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QUANTUM MECHANICS

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Chapter - 1

The Linear Vector Space

The Linear Vector Space: A linear vector space consists of a set of vectors $(|\Psi\rangle, |\phi\rangle, |\xi\rangle)$ & a set of scalars $(a, b, c, \ldots\ldots)$ which is closed under two operations:

(i) Vector addition

(ii) Scalar multiplication

Vector Addition

→ If $|\Psi\rangle$&$|\phi\rangle$ are two vectors of a LVS then their sum is also a vector of the same LVS

→ Commutativity: $|\Psi\rangle + |\phi\rangle = |\phi\rangle + |\Psi\rangle$

→ Associativity: $(|\Psi\rangle + |\phi\rangle) + |\xi\rangle = |\Psi\rangle + (|\phi\rangle + |\xi\rangle)$

→ Existance of zero or Null vector: For every vector $|\Psi\rangle$ there must exist a zero vector $|0\rangle$such that $|\Psi\rangle + |-\Psi\rangle = 0$

Scalar Multiplication

Multiplication of vectors by scalars has these following properties:

→ The product of a scalar with a vector gives another vector from the same LVS.

$$a|\Psi\rangle = |\phi\rangle$$

In general if $|\Psi\rangle$ & $|\phi\rangle$ are two vectors of the space, any linear combination $a|\Psi\rangle + b|\phi\rangle$ is also a vector of the same space, a & b being scalars.

→ Scalar multiplication is distributive with respect to vector addition $(a[|\Psi\rangle + |\phi\rangle] = a|\Psi\rangle + a|\phi\rangle)$ & scalar addition $([a + b]|\Psi\rangle + a|\Psi\rangle + b|\Psi\rangle)$

→ Associativity with respect to ordinary multiplication of scalars

$$a(b|\Psi\rangle) = (ab)|\Psi\rangle$$

→ Multiplication by the scalars 0 & 1 has the effect you would expect

$$0|\Psi\rangle = |0\rangle \;\&\; 1|\Psi\rangle = |\Psi\rangle$$

The Hilbert Space:- A Hilbert space consists of a set of vectors $(|\Psi\rangle, |\phi\rangle, |\xi\rangle \ldots.)$ & a set of scalars (a, b,c ,….) which satisfy the following four properties

(A) A Hilbert space is a linear vector space

(B) Hilbert space has a defined scalar product (also known as inner product)

(C) Hilbert space is separable

(D) Hilbert space is complete i.e. any Cauchy sequence of elements in Hilbert space converges to an element that also belongs to the Hilbert space.

Dirac's Bra-ket Notation

Dirac denoted the vectors of a Hilbert space by the sign $|\Psi\rangle$ which he called a ket-vector or simply a ket.

As we know from linear algebra that corresponding to every vector space there exists a dual vector space. Dirac denoted the elements of a dual vector space by the symbol $\langle\Psi|$. Which he called a bra-vector or simply a bra. We postulate that corresponding to every ket$|\Psi\rangle$ in Hilbert space there exists a bra to the $\langle\Psi|$ in dual Hilbert space. Therefore kets belong to the Hilbert space H & the correspond bras belong to the dual Hilbert space H_D.

There is a one to one correspondence between ket space (Hilbert space) & Bra space (dual Hilbert space)

$$|\Psi\rangle \overleftrightarrow{DC} \langle\Psi|$$

$$a|\Psi\rangle + b|\phi\rangle \overleftrightarrow{DC} \quad a^*\langle\Psi| + b^*\langle\phi|$$

$$a|\Psi\rangle = |\mathrm{a}\Psi\rangle$$

$$\langle\mathrm{a}\Psi| = a^*\langle\Psi|$$

Inner product:- We now define inner product of a bra & a ket. The product is written as a bra standing on the left & a ket standing on the right. For example

$$\langle\Psi|\phi\rangle = (\langle\Psi|).(|\phi\rangle)$$

Bra ket

The product is in general a complex number. Notice that in forming an inner product we always take one vector from the bra space & one vector from the ket space.

Properties

$\rightarrow \langle\Psi|\phi\rangle = \langle\phi|\Psi\rangle^*$

Therefore $\langle\Psi|\phi\rangle$&$\langle\phi|\Psi\rangle$ are complex conjugate of each other.

$\rightarrow\ \langle\Psi|\Psi\rangle \geq 0$ and Real

Where the equality sign holds only if $|\Psi\rangle$ is a null ket. This property is known as the postulate of positive definite metric. From a physicist's point of view this postulate is essential for the probabilistic interpretation of quantum mechanics

Given a ket $|\Psi\rangle$ is not a null ket, we can form a normalized ket $|\widetilde{\Psi}\rangle$ where $|\widetilde{\Psi}\rangle = \frac{|\Psi\rangle}{\sqrt{\langle\Psi|\Psi\rangle}}$. Quite generally $\sqrt{\langle\Psi|\Psi\rangle}$ is known as the norm of $|\Psi\rangle$ analogous to the magnitude of a vector in Euclidean vector space

→ Sechwarz inequality: $|\langle\Psi|\phi\rangle|^2 \leq \langle\phi|\phi\rangle$ if $|\Psi\rangle$&$|\phi\rangle$ are linearly dependent ($|\Psi\rangle = a|\phi\rangle$) this relation becomes an equality:

→ Triangle inequality: $\sqrt{\langle\Psi+\phi|\Psi+\phi\rangle} \leq \sqrt{\langle\Psi|\Psi\rangle} + \sqrt{\langle\phi|\phi\rangle}$if $|\Psi\rangle$&$|\phi\rangle$ are linearly dependent $|\Psi\rangle = a|\phi\rangle$& the proportionally scalar a is real & positive the triangle inequality becomes an equality meaning of inner product.

$\langle\phi|\Psi\rangle$ means the projection of the ket vector $|\Psi\rangle$ along the direction of the ket vector $|\phi\rangle$.

∴ If $\langle\phi|\Psi\rangle = 0$ then the two kets $|\phi\rangle$&$|\Psi\rangle$ are said to be orthogonal. i.e. there is no projection of one vector along the $[\langle\Psi|\phi\rangle = 0\ implies\ \langle\phi|\Psi\rangle = 0]$

Two kets $|\Psi\rangle$ & $|\phi\rangle$ are said to be orthonormal if mutually orthogonal & normalized to unity $\langle\Psi|\phi\rangle = 0$; $\langle\Psi|\Psi\rangle = 1$; $\langle\phi|\phi\rangle = 1$

A set of vectors $\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle \ldots\ldots |\phi_N\rangle\}$ in a vector space v is said to be linearly independent if the only possible solution of the equation

$$\sum_{n=1}^{N} a_n |\phi_n\rangle = 0 \text{ is } a_1 = a_2 = a_3 = \cdots . = a_N = 0$$

∴ we can say that, a set of vectors $\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, \ldots., |\phi_N\rangle\}$ is said to be linearly independent of none of them can be expressed as a linear combination of the others.

A set of vectors $\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, \ldots\ldots, |\phi_N\rangle\}$ is said to be complete OR is said to span a vector space V if any arbitrary vector $|\Psi\rangle$ belonging to that space can be expressed as a linear combination of the members (elements) of the set.

∴ if $|\Psi\rangle \in V$ then $|\Psi\rangle = \sum_{n=1}^{N} C_n |\phi_n\rangle$

A vector space is said to be N-dimensional & is denoted by V^N if maximum number of linearly independent vectors that can be found in that space is equal to N.

Basis: Any arbitrary non trivial (non-zero) vectors $|\Psi\rangle$ in an N-dimensional vector space V^N can be expressed uniquely as a linear combination of N linearly independent vectors in V^N.

A set of N linearly independent vectors $\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, \ldots., |\phi_n\rangle\}$ is said to form a basis of a vector space V^N if any arbitrary vector belonging to that space can be expressed as a linear combination of the members (elements) of the set.

Therefore a set of linearly independent vectors that spans the vector space is said to form a Basis. Actually the set is called the basis & the elements of the set are called basis vectors. The number of basis vectors in a basis defines the dimension of the vector space.

$\therefore$ If $|\Psi\rangle \in V^N$

Then we can write $|\Psi\rangle = \sum_{n=1}^{N} C_n |\phi_N\rangle$

Where $|\phi_n\rangle$ are the basis vectors $(n = 1,2,3, \ldots . N)$,

$|\Psi\rangle$ any arbitrary vector belonging to V^N

c_n are scalars called the coefficients of expansion of the vector $|\Psi\rangle$ in this basis. More accurately c_n is the projection (component) of the vector $|\Psi\rangle$ along the direction of the vector $|\phi_n\rangle$.

We can find an infinite no. of such sets (called basis) in a vector space each containing exactly N number of basis vectors (N= dimension of the vector space V^N). Therefore, the choice of basis in a vector space is not unique but the number of basis vectors sin any basis of a vector space must be equal to the dimension of a vector space. As for example, we can consider three-dimensional Euclidean space where in an infinite number of basis. Out of them 3 bases are very popular

$$\{\hat{\imath}, \hat{\jmath}, \hat{k}\}; \{\hat{r}, \hat{\theta}, \hat{\phi}\}; \{\hat{p}, \hat{\phi}, \hat{z}\}$$

$\vec{A} = A_x\hat{\imath} + A_y\hat{\jmath} + A_z\hat{k}$where A_x, A_y, A_z are the coeff of expansion in basis $\{\hat{\imath}, \hat{\jmath}, \hat{k}\}$

$\vec{A} = A_r\hat{r} + A_\theta\hat{\theta} + A_\phi\hat{\phi}$ where A_r, A_θ, A_ϕ are the coeff of expansion in basis $\{\hat{r}, \hat{\theta}, \hat{\phi}\}$

$\vec{A} = A_p\hat{p} + A_\phi\hat{\phi} + A_z\hat{z}$ where A_p, A_ϕ, A_z are the coeff of expansion in basis $\{\hat{p}, \hat{\phi}, \hat{z}\}$

There the choice of Basis in a vector space is not unique but the expansion of a vector in a given basis is unique.

Singular → Basis

Plural → Bases

Of course there are infinite number of bases in a given vector space but the expansion of a vector in terms of a given basis is unique.

If the dimension N of a vector space V^N is finite the space is called finite dimensional but if N is infinite then the space is called infinite dimensional vector space.

In a finite dimensional vector space V^N every basis has the same number of elements Also any linearly independent set of N vectors would form a basis. These properties are not shared by infinite dimensional spaces: any linearly independent set having infinite number of elements is not a basis in such a space.

Let the set $\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, \ldots\ldots, |\phi_N\rangle\}$ forms a basis of the vector space V^N then we can represent this basis set as $\{|\phi_n\rangle\}$

Let me tell you – Every physical state of a quantum mechanical system can be represented by a vector (called state vector) belonging to an abstract vector space called state space or ket space of the system. Any vector of this vector or simply ket& is represented by the symbol "$1\rangle$" inside which is placed a distinctive sign which enables us to distinguish the corresponding ket from all others, for example $|\Psi\rangle$.

Now if $|\Psi\rangle$ represent a certain physical state of the quantum mechanical system then $c|\Psi\rangle$ represents the same physical state of the quantum mechanical system, where c = non-zero complex quantity. $c|\Psi\rangle = |\Psi\rangle c$

If c = zero the $c|\Psi\rangle$ is a null ket.

If $|\Psi\rangle$ represents a particular state of the system

& $|\phi\rangle$ represents another state of the system

Then $|\xi\rangle = a|\Psi\rangle + b|\phi\rangle$ also represents a state of the system different from $|\Psi\rangle$&$|\phi\rangle$. Therefore $|\xi\rangle$ belongs to the same state space (as we also have seen this in the properties of LVS)

Discrete Basis: A set of ket vectors (discrete) $\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, \ldots., |\phi_N\rangle\}$ is said to be orthonormal if $\langle\phi_m|\phi_n\rangle = \delta_{mn}$

Where $\delta_{mn} = \begin{matrix} 1 & for & m = n \\ 0 & for & m \neq n \end{matrix}\Big\}$ ⇒Kronecker delta

A set of discrete orthonormal kets is said to form a basis in the Hilbert space if any arbitrary ket can be represented as a linear combination of them.

$$|\Psi\rangle = \sum_{n=1}^{N} c_n |\phi_n\rangle$$

$$\Rightarrow \langle\phi_m|\Psi\rangle = \sum_{n=1}^{N} c_n \langle\phi_m|\phi_n\rangle = \sum_{n=1}^{N} c_n \delta_{mn} = c_m$$

$$\therefore |\Psi\rangle = \sum_{n=1}^{N} (\langle\phi_n|\Psi\rangle) \Rightarrow \sum_{n=1}^{N} |\phi_n\rangle (\langle\phi_n|\Psi\rangle)$$

$$= \left\{\sum_{n=1}^{N} |\phi_n\rangle \langle\phi_n|\right\} |\Psi\rangle$$

$$\therefore \sum_{n=1}^{N} |\phi_n\rangle \langle\phi_n| = \hat{I}$$

This relation is known as completeness relation or closure in discrete basis.

Continuous basis:- A set of linearly independent vectors $\{|\phi_\alpha\rangle\}$ is said to form a complete orthonormal basis in the Hilbert space if any arbitrary ket belonging to that Hilbert space can be written as a linear combination of them.

$$|\Psi\rangle = \int c(\alpha) |\phi_\alpha\rangle d\alpha$$

& orthonormality⇒ $\langle\phi_{\alpha'}|\phi_\alpha\rangle = \delta(\alpha - \alpha')$Dirac's delta it can be seen that for a continuous basis $\langle\phi_\alpha|\phi_\alpha\rangle$ doesn't exist: The $|\phi_\alpha\rangle$ has an infinite norm & therefore doesn't belong to the Hilbert space. But a linear combination of these basis kets is normalized, hence the vectors of the Hilbert space can still be expanded over the basis $\{|\phi_\alpha\rangle\}$.

$$\therefore |\Psi\rangle = \int c(\alpha) |\phi_\alpha\rangle d\alpha$$

$$\Rightarrow \langle\phi_{\alpha'}|\Psi\rangle\rangle = \int c(\alpha) \langle\phi_{\alpha'}|\langle\phi_\alpha\rangle\rangle d\alpha$$

$$= \int c(\alpha) \delta(\alpha - \alpha') d\alpha = c(\alpha')$$

$$\therefore |\Psi\rangle = \int \langle\phi_\alpha|\Psi\rangle |\phi_\alpha\rangle d\alpha$$

$$= \int |\phi_\alpha\rangle \langle\phi_\alpha|\Psi\rangle d\alpha = \left\{\int |\phi_\alpha\rangle \langle\phi_\alpha| d\alpha\right\} |\Psi\rangle$$

$$\therefore \int |\phi_\alpha\rangle \langle\phi_\alpha| d\alpha = \hat{I}$$

This relation is known as completeness relation or closure in continuous basis

Operators

An operator A is a mathematical rule that when applied to a ket$|\Psi\rangle$ transforms it into another ket $|\phi\rangle$ of the same space & when it acts on a bra $\langle\xi|$ transoforms it into another bra $\langle x|$ of the same Dual-space.

$\hat{A}|\Psi\rangle = |\phi\rangle \qquad \langle\xi|\hat{A} = \langle x|$

An operator acts on a ket from the left side & acts on a bra from the right side

Examples:-

(1) Identity operates: It operates on a ket& returns the same ket$\hat{I}|\Psi\rangle = |\Psi\rangle$

(2) null operator: If for any arbitrary ket$|\Psi\rangle\hat{A}|\Psi\rangle = 0$ then $\hat{A}$ is a null operator

(3) parity operator: $\hat{\pi}\Psi(\vec{r}) = \Psi(-\vec{r})$

Properties of Operators:

→ Operators can be added; addition operations are commutative & associative

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

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

→ Product of two operators in general not commutative in nature $\hat{A}\hat{B} \neq \hat{B}\hat{A}$. Howeverproduct of operators is associate

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

→ When product $\hat{A}\hat{B}$ operates on a ket $|\Psi\rangle$ (the order of application is important), the operator $\hat{B}$ acts first on $|\Psi\rangle$& then $\hat{A}$ acts on the new ket $(\hat{B}|\Psi\rangle)$

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

→ When an operator $\hat{A}$ is sandwiched between a bra $\langle\phi|$& a ket $|\Psi\rangle$, it yields in general a complex number: $\langle\phi|\hat{A}|\Psi\rangle =$ complex quantity. In evaluating $\langle\phi|\hat{A}|\Psi\rangle$ it doesn't matter if one first applies $\hat{A}$ to the ket then takes the bra-ket or one first applies $\hat{A}$ to the bra & then takes the bra-ket.

$\therefore \langle\phi|A|\Psi\rangle = (\langle\phi|\hat{A})|\Psi\rangle = \langle\phi|(\hat{A}|\Psi\rangle)$

$\rightarrow \hat{A}^m + \hat{A}^n = \hat{A}^{m+n}$

Linear Operators:- AN operator $\hat{A}$ is said to be linear of for any arbitrary kets$|\Psi_1\rangle$&$|\Psi_2\rangle$& for any complex numbers a_1& a_2

$$\hat{A}(a_1|\Psi_1\rangle + a_2|\Psi_2\rangle) = a_1\hat{A}|\Psi_1\rangle + a_2\hat{A}|\Psi_2\rangle$$

Note:- The quantity $|\phi\rangle\langle\Psi|$ is a linear operator in Dirac's notation known as outer product. When $|\phi\rangle\langle\Psi|$ is applied to a ket $|\xi\rangle$ we obtain another ket along the direction of $|\phi\rangle$

$$(|\phi\rangle\langle\Psi|)|\xi\rangle = |\phi\rangle\langle\Psi|\xi\rangle = \langle\Psi|\xi\rangle|\phi\rangle$$

& when$|\phi\rangle\langle\Psi|$ is applied to a bra $\langle\xi|$ we obtain another bra along the direction of

$$\langle\xi|(|\phi\rangle\langle\Psi|) = \langle\xi|\phi\rangle\langle\Psi|$$

(2) Products of types $|\phi\rangle\hat{A}$ or $\hat{A}\langle\phi|$ are forbidden they hold no physical meanings.

Hermitian Adjoint:- The Hermitian Adjoint of a complex number a is the complex conjugate of this number: $a^+ = a^*$. The hermitian adjoint of an operator $\hat{A}$ is $\hat{A}^+$& is defined by the relation

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

Therefore:

(1) $\left(\hat{A}^{+}\right)^{+} = \hat{A}$

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

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

(4) $(|\phi\rangle\langle\Psi|)^{+} = |\Psi\rangle\langle\phi|$

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

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

(7) $\hat{A}|\Psi\rangle = \left|\hat{A}\Psi\right\rangle$

(8) $\left(\hat{A}|\Psi\rangle\right)^{+} = \langle\Psi|\hat{A}^{+} = \left\langle\hat{A}\Psi\right|$

(9) $\langle\Psi|A|\phi\rangle = \langle A^{+}|\Psi|\phi\rangle = \left\langle\Psi\middle|\hat{A}\middle|\phi\right\rangle$

(10) $[\exp(\lambda AB)]^{+} = \exp(\lambda^{*}B^{+}A^{+})$

Eigenvalues & eigenvectors of an operators:

If an operator $\hat{A}$ operates on a ket $|\Psi\rangle$ & returns the same ket $|\Psi\rangle$ with a multiplicative scalar λ then we say that $|\Psi\rangle$ is an eigenvector of $\hat{A}$ with eigenvalues λ

$$\hat{A}|\Psi\rangle = \lambda|\Psi\rangle$$

- If corresponding to a certain eigenvalue of an operator there exists only one linearly independent eigenvector then that eigenvalue is said to be non-degenerate.
- If corresponding to a certain eigenvalue of an operator there exists n number of linearly independent eigenvectors then that eigenvalues is said to be degenerate with the degree of degeneracy n.
- The collection of all the eigenvalues of an operator is called its spectrum.
- If $\hat{A}|\Psi\rangle = \lambda|\Psi\rangle$ then it implies that $\hat{A}^{n}|\Psi\rangle = \lambda^{n}|\Psi\rangle$ and $F\left(\hat{A}\right)|\Psi\rangle = F(\lambda)|\Psi\rangle$
  for instance, we have $\hat{A}|\Psi\rangle = \lambda|\Psi\rangle$
  $\Rightarrow e^{i\hat{A}}|\Psi\rangle = e^{i\lambda}|\Psi\rangle$

Commutator Algebra:

The commutator of two operators $\hat{A}\&\hat{B}$ is defined as $\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}$

The anti-commutator of two operators $\hat{A}\&\hat{B}$ is defined as $\left\{\hat{A},\hat{B}\right\} = \hat{A}\hat{B} + \hat{B}\hat{A}$

Properties of Commutators:

If $\hat{A}$ & $\hat{B}$ are two linear operators then,

(1) $[A,B] = \hat{A}\hat{B} - \hat{B}\hat{A} = -\left[\hat{B},\hat{A}\right]$

(2) $\left[\hat{A},\hat{B}+\hat{C}\right] = \left[\hat{A},\hat{B}\right] + \left[\hat{A},\hat{C}\right]$

(3) $\left[k\hat{A},\hat{B}\right] = \left[\hat{A},k\hat{B}\right] = k\left[\hat{A},\hat{B}\right]$

(4) $[A+B,C] = \left[\hat{A},\hat{C}\right] + \left[\hat{B},\hat{C}\right]$

(5) $\left[\hat{A},\hat{B},\hat{C}\right] = \left[\hat{A},\hat{B}\right]\hat{C} + \hat{B}[A,C]$

(6) $\left[\hat{A},\hat{B},\hat{C}\right] = [A,C]B + A\left[\hat{B},\hat{C}\right]$

(7) $\left[\hat{A},\hat{B}\hat{C}\hat{D}\right] = \left[\hat{A},\hat{B}\right]\hat{C}\hat{D} + \hat{B}\left[\hat{A},\hat{C}\hat{D}\right] = [A,B]\hat{C}\hat{D} + \hat{B}\left[\hat{A},\hat{C}\right]\hat{D} + \hat{B}\hat{C}\left[\hat{A},\hat{D}\right]$

(8) $\left[\hat{A}\hat{B},\hat{C}\hat{D}\right] = [AB,C]D = C[AB,D] = [A,C]BD + \hat{A}\left[\hat{B},\hat{C}\right]\hat{D} + \hat{C}\left[\hat{A},\hat{D}\right]\hat{B} + \hat{C}\hat{A}\left[\hat{B},\hat{D}\right]$

(9) $\left[\hat{A},\hat{A}\right] = 0$

(10) $\left[\hat{A},\hat{C}\right]=0$ (where c is a constant number)

(11) $\left[\hat{A},F\left(\hat{A}\right)\right]=0$

(12) $\left[F\left(\hat{A}\right),G\left(\hat{A}\right)\right]=0$

(13) If $[A,B]=0\Rightarrow[B,F(A)]=0$

Hermitian Operator:-

An operator $\hat{A}$ is said to be Hermitian

If $\hat{A}=\hat{A}^{+}$ or $\langle\phi|A|\Psi\rangle=\langle\phi|A^{+}|\Psi\rangle=\langle A|\phi|\Psi\rangle=\langle\Psi|A|\phi\rangle^{*}$

Theorem 1 The eigenvalues of a Hermitian operator are real. Let $\hat{A}$ be a hermitian operator $\left(\hat{A}^{+}=\hat{A}\right)$. If $|\Psi_n\rangle$ be an eigenvector of the operator $\hat{A}$ with eigenvalue a_n then, $\hat{A}|\Psi_n\rangle=a_n|\Psi_n\rangle\rightarrow(1)$

Taking hermitian conjugate of equation (1)

$$|\Psi_n\rangle\hat{A}^{+}=a_n^{*}\langle\Psi_n|$$

$\Rightarrow\langle\Psi_n|\hat{A}=a_n^{*}\langle\Psi_n|$ ..... (2)

Multiplying $\langle\Psi_n|$ from left side of eq. (1) we get

$\left\langle\Psi_n\middle|\hat{A}\middle|\Psi_n\right\rangle=a_n\langle\Psi_n|\Psi_n\rangle$ .... (3)

Multiplying $|\Psi_n\rangle$ from right side of eq (2) we get

$$\langle\Psi_n|A|\Psi_n\rangle=a_n^{*}\langle\Psi_n|\Psi_n\rangle=0$$

If $|\Psi_n\rangle$ is not a null ket then $\langle\Psi_n|\Psi_n\rangle>0$

If $|\Psi_n\rangle$ is not a null ket then $\langle\Psi_n|\Psi_n\rangle>0$

$\therefore a_n=a_n^{*}$ $\therefore$ all eigenvalues of $\hat{A}$ are real.

Theorem 2 Eigenvectors of a hermitian operator corresponding to different eigenvalues are mutually orthogonal.

Let $|\Psi_m\rangle$ and $|\Psi_n\rangle$ are two eigenvectors of a hermitian operator $\hat{A}$ corresponding to the eigenvalues a_m&a_n respectively.

Here $a_m\neq a_n$&$\hat{A}^{+}=\hat{A}\hat{A}|\Psi_n\rangle=a_n|\Psi_n\rangle\rightarrow(1)$

$\Rightarrow\langle\Psi_n|\hat{A}^{+}=a_n^{*}\langle\Psi_n|$

$\Rightarrow\langle\Psi_n|\hat{A}=a_n\langle\Psi_n|(\because a_n\ is\ real)$

$\Rightarrow\left\langle\Psi_n\middle|\hat{A}\middle|\Psi_m\right\rangle=a_n\langle\Psi_n|\Psi_m\rangle$ .... (2)

Again, $\hat{A}|\Psi_m\rangle=a_m|\Psi_m\rangle$ .... (3)

$\Rightarrow\left\langle\Psi_n\middle|\hat{A}\middle|\Psi_m\right\rangle=a_m\langle\Psi_n|\Psi_m\rangle$ .... (4)

From equations (2) & (4) we get

$$(a_m-a_n)\langle\Psi_n|\Psi_m\rangle=0$$

$\because a_m\neq a_n\therefore(a_m-a_n)\neq0$ so $\langle\Psi_n|\Psi_m\rangle=0$

$\therefore$ eigenvectors of a Hermitian operator corresponding to different eigenvalues are mutually orthogonal.

NOTE: what can we infer about the eigenvectors of a Hermitian operator corresponding to the same eigenvalue are degenerate states mutually orthogonal. Well the answer is they may be orthogonal or may not be orthogonal. If they are not you can always make them orthogonal by using Gram-Schmidt orthonormalization procedure.

Theorem 3 The eigenvectors of a hermitian operator from a complete orthonormal basis of the Hilbert space. And this basis is known as the eigenbasis of this operator. The matrix representation of this operator in its own eigenbasis is a diagonal matrix with the elements in the principal diagonal as its eigenvalues.

This eigenbasis is unique if the operator has no degenerate eigenvalues & not unique (infact it is infinite) if there is any degeneracy.

Theorem 4. If $\hat{A}\ \&\ \hat{B}$ are two commutating hermitian operators then, any eigenvector of $\hat{A}$ corresponding to a non-degenerate eigenvalue is also an eigenvector of $\hat{B}$

$[\hat{A}, \hat{B}] = 0 \Rightarrow \hat{A}\hat{B} = \hat{B}A$ ..... (1)

Let $|\Psi_n\rangle$ be an eigenvector of $\hat{A}$ corresponding to the non-degenerate eigenvalue a_n

$\hat{A}|\Psi_n\rangle = a_n|\Psi_n\rangle$ ..... (2)

Operating $\hat{B}$ from right side of eq (2) we get

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

$\Rightarrow \hat{A}\hat{B}|\Psi_n\rangle = a_n(\hat{B}|\Psi_n\rangle)$ $[\because \hat{A}\hat{B} = \hat{B}\hat{A}]$

$\Rightarrow \hat{A}(\hat{B}|\Psi_n\rangle) = a_n(\hat{B}|\Psi_n\rangle)$

$\therefore (\hat{B}|\Psi_n\rangle)$ is also a eigenvector of $\hat{A}$ with the same eigenvalue a_n. But since a_n is a non-degenerate eigenvalue so there exists only one linearly independent eigenvector of $\hat{A}$ corresponding to a_n. $\therefore |\Psi_n\rangle$&$\hat{B}|\Psi_n\rangle$ must be linearly dependent

$\therefore \hat{B}|\Psi_n\rangle = \lambda|\Psi_n\rangle$

$\therefore |\Psi_n\rangle$ is also an eigenvector of $\hat{B}$ corresponding to the eigenvalue λ.

Matrix Representation of kets Bras:

Let us consider a set of discrete vectors $\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, \ldots., |\phi_N\rangle\}$ which form a complete orthonormal basis of N-dimensional Hilbert space.

Any arbitrary vector belongingto that basis can be represented in this basis as

$$|\Psi\rangle = \hat{\imath}|\Psi\rangle = \left(\sum_{n=1}^{N}|\phi_n\rangle\langle\phi_n|\right)|\Psi\rangle = \sum_{n=1}^{N}(\langle\phi_n|\Psi\rangle)\,|\phi_n\rangle$$

$$= \sum_{n=1}^{N} c_n\,|\phi_n\rangle$$

$c_n = \langle\phi_n|\Psi\rangle =$ The projection of the vector $|\Psi\rangle$ along the vector $|\phi_n\rangle$ so within the basis $\{|\phi_n\rangle\}$ the ket $|\Psi\rangle$ is represented by the set of its components c_1, c_2, c_3.....

Along $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle$..... respectively.

$$\therefore |\Psi\rangle = \begin{bmatrix}\langle\phi_1|\Psi\rangle\\ \langle\phi_2|\Psi\rangle\\ \langle\phi_3|\Psi\rangle\\ \vdots\\ \langle\phi_N|\Psi\rangle\end{bmatrix}_{N\times 1} = \begin{bmatrix}c_1\\ c_2\\ c_3\\ \vdots\\ c_N\end{bmatrix}_{N\times 1}$$

Bra $\langle\Psi|$ can be represented by a row vector $\langle\Psi| = (|\Psi\rangle)^+$

$\therefore \langle\Psi_1| = [\langle\phi_1|\Psi\rangle^*\langle\phi_2|\Psi\rangle^* \ldots..\langle\phi_N|\Psi\rangle^*]_{1\times N}$

$= [c_1^*, c_2^*, c_3^*, , \ldots\ldots., c_N^*]_{1\times N}$

Matrix Representation of an operator in the basis $\{|\phi_n\rangle\}$

For each linear operator $\hat{A}$ we can write

$$\hat{A} = \hat{I}\hat{A}\hat{I} = \left(\sum_{m=1}^{N}|\phi_m\rangle|\phi_m\rangle\right)\hat{A}\left(\sum_{n=1}^{N}|\phi_n\rangle\langle\phi_n|\right)$$

$$= \sum_{m=1}^{N}\sum_{n=1}^{N}|\phi_m\rangle\langle\phi_m|\hat{A}|\phi_n\rangle\langle\phi_n| = \sum_{m=1}^{N}\sum_{n=1}^{N}\langle\phi_m|A|\phi_n\rangle\,|\phi_m\rangle\langle\phi_n|$$

$$= \sum_{m=1}^{N}\sum_{n=1}^{N}A_{mn}\,|\phi_m\rangle\langle\phi_n|$$

Where $A_{mn} = \langle\phi_m|\hat{A}|\phi_n\rangle$

Is the element of the matrix belonging to mth row & nth columns.

Let $\{|\phi_1\rangle, |\phi_2\rangle\}$ form a complete orthonormal basis of a two-dimensional Hilbert space where $|\phi_1\rangle = \binom{1}{0}$&$|\phi_2\rangle = \binom{0}{1}$

$$\therefore \hat{A} = \sum_{m=1}^{N}\left(\sum_{n=1}^{N} A_{mn}\,|\phi_m\rangle|\phi_n\rangle\right) = \sum_{m=1}^{N}\left(A_{m_1}|\phi_m\rangle\langle\phi_1| + A_{m_2}|\phi_m\rangle\langle\phi_2|\right)$$

$$= A_{11}|\phi_1\rangle\langle\phi_2| + A_{12}|\phi_1\rangle\langle\phi_2| + A_{21}|\phi_2\rangle\langle\phi_1| + A_{22}|\phi_2\rangle\langle\phi_2|$$

$$= A_{11}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} + A_{12}\begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix} + A_{21}\begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix} + A_{22}\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}$$

$$= \begin{bmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{bmatrix}$$

Q. Prove that matrix Representation of an operator $\hat{A}$in its own eigen basis is a diagonal matrix with the elements in the principal diagonal is its eigenvalues.

$$\hat{A}|\phi_n\rangle = a_n|\phi_n\rangle\langle\phi_m|\phi_n\rangle = \delta_{mn}$$

$$\hat{A} = \hat{I}\hat{A}\hat{I} = \left(\sum\nolimits_{m=1}^{N}|\phi_m\rangle\langle\phi_n|\right)\hat{A}\left(\sum_{n=1}^{N}|\phi_n\rangle\langle\phi_n|\right)$$

$$= \sum_{m=1}^{N}\sum_{n=1}^{N}\langle\phi_m|\hat{A}|\phi_n\rangle\,(|\phi_m\rangle\langle\phi_n|) = \sum_{m=1}^{N}\sum_{n=1}^{N} a_n\,\delta_{mn}|\phi_m\rangle\langle\phi_n|$$

$$= \sum_{m=1}^{N} a_m\,(|\phi_m\rangle\langle\phi_m|)$$

This represents a diagonal matrix with a_m as the diagonal elements.

Projection operator: An operator $\hat{p}$ is said to be a projection operator if its Hermitian$(\hat{p}^+ = \hat{p})$& idempotent $(\hat{p}^2 = \hat{p})$.

Q. Show that $|\Psi\rangle\langle\Psi|$ is a projection operator only if $|\Psi\rangle$ is normalized

Solution:-$\hat{p} = |\Psi\rangle\langle\Psi|$

$\therefore \hat{p}^+ = (|\Psi\rangle\langle\Psi|)^+ = (\langle\Psi|)^+(|\Psi\rangle)^+ = |\Psi\rangle\langle\Psi| = \hat{p}$

$\hat{p}^2 = \hat{p}.\hat{p} = (|\Psi\rangle\langle\Psi|).(|\Psi\rangle\langle\Psi|) = |\Psi\rangle(\langle\Psi||\Psi\rangle)\langle\Psi|$

$= |\Psi\rangle\langle\Psi|(\because \langle\Psi|\Psi\rangle = 1)$

$= \hat{p}$

Since $\hat{p}$ is hermitian & idempotent so $\hat{p}$ is a projection operator.

Example: Let us consider $\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, |\phi_4\rangle\}$forms a complete orthonormal basis in 4-dimensional Hilbert space. Therefore any arbitrary vector $|\Psi\rangle$ be written as a linear combination of these four basis vectors: $|\Psi\rangle = \sum_{n=1}^{4} c_n\,|\phi_n\rangle$

Then $\hat{p} = |\phi_2\rangle\langle\phi_2|$ is a projection vectors as $\hat{p}|\Psi\rangle = c_2|\phi_2\rangle$

$\hat{p}$ when operates on $|\Psi\rangle$ it picks out the component (or projection) of $|\Psi\rangle$ along the direction of the vector $|\phi_2\rangle$.

Properties of Projection Operator:

(1) The product of two commutating projection operators $\hat{p}_1$&$\hat{p}_2$ is also projection operator.

(2) Two projection operators are said to be orthogonal if their product is zero.

$\therefore \hat{p}_1 \perp \hat{p}_2$ if $\hat{p}_1.\hat{p}_2 = (|\Psi\rangle\langle\Psi|)(|\phi\rangle\langle\phi|)$

$= |\Psi\rangle(\langle\Psi||\phi\rangle)\langle\phi| = 0$

$\hat{p}_1 = |\Psi\rangle\langle\Psi|$

$\hat{p}_2 = |\phi\rangle\langle\phi|$ i.e. if $\langle\Psi|\phi\rangle = 0$

(3) For a sum of projection operators $\hat{p}_1 + \hat{p}_2 + \hat{p}_3 + \cdots$ to be a projection operator it is necessary & sufficient that these projection operators be mutually orthogonal.

Eigenvalues & Eigenvectors of a projection operator Let $|\Psi\rangle$ is an eigenvector of the projection operator $\hat{p}(= |\phi\rangle\langle\phi|)$ with eigenvalue λ. Then