Chapter 1

Tools of Quantum Mechanics

4. Operators and Matrices

An operator $\hat{A}$ is the mathematical rule that when applied to a ket $|\phi\rangle$ will transformed into another $|\psi\rangle$ of the same space and when it acts on a any bra $\langle\chi|$ it transforms it into another bra $\langle\phi|$. that means $\hat{A}|\phi\rangle = |\psi\rangle$ and $\langle\chi|\hat{A} = \langle\phi|$

Similar definition is also applied on function as $\hat{A}\phi(r) = \psi(r)$

Basic example of operators Example of Operator:

Identity operator $I|\psi\rangle = |\psi\rangle$

Parity operator $\pi|\psi(r)\rangle = |\psi(-r)\rangle$

Gradient operator $\nabla\psi(r)$

Linear momentum operator $P(\psi\rangle = -i\hbar\nabla\psi(\vec{r})$

Linear Operator: $\hat{A}$ is linear operator if

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

$\hat{A}\left(c|\phi\rangle\right)=c\hat{A}|\phi\rangle$

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

$\hat{A}(a_1|\psi_1\rangle+a_2|\psi_2\rangle=a_1\hat{A}|\psi_1\rangle+a_2\hat{A}|\psi_2\rangle$

$\left(\langle\psi_1|a_1+\langle\psi_2|a_2\right)\hat{A}=\langle\psi_1|\hat{A}a_1+\langle\psi_2|\hat{A}a_2$

If two operators are $\hat{A}$ and $\hat{B}$ then $\hat{A}\hat{B}$ is product of operator**.** Product of two linear operator $\hat{A}$ and $\hat{B}$ written $\hat{A}\hat{B}$ which is defined $(AB)|\psi\rangle=A(B|\psi\rangle)$

In general, $\hat{A}\hat{B}\neq\hat{B}\hat{A}$

Matrix representation of operator Any operator $\hat{A}$ can be represented in square matrix of order $N\times N$ in a basis of $|\phi_1\rangle,|\phi_2\rangle....|\phi_i\rangle....|\phi_j\rangle......|\phi_N\rangle$ with matrix element $A_{i,j}=\langle\phi_i|A|\phi_j\rangle$

Hermitian Adjoint of Operator

If operator $\hat{A}$ is defined as $\hat{A}|\phi\rangle=|\psi\rangle$ then $\langle\phi|\hat{A}^\dagger=\langle\psi|$ where $\hat{A}^\dagger$ is identified as Hermitian conjugate of operator $\hat{A}^\dagger$. Hermitian conjugate $A^\dagger$ of matrix *A* can be find in two step.

Step I: Find transpose of $\hat{A}$ i.e. Convert row into column ie $\hat{A}^T$

Step II: Then take complex conjugate to each element of $\hat{A}^T$ i.e. $\hat{A}^\dagger=\left(\hat{A}^T\right)^*$.

Properties of Hermitian adjoint operator $\hat{A}^\dagger$

- $(\hat{A}^\dagger)^\dagger=\hat{A}$
- $(\hat{A}^n)^\dagger=\left(\hat{A}^\dagger\right)^n$
- $(a\hat{A})^\dagger=a^*\hat{A}^\dagger$
- $(\hat{A}+\hat{B})^\dagger=\hat{A}^\dagger+\hat{B}^\dagger$
- $(\hat{A}\hat{B})^\dagger=\hat{B}^\dagger\hat{A}^\dagger$

Proof of $(\hat{A}\hat{B})^\dagger=\hat{B}^\dagger\hat{A}^\dagger$

Let us assume $\hat{A}\hat{B}|\phi\rangle=|\psi\rangle\Rightarrow\langle\phi|\left(\hat{A}\hat{B}\right)^\dagger=\langle\psi|$

In this process $\hat{B}|\phi\rangle=|\xi\rangle\Rightarrow\langle\phi|\hat{B}^\dagger=\langle\chi|$

$\hat{A}\hat{B}|\phi\rangle=\hat{A}|\chi\rangle=|\psi\rangle\Rightarrow\langle\chi|\hat{A}^\dagger=\langle\psi|\Rightarrow\langle\phi|\hat{B}^\dagger\hat{A}^\dagger=\langle\psi|$ so we can conclude $\left(\hat{A}\hat{B}\right)^\dagger=\hat{B}^\dagger\hat{A}^\dagger$

Eigen value of operator:

If A operator is defined such that $\hat{A}|\phi\rangle = \lambda|\phi\rangle$ then

λ is said to be eigen value and $|\phi\rangle$ is said to be eigen vector corresponding to operator.

$\left(\hat{A}-\lambda\hat{I}\right)|\phi\rangle = 0$, $|\phi\rangle \neq 0$ so $\left|\hat{A}-\lambda\hat{I}\right| = 0$ identify as characteristic equation

The values of λ satisfying the characteristic equation are known as eigen value if λ is non repeated then it is non degenerate eigen value and if λ is repeated then it is degenerate eigen value.

If the $N\times N$ matrix $\rightarrow N$ value of λ

For the given value of $\lambda = \lambda_n$ if any column vector $|\phi_n\rangle$ will satisfy $A|\phi_n\rangle = \lambda_n|\phi_n\rangle$ then $|\phi_n\rangle$ is identified as eigen vector corresponds is eigen value λ_n. In Quantum Mechanics one should always find orthonormal set of eigen vectors such that it can make complete basis. For non-degenerate eigen values one can make unique set of orthonormal eigen state but for degenerate eigen values there may be more than one set of orthonormal vectors.

Hermitian Operators

An operator is said to be Hermitian if Hermitian adjoint is same operators which means $\hat{A}^\dagger = \hat{A}$ i.e., Matrix element $\langle\phi_i|\hat{A}|\phi_j\rangle = (\langle\phi_j|\hat{A}|\phi_i\rangle)^*$ which can be also written as

$$\int_{-\infty}^{\infty}\phi(x)\left(\hat{A}\psi(x)\right)^* dx = \int_{-\infty}^{\infty}\psi^*(x)\hat{A}\phi(x)dx$$

- The eigen values of Hermitian matrix is real

  $\hat{A}|\phi_n\rangle = \lambda_n|\phi_n\rangle \Rightarrow \langle\phi_n|\hat{A}^\dagger = \lambda_n^*\langle\phi_n|$

  Now $\langle\phi_n|\hat{A}|\phi_n\rangle = \lambda_n\langle\phi_n|\phi_n\rangle \Rightarrow \langle\phi_n|\hat{A}^\dagger|\phi_n\rangle = \lambda_n^*\langle\phi_n|\phi_n\rangle$ hence $\hat{A}$ is Hermitian then $\hat{A} = \hat{A}^\dagger$ then $\langle\phi_n|\hat{A}|\phi_n\rangle = \lambda_n\langle\phi_n|\phi_n\rangle \Rightarrow \langle\phi_n|\hat{A}|\phi_n\rangle = \lambda_n^*\langle\phi_n|\phi_n\rangle$ equating both side we will get $\lambda_n = \lambda_n^*$ which means eigen values are real

- The eigen vectors corresponding to different eigen values are orthogonal.

$\hat{A}|\phi_n\rangle = \lambda_n|\phi_n\rangle \Rightarrow \langle\phi_m|\hat{A}|\phi_n\rangle = \lambda_n\langle\phi_m|\phi_n\rangle$

$\hat{A}|\phi_m\rangle = \lambda_m|\phi_m\rangle \Rightarrow \langle\phi_m|\hat{A}^\dagger = \lambda_m^*\langle\phi_m|$ where $m\neq n$ $\Rightarrow \langle\phi_m|\hat{A}^\dagger|\phi_n\rangle = \lambda_m^*\langle\phi_m|\phi_n\rangle$ hence $\hat{A}$ is Hermitian then $\hat{A} = \hat{A}^\dagger$ $\Rightarrow \langle\phi_m|\hat{A}|\phi_n\rangle = \lambda_m^*\langle\phi_m|\phi_n\rangle$

$\langle\phi_m|\hat{A}|\phi_n\rangle - \langle\phi_m|\hat{A}|\phi_n\rangle = \left(\lambda_n-\lambda_m^*\right)\langle\phi_m|\phi_n\rangle \Rightarrow \left(\lambda_n-\lambda_m^*\right)\langle\phi_m|\phi_n\rangle = 0 \quad m\neq n$

so $(\lambda_n \neq \lambda_m^*)$ i.e. $\langle \phi_m | \phi_n \rangle = 0$ which means eigen vectors corresponds to different eigen values are orthogonal

Some important operator and its property

Position Operator $(\hat{X})$**:** Mathematically position operator is defined as $\hat{X}\psi(x) = x\psi(x)$

Momentum Operators$(\hat{P})$**:** It is Mathematically define as $\hat{P} = -i\hbar\nabla$ the eigen value of Momentum operator is momentum

Hamiltonian Operator $(\hat{H})$**:** It is defined as $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(x,y,z)$ The eigen value of Hamiltonian operator is Energy.

Parity Operator $(\hat{\pi})$**:** A Parity Operator (also called **parity inversion**) is the flip in the sign of spatial coordinate In three dimensions, it can also refer to the simultaneous flip in the sign of all three spatial coordinates (a Point reflection).

Mathematically it is defined as $\hat{\pi}\psi(x,y,z) = \psi(-x,-y,-z)$.

If $\hat{\pi}\psi(x,y,z) = \psi(-x,-y,-z) = \psi(x,y,z)$ then wave function is said to be symmetric or even symmetry, so even parity have eigen value 1

If $\hat{\pi}\psi(x,y,z) = \psi(-x,-y,-z) = -\psi(x,y,z)$ then wave function is said to be Antisymmetric symmetric or odd symmetry ,so even parity have eigen value -1

So eigen value of parity is either $+1$ or -1.

Translation Operator $\hat{T}(a)$**:** The translation operator moves particles and fields by the amount a Therefore, if a particle is in an eigen state of the Position operator (i.e., $\psi(x)$ precisely located at the position x then after operating $\hat{T}(a)$ on it, the particle is at the position $x+a$. $\hat{T}\psi(x) = \psi(x+a)$. Momentum operator is generator of translation operator. It is defined as $T = \exp\left(\frac{i\hat{P}_x a}{\hbar}\right)$, where $\hat{P}_x = \frac{\partial}{\partial x}$

$$T\psi(x) = \exp\left(\frac{i\hat{P}_x a}{\hbar}\right)\psi(x) \Rightarrow \exp\left(a\frac{\partial}{\partial x}\right)\psi(x) = \sum_{N=0}^{N}\frac{1}{\lfloor N}\left(a\frac{\partial}{\partial x}\right)^N \psi(x)$$

$$\hat{T}\psi(x) = \psi(x) + a\frac{\partial\psi}{\partial x} + \frac{1}{2}a^2\frac{\partial^2\psi}{\partial x^2}.... = \psi(x+a)$$

Projection operator and completeness relation

If we want to project any vector $|\psi\rangle$ in direction of $|\phi_i\rangle$ then we need projection operator which is define as $\hat{p}_i = |\phi_i\rangle\langle\phi_i|$. In general, $\langle\phi_i|\phi_j\rangle = \delta_{i,j}$

$\hat{p}_i|\psi\rangle = |\phi_i\rangle\langle\phi_i|\psi\rangle = c_i|\phi_i\rangle$ where c_i is complex number.

hence $\langle\phi_i|\phi_i\rangle = 1$ $\hat{p}_i^2 = \hat{p}_i.\hat{p}_i = |\phi_i\rangle\langle\phi_i| = \hat{p}_i \Rightarrow \hat{p}_i^2 = \hat{p}_i \Rightarrow \hat{p}_i = O$ null operator or $p_i = I$ identity operator . so eigen value of projection operator is 0 or 1

if we have $\langle\phi_i|\phi_j\rangle = \delta_{i,j}$ and $\sum_{i=1}^{N} p_i = I \Rightarrow \sum_{i=1}^{N}|\phi_i\rangle\langle\phi_i| = I$ is identify as completeness relation in quantum mechanics. The completeness relation can be use to write any ket vector $|\psi\rangle$ in a orthonormal basis of $|\phi_1\rangle, |\phi_2\rangle ... |\phi_i\rangle ... |\phi_j\rangle .... |\phi_N\rangle$ as $|\psi\rangle = I|\psi\rangle = \sum_{i=1}^{N}|\phi_i\rangle\langle\phi_i|\psi\rangle = |\psi\rangle = \sum_{i=1}^{N} c_i|\phi_i\rangle$

where $\langle\phi_i|\psi\rangle = c_i$

In quantum mechanics orthonormal set of eigen values of Hermitian operators will make complete basis.

Example: If $\hat{A}$ is an operator $\hat{A} = \hat{D}_x + \hat{X}$, where $\hat{D}_x\psi(x) = \frac{d\psi}{dx}$ and $\hat{X}\psi(x) = x\psi(x)$ find equivalent of $\hat{A}^2$.

Solution: $\hat{A}^2 = \left(\hat{D}_x + \hat{X}\right)^2 = \left(\hat{D}_x + \hat{X}\right)\left(\hat{D}_x + \hat{X}\right)$

$$A^2\psi(x) = \left(\frac{d}{dx} + \hat{X}\right)\left(\frac{d}{dx} + \hat{X}\right)\psi(x) = \frac{d^2\psi(x)}{dx} + \hat{X}\frac{d\psi(x)}{dx} + \psi(x) + \frac{\hat{X}d\psi(x)}{dx} + \hat{X}^2\psi(x)$$

$$A^2\psi(x) = \frac{d^2\psi}{dx^2} + 2x\frac{d\psi}{dx} + x^2\psi(x) + \psi(x)$$

$$\Rightarrow A^2 \equiv \frac{d^2}{dx^2} + 2x\frac{d}{dx} + x^2 + 1 \Rightarrow \hat{A}^2 = \hat{D}_x^2 + 2\hat{X}\hat{D}_x + \hat{X}^2 + I$$

Example: If $\hat{D}_x$ is defined as $\frac{\partial}{\partial x}$ and $\psi(x) = A\sin\frac{n\pi x}{a}$

(a) operate $\hat{D}_x$ and $\psi(x)$

(b) operate $\hat{D}_x^2$ on $\psi(x)$

(c) which one of the above given eigen value problem.

Solution: (a) $\hat{D}_x\psi(x)=\frac{\partial}{\partial x}A\sin\frac{n\pi x}{a}=A\frac{n\pi}{a}\cos\frac{n\pi x}{a}$

(b) $\hat{D}_x^2\psi(x)=\frac{\partial^2}{\partial x^2}A\sin\frac{n\pi x}{a}=A\left(-\frac{n^2\pi^2}{a^2}\right)\sin\frac{n\pi x}{a}$

$$\hat{D}_x^2\psi(x)=-\frac{n^2\pi^2}{a^2}A\sin\frac{n\pi x}{a}$$

(c) when $\hat{D}_x^2$ operate on $\hat{D}_x^2\psi(x)=-\frac{n^2\pi^2}{a^2}\psi(x)$

So operation of $\hat{D}_x^2(x)$ on $\psi(x)=A\sin\frac{n\pi x}{a}$ give eigen value problem with eigen value $-\frac{n^2\pi^2}{a^2}$

Example: The momentum operator in one dimension is defined as $\hat{P}_x=-i\hbar\frac{\partial}{\partial x}$.

(a) If p is eigen value of momentum operator find corresponding the eigen function.

(b) If particle is confine between $-\frac{l}{2}\le x\le\frac{l}{2}$ then write down Normalized eigen state.

Solution: (a) Let us assume $\psi(x)$ is eigen function of momentum operator with eigen value p.

$\hat{P}_x\psi(x)=p\psi\Rightarrow -i\hbar\frac{\partial\psi}{\partial x}=p\psi\Rightarrow -i\hbar\int\frac{\partial\psi}{\psi}=p\int dx\Rightarrow\psi=A\exp\left(\frac{ipx}{\hbar}\right)$ where A is normalized constant.

(b) $\int_{-\frac{l}{2}}^{\frac{l}{2}}\psi^*(x)\psi(x)dx\Rightarrow|A|^2\int_{-\frac{l}{2}}^{\frac{l}{2}}\exp\frac{-ipx}{\hbar}.\exp\frac{ipx}{\hbar}dx=1\Rightarrow A=\frac{1}{\sqrt{l}}$

The normalized wave function is given as $\psi(x)=\begin{cases}\frac{1}{\sqrt{l}}\exp\frac{ipx}{\hbar}, -\frac{l}{2}\le x\le\frac{l}{2}\\ 0,\quad otherwise\end{cases}$

Example: Two operators are given as $\hat{A}=\begin{pmatrix}1&0&0\\0&7&-3i\\0&3i&5\end{pmatrix}$ and $\hat{B}=\begin{pmatrix}0&-i&3i\\-i&0&i\\3i&i&0\end{pmatrix}$, which of following have real eigen values.

Solution: $\hat{A}=\begin{pmatrix}1&0&0\\0&7&-3i\\0&3i&5\end{pmatrix}$ $\hat{A}^\dagger=\begin{pmatrix}1&0&0\\0&7&-3i\\0&3i&5\end{pmatrix}$

$\hat{A}^{\dagger} = \hat{A}$ so A is Hermitian so it has real eigen value

$$\hat{B} = \begin{pmatrix} 0 & -i & -3i \\ -i & 0 & i \\ 3i & i & 0 \end{pmatrix} \qquad \hat{B}^{\dagger} = \begin{pmatrix} 0 & -i & -3i \\ i & 0 & -i \\ -3i & -i & 0 \end{pmatrix}$$

$\hat{B}^{\dagger} = -\hat{B}$ So, it is not Hermitian rather it is Anti-Hermitian so its eigen values are not real.

Example: If $\hat{S}$ operator is defined as $\hat{S}|u_1\rangle = |u_3\rangle$, $\hat{S}|u_2\rangle = |u_2\rangle$, $\hat{S}|u_3\rangle = |u_1\rangle$. It is given $\langle u_i | u_j\rangle = \delta_{ij}$ represent operator $\hat{S}$ in basis of $|u_1\rangle, |u_2\rangle$ and $|u_3\rangle$.

Solution: The Matrix $\hat{S} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix}$

Where matrix element $S_{ij} = \langle u_i | \hat{S} | u_j\rangle$

$$S_{11} = \langle u_1 | \hat{S} | u_1\rangle = \langle u_1 | u_3\rangle = 0 \qquad S_{12} = \langle u_1 | \hat{S} | u_2\rangle = \langle u_1 | u_2\rangle = 0$$

$$S_{13} = \langle u_1 | \hat{S} | u_3\rangle = \langle u_1 | u_3\rangle = 1 \qquad S_{21} = \langle u_2 | \hat{S} | u_1\rangle = \langle u_2 | u_3\rangle = 0$$

$$S_{22} = \langle u_2 | \hat{S} | u_2\rangle = \langle u_2 | u_2\rangle = 1 \qquad S_{23} = \langle u_2 | \hat{S} | u_3\rangle = \langle u_2 | u_1\rangle = 0$$

$$S_{31} = \langle u_3 | \hat{S} | u_1\rangle = \langle u_3 | u_3\rangle = 1 \qquad S_{32} = \langle u_3 | \hat{S} | u_2\rangle = \langle u_3 | u_2\rangle = 0$$

$$S_{33} = \langle u_3 | \hat{S} | u_3\rangle = \langle u_3 | u_1\rangle = 0$$

$$\hat{S} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

Example: If $\hat{A}$ operator is given by $\hat{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

(a) Find eigen value and eigen vector of $\hat{A}$.

(b) Normalized there eigen vector.

(c) Prove both eigen vector are orthogonal.

Solution: (a) $A=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$ for eigen value

$$|A-\lambda I|=0$$

$$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}-\lambda\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}=0 \Rightarrow \begin{vmatrix}-\lambda & 1\\ 1 & -\lambda\end{vmatrix}=0 \Rightarrow \lambda=1, \text{ and } \lambda=-1,$$

The eigen vector corresponding to $\lambda=1,$

$$A=|u_1\rangle=\lambda|u_1\rangle$$

$$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix}=\begin{pmatrix}a\\ b\end{pmatrix}\Rightarrow a=b$$

So eigen vector corresponds to $\lambda=1,\ |u_1\rangle=\begin{pmatrix}a\\ a\end{pmatrix}$

eigen vector corresponds to $\lambda=-1$

$$A|u_2\rangle=\lambda|u_2\rangle$$

$$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix}=-1\begin{pmatrix}a\\ b\end{pmatrix}\Rightarrow a=-b\Rightarrow|u_2\rangle=\begin{pmatrix}a\\ -a\end{pmatrix}$$

(b) For normalised eigen vector.

$$\langle u_1|u_1\rangle=1 \qquad \langle u_2|u_2\rangle=1$$

$$|u_1\rangle=\begin{pmatrix}a\\ a\end{pmatrix} \qquad \langle u_1|=\begin{pmatrix}a & a\end{pmatrix}$$

$$\langle u_1|u_1\rangle=a^2+a^2=1=a=\frac{1}{\sqrt{2}}\quad |u_1\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix}$$

Similarly, $|u_2\rangle=\begin{pmatrix}a\\ -a\end{pmatrix}$ and $\langle u_2|=(a,\ -a)$

$$\langle u_2|u_2\rangle=(a,\ -a)\begin{pmatrix}a\\ -a\end{pmatrix}=1\Rightarrow a^2+a^2=1\Rightarrow a=\frac{1}{\sqrt{2}}\Rightarrow|u_2\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix}$$

(c) For orthogonality $\langle u_1|u_2\rangle=\langle u_2|u_1\rangle=0$

$$\frac{1}{\sqrt{2}}(1\quad 1)\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix}=0 \qquad \frac{1}{\sqrt{2}}(1\quad -1)\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix}=0$$

Example: (a) Find the eigen value and orthonormal eigen vectors of operator $\hat{A}=\begin{pmatrix}2&0&0\\0&0&1\\0&1&0\end{pmatrix}$

(b) Prove that eigen vectors of $\hat{A}$ are satisfying completeness relation

$$\left|\hat{A}-\lambda\hat{I}\right|=0\Rightarrow\begin{vmatrix}2-\lambda&0&0\\0&-\lambda&1\\0&1&-\lambda\end{vmatrix}=0\Rightarrow(2-\lambda)(\lambda^2-1)=0$$

Solution: Eigen values are $\lambda_1=2,\lambda_2=1,\lambda_3=-1$ hence they are non-repeated they are nondegenerate eigen values

Now let us find Eigen vector for eigen value $\lambda_1=2$, which is $|\phi_1\rangle=\begin{pmatrix}a_1\\b_1\\c_1\end{pmatrix}$

$$\hat{A}|\phi_1\rangle=\lambda_1|\phi_1\rangle\Rightarrow\begin{pmatrix}2&0&0\\0&0&1\\0&1&0\end{pmatrix}\begin{pmatrix}a_1\\b_1\\c_1\end{pmatrix}=2\begin{pmatrix}a_1\\b_1\\c_1\end{pmatrix}$$

$2a_1=2a_1$, $c_1=2b_1, b_1=2c_1$ the solutions are $b_1=c_1=0$ and a_1 can be any arbitrary value so $|\phi_1\rangle=\begin{pmatrix}a_1\\0\\0\end{pmatrix}$ we can find value of a_1 with normalization condition $\langle\phi_1|\phi_1\rangle=1$ Normalization to get one specific vector

$$\begin{pmatrix}a_1^*&0&0\end{pmatrix}\begin{pmatrix}a_1^*\\0\\0\end{pmatrix}=1\Rightarrow|a_1|^2=1\Rightarrow a_1=1$$

Now let us find Eigen vector for eigen value $\lambda_2=1$, which is $|\phi_2\rangle=\begin{pmatrix}a_2\\b_2\\c_2\end{pmatrix}$

$$\hat{A}|\phi_2\rangle=\lambda_2|\phi_2\rangle\Rightarrow\begin{pmatrix}2&0&0\\0&0&1\\0&1&0\end{pmatrix}\begin{pmatrix}a_2\\b_2\\c_2\end{pmatrix}=1\begin{pmatrix}a_2\\b_2\\c_2\end{pmatrix}$$

$$\begin{pmatrix}2&0&0\\0&0&1\\0&1&0\end{pmatrix}\begin{pmatrix}a_2\\b_2\\c_2\end{pmatrix}=\begin{pmatrix}a_2\\b_2\\c_2\end{pmatrix}\Rightarrow 2a_2=a_2\Rightarrow a_2=0\ c_2=b_2, b_2=c_2\Rightarrow b_2=c_2$$

$|\phi_2\rangle = \begin{pmatrix} 0 \\ b_2 \\ b_2 \end{pmatrix}$ the value of b_2 can be found with normalization condition

$$\langle \phi_2 | \phi_2 \rangle = \begin{pmatrix} 0 & b_2 & b_2 \end{pmatrix} \begin{pmatrix} 0 \\ b_2 \\ b_2 \end{pmatrix} = 2|b_2|^2 = 1 \Rightarrow b_2 = \frac{1}{\sqrt{2}} \quad |\phi_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

Now we will find eigen vector for eigen value $\lambda_3 = -1$ which is $|\phi_3\rangle = \begin{pmatrix} a_3 \\ b_3 \\ c_3 \end{pmatrix}$

$$\hat{A}|\phi_3\rangle = \lambda_3 |\phi_3\rangle \Rightarrow \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a_3 \\ b_3 \\ c_3 \end{pmatrix} = -1 \begin{pmatrix} a_3 \\ b_3 \\ c_3 \end{pmatrix}$$

$$2a_3 = -a_3 \Rightarrow a_3 = 0 \;, c_3 = -b_3, b_3 = -c_3 \; |\phi_3\rangle = \begin{pmatrix} 0 \\ b_3 \\ -b_3 \end{pmatrix}$$

The value of b_3 can be found from normalization condition

$$\langle \phi_3 | \phi_3 \rangle = \begin{pmatrix} 0 & b_3^* & -b_3^* \end{pmatrix} \begin{pmatrix} 0 \\ b_3 \\ -b_3 \end{pmatrix} = 1 \Rightarrow b_3 = 1 \quad |\phi_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$$

$|\phi_1\rangle, |\phi_2\rangle$ and $|\phi_3\rangle$ are orthogonal set.

$$|\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2| + |\phi_3\rangle\langle\phi_3| = I$$

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} + \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} \\ 0 & -\frac{1}{2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

If Eigen value is non-degenerate, then one can find unique set of orthonormal basis vector.

Example: Find the eigen values of operator $\hat{A}=\begin{vmatrix}1&0&0\\0&0&1\\0&1&0\end{vmatrix}$

Find two set of orthonormal eigen vectors.

Solution: $\left[\hat{A}-\lambda I\right]=0\Rightarrow\begin{vmatrix}1-\lambda&0&0\\0&-\lambda&1\\0&1&-\lambda\end{vmatrix}=0\Rightarrow(1-\lambda)\left(\lambda^2-1\right)=0\ \Rightarrow\lambda_1=-1,\lambda_2=1,=\lambda_3=1$

Hence $\lambda_2=\lambda_3=1$ so eigen value 1 is doubly degenerate.

Eigen vectors for $\lambda_1=-1$ is $|\phi_1\rangle=\begin{pmatrix}a_1\\b_1\\c_1\end{pmatrix}$

$$\hat{A}|\phi_1\rangle=\lambda_1|\phi_1\rangle\Rightarrow\begin{pmatrix}1&0&0\\0&0&1\\0&1&0\end{pmatrix}\begin{pmatrix}a_1\\b_1\\c_1\end{pmatrix}=-1\begin{pmatrix}a_1\\b_1\\c_1\end{pmatrix}\Rightarrow a_1=-a_1\Rightarrow a_1=0\ ,c_1=-b_1 \text{ or } b_1=-c_1$$

$|\phi_1\rangle=\begin{pmatrix}0\\b_1\\-b_1\end{pmatrix}$ using normalization condition $\langle\phi_1|\phi_1\rangle=1\Rightarrow b_1=\frac{1}{\sqrt{2}}$ so $|\phi_1\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\end{pmatrix}$

Hence $\lambda_1=-1$ is non degenerate Eigen value it has unique normalized vector.

Now we well find eigen vector for eigen value $\lambda=1$ .which is doubly degenerate so there may be infinite set of normalized eigen vectors but it is not necessary that they are orthogonal .so for $\lambda_2=1$ we need to choose two normal vectors which are orthogonal in nature

$$\hat{A}|\phi_2\rangle=\lambda_2|\phi_2\rangle\Rightarrow\begin{pmatrix}1&0&0\\0&0&1\\0&1&0\end{pmatrix}\begin{pmatrix}a_2\\b_2\\c_2\end{pmatrix}=1\begin{pmatrix}a_2\\b_2\\c_2\end{pmatrix}\Rightarrow a_2=a_2\,,c_2=b_2\ \ b_2=c_2$$

$|\phi_2\rangle=\begin{pmatrix}a_2\\b_2\\b_2\end{pmatrix}$ where a_2 and b_2 has arbitrary number so there is possibility of infinite normalized vector.

Similarly, for $\lambda_3=1$

$$\hat{A}|\phi_3\rangle=\lambda_3|\phi_3\rangle\Rightarrow\begin{pmatrix}1&0&0\\0&0&1\\0&1&0\end{pmatrix}\begin{pmatrix}a_3\\b_3\\c_3\end{pmatrix}=1\begin{pmatrix}a_3\\b_3\\c_3\end{pmatrix}\Rightarrow a_3=a_3\,,c_3=b_3\ \ b_3=c_3$$

$|\phi_3\rangle = \begin{pmatrix} a_3 \\ b_3 \\ b_3 \end{pmatrix}$ where a_3 and b_3 has arbitrary number, so there is possibility of infinite normalized vector

We can easily conclude $|\phi_2\rangle$ and $|\phi_3\rangle$ are vectors in same plane with is surely orthogonal to $|\phi_1\rangle$.

Now we need to choose two set of orthonormal vectors which are in same plane where $|\phi_1\rangle$ is uniquely defined for all set.

Set I: We can choose $a_2 = 1$, $|\phi_2\rangle = \begin{pmatrix} 1 \\ b_2 \\ b_2 \end{pmatrix}$

from normalization condition we can find $b_2 = 0$ so $|\phi_2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$

Now we can not choose $|\phi_3\rangle = \begin{pmatrix} a_3 \\ b_3 \\ b_3 \end{pmatrix}$ it must be orthogonal to $|\phi_2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$

$\langle \phi_2 | \phi_3 \rangle = 0 \; \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} a_2 \\ b_2 \\ b_2 \end{pmatrix} = 0 \Rightarrow a_2 = 0$ so $|\phi_3\rangle$ must be in form of $|\phi_3\rangle = \begin{pmatrix} 0 \\ b_3 \\ b_3 \end{pmatrix}$

from normalization condition we can get $|\phi_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$

So, first set of orthonormal vectors are corresponds to eigen value $-1, 1, 1$ is

$|\phi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$, $|\phi_2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |\phi_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$. Again we can easily check these vectors make complete basis.

Set II: Again eigen value of nondegenerate eigen vector is $|\phi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$ which is uniquely defined but we can choose another set of orthonormal eigen vectors for degenerate eigen value $\lambda_2 = \lambda_3 = 1$ $|\phi_2\rangle = \begin{pmatrix} a_2 \\ b_2 \\ b_2 \end{pmatrix}$ and $|\phi_3\rangle = \begin{pmatrix} a_3 \\ b_3 \\ b_3 \end{pmatrix}$

We can choose arbitrary $|\phi_2\rangle = \begin{pmatrix} a_2 \\ b_2 \\ b_2 \end{pmatrix}$ by putting $a_2 = \frac{1}{2}$, $|\phi_2\rangle = \begin{pmatrix} 1/2 \\ b_2 \\ b_2 \end{pmatrix}$

From normalization condition $\langle\phi_2|\phi_2\rangle = \frac{1}{4} + 2b_2 = 1$ $b_2 = \sqrt{\frac{3}{8}}$ so $|\phi_2\rangle = \begin{pmatrix} 1/2 \\ \sqrt{3/8} \\ \sqrt{3/8} \end{pmatrix}$

Now $|\phi_3\rangle = \begin{pmatrix} a_3 \\ b_3 \\ b_3 \end{pmatrix}$ cannot be chosen arbitrary it must be orthogonal to $|\phi_2\rangle = \begin{pmatrix} 1/2 \\ \sqrt{3/8} \\ \sqrt{3/8} \end{pmatrix}$

$$\langle\phi_2|\phi_3\rangle = 0 \Rightarrow \begin{pmatrix} \frac{1}{2} & \sqrt{\frac{3}{8}} & \sqrt{\frac{3}{8}} \end{pmatrix}\begin{pmatrix} a_3 \\ b_3 \\ b_3 \end{pmatrix} = 0 \Rightarrow \frac{1}{2}a_3 + 2\sqrt{\frac{3}{8}}b_3 = 0 \Rightarrow a_3 = -b_3 4\sqrt{\frac{3}{8}}$$

$|\phi_3\rangle = \begin{pmatrix} -b_3 4\sqrt{\frac{3}{8}} \\ b_3 \\ b_3 \end{pmatrix}$ the value of b_3 can be found with normalization condition

$$\langle\phi_3|\phi_3\rangle = 1 \Rightarrow = 16 \times \frac{3}{8}b_3^2 + 2b_3^2 = 1 \Rightarrow 8b_3^2 = 1 \Rightarrow b_3 = \sqrt{\frac{1}{8}} \Rightarrow |\phi_3\rangle = \begin{pmatrix} -\sqrt{3/2} \\ 1/\sqrt{8} \\ 1/\sqrt{8} \end{pmatrix}$$

So second set of orthonormal vectors corresponding to eigen values are $\lambda_1 = -1, \lambda_2 = 1$ and $\lambda_2 = 1$ are $|\phi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$ $|\phi_2\rangle = \begin{pmatrix} 1/2 \\ \sqrt{3/8} \\ \sqrt{3/8} \end{pmatrix}$ $|\phi_3\rangle = \begin{pmatrix} -\sqrt{3/2} \\ 1/\sqrt{8} \\ 1/\sqrt{8} \end{pmatrix}$ which will also make complete basis.

Example: Operate Parity operator π on functions $\psi_1 = \sin x$ $\psi_2 = \cos x$ and $\psi_3 = \sin x + \cos x$, also discuss parity symmetry of each function.

Solution: $\pi\psi_1 = \pi \sin x = \sin(-x) = -\sin x = -\psi_1$ which is antisymmetric so eigen value is -1.

$\pi\psi_2 = \pi \cos x = \cos(-x) = \cos x = \psi_2$ which is symmetric so eigen value is 1.

$\pi\psi_3 = \pi \sin x + \pi \cos x = \sin(-x) + \cos(-x) = -\sin x + \cos x \neq \psi_3$ so ψ_3 is not eigen function of parity operator.