Density Matrices

- Density Matrices represent a <u>broader class</u> of quantum states and quantum statevectors.

- Density matrices can describe states of <u>isolated parts</u> of systems, such as the state of one system that happens to be entangled with another system that we wish to ignore.

- Probabilistic states can be represented by density matrices, allowing quantum and classical information to be described together within a <u>single mathematical framework</u>.

Definition of density matrices :-

Suppose that X is a system and Σ is its classical state set.
$\hookrightarrow$ finite & non-empty.

A density matrix describing of a state of X is a matrix with complex entries whose rows and columns have been placed ~~with~~ in correspondence with Σ.

$\rightarrow$ sum of diagonal entries

1. Density matrices must have unit Trace $\boxed{Tr(\rho) = 1}$.
2. Density matrices must be positive semidefinite : $\boxed{\rho \geq 0}$.

- Trace :

$$Tr\begin{pmatrix} \alpha_{0,0} & \alpha_{0,1} & \cdots & \alpha_{0,n-1} \\ \alpha_{1,0} & \alpha_{1,1} & \cdots & \alpha_{1,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{n-1,0} & \alpha_{n-1,1} & \cdots & \alpha_{n-1,n-1} \end{pmatrix} = \alpha_{0,0} + \alpha_{1,1} + \alpha_{2,2} \cdots \alpha_{n-1,n-1}$$

Trace is a linear f^n : $\boxed{Tr(\alpha A + \beta B) = \alpha\, Tr(A) + \beta\, Tr(B)}$

- positive semidefinite :-

This property can be expressed in several different ways

- There exist matrix M such that $\rho = M^{+} M$
- The matrix ρ is Hermitian, meaning that $\rho = \rho^{+}$, and all it's eigenvalues are non-negative real numbers.
- For every complex vector $|\psi\rangle$ we have $\langle\psi|\rho|\psi\rangle \geq 0$.

Then we can say $\rho \geq 0$.

Example of a positive semidefinite :-

Choosing Random $M = \begin{pmatrix} -4-9i & 8 & 2+9i \\ -7 & -4-9i & -9+7i \\ 1-5i & 8-6i & -4i \end{pmatrix}$

$$\therefore M^{+} = \begin{pmatrix} -4+9i & \cancel{8}-7 & 1+5i \\ \cancel{2-9i}\ 8 & -4+9i & 8+6i \\ 2-9i & -9-7i & 4i \end{pmatrix}$$

$$M^{T}M = \begin{pmatrix} -4+9i & -7 & 1+5i \\ 8 & -4+9i & 8+6i \\ 2-9i & -9-7i & 4i \end{pmatrix} \begin{pmatrix} -4-9i & 8 & 2+9i \\ -7 & -4-9i & -9+7i \\ 1-5i & 8-6i & -4i \end{pmatrix}$$

$$= \begin{pmatrix} 172 & 34+169i & -6-71i \\ 39-169i & 261 & 13-69i \\ -6+71i & 13+69i & 231 \end{pmatrix} \longrightarrow \text{semi definite matrix}$$

Examples of density matrices :-

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} \quad \begin{pmatrix} 3/4 & i/8 \\ -i/8 & 1/4 \end{pmatrix} \quad \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

- For a given density matrix both the rows and ~~column~~ columns correspond to ~~the~~ classical states.
- Diagonal entries are the probabilities of each classical state to appear from a standard basis measurement.
- Off-Diagonal entries describe how two corresponding states are in quantum superposition.

Connection to state vectors :-

A quantum state $|\psi\rangle$ is a column vector having euclidean norm 1.

Here, the density matrix representation of the same state :

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

eigenvalues: 1, 0, 0, 0, ...

States that are represented by density matrices are called <u>pure states</u>.

Ex - $|+i\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 1/\sqrt{2} \end{pmatrix}$ $\quad |+i\rangle\langle +i| = \begin{pmatrix} 1/\sqrt{2} \\ i/\sqrt{2} \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & -i/\sqrt{2} \end{pmatrix} = \begin{pmatrix} 1/2 & -i/2 \\ i/2 & 1/2 \end{pmatrix}$

$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\quad |0\rangle\langle 0| = \cancel{\begin{pmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{pmatrix}} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$

$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $\quad |1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

$|+\rangle = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$ $\quad |+\rangle\langle +| = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$

$|-\rangle = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}$ $\quad |-\rangle\langle -| = \begin{pmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{pmatrix}$

There is <u>no global phase degeneracy</u> for density matrices : two quantum states are identical if and only if their density matrix representations are equal.

Ex $\rightarrow$ $|\phi\rangle = e^{i\theta}|\psi\rangle$

$$\therefore |\phi\rangle\langle\phi| = (e^{i\theta}|\psi\rangle)(e^{i\theta}|\psi\rangle)^{\dagger}$$

$$= e^{i(\theta-\theta)}|\psi\rangle\langle\psi|$$

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

Probabilistic selections

Convex combination of density matrices represent probabilistic selections of quantum states.

Let ρ and σ be density matrices representing quantum states of a system and suppose we prepare the system in state ρ with probability $p \in [0,1]$ and σ with probability $1-p$.

The resulting state is represented by this density matrix:

$$p\rho + (1-p)\sigma$$

In general, $\rho_0, \rho_1, \rho_2 \dots \rho_{m-1}$ be density matrices, let $(p_0, p_1, p_2 \dots p_{m-1})$ be the probability vector.

$\therefore$ The resulting state is represented by this density matrix:-

$$\sum_{k=0}^{m-1} p_k \rho_k$$

→ convex combination (where coeff form a probability vector)

Set of all density matrices corresponding to a given system is a convex set.

Ex- A qubit is prepared in the state $|0\rangle$ with probability $1/2$ and in the state $|+\rangle$ with probability $1/2$.

$$\frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|+\rangle\langle +| = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$$

$$= \begin{pmatrix} 3/4 & 1/4 \\ 1/4 & 1/4 \end{pmatrix}$$

Completely mixed states:-

Suppose we set the state of a qubit to be $|0\rangle$ or $|1\rangle$ randomly, each with probability $1/2$.

$\therefore$ Density matrix representation of the same state:-

$$\frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} = \frac{1}{2}I$$

This is known as ~~mixed~~ the completely mixed state - It represents complete uncertainty about the state of a qubit.

Suppose in place of the states $|0\rangle$ and $|1\rangle$, we'll use the states $|+\rangle$ and $|-\rangle$

$$\frac{1}{2}|+\rangle\langle+| + \frac{1}{2}|-\rangle\langle-| = \frac{1}{2}\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{pmatrix}$$

$$= \frac{1}{2} I$$

$\therefore$ The two states cannot be distinguished by measuring the qubit.

Probabilistic states

Probabilistic states are represented by convex combinations of density matrices.

Ex -

Suppose the classical state set X is $\{0, 1, \ldots, n-1\}$

we can identify the probabilistic state of X represented by the probability vector $(p_0, p_1, \cdots p_{n-1})$ with this density matrix.

$$\rho = \sum_{k=0}^{n-1} p_k |k\rangle\langle k| = \begin{pmatrix} p_0 & 0 & \cdots & 0 \\ 0 & p_1 & \cdots & \vdots \\ \vdots & \vdots & \ddots & 0 \\ 0 & \cdots & 0 & p_{n-1} \end{pmatrix}$$

Bloch Sphere

Upto a global phase, every qubit quantum state vector is equivalent to

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle \qquad \begin{array}{l}\theta \in [0,\pi] \\ \phi \in [0,2\pi)\end{array}$$

If $\theta = 0$ or $\theta = \pi$, then ϕ is irrelevant.

If $\theta \in (0,\pi)$, then ϕ is unique.

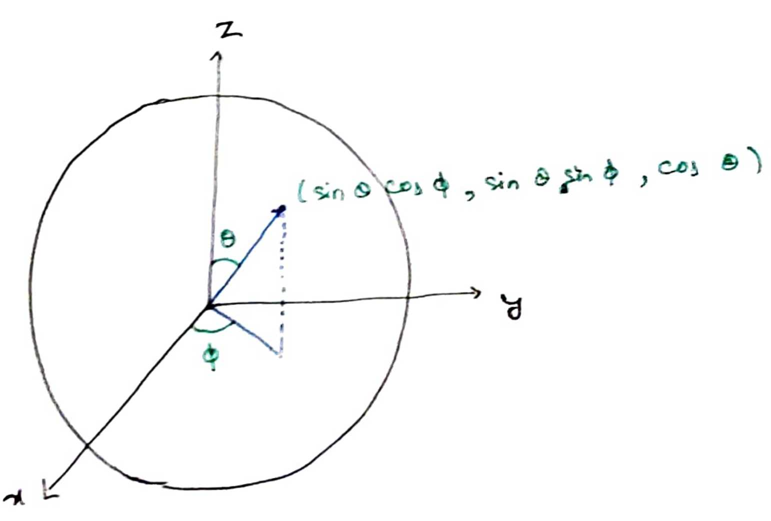
The density matrix :

$$|\psi\rangle\langle\psi| = \begin{bmatrix} \cos^2\left(\frac{\theta}{2}\right) & e^{-i\phi}\cos\left(\frac{\theta}{2}\right)\sin\left(\theta/2\right) \\ e^{i\phi}\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right) & \sin^2\left(\frac{\theta}{2}\right) \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1+\cos\theta}{2} & (\cos(\phi) - i\sin\phi)\,\frac{\sin\theta}{2} \\ \cancel{\cos\phi + i\sin\theta)}\;(\cos\phi + i\sin\phi)\,\frac{\sin\theta}{2} & \frac{1-\cos\theta}{2} \end{bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix} 1+\cos\theta & \sin\theta\cos\phi - i\sin\theta\sin\phi \\ \cancel{\cos\phi}\;\sin\theta\cos\phi + i\sin\theta\sin\phi & 1-\cos\theta \end{bmatrix}$$

$$= \frac{1}{2}\left[I + \sin\theta\cos\phi\,\sigma_x + \sin\theta\sin\phi\,\sigma_y + \cos(\theta)\,\sigma_z\right]$$

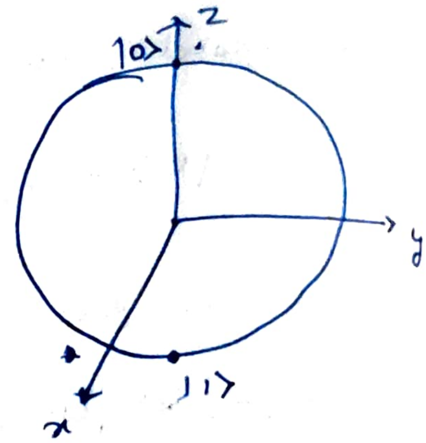


$$|0\rangle = \cos(0)\,|0\rangle + e^{i\phi}\sin(0)\,|1\rangle$$

$$|0\rangle\langle 0| = \frac{I + \sigma_z}{2}$$

$$|1\rangle = \cos\left(\frac{\pi}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\pi}{2}\right)|1\rangle$$

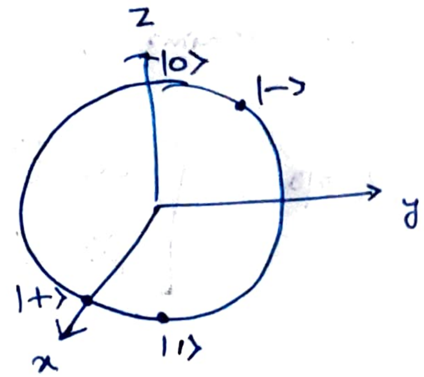
$$|1\rangle\langle 1| = \frac{I - \sigma_z}{2}$$



$$|+\rangle = \cos\left(\frac{\pi/2}{2}\right)|0\rangle + e^{i0}\sin\left(\frac{\pi/2}{2}\right)|1\rangle$$

$$|+\rangle\langle +| = \frac{I + \sigma_x}{2}$$

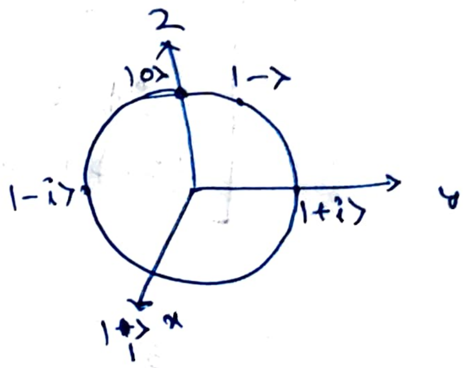
$$|-\rangle\langle -| = \frac{I - \sigma_x}{2}$$



$$|+i\rangle = \cos\left(\frac{\pi/2}{2}\right)|0\rangle + e^{i\frac{\pi}{2}}\sin\left(\frac{\pi/2}{2}\right)|1\rangle$$

$$|+i\rangle\langle +i| = \frac{I + \sigma_y}{2}$$

$$|-i\rangle\langle -i| = \frac{I - \sigma_y}{2}$$



Multiple Systems

Density matrices can represent states of multiple systems:

- Multiple system are viewed as single, compound systems.
- The rows and columns of density matrices for multiple systems correspond to cartesian products of the classical states sets of the individual systems.

Example :-

$$|\phi^+\rangle\langle\phi^+| = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 0 \\ 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{bmatrix}$$

$$|\phi^-\rangle\langle\phi^-| = \begin{bmatrix} 1/2 & 0 & 0 & -1/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1/2 & 0 & 0 & 1/2 \end{bmatrix}$$

$$|\psi^+\rangle\langle\psi^+| = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \qquad |\psi^-\rangle\langle\psi^-| = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/2 & -1/2 & 0 \\ 0 & -1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$