Chapter 2

Mathematical Tools of Quantum Mechanics

In this chapter we deal with the mathematical machinery required to study quantum mechanics. Here we will limit ourselves to only those issues that are relevant to the formalism of quantum mechanics.

Schrödinger equation has a structure of linear equation. In quantum mechanics we deal with operators that are linear and wavefunctions belong to abstract Hilbert space.

Quantum mechanics was formulated in two different ways. Schrodinger's wave mechanics for continuous basis and Heisenberg's matrix mechanics for discrete basis.

The Hilbert Space and Wave Functions

The Linear Vector Space

It consists of two sets of elements and two algebraic rules

i) a set of vectors $\psi, \phi, \chi, \ldots$ and a set of scalars $a, b, c, \ldots$

ii) a rule for vector addition and a rule for scalar multiplication.

Addition rule: Addition rule has the properties and structure of abelian group.

- If ψ and ϕ are vectors of a space, then $\psi+\phi$ is also a vector of the same space.
- Vector addition is commutative $\psi+\phi = \phi+\psi$
- Vector addition is associative $(\psi+\phi)+\chi = \psi+(\phi+\chi)$
- There exists a null (or zero) vector with the property that
  $0+\psi = \psi+0 = \psi$
- For every vector ψ there is an associative symmetric vector $(-\psi)$ such that $\psi+(-\psi) = (-\psi)+\psi = 0$

Scalar Multiplication Rule The product of any scalar with any vector is another vector i.e $a\psi = \phi$. In general if ψ and ϕ are two vectors of the space, then any linear combination $a\psi + b\phi$ is also a vector in the same space. Here 'a' and 'b' are scalars.

- Scalar multiplication is distributive w.r.t addition

$$a(\psi+\phi) = a\psi + a\phi, \qquad (a+b)\psi = a\psi + b\psi$$

- It is associative w.r.t ordinary multiplication of scalars.

$$ab(\psi) = (ab)\psi$$

- For each element ψ there must exists a unitary scalar 'I' and a zero scalar '0' such that

$$I\psi = \psi I = \psi \qquad \text{and} \qquad 0\psi = \psi 0 = 0$$

The Hilbert Space

A Hilbert space ($\mathcal{H}$) consists of a set of vectors $\psi, \phi, \chi, \ldots$ and a set of scalars a, b, c, ... having the following properties

- $\mathcal{H}$ is a linear space: A Hilbert space is a linear vector space having few additional properties.
- Hilbert space has a defined scalar product that is strictly positive.

The scalar product of an element ψ with another element ϕ is generally a complex number. It can be represented as $(\psi,\phi) = \psi^*\phi$ = complex number

The order of the product is important i.e

$$(\psi,\phi) = \psi^*\phi$$

&

$$(\phi,\psi) = \phi^*\psi$$

} both the products are not equal.

Scalar product has the following properties.

i) The scalar product of ψ and ϕ is equal to the complex conjugate of the scalar product of ϕ with ψ i.e.,

$$(\psi,\phi) = (\phi,\psi)^*$$

(ii) The scalar product of ϕ with $\psi = a\psi_1 + b\psi_2$ (second vector) is linear

$$(\phi, a\psi_1 + b\psi_2) = (\phi, a\psi_1) + (\phi, b\psi_2)$$

$$= \phi^* a\psi_1 + \phi^* b\psi_2 = a\phi^*\psi_1 + b\phi^*\psi_2$$

it is antilinear w.r.t the first vector if $\phi = a\phi_1 + b\phi_2$ i.e.,

$$(a\phi_1 + b\phi_2, \psi) = (a\phi_1, \psi) + (b\phi_2, \psi)$$

$$= a^*(\phi_1, \psi) + b^*(\phi_2, \psi)$$

(iii) The scalar product of a vector ψ with itself must not be zero

$$(\psi,\psi) = \|\psi\|^2 \geq 0,$$

and it is equal to zero only when $\psi = 0$. This is also known as positive definitness.

- Hilbert spaces are separable, so they contain a countable, dense, subset. There exists a Cauchy sequence $\psi_n \in \mathcal{H}$ $(n = 1, 2, 3, \ldots)$ such that for every ψ of $\mathcal{H}$ and $\epsilon > 0$, there exists atleast one ψ_n of the sequence for which

$$\|\psi - \psi_n\| < \epsilon$$

- Hilbert spaces are complete (no gaps). So every Cauchy sequence $\psi_n \in \mathcal{H}$ converges to an element of $\mathcal{H}$ i.e., for any ψ_n

$$\lim_{n,m \to \infty} \|\psi_n - \psi_m\| = 0,$$

defining a unique limit ψ of $\mathcal{H}$ such that

$$\lim_{n \to \infty} \|\psi - \psi_m\| = 0$$

Dual Hilbert Space

considering the scalar product $(\phi, \psi) = \phi^* \psi$, the second factor, ψ, belongs to Hilbert space $\mathcal{H}$, whereas, the first vector belongs to its dual Hilbert space $\mathcal{H}_d$. The existence of this dual space is due to the fact that scalar product is non-commutative i.e., $(\phi, \psi) \neq (\psi, \phi)$ (according to linear algebra, every vector space can be associated with a dual vector space.

Linearly Independent and Dependent Vectors

The linear combination of N non-zero vectors $\phi_1, \phi_2, \ldots, \phi_N$ can be written as

$$a_1 \phi_1 + a_2 \phi_2 + a_3 \phi_3 + \cdots + a_N \phi_N = \sum_{i=1}^{N} a_i \phi_i \longrightarrow (1)$$

They will be linearly independent if and only if

$$\sum_{n=1}^{N} a_i \phi_i = 0 \longrightarrow (2)$$

and is possible only when $a_1 = a_2 = a_3 = \cdots = a_N = 0$.

If λ is a vector and it will be linearly independent of the vectors set given by eq. (1), if it can not be written as a linear combination of them. For example, in 3D, the unit vector $\hat{k}$ is linearly independent of $\hat{i}$ and $\hat{j}$. But any vector in the xy-plane is linearly dependent on $\hat{i}$ and $\hat{j}$. So we can also say, a set of vectors is linearly independent, if each one is linearly independent of all the rest.

Considering eq.(2), if among the set of scalars i.e $a_1, a_2, a_3, \cdots, a_N$, which are not all zero, then any of the vectors, say, ϕ_n, can be expressed as the linear combination of the others and mathematically we can write as

$$\phi_n = \sum_{i=1}^{N-1} a_i \phi_i + \sum_{i=n+1}^{N} a_i \phi_i \longrightarrow (3)$$

and the set $\{\phi_i\}$ is said to be linearly dependent.

Dimensions of Vector Space

The dimension of a vector space is given by the maximum number of linearly independent vectors a space can have. For example there are N linearly independent vectors $(\phi_1, \phi_2, \phi_3, \cdots, \phi_N)$ in a space, then the space is said be N dimentional. In N-dimensional vector space, any vector ψ can be expanded as a linear combination of its linearly independent vectors as

$$\psi = \sum_{i=1}^{N} a_i \phi_i, \longrightarrow (4)$$

here a_i, the expansion co-efficients, are called the components of the vector ψ. Each component is given by the scalar product of ψ with the corresponding vector (base vector) as

$$a_i = (\phi_i, \psi)$$

Basis

The basis of a vector space is a set of maximum linearly independent vectors that the space can have. This set of linearly independent vector i.e $\phi_1, \phi_2, \phi_3, \ldots, \phi_N$ are called the basis of the vector space, while these vectors $\phi_1, \phi_2, \ldots, \phi_N$ are called base vectors. In short these basis are written as $\{\phi_n\}$.

The choice of the set of these linearly independent vectors is arbitrary, but it is convenient to choose them orthonormal i.e their scalar product satisfy the following relation

$$(\phi_i, \phi_j) = \delta_{ij} = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases}$$

The basis is said to be complete, if it spans the entire space, i.e., there is no need to introduce any additional base vector.

Square Integrable Functions: Wave Functions

Considering the function spaces, in which the vectors are (complex) functions of x and their scalar product is represented by integrals. The scalar product of two functions $\psi(x)$ and $\phi(x)$ is given by

$$(\psi, \phi) = \int \psi^*(x)\, \phi(x)\, dx \longrightarrow (1)$$

The scalar product exists only if the integral remains convergent. To achieve this, we select only those fuctions for which the scalar product (ψ, ϕ) remains finite.

The function $\psi(x)$ is said to be square integrable if the scalar product of $\psi(x)$ with itself

$$(\psi, \psi) = \int \psi^*(x)\psi(x)\, dx = \int |\psi(x)|^2 dx \longrightarrow (2)$$

is finite.

It is to be noted that space of square integrable functions possesses the properties of Hilbert space. For example, any linear combination of square integrable functions is also a square integrable function and satisfies all the properties of Hilbert space.

Since a square integrable function can be expanded in terms of infinite number of linearly independent function, so the dimension of the Hilbert space of square integrable functions is infinite.

The wave function $\psi(\vec{r}, t)$ in quantum mechanics is also square integrab and mathematically

$$\int |\psi(\vec{r}, t)|^2 d^3r = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} |\psi(\vec{r}, t)| dz = 1 \longrightarrow (3)$$

represents the probability of finding the particle at time 't' in a volume of d^3r somewhere in space is equal to 1. The wave function satisfying the condition given by eq. (3) is called normalized or squale integrable.

Dirac Notation

Quantum mechanically the physical state of a system is represented by elements of Hilbert space and they are called state vectors. These state vectors are represented in different bases using function expansions. It is the same process by which we represent a vector in various coordinate systems e.g in Cartesian or in cylinderical or in spherical coordinate system. In fact, the meaning of a vector is independent of the coordinate system used to find its components.

To free state vectors from cooodinate meaning, Dirac introduced the concept of kets, bras and bra-kets.

Kets: elements of a vector space The state vector ψ can be denoted by a symbol $|\psi\rangle$ and is called a ket vector or simply a ket. They belong to Hilbert space $\mathcal{H}$ or to the ket space.

Bras: elements of a dual space The elements of a dual space ($\mathcal{H}_d$) like ψ^*, ϕ^* are represented by a symbol $\langle|$ called a bra vector or bra. So ψ^* is represented by $\langle\psi|$. It must be noted that for every ket there exists a unique bra.

Bra-ket: Notation for scalar product According to Dirac, the scalar or inner product is represented by $\langle|\rangle$, which is called bra-ket, for example

$$(\psi, \phi) \longrightarrow \langle\psi|\phi\rangle$$

Wave functions and Dirac's notation Wave functions like kets are members of Hilbert space and $\psi(\vec{r}, t)$ can be represented by $|\psi\rangle$. Like wave function, kets also contain all the information about the system to be represted. The only difference between these two notations is that kets are coordinate independent. If we want to caculate the probability of finding a particle at some position in space, we must have to use the appropriate coordinate representation. So to achieve the wave functions $\psi(x)$ of a particle from a ket, we take the inner product of ket with x coordinate i.e

$$\psi(x) = \langle x|\psi\rangle$$

and the scalar product of $\langle\phi|\psi\rangle$ is given by

$$\langle\phi|\psi\rangle = \int \phi^*(x)\,\psi(x)\,dx$$

Similarly for a 3-D time dependent wave function $\psi(\vec{r}, t)$ we have

$$\psi(\vec{r}, t) = \langle\vec{r}\,t|\psi\rangle$$

and

$$\langle\phi|\psi\rangle = \int \phi^*(\vec{r}, t)\,\psi(\vec{r}, t)\,d^3r.$$

If we want to express a wave function in momentum space i.e; $\psi(\vec{p})$ then

$$\psi(\vec{p}) = \langle\vec{p}|\psi\rangle$$

Properties of kets, bras and bra-kets

1) Every ket has a corresponding bra

$$|\psi\rangle \longleftrightarrow \langle\psi|$$

$$|\psi\rangle^* = \langle\psi|$$
$$\langle\psi|^* = |\psi\rangle$$

There is one to one correspondence between bras and kets.

$$a|\psi\rangle + b|\phi\rangle \longleftrightarrow a^*\langle\psi| + b^*\langle\phi|$$

Here 'a' and 'b' are complex numbers. Also

$$|a\psi\rangle = a|\psi\rangle \quad \& \quad \langle a\psi| = a^*\langle\psi|$$

2) Properties of scalar product: As we have learned that scalar product is a complex number and ordering of vectors in product is important. As

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

when $|\psi\rangle$ and $|\phi\rangle$ are real then

$$\langle\psi|\phi\rangle = \langle\phi|\psi\rangle$$

The proof of (a) is as follows

$$\langle\phi|\psi\rangle^* = \left(\int \phi^*(\vec{r},t)\,\psi(\vec{r},t)\,d^3r\right)^*$$

$$= \int \psi^*(\vec{r},t)\,\phi(\vec{r},t)\,d^3r = \langle\psi|\phi$$

* There are few other properties of inner product which are

i) $\langle\psi|a_1\psi_1 + a_2\psi_2\rangle = \langle\psi|a_1\psi_1\rangle + \langle\psi|a_2\psi_2\rangle$

$= a_1\langle\psi|\psi_1\rangle + a_2\langle\psi|\psi_2\rangle$

ii) $\langle a_1\phi_1 + a_2\phi_2|\psi\rangle = \langle a_1\phi_1|\psi\rangle + \langle a_2\phi_2|\psi\rangle$

$= a_1^*\langle\phi_1|\psi\rangle + a_2^*\langle\phi_2|\psi\rangle$

iii) $\langle a_1\phi_1 + a_2\phi_2|b_1\psi_1 + b_2\psi_2\rangle = \langle a_1\phi_1|b_1\psi_1\rangle + \langle a_1\phi_1|b_2\psi_2\rangle + \langle a_2\phi_2|b_1\psi_1\rangle + \langle a_2\phi_2|b_2\psi_2\rangle$

$= a_1^* b_1\langle\phi_1|\psi_1\rangle + a_1^* b_2\langle\phi_1|\psi_1\rangle + a_2^* b_1\langle\phi_2|\psi_1\rangle + a_2^* b_2\langle\phi_2|\psi_2\rangle$

3) The norm is real and positive

The norm $\langle\psi|\psi\rangle$ is real and is zero only when $|\psi\rangle = 0$. If $|\psi\rangle$ is normalized then $\langle\psi|\psi\rangle = 1$

4) Schwarz Inequality For any two state vectors $|\psi\rangle$ and $|\phi\rangle$, we can show that

$$|\langle\psi|\phi\rangle|^2 \leq \langle\psi|\psi\rangle\langle\phi|\phi\rangle$$

If $|\psi\rangle$ and $|\phi\rangle$ are linearly dependent, this relation becomes equality i.e.,

$$|\langle\psi|\phi\rangle|^2 = \langle\psi|\psi\rangle\langle\phi|\phi\rangle$$

This property is analogous to the following property in real space

$$|\vec{A}\cdot\vec{B}|^2 \leq |\vec{A}|^2|\vec{B}|^2$$

5) Triangular Inequality Mathematically

$$\sqrt{\langle\psi+\phi|\psi+\phi\rangle} \leq \sqrt{\langle\psi|\psi\rangle}+\sqrt{\langle\phi|\phi\rangle}$$

In case when both $|\psi\rangle$ and $|\phi\rangle$ are linearly dependent then

$$\sqrt{\langle\psi+\phi|\psi+\phi\rangle} = \sqrt{\langle\psi|\psi\rangle}+\sqrt{\langle\phi|\phi\rangle}$$

6) Orthogonal States Two ket vectors $|\psi\rangle$ and $|\phi\rangle$ are said to orthogonal if $\langle\psi|\phi\rangle = 0$

7) Orthonormal States Two kets $|\psi\rangle$ and $|\phi\rangle$ are said to be orthonormal, if they are orthogonal and both have unit norm

$$\langle\psi|\phi\rangle = 0 \qquad \langle\psi|\psi\rangle = 1 \qquad \langle\phi|\phi\rangle = 1$$

8) Forbidden Quantities If $|\psi\rangle$ and $|\phi\rangle$ belongs to the same vector (Hilbert) space then the product of the forms $|\psi\rangle|\phi\rangle$ or $\langle\psi|\langle\phi|$ are not allowed. However, if $|\psi\rangle$ and $|\phi\rangle$ belongs to two different vector spaces then the product $|\psi\rangle|\phi\rangle$ represented as $|\psi\rangle\otimes|\phi\rangle$, called the tensor product is allowed.

Operators

General Definition An operator is a mathematical rule when applied to a ket $|\psi\rangle$ or bra $\langle\psi|$, transforms it to another ket $|\psi'\rangle$ or bra $\langle\psi'|$. Sometimes when an operator operator operates on a ket or bra, it leaves the ket or bra unchanged. Mathematically an operator is represented by putting a hat over the operator symbol i.e $\hat{A}$, $\hat{x}$, $\hat{p}$ etc.

Now

$$\hat{A}|\psi\rangle = |\psi'\rangle$$

$$\langle\phi|\hat{A} = \langle\phi'|$$

A similar defination applies to the wave functions

$$\hat{A}\,\psi(\vec{r}) = \psi'(\vec{r})$$

Few examples of operators: Unity operator leaves the ket unchanged

$$\hat{I}|\psi\rangle = |\psi\rangle$$

The gradient operator: $\vec{\nabla}\psi(\vec{r}) = \left(\frac{\partial\psi(\vec{r})}{\partial x}\right)\hat{i} + \left(\frac{\partial\psi(\vec{r})}{\partial y}\right)\hat{j} + \left(\frac{\partial\psi(\vec{r})}{\partial z}\right)\hat{k}$

The linear momentum operator: $\hat{p}\psi(\vec{r}) = -i\hbar\vec{\nabla}\psi(\vec{r})$

Since momentum is a vector quantity so $\hat{\vec{P}} = \hat{P}_x\hat{i} + \hat{P}_y\hat{j} + \hat{P}_z\hat{k}$

Also $\hat{P}_x = -i\hbar\frac{\partial}{\partial x}$, $\hat{P}_y = -i\hbar\frac{\partial}{\partial y}$, and $\hat{P}_z = -i\hbar\frac{\partial}{\partial z}$

So $\hat{\vec{P}} = -i\hbar\frac{\partial}{\partial x}\hat{i} - i\hbar\frac{\partial}{\partial y}\hat{j} - i\hbar\frac{\partial}{\partial z}\hat{k} = -i\hbar\left(\frac{\partial}{\partial x}\hat{i} + \frac{\partial}{\partial y}\hat{j} + \frac{\partial}{\partial z}\hat{k}\right)$

So $\hat{\vec{P}} = -i\hbar\vec{\nabla}$

ANGULAR MOMENTUM OPERATOR. Angular momentum is defined as

$\vec{L} = \vec{R}\times\vec{P}$ and in operator form we have

$\hat{\vec{L}} = \hat{\vec{R}}\times\hat{\vec{P}} = -i\hbar(\vec{r}\times\vec{\nabla})$

OPERATOR FOR ENERGY It is represented by $\hat{E}$ and its value is given by

$$\vec{E} = i\hbar\frac{\partial}{\partial t}$$

The laplacian operator: $\nabla^2\psi(\vec{r}) = \frac{\partial^2\psi(\vec{r})}{\partial x^2} + \frac{\partial^2\psi(\vec{r})}{\partial y^2} + \frac{\partial^2\psi(\vec{r})}{\partial z^2}$

The parity operator: $\hat{P}\psi(\vec{r}) = \psi(-\vec{r})$

Product of operators

The product of two operators is generally non commutative

i.e., $\hat{A}\hat{B} \neq \hat{B}\hat{A}$

It obeys associative property

$$\hat{A}\hat{B}\hat{C} = \hat{A}(\hat{B}\hat{C}) = (\hat{A}\hat{B})\hat{C}$$

The square of an operator is defined as

$$\hat{A}^2 = \hat{A}\hat{A}$$

so $\hat{A}^2|\psi\rangle = \hat{A}(\hat{A}|\psi\rangle)$

and $\hat{A}^n = \hat{A}\hat{A}^{n-1} = \hat{A}\hat{A}\hat{A}^{n-2} = \underbrace{\hat{A}\hat{A}\hat{A}\cdots\hat{A}}_{n\text{-times}}$

Order does matters when the product $\hat{A}\hat{B}$ operates on ket $|\psi\rangle$

$$\hat{A}\hat{B}|\psi\rangle = \hat{A}(\hat{B}|\psi\rangle)$$

The operator $\hat{B}$ first acts on $|\psi\rangle$ and $\hat{A}$ acts on new ket $(\hat{B}|\psi\rangle)$

The expression $\langle\phi|\hat{A}|\psi\rangle$ = complex number. It can also be purely real number or purely imaginary.

If we apply this operator to a ket $|\psi'\rangle$ we get another ket

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

wher $\langle\psi|\psi'\rangle = a =$ complex number.

○ The products of type $|\psi\rangle\hat{A}$ or $\hat{A}\langle\psi|$ are not allowed as they don't carry any physical meanings. It must be remembered that an operator act on a ket $|\rangle$ from left side and on a bra $\langle|$ from right side.

Hermitioan Adjoint

The Hermitian adjoint of scalars, vectors (bras, kets, inner products) and operators is defined as follows

i) Replace constants by their complex conjugates $a^{+} = a^{*}$

ii) Replace kets with their corresponding bras $|\psi\rangle^{+} = \langle\psi|$

iii) Replace bras by their corresponding kets $(\langle\psi|)^{+} = |\psi\rangle$

iv) Replace operator with their adjoints $(\hat{A})^{+} = \hat{A}^{+}$

For example $\langle\phi|\hat{A}|\psi\rangle^{*} = \langle\psi|\hat{A}^{+}|\phi\rangle$

Note: here the terms "adjoint" and "conjugate" are used indiscriminately.

Properties of Hermitian conjugate rules

$$(\hat{A}^{+})^{+} = \hat{A}$$

$$(a\hat{A})^{+} = a^{*}\hat{A}^{+}$$

$$(\hat{A}^{n})^{+} = (\hat{A}^{+})^{n}$$

$$(\hat{A} + \hat{B} + \hat{C} + \hat{D})^{+} = \hat{A}^{+} + \hat{B}^{+} + \hat{C}^{+} + \hat{D}^{+}$$

$$(\hat{A}\hat{B}\hat{C}\hat{D})^{+} = \hat{D}^{+}\hat{C}^{+}\hat{B}^{+}\hat{A}^{+}$$

$$(\hat{A}\hat{B}\hat{C}\hat{D}|\psi\rangle)^{+} = \langle\psi|\hat{D}^{+}\hat{C}^{+}\hat{B}^{+}\hat{A}^{+}$$

Also $(|\psi\rangle\langle\phi|)^{+} = |\phi\rangle\langle\psi|$

$|a\hat{A}\psi\rangle = a\hat{A}|\psi\rangle$ } very important to note.

& $\langle a\hat{A}\psi| = \hat{a}^{*}\langle\psi|\hat{A}^{+}$

also $\langle a\hat{A}^{+}\psi| = a^{*}\langle\psi|(\hat{A}^{+})^{+} = a^{*}\langle\psi|\hat{A}$

using the above relations we can also write

$$\langle\psi|\hat{A}|\phi\rangle = \langle\psi\hat{A}^{+}|\phi\rangle = \langle\psi|\hat{A}\phi\rangle$$

Hermitian and Skew-Hermitian Operators

An operator $\hat{A}$ is said to be Hermitian, if it is equal to its adjoint i.e,

$$\hat{A}^{\dagger} = \hat{A}$$

Incase of mixed expression

$$\langle \phi | \hat{A} | \psi \rangle^{\dagger} = \langle \psi | \hat{A}^{\dagger} | \phi \rangle \quad \text{or} \quad \langle \psi | \hat{A} | \phi \rangle$$

An operator $\hat{B}$ is said to skew-Hermitian or anti-Hermitian if

$$\hat{B}^{\dagger} = -\hat{B}$$

so

$$\langle \psi | \hat{B} | \phi \rangle = -\langle \phi | \hat{B} | \psi \rangle^{*}$$

It must be remembered that hermitian adjoint of an operator is not equal to its complex conjugate i.e $\hat{A}^{\dagger} \neq \hat{A}^{*}$

Projection Operator

An operator is said to projection operator if it is Hermitian and equal to its square i.e.,

$$\hat{P}^{\dagger} = \hat{P} \quad \& \quad \hat{P}^{2} = \hat{P}$$

e.g; the unit operator $\hat{I}$ is an example of projection operator

$$\hat{I}^{\dagger} = \hat{I} \quad \& \quad \hat{I}^{2} = \hat{I}$$

Propertis of projection operators.

i) The product of two commuting projection operators is also a projection operator. Since

$$(\hat{P}_1 \hat{P}_2)^{\dagger} = \hat{P}_2^{\dagger} \hat{P}_1 = \hat{P}_2 \hat{P}_1 = \hat{P}_1 \hat{P}_2 \quad \because \text{Commuting and Hermitian}$$

$$(\hat{P}_1 \hat{P}_2)^2 = \hat{P}_1 \hat{P}_2 \hat{P}_1 \hat{P}_2 = \hat{P}_1^2 \hat{P}_2^2 = \hat{P}_1 \hat{P}_2 \quad (\text{As } \hat{P}_1 \,\&\, \hat{P}_2 \text{ are projection operators})$$

ii) The sum of two projecting operators is generally not a projection operator.

iii) Two projection operators are said to orthogonal if their product is zero.

iv) For sum of projection operators to be a projection operator i.e $\hat{P} = \hat{P}_1 + \hat{P}_2 + \hat{P}_3 + \dots$, it is necessary and sufficient that all these projection operators are mutually orthogonal.

Example 2.7

Show that the operator $|\psi\rangle\langle\psi|$ is a projection operator only when $|\psi\rangle$ is normalized.

Solution: First property that it is Hermitian $(|\psi\rangle\langle\psi|)^{\dagger} = |\psi\rangle\langle\psi|$

Second property $(\hat{P}^2 = \hat{P})$ i.e $(|\psi\rangle\langle\psi|)^2 = (|\psi\rangle\langle\psi|)(|\psi\rangle\langle\psi|) = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi|$

since $|\psi\rangle$ is normalized i.e $\langle\psi|\psi\rangle = 1$.

Commutator Algebra

The commutation relation between two operators $\hat{A}$ and $\hat{B}$ is reprosted as

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \longrightarrow (a)$$

and the anti-Commutator is given by

$$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$$

Two operators are said to commute, if their commutator is equal to zero. This means that (a) will be equal to zero i.e

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0$$

This relation also leads to

$$\hat{A}\hat{B} = \hat{B}A$$

Examples $\left[x, \frac{\partial}{\partial x}\right] = ?$

$$\left[x, \frac{\partial}{\partial x}\right] = x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x$$

Multiply both sides from right with $\psi(x)$

$$\left[x, \frac{\partial}{\partial x}\right]\psi(x) = \left(x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x\right)\psi(x)$$

$$\left[x, \frac{\partial}{\partial x}\right]\psi(x) = x\frac{\partial \psi}{\partial x} - \frac{\partial}{\partial x}(x\psi(x))$$

$$= x\frac{\partial \psi}{\partial x} - \psi - x\frac{\partial \psi}{\partial x}$$

$$\left[x, \frac{\partial}{\partial x}\right]\psi(x) = -\psi(x)$$

or

$$\left[x, \frac{\partial}{\partial x}\right] = -1$$

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

To prove this we have $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$

so L.H.S

$$\left[\hat{x}, -i\hbar\frac{\partial}{\partial x}\right] = -i\hbar\left[\hat{x}, \frac{\partial}{\partial x}\right] \quad \text{sin} \quad \left[\hat{x}, \frac{\partial}{\partial x}\right] = -1$$

so

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

Similarly $[\hat{y}, \hat{p}_y] = i\hbar$, $[\hat{z}, \hat{p}_z] = i\hbar$

Properties of commutators

i) Antisymmetry $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = -(\hat{B}\hat{A} - \hat{A}\hat{B}) = -[\hat{B},\hat{A}]$

ii) Linearity: $[\hat{A}, \hat{B}+\hat{C}+\hat{D}+\hat{E}+\cdots] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}] + [\hat{A},\hat{D}] + \cdots\cdots$

iii) Hermitian Conjugate: $[\hat{A},\hat{B}]^{\dagger} = [\hat{B}^{\dagger}, \hat{A}^{\dagger}]$

iv) Distributivity: $[\hat{A},\hat{B}\hat{C}] = [\hat{A},\hat{B}]\hat{C} + \hat{B}[\hat{A},\hat{C}]$

$[\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B}$

v) Jacobi identity: $[\hat{A},[\hat{B},\hat{C}]] + [\hat{B},[\hat{C},\hat{A}]] + [\hat{C},[\hat{A},\hat{B}]] = 0$ * using cyclic order

vi) Repeated application of distributivity property we can find general expressions

$$[\hat{A},\hat{B}^n] = \sum_{j=0}^{n-1} \hat{B}^j [\hat{A},\hat{B}] \hat{B}^{n-j-1}$$

&

$$[\hat{A}^n,\hat{B}] = \sum_{j=0}^{n-1} \hat{A}^{n-j-1} [\hat{A},\hat{B}] \hat{A}^j$$

vii) Operators commute with scalars i.e

$$[\hat{A}, a] = 0$$

The Expectaion or Mea Value of an Operator

The expectation or mean value of an operator $\hat{A}$, represented by $\langle \hat{A} \rangle$, w.r.t stat $|\psi\rangle$ is given by

$$\langle \hat{A} \rangle = \frac{\langle \psi|\hat{A}|\psi\rangle}{\langle \psi|\psi\rangle} = \int_{-\infty}^{+\infty} \psi^*(x)\hat{A}\psi(x)dx \Big/ \int_{-\infty}^{+\infty} \psi^*(x)\psi(x)dx$$

If the state $|\psi\rangle$ is normalized i.e., $\langle \psi|\psi\rangle = 1$ then

$$\langle \hat{A} \rangle = \langle \psi|\hat{A}|\psi\rangle$$

Similarly the expectation value of square of an operator i.e $\langle \hat{A}^2 \rangle$ is

$$\langle \hat{A}^2 \rangle = \frac{\langle \psi|\hat{A}^2|\psi\rangle}{\langle \psi|\psi\rangle}$$

Similarly the expectation of momentum operator is

$$\langle \hat{p} \rangle = \frac{\langle \psi|\hat{p}_x|\psi\rangle}{\langle \psi|\psi\rangle} = \frac{\int_{-\infty}^{+\infty} \psi^*(x)\hat{p}_x\psi(x)dx}{\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx} = -i\hbar \frac{\int_{-\infty}^{+\infty} \psi^*(x)\frac{\partial}{\partial x}\psi(x)dx}{\int_{-\infty}^{+\infty} |\psi(x)|^2 dx}$$

Uncertainty Relation Between Two Operators

Using the commutator algebra we can find the uncertainties in the product of two operators $\hat{A}$ and $\hat{B}$ (a formal derivation of Heisenburg's uncertainty relation).
Let $\langle \hat{A} \rangle$ and $\langle \hat{B} \rangle$ denotes the expectation values of two operator $\hat{A}$ and $\hat{B}$. It is further assumed that both the operators are Hermitian i.e $\hat{A}^{\dagger} = \hat{A}$ and $\hat{B}^{\dagger} = \hat{B}$ w.r.t to a normalized state vector $|\psi\rangle$ i.e $\langle \psi|\psi\rangle = 1$. so

$$\langle \hat{A} \rangle = \langle \psi|\hat{A}|\psi\rangle \quad \text{and} \quad \langle \hat{B} \rangle = \langle \psi|\hat{B}|\psi\rangle$$

Introducing $\Delta\hat{A}$ and $\Delta\hat{B}$ as

$$\Delta\hat{A} = \hat{A} - \langle\hat{A}\rangle \quad , \quad \Delta\hat{B} = \hat{B} - \langle\hat{B}\rangle \longrightarrow (1)$$

both expressions in eq.(1) shows the deviation of the measurement of any operator $\hat{A}$ from its mean value $\langle\hat{A}\rangle$.

$$\begin{cases} (a+b)^2 = a^2 + 2ab + b^2 \\ (a-b)^2 = a^2 - 2ab + b^2 \end{cases}$$

Now $(\Delta\hat{A})^2 = \hat{A}^2 - 2\hat{A}\langle A\rangle + \langle\hat{A}\rangle^2$

Similarly $(\Delta B)^2 = \hat{B}^2 - 2\hat{B}\langle\hat{B}\rangle + \langle\hat{B}\rangle^2$

(The expectation value is a scalar i.e a number)

Now taking the expectation values of $(\Delta\hat{A})^2$ and $(\Delta\hat{B})^2$ w.r.t state $|\psi\rangle$

$$\langle\psi|\Delta\hat{A}^2|\psi\rangle = \langle\psi|\hat{A}^2 - 2\hat{A}\langle\hat{A}\rangle + \langle\hat{A}\rangle^2|\psi\rangle$$

$$= \langle\psi|\hat{A}^2|\psi\rangle - 2\langle\hat{A}\rangle\langle\psi|\hat{A}|\psi\rangle + \langle\hat{A}\rangle^2\langle\psi|\psi\rangle$$

$$\langle(\Delta\hat{A})^2\rangle = \langle\hat{A}^2\rangle - 2\langle\hat{A}\rangle\langle\hat{A}\rangle + \langle\hat{A}\rangle^2$$

$$= \langle\hat{A}^2\rangle - 2\langle\hat{A}\rangle^2 + \langle\hat{A}\rangle^2$$

$$\langle(\Delta\hat{A})^2\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$$

similarly

$$\langle(\Delta B)^2\rangle = \langle\hat{B}^2\rangle - \langle\hat{B}\rangle^2$$

or $\Delta A = \sqrt{\langle(\Delta\hat{A})^2\rangle} = \sqrt{\langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2} \longrightarrow (2)$

and $\Delta B = \sqrt{\langle(\Delta B)^2\rangle} = \sqrt{\langle\hat{B}^2\rangle - \langle\hat{B}\rangle^2} \longrightarrow (3)$

Now operating the operators defined by eq(1) on $|\psi\rangle$

$$\left.\begin{aligned} |\chi\rangle &= \Delta A|\psi\rangle = (\hat{A} - \langle\hat{A}\rangle)|\psi\rangle \\ \& \quad |\phi\rangle &= \Delta B|\psi\rangle = (\hat{B} - \langle\hat{B}\rangle)|\psi\rangle \end{aligned}\right\} \longrightarrow (4)$$

The Schwarz inequality for the states $|\chi\rangle$ and $|\phi\rangle$ is given by

$$\langle\chi|\chi\rangle\langle\phi|\phi\rangle \geq |\langle\chi|\phi\rangle|^2 \longrightarrow (5)$$

since $\hat{A}$ and $\hat{B}$ are Hermitian, so $\Delta\hat{A}$ and $\Delta\hat{B}$ must also be Hermitian i.e

$$\Delta\hat{A}^{\dagger} = \hat{A}^{\dagger} - \langle\hat{A}\rangle = \hat{A} - \langle\hat{A}\rangle$$

and

$$\Delta\hat{B}^{\dagger} = \hat{B}^{\dagger} - \langle\hat{B}\rangle = \hat{B} - \langle\hat{B}\rangle$$

using this along with eq.(4) we can show that

$$\langle\chi|\psi\rangle = \langle\psi|(\Delta\hat{A})^2|\psi\rangle$$

As $\langle\chi|\chi\rangle = (\langle\psi|(\hat{A}^{\dagger} - \langle\hat{A}\rangle)(\hat{A} - \langle\hat{A}\rangle)|\psi\rangle = (\langle\psi|(\hat{A} - \langle\hat{A}\rangle)((\hat{A} - \langle\hat{A}\rangle)|\psi\rangle$

$$\left.\begin{aligned} \langle\chi|\chi\rangle &= \langle\psi|\Delta\hat{A}\Delta\hat{A}|\psi\rangle = \langle\psi|(\Delta\hat{A})^2|\psi\rangle = \langle(\Delta\hat{A})^2\rangle \\ \text{Similarly } \langle\phi|\phi\rangle &= \langle\psi|\Delta\hat{B}\Delta\hat{B}|\psi\rangle = \langle\psi|(\Delta\hat{B})^2|\psi\rangle = \langle(\Delta\hat{B})^2\rangle \\ \langle\chi|\phi\rangle &= \langle\psi|\Delta\hat{A}\Delta\hat{B}|\psi\rangle = \langle(\Delta\hat{A}\Delta\hat{B})\rangle \end{aligned}\right\} \longrightarrow (6)$$

So Schwarz inequality can be written as

$$\langle (\Delta\hat{A})^2\rangle \langle (\Delta\hat{B})^2\rangle \geq |\langle \Delta\hat{A}\Delta\hat{B}\rangle|^2 \longrightarrow (7)$$

we can write the term on the R.H.S as

$$\Delta\hat{A}\Delta\hat{B} = \frac{1}{2}[\Delta\hat{A}, \Delta\hat{B}] + \frac{1}{2}\{\Delta\hat{A}, \Delta\hat{B}\}$$

(see the properties of Hermitian and anti-Hermitian operators in commutator topic)

$$= \frac{1}{2}[\hat{A}, \hat{B}] + \frac{1}{2}\{\Delta\hat{A}, \Delta\hat{B}\} \longrightarrow (8)$$

Since $[\hat{A}, \hat{B}]$ is anti-Hermitian and $\{\Delta\hat{A}, \Delta\hat{B}\}$ is Hermitian, as the expectation value of an anti-Hermitian operator is purely imaginary and that of Hermitian operator is real. The expectation value of $\Delta\hat{A}\Delta\hat{B}$ in equation (8) becomes equal to the sum of real part $\frac{\langle\{\Delta\hat{A}, \Delta\hat{B}\}\rangle}{2}$ and imaginary part $\langle[\hat{A}, \hat{B}]\rangle/2$, so

$$|\langle \Delta\hat{A}\Delta\hat{B}\rangle|^2 = \frac{1}{4}|\langle[\hat{A}, \hat{B}]\rangle|^2 + \frac{1}{4}|\langle\{\Delta\hat{A}, \Delta\hat{B}\}\rangle|^2$$

the last term is merely a positive real number, so we can write

$$|\langle \Delta\hat{A}\Delta\hat{B}\rangle|^2 \geq \frac{1}{4}|\langle[\hat{A}, \hat{B}]\rangle|^2 \longrightarrow (9)$$

Comparing eqns. (7) & (9) we have

$$\langle (\Delta\hat{A})^2\rangle \langle (\Delta\hat{B})^2\rangle \geq \frac{1}{4}|\langle[\hat{A}, \hat{B}]\rangle|^2$$

Taking the square root on both sides, we get

$$\boxed{\Delta A \Delta B \geq \frac{1}{2}|\langle[\hat{A}, \hat{B}]\rangle|}$$

This uncertainty relation plays an important role in the formalism of quantum mechanics.