger$ and $\hat{\mathcal{A}}$. Following equation 1.49, the Hermitian adjoint operator is defined as

  $$\langle w|\hat{\mathcal{A}}|u\rangle^* = \langle u|\hat{\mathcal{A}}^\dagger|w\rangle.$$

  The insertion of the identity operator

  $$\hat{\mathcal{I}} = \sum_{i=1}^{n} |e_i\rangle\langle e_i|,$$

  at the appropriate places in the term $\langle w|\hat{\mathcal{A}}|u\rangle$ leads to

  $$\langle w|\hat{\mathcal{A}}|u\rangle = \langle w|\hat{\mathcal{I}}\hat{\mathcal{A}}\hat{\mathcal{I}}|u\rangle = \sum_{i=1}^{n}\sum_{j=1}^{n} \langle w|e_j\rangle\langle e_j|\hat{\mathcal{A}}|e_i\rangle\langle e_i|u\rangle$$

  $$\Longrightarrow \langle w|\hat{\mathcal{A}}|u\rangle = \sum_{i=1}^{n}\sum_{j=1}^{n} w_j^* A_{ji} u_i.$$

  Taking the complex conjugate both sides

  $$\langle w|\hat{\mathcal{A}}|u\rangle^* = \sum_{i=1}^{n}\sum_{j=1}^{n} w_j A_{ji}^* u_i^* = \sum_{i=1}^{n}\sum_{j=1}^{n} u_i^* A_{ij}^\dagger w_j.$$

  The last term of the matrix element, $A_{ij}^\dagger$, is resulted from the expression 1.49 as

  $$A_{ji}^* = \langle j|\hat{\mathcal{A}}|i\rangle^* = \langle i|\hat{\mathcal{A}}^\dagger|j\rangle.$$

  Thus,

  $$A_{ij}^\dagger = A_{ji}^*.$$

  implies that the matrix elements of the Hermitian adjoint of $\hat{\mathcal{A}}$ are obtained by interchanging rows and columns and then taking their complex conjugate.

- In case of a real operator,

  $$A_{ij}^{\dagger} = A_{ji},$$

  the Hermitian adjoint is obtained just by interchanging the rows and columns of its matrix elements.

- **Hermitian operator representation**: A Hermitian operator, $\hat{\mathcal{Q}}$, is defined as an operator that is equal to its Hermitian adjoint and is expressed as

  $$\langle w|\hat{\mathcal{Q}}|u\rangle^* = \langle u|\hat{\mathcal{Q}}|w\rangle. \tag{1.54}$$

  This implies that $\hat{\mathcal{Q}} = \hat{\mathcal{Q}}^{\dagger}$. In matrix notation, it is expressed as

  $$A_{ij} = A_{ji}^*,$$

  both i and j vary, respectively, $1 \leq i \leq n$ and $1 \leq j \leq n$. Importantly, the Hermiticity of an operator is independent of the specific choice of bases in the Hilbert space. In quantum mechanics, such operators generally represent some physical observables.

- **Characteristics of Hermitian operator** Each dynamical observable is defined by a specific operator. These operators must be Hermitian so that the observables are real in character. The physical measurement of a dynamical variable in a particular state yields an eigenvalue of its operator and permits the validity of that eigenstate of a physical system. Here we use the notations, $\{|q_i\rangle; i = 1, 2, ..., n\}$ for the set of eigenstates with corresponding eigenvalues $\{\lambda_i; i = 1, 2, ..., n\}$.

  (a) **The eigenvalues of Hermitian operators are always real**: An eigenvalue equation is defined as an expression in which an operator $\hat{\mathcal{Q}}$ operates on a **ket** vector $|q_i\rangle$ to generate an eigenvalue λ_i times the same **ket** vector, i.e.,

  $$\hat{\mathcal{Q}}|q_i\rangle = \lambda_i|q_i\rangle. \tag{1.55}$$

  Next, operating $\hat{\mathcal{Q}}$ on a **bra** vector $\langle q_i|$ generates a complex conjugate eigenvalue λ_i^*, i.e.,

  $$\langle q_i|\hat{\mathcal{Q}}^{\dagger} = \langle q_i|\hat{\mathcal{Q}} = \lambda_i^*\langle q_i|. \tag{1.56}$$

  Now multiplying on both sides of the equation 1.55 from the left by a **bra** vector $\langle q_i|$ and equation 1.56 from the right by a **ket** vector $|q_i\rangle$; and then subtract the resulting equations, we get

  $$0 = \left(\lambda_i - \lambda_i^*\right)\langle q_i|q_i\rangle. \tag{1.57}$$

  In equation 1.57 either $\left(\lambda_i - \lambda_i^*\right)$=0 or $\langle q_i|q_i\rangle$=0. Since the square of the norm, i.e., $\langle q_i|q_i\rangle \neq$0, therefore, $\left(\lambda_i - \lambda_i^*\right)$=0. This implies that

  $$\lambda_i = \lambda_i^*, \tag{1.58}$$

  the eigenvalues of Hermitian operators are always real.

(b) **The eigenstates of the Hermitian operator belonging to distinct eigenvalues are mutually orthogonal**: Consider two distinct eigenstates, $|q_i\rangle$ and $|q_j\rangle$ belonging, respectively, to eigenvalues λ_i and λ_j. Again, the operator $\hat{\mathcal{Q}}$ operates on a **ket** vector $|q_i\rangle$ gives

$$\hat{\mathcal{Q}}|q_i\rangle = \lambda_i|q_i\rangle. \tag{1.59}$$

Also, operating $\hat{\mathcal{Q}}$ on a **bra** vector $\langle q_j|$ generates a real eigenvalue λ_j, i.e.,

$$\langle q_j|\hat{\mathcal{Q}}^\dagger = \langle q_j|\hat{\mathcal{Q}} = \lambda_j\langle q_j|. \tag{1.60}$$

Here, multiplying on both sides of the equation 1.59 from the left by a **bra** vector $\langle q_j|$ and equation 1.60 from the right by a **ket** vector $|q_i\rangle$; and then subtracting the resulting expressions leads to

$$0 = \Big(\lambda_i - \lambda_j\Big)\langle q_j|q_i\rangle. \tag{1.61}$$

Because $\lambda_i \neq \lambda_j$, therefore,

$$\langle q_j|q_i\rangle = 0, \tag{1.62}$$

and it ensures that the eigenstates of the Hermitian operator belonging to distinct eigenvalues are mutually orthogonal.
Conventionally, an orthonormalized set of eigenvectors $\{|q_i\rangle; i = 1, 2, ..., n\}$, i.e.,

$$\langle q_j|q_i\rangle = \delta_{ji}, \tag{1.63}$$

form a complete set of bases in the Hilbert space of a physical system.

Ex. 1.3 — In a quantum mechanical system, if two or more different eigenstates of a Hermitian operator have the same eigenvalue, then these eigenstates are said to be degenerate. Given two linearly independent eigenvectors $|q_1\rangle$ and $|q_2\rangle$ corresponding to two fold, degenerate states with eigenvalue λ of the Hermitian operator $\hat{\mathcal{Q}}$. Construct an orthonormal eigenvectors $|v_i\rangle$ i=1,2 corresponding to the same eigenvalue λ.

Answer (Ex. 1.3) — Since $|q_1\rangle$ and $|q_2\rangle$ are two linearly independent eigenvectors of the operator $\hat{\mathcal{Q}}$ having the same eigenvalue λ, i.e,

$$\hat{\mathcal{Q}}|q_1\rangle = \lambda|q_1\rangle$$
$$\hat{\mathcal{Q}}|q_2\rangle = \lambda|q_2\rangle.$$

We start with the normalization of the first eigenvector $|q_1\rangle$, i.e.,

$$|q_1'\rangle = \frac{|q_1\rangle}{\sqrt{\langle q_1|q_1\rangle}},$$

and defined by a linear combination

$$|q\rangle = |q_2\rangle + \alpha|q_1'\rangle.$$

The constant α is obtained by using the orthogonalization constraint between the vectors $|q_1'\rangle$ and $|q\rangle$, i.e.,

$$\langle q_1'|q\rangle = 0,$$

and it gives

$$\alpha = -\langle q_1' | q_2 \rangle.$$

Thus, knowing the complex coefficient α, the normalized eigenstate $|q\rangle$ is obtained, i.e.,

$$|q_2'\rangle = \frac{|q\rangle}{\sqrt{\langle q|q\rangle}}.$$

Hence, from the linearly independent eigenstates $|q_1\rangle$ and $|q_2\rangle$ of two fold degenerate eigenvalue λ of the Hermitian operator $\hat{\mathcal{Q}}$, we have been able to construct two orthonormal eigenstates $|q_1'\rangle$ and $|q_2'\rangle$, corresponding to the same eigenvalues λ. This formalism can also be generalized to the case of any fold degeneracy in a quantum system.
Interesting enough to notice here that the mutually orthonormal eigenstates of a Hermitian operator define a complete set of bases of the Hilbert space. Further, the uniqueness of this set is determined by non-degenerate eigenvalues. It loses the unique character even if a single degenerate eigenstate exists in a quantum system.

1.2.4 Postulates of quantum mechanics

The above discussion leads to the following postulates, which lay down the foundation stone for developing the formalism of quantum systems.

- **Postulate 1** The elements of a complex vector space describe the possible state of a physical system.
- **Postulate 2** Each measurement of a physical quantity is defined by an observable, which is specified by a Hermitian operator, i.e., there is one-to-one correspondence between the observables and Hermitian operators.
- **Postulate 3** The eigenvalues of the Hermitian operator provide the only possible outcomes of the observable.
- **Postulate 4** For the quantum state $|u\rangle$, the probability of measuring an observable having value λ_q is defined as

$$Probability(\lambda_q) = |\langle q|u\rangle|^2. \tag{1.64}$$

  Here, $|q\rangle$ is an eigenvector of the corresponding Hermitian operator with eigenvalue λ_q.

1.2.5 Anti-hermitian Operator and its Properties

An anti-hermitian operator is defined as an operator that is equal to the negative of its Hermitian adjoint, i.e.,

$$\hat{\mathcal{X}} = -\hat{\mathcal{X}}^\dagger. \tag{1.65}$$

Its characteristics are as follows:

(a) **The expectation value of an Anti-hermitian operator is imaginary**: The expectation value is the probabilistic result of the measurements of an experiment. It implies that the expectation value is not the most probable value of the measurements; indeed, it reflects the average value of all measurements of an experiment.

Let $\hat{\mathcal{X}}$ be an Anti-hermitian operator and its expectation value is expressed as

$$\langle\hat{\mathcal{X}}\rangle = \langle u|\hat{\mathcal{X}}|u\rangle, \tag{1.66}$$

where $|u\rangle$ is normalized **ket** vector. Using the definition of Anti-hermitian operator, we get

$$\begin{aligned}
\langle\hat{\mathcal{X}}\rangle &= \langle u|-\hat{\mathcal{X}}^\dagger|u\rangle \\
\langle\hat{\mathcal{X}}\rangle &= -\langle u|\hat{\mathcal{X}}^\dagger|u\rangle \\
\implies \langle\hat{\mathcal{X}}\rangle &= -\langle u|\Big(\hat{\mathcal{X}}|u\rangle\Big)^* = -\langle u|\hat{\mathcal{X}}|u\rangle^* \\
\implies \langle\hat{\mathcal{X}}\rangle &= -\langle\hat{\mathcal{X}}\rangle^*.
\end{aligned}$$

Thus, the expectation value of an Anti-hermitian operator is purely imaginary. On the other hand, the expectation value of the Hermitian operator, obtained by using similar steps, comes out to be real.

(b) **The eigenvalues of an Anti-hermitian operator are imaginary in character**
Let the eigenvalue of an Anti-hermitian operator $\hat{\mathcal{X}}$ operates on a **ket** vector $|u\rangle$ be x_i, i.e.,

$$\hat{\mathcal{X}}|u\rangle = x_i|u\rangle. \tag{1.67}$$

Multiply equation 1.67 from the left by **bra** vector $\langle u|$, we get

$$\begin{aligned}
\langle u|\hat{\mathcal{X}}|u\rangle &= x_i\langle u|u\rangle \\
\implies \Big[\Big(\langle u|\hat{\mathcal{X}}^\dagger\Big)|u\rangle\Big]^* &= x_i\langle u|u\rangle \\
\implies \Big[\Big(\langle u|-\hat{\mathcal{X}}\Big)|u\rangle\Big]^* &= x_i\langle u|u\rangle \\
\implies -\Big[\langle u|\Big(\hat{\mathcal{X}}|u\rangle\Big)\Big]^* &= x_i\langle u|u\rangle \\
\implies -x_i^*\langle u|u\rangle^* &= x_i\langle u|u\rangle \\
\implies -x_i^*\langle u|u\rangle &= x_i\langle u|u\rangle \\
\implies 0 &= \Big(x_i + x_i^*\Big)\langle u|u\rangle.
\end{aligned}$$

Since the eigenvector $|u\rangle$ cannot be zero and also, the inner product $\langle u|u\rangle$ is positive. Therefore, $x_i^* = -x_i$, hence the eigenvalues of an Anti-hermitian operator are purely imaginary in character.

(c) **The eigenvectors of Anti-hermitian operator belonging to distinct eigenvalues are mutually orthogonal in character**: Reconsidering the eigenvalue equations in which an Anti-hermitian operator $\hat{\mathcal{X}}$ operates on two different **ket** vectors $|u\rangle$ and $|v\rangle$ to generate distinct eigenvalues x_1 and x_2, respectively, i.e.,

$$\hat{\mathcal{X}}|u\rangle = x_1|u\rangle, \tag{1.68}$$

$$\hat{\mathcal{X}}|v\rangle = x_2|v\rangle. \tag{1.69}$$

The dual correspondence of equation 1.69 is

$$\langle v|\hat{\mathcal{X}}^\dagger = x_2^*\langle v|. \tag{1.70}$$

By the definition of the Anti-hermitian operator, equation 1.70 becomes

$$-\langle v|\hat{\mathcal{X}} = x_2^*\langle v|. \tag{1.71}$$

Pre-multiplying the equation 1.68 by a **bra** vector $\langle v|$ and the post-multiplication of equation 1.71 by the **ket** vector $|u\rangle$ and then adding the resulting expressions lead to

$$0 = \Big(x_1 + x_2^*\Big)\langle v|u\rangle. \tag{1.72}$$

Since eigenvalues x_1 and x_2 are distinct, therefore, $\Big(x_1 + x_2^*\Big) \neq 0$. Hence,

$$\langle v|u\rangle = 0, \tag{1.73}$$

the eigenvectors of Anti-hermitian operator belonging to distinct eigenvalues are mutually orthogonal in character.

(d) **The commutator of two Hermitian operator is Anti-hermitian in character but the reverse is not true**: Let $\hat{\mathcal{Q}}_1$ and $\hat{\mathcal{Q}}_2$ be two Hermitian operators. The hermitian adjoint to their commutator gives

$$\begin{aligned}
\Big[\hat{\mathcal{Q}}_1, \hat{\mathcal{Q}}_2\Big]^\dagger &= \Big(\hat{\mathcal{Q}}_1\hat{\mathcal{Q}}_2 - \hat{\mathcal{Q}}_2\hat{\mathcal{Q}}_1)^\dagger \\
\implies \Big[\hat{\mathcal{Q}}_1, \hat{\mathcal{Q}}_2\Big]^\dagger &= \Big(\hat{\mathcal{Q}}_1\hat{\mathcal{Q}}_2\Big)^\dagger - \Big(\hat{\mathcal{Q}}_2\hat{\mathcal{Q}}_1)^\dagger \\
\implies \Big[\hat{\mathcal{Q}}_1, \hat{\mathcal{Q}}_2\Big]^\dagger &= \hat{\mathcal{Q}}_2^\dagger\hat{\mathcal{Q}}_1^\dagger - \hat{\mathcal{Q}}_1^\dagger\hat{\mathcal{Q}}_2^\dagger \\
\implies \Big[\hat{\mathcal{Q}}_1, \hat{\mathcal{Q}}_2\Big]^\dagger &= \hat{\mathcal{Q}}_2\hat{\mathcal{Q}}_1 - \hat{\mathcal{Q}}_1\hat{\mathcal{Q}}_2 \\
\implies \Big[\hat{\mathcal{Q}}_1, \hat{\mathcal{Q}}_2\Big]^\dagger &= -\Big(\hat{\mathcal{Q}}_1\hat{\mathcal{Q}}_2 - \hat{\mathcal{Q}}_2\hat{\mathcal{Q}}_1\Big) = -\Big[\hat{\mathcal{Q}}_1, \hat{\mathcal{Q}}_2\Big].
\end{aligned}$$

Thus, the commutator of two Hermitian operators is Anti-hermitian in character.

Now consider two Anti-hermitian operators, $\hat{\mathcal{X}}_1$ and $\hat{\mathcal{X}}_2$ and their commutator gives

$$\begin{aligned}
\Big[\hat{\mathcal{X}}_1, \hat{\mathcal{X}}_2\Big]^\dagger &= \Big(\hat{\mathcal{X}}_1\hat{\mathcal{X}}_2 - \hat{\mathcal{X}}_2\hat{\mathcal{X}}_1)^\dagger \\
\implies \Big[\hat{\mathcal{X}}_1, \hat{\mathcal{X}}_2\Big]^\dagger &= \Big(\hat{\mathcal{X}}_1\hat{\mathcal{X}}_2\Big)^\dagger - \Big(\hat{\mathcal{X}}_2\hat{\mathcal{X}}_1)^\dagger \\
\implies \Big[\hat{\mathcal{X}}_1, \hat{\mathcal{X}}_2\Big]^\dagger &= \hat{\mathcal{X}}_2^\dagger\hat{\mathcal{X}}_1^\dagger - \hat{\mathcal{X}}_1^\dagger\hat{\mathcal{X}}_2^\dagger \\
\implies \Big[\hat{\mathcal{X}}_1, \hat{\mathcal{X}}_2\Big]^\dagger &= -\hat{\mathcal{X}}_2\Big(-\hat{\mathcal{X}}_1\Big) - \Big(-\hat{\mathcal{X}}_1\Big)\Big(-\hat{\mathcal{X}}_2\Big) \\
\implies \Big[\hat{\mathcal{X}}_1, \hat{\mathcal{X}}_2\Big]^\dagger &= -\Big(\hat{\mathcal{X}}_1\hat{\mathcal{X}}_2 - \hat{\mathcal{X}}_2\hat{\mathcal{X}}_1\Big) = -\Big[\hat{\mathcal{X}}_1, \hat{\mathcal{X}}_2\Big].
\end{aligned}$$

Thus, the commutator of two Anti-hermitian operators is Anti-hermitian in character.

(e) **Any arbitrary operator can be expressed as a sum of a Hermitian operator and an Anti-hermitian operator**: Let an arbitrary operator $\hat{\mathcal{F}}$ operate on a $|u\rangle$ to give a complex eigenvalue α, i.e.,

$$\begin{aligned}
\hat{\mathcal{F}}|u\rangle &= \alpha|u\rangle, \\
\implies \hat{\mathcal{F}}|u\rangle &= (p + \iota q)|u\rangle.
\end{aligned}$$

Here, both p and q are real numbers.

By hypothesis, the Hermitian $\hat{\mathcal{Q}}$ and Anti-hermitian $\hat{\mathcal{X}}$ operators acting on a $|u\rangle$ give, respectively, real (p) and imaginary (ιq) eigenvalues as

$$\hat{\mathcal{Q}}|u\rangle = p|u\rangle,$$
$$\hat{\mathcal{X}}|u\rangle = \iota q|u\rangle.$$

As a result,

$$\hat{\mathcal{F}}|u\rangle = \left(\hat{\mathcal{Q}} + \hat{\mathcal{X}}\right)|u\rangle,$$
$$\implies \hat{\mathcal{F}} = \hat{\mathcal{Q}} + \hat{\mathcal{X}}.$$

Taking the Hermitian adjoint both sides

$$\hat{\mathcal{F}}^\dagger = \left(\hat{\mathcal{Q}} + \hat{\mathcal{X}}\right)^\dagger,$$
$$\implies \hat{\mathcal{F}}^\dagger = \hat{\mathcal{Q}}^\dagger + \hat{\mathcal{X}}^\dagger,$$
$$\implies \hat{\mathcal{F}}^\dagger = \hat{\mathcal{Q}} - \hat{\mathcal{X}}.$$

The addition and subtraction of operators $\hat{\mathcal{F}}$ and $\hat{\mathcal{F}}^\dagger$, gives

$$\hat{\mathcal{Q}} = \frac{1}{2}\left(\hat{\mathcal{F}} + \hat{\mathcal{F}}^\dagger\right),$$
$$\hat{\mathcal{X}} = \frac{1}{2}\left(\hat{\mathcal{F}} - \hat{\mathcal{F}}^\dagger\right).$$

The Hermiticity and anti-Hermiticity, respectively, of the operators $\hat{\mathcal{Q}}$ and $\hat{\mathcal{X}}$ can easily be verified by taking the adjoint of these operators, i.e.,

$$\hat{\mathcal{Q}}^\dagger = \frac{1}{2}\left(\hat{\mathcal{F}}^\dagger + \hat{\mathcal{F}}\right) = \hat{\mathcal{Q}},$$
$$\hat{\mathcal{X}}^\dagger = \frac{1}{2}\left(\hat{\mathcal{F}}^\dagger - \hat{\mathcal{F}}\right) = -\hat{\mathcal{X}}.$$

Thus, any arbitrary operator in the Hilbert space can be expressed as a sum of a Hermitian operator and an Anti-hermitian operator.

1.2.6 Unitary Operator and its Characteristics

An operator $\hat{\mathcal{U}}$ is defined as a Unitary operator if it commutes with its Hermitian adjoint $\hat{\mathcal{U}}^\dagger$ and, also, $\hat{\mathcal{U}}^\dagger$ acts as an inverse for $\hat{\mathcal{U}}$, i.e.,

$$\hat{\mathcal{U}}\hat{\mathcal{U}}^\dagger = \hat{\mathcal{U}}^\dagger\hat{\mathcal{U}} = \hat{\mathcal{I}}. \tag{1.74}$$

Here, $\hat{\mathcal{I}}$ is an identity operator. The characteristics of Unitary operator are discussed below.

(a) **The eigenvalues of a Unitary operator are complex numbers and its eigenstates corresponding to non-degenerate eigenvalues are mutually orthogonal**: Let $|u_i\rangle$ and $|u_j\rangle$ be the eigenstates of $\hat{\mathcal{U}}$ operator with corresponding eigenvalues α_i and α_j. We then have

$$\left(\langle u_j|\hat{\mathcal{U}}^\dagger\right)\left(\hat{\mathcal{U}}|u_i\rangle\right) = \alpha_j^*\alpha_i\langle u_j|u_i\rangle.$$