

Density Matrix

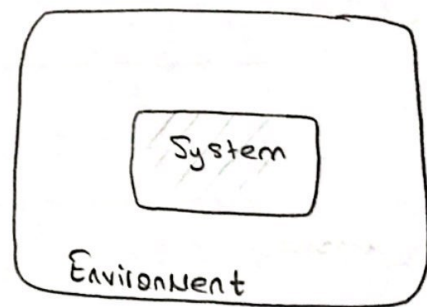
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Need \rightarrow Generalize notion of quantum state

Till now $|\psi\rangle \in \mathcal{H}$ for isolated system

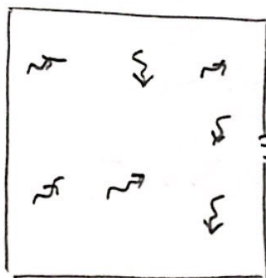
New situation systems are not isolated.

Another new situation:



Statistical mixture of state

gas of photons



N qubits possible states:

$\left\{ \begin{array}{l} |\psi_1\rangle \\ p_1 \end{array} \right\} \quad \left\{ \begin{array}{l} |\psi_2\rangle \\ p_2 \end{array} \right\} \quad \dots \quad \left\{ \begin{array}{l} |\psi_k\rangle \\ p_k \end{array} \right\}$

$$0 \leq p_i \leq 1, \quad \sum_{i=1}^k p_i = 1$$

① Description of Statistical Mixtures

Def: Stat. mixture is an ensemble of states $|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_k\rangle \in \mathcal{H}$
 with each state drawn with probabilities $p_1, p_2, p_3, \dots, p_k$.

$$(0 \leq p_i \leq 1, \quad \sum_{i=1}^k p_i = 1)$$

The Density Matrix of the statistical mixture is

$$\rho \stackrel{\text{def}}{=} \sum_{i=1}^k p_i \underbrace{|\varphi_i\rangle\langle\varphi_i|}_{\text{Projector matrix onto } |\varphi_i\rangle}$$

Dimension of ρ is $[\dim \mathcal{H} \times \dim \mathcal{H}]$

Properties: 1) $\rho \geq 0$ positive semi-definite $\left\{ \begin{array}{l} \text{All eigenvalues are } \geq 0 \\ \langle \psi | \rho | \psi \rangle \geq 0 \end{array} \right.$

2) $\rho^\dagger = \rho$ hermitian \rightarrow eigenvalues are real

$$3) \text{Tr } \rho = 1$$

$$\text{Tr } \rho = \sum_{i=1}^k p_i \underbrace{\text{Tr } |\varphi_i\rangle\langle\varphi_i|}_1 = 1$$

$$\frac{\text{Tr}(\langle \psi | \rho | \psi \rangle)}{\langle \psi | \psi \rangle} = 1$$

sum of the diagonal elements (eigenvalues?)

②

Cyclicity of Trace: $\text{Tr}(AB) = \text{Tr}(BA)$

$$\text{Tr}(|\varphi_i\rangle\langle\varphi_i|) = \text{Tr}(\langle\varphi_i|\varphi_i\rangle) = 1$$

Lemma: Any square matrix ρ with the properties $\rho^\dagger = \rho$, $\rho \geq 0$, $\text{Tr} \rho = 1$ is a density matrix for some statistical mixture,

$$\rho = \sum_{i=1}^k p_i |\varphi_i\rangle\langle\varphi_i|$$

for some $(|\varphi_1\rangle, |\varphi_2\rangle, \dots, |\varphi_k\rangle, p_1, \dots, p_k)$
probabilities

Proof: Since $\rho^\dagger = \rho$ the spectral Thm says that

Real eigenvalues & eigenvectors form an orthonormal basis.

$$\rho |\chi_\alpha\rangle = \lambda_\alpha |\chi_\alpha\rangle, \quad \lambda_\alpha \in \mathbb{R}, \quad \langle\chi_\alpha|\chi_\beta\rangle = \delta_{\alpha\beta}$$

Thus

$$\rho = \sum_{\alpha=1}^D \lambda_\alpha |\chi_\alpha\rangle\langle\chi_\alpha|$$

since $\rho \geq 0$: $0 \leq \lambda_\alpha$

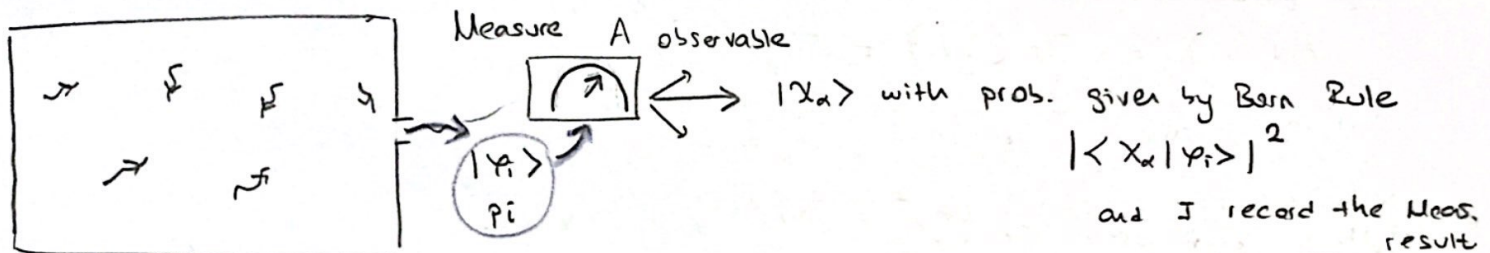
$$\text{Tr} \rho = 1 = \sum_{\alpha} \lambda_\alpha \Rightarrow \lambda_\alpha \leq 1 \quad (3)$$

$$g|x_\alpha\rangle = \lambda_\alpha |x_\alpha\rangle$$

$$g|x_\alpha\rangle\langle x_\alpha| = \lambda_\alpha |x_\alpha\rangle\langle x_\alpha|$$

$$g \left[\sum_\alpha |x_\alpha\rangle\langle x_\alpha| \right] = \sum_\alpha \lambda_\alpha |x_\alpha\rangle\langle x_\alpha|$$

II



Average of A over measurement = $\text{Tr}(Ag)$

$\langle A \rangle$
 $A \psi(A)$

$E(f(x)) = \int dx f(x) p(x) \rightarrow \text{Analogy}$

p_α

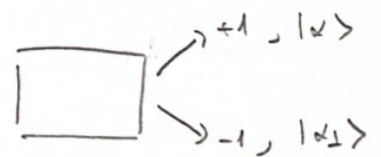
$A^\dagger = A$ has spectral decomposition $A |x_0\rangle = \lambda_0 |x_0\rangle$

$$A = \sum_{\alpha} \lambda_{\alpha} |x_{\alpha}\rangle \langle x_{\alpha}|$$

According to Meas. postulate, I modeled the Meas. apparatus by the orthonormal basis $\{ |x_{\alpha}\rangle \}_{\alpha=1, \dots, \dim \mathcal{H}}$

(Previously)

Polarization obs. $A = (+1) |\alpha\rangle \langle \alpha| + (-1) |\alpha_{\perp}\rangle \langle \alpha_{\perp}|$



$$Av(A) = \sum_i p_i \sum_{\alpha} \lambda_{\alpha} |\langle x_{\alpha} | \psi_i \rangle|^2$$

(Conditional on state being measured is $|\psi_i\rangle$, the avg. is $\sum_{\alpha} \lambda_{\alpha} |\langle x_{\alpha} | \psi_i \rangle|^2$)

$$Av(A) = \sum_{\alpha} \lambda_{\alpha} \sum_i p_i \langle x_{\alpha} | \psi_i \rangle \langle \psi_i | x_{\alpha} \rangle = \sum_{\alpha} \lambda_{\alpha} \langle x_{\alpha} | \left(\sum_i p_i |\psi_i\rangle \langle \psi_i| \right) | x_{\alpha} \rangle$$

$$= \sum_{\alpha} P_{\alpha} \langle x_{\alpha} | g | x_{\alpha} \rangle = \text{Tr} \left(g \underbrace{\sum_{\alpha} P_{\alpha} |x_{\alpha}\rangle \langle x_{\alpha}|}_A \right)$$

$$\text{Tr}(\langle x_{\alpha} | \overbrace{g}^? | x_{\alpha} \rangle) = \text{Tr}(g | x_{\alpha} \rangle \langle x_{\alpha} |)$$

$$\text{Tr}(AB) = \text{Tr}(BA)$$

$$\boxed{A_V(A) = \text{Tr}(gA) = \text{Tr}(Ag)}$$

$$\begin{aligned} \text{Variance of } A : (\Delta A)^2 &= A_V(A^2) - (A_V(A))^2 \\ &= \text{Tr}(gA^2) - (\text{Tr} gA)^2 \end{aligned}$$

$$\text{Var}(x) = \int dx x^2 p(x) - \left(\int dx x p(x) \right)^2 \rightarrow \text{Analogy}$$

Measurements & Density Matrix

System (statistical mix) described by ρ

Measurement with apparatus with basis $\{|X_\alpha\rangle\} \Leftrightarrow \{\overset{\text{projector}}{P_\alpha} = |X_\alpha\rangle\langle X_\alpha|\}$

If initially state is $|\varphi_i\rangle \rightarrow$ after meas. $\frac{P_\alpha |\varphi_i\rangle}{\|P_\alpha |\varphi_i\rangle\|} = |X_\alpha\rangle$

Initially $\rho = \sum_{i=1}^k p_i |\varphi_i\rangle\langle\varphi_i|$ what is the DM after the meas?

$$\rho^{\text{after}} = \sum_{i=1}^k p_i \left(\frac{P_\alpha |\varphi_i\rangle\langle\varphi_i| P_\alpha}{\|P_\alpha |\varphi_i\rangle\| \|P_\alpha |\varphi_i\rangle\|} \right)$$

$$\rho^{\text{after}} = \sum_{i=1}^k p_i \frac{|X_\alpha\rangle\langle X_\alpha| \overset{\uparrow}{P_\alpha |\varphi_i\rangle} \langle\varphi_i| P_\alpha}{\langle\varphi_i| X_\alpha\rangle\langle X_\alpha|\varphi_i\rangle} = \sum_{i=1}^k p_i \underbrace{|X_\alpha\rangle\langle X_\alpha|}_{P_\alpha}$$

$\langle\varphi_i| P_\alpha P_\alpha |\varphi_i\rangle = \langle\varphi_i| X_\alpha\rangle\langle X_\alpha|\varphi_i\rangle$

$$\rho^{\text{after}} = \left(\sum_i p_i \right) |X_\alpha\rangle\langle X_\alpha| = P_\alpha$$

$$g \longrightarrow \left[\text{circular arrow} \right] \longrightarrow g^{\text{after}} = \frac{P_\alpha g P_\alpha}{\text{Tr}(P_\alpha g P_\alpha)} = \frac{|X_\alpha\rangle\langle X_\alpha| g |X_\alpha\rangle\langle X_\alpha|}{\text{Tr}(|X_\alpha\rangle\langle X_\alpha| g |X_\alpha\rangle\langle X_\alpha|)}$$

$\underbrace{\langle X_\alpha | X_\alpha \rangle}_1 \underbrace{\langle X_\alpha | g | X_\alpha \rangle}_{\text{some number}}$

$$g^{\text{after}} = \frac{|X_\alpha\rangle\langle X_\alpha| g |X_\alpha\rangle\langle X_\alpha|}{\langle X_\alpha | g | X_\alpha \rangle} = |X_\alpha\rangle\langle X_\alpha|$$

Prob. to get $|X_\alpha\rangle\langle X_\alpha| = \text{Tr}(P_\alpha g)$

$$\text{Tr}(P_\alpha g P_\alpha) = \text{Tr}(P_\alpha^2 g) = \text{Tr}(P_\alpha g) = \text{Tr}(|X_\alpha\rangle\langle X_\alpha| g) = \text{Tr}(\langle X_\alpha | g | X_\alpha \rangle)$$

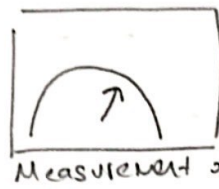
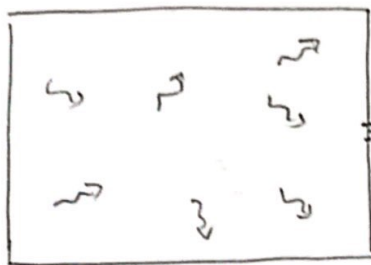
$$g = \sum_i p_i | \psi_i \rangle \langle \psi_i |$$

$$\text{Average} \leftarrow \langle X_\alpha | g | X_\alpha \rangle = \sum_i p_i \underbrace{\langle X_\alpha | \psi_i \rangle \langle \psi_i | X_\alpha \rangle}_{|\langle X_\alpha | \psi_i \rangle|^2} = \sum_i p_i |\langle X_\alpha | \psi_i \rangle|^2$$

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Density Matrix - Review

System statistical mixture of states



$|x_\alpha\rangle, \lambda_\alpha$ with probability $|\langle x_\alpha | \psi_i \rangle|^2$

$$A = \sum_{\alpha} \lambda_{\alpha} |x_{\alpha}\rangle \langle x_{\alpha}|$$

$|\psi_1\rangle, |\psi_2\rangle, \dots, |\psi_k\rangle$
 $p_1 \quad p_2 \quad p_k$

$$A_V(A) = \sum_{i=1}^k p_i \sum_{\alpha} \lambda_{\alpha} |x_{\alpha}\rangle \langle x_{\alpha}| \Rightarrow A_V(A) = \text{Tr}(A \rho) \text{ with } \rho = \sum_{i=1}^k p_i |\psi_i\rangle \langle \psi_i|$$

convex combination of states in the mixture.

(ρ = Density Matrix (DM) = Mixed states)

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Terminology: **Pure States** \rightarrow usual vectors of Hilbert space $|\psi\rangle \in \mathcal{H}$
 $\Leftrightarrow |\psi\rangle\langle\psi| = \rho_\psi = \{|\psi\rangle, p=1\}$

Mixed States \rightarrow Density matrices of stat. mixture
 $\{|\psi_1\rangle, \dots, |\psi_k\rangle, p_1, \dots, p_k\}$
 $\rho = \sum_{i=1}^k p_i |\psi_i\rangle\langle\psi_i|$

Remark $\rho^2 = \rho \rightarrow$ Pure state

but in general $\rho^2 \neq \rho$

Measurement of a Mixed state

$\rho \rightarrow$ 
 $\{ |u_\alpha\rangle\langle u_\alpha| = P_\alpha$
 $\alpha = 1, \dots, D \}$
 orthonormal basis

\rightarrow $|u_\alpha\rangle\langle u_\alpha|$ with
 $\text{prob}(\alpha) = \text{Tr}(\rho P_\alpha) = \langle u_\alpha | \rho | u_\alpha \rangle$

$$\rho_{\psi} = |\psi\rangle\langle\psi| \rightarrow \text{prob } \alpha = \langle v_{\alpha} | \psi \rangle \langle \psi | v_{\alpha} \rangle = |\langle v_{\alpha} | \psi \rangle|^2 \rightarrow \text{Born Rule}$$

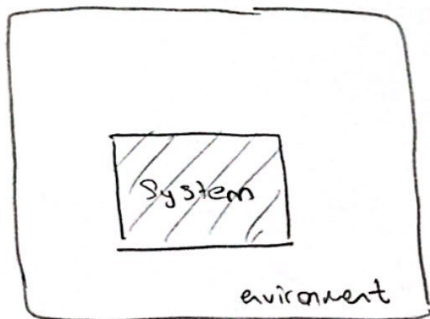
Pure states

$$|v_{\alpha}\rangle\langle v_{\alpha}| = \frac{P_{\alpha} \rho P_{\alpha}}{\text{Tr}(P_{\alpha} \rho P_{\alpha})} = \frac{P_{\alpha} \rho P_{\alpha}}{\text{Tr}(\rho P_{\alpha})}$$

Density Matrix after the measurement

$\int P_{\alpha}^2 = \rho P_{\alpha}$

Projected from both sides
(for states (vectors) only, one projection is enough)



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

description of S
only involves ρ_S

(eliminate degrees of freedom of environment)

Density Matrix of one qubit

State vector of 1 qubit

$$\mathcal{H} = \mathbb{C}^2$$

$$\rho = \frac{a_0}{2} I + \frac{a_1}{2} \sigma_x + \frac{a_2}{2} \sigma_y + \frac{a_3}{2} \sigma_z$$

$$|\psi\rangle = \cos\frac{\theta}{2} |0\rangle + \sin\frac{\theta}{2} e^{i\phi} |1\rangle$$

$$I, \sigma_x, \sigma_y, \sigma_z$$

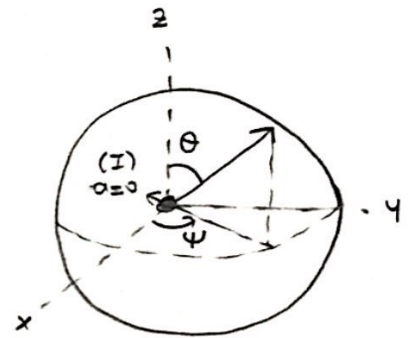
$$I, x, y, z$$

Pauli Matrices

$$\rho^\dagger = \rho \Rightarrow a_0, a_1, a_2, a_3 \Rightarrow \text{real}$$

$$\text{Tr } \rho = 1 \Rightarrow a_0 = 1$$

$$\rho \geq 0 \Rightarrow \|\vec{a}\| \leq 1$$



$$\rho = \frac{1}{2} (I + \vec{a} \cdot \vec{\sigma})$$

$$\vec{a} = r (\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta)$$

↳

$$0 \leq r \leq 1$$

If $r=1$ then $\rho^2 = \rho \Rightarrow \rho = |\psi\rangle\langle\psi|$ (pure state) on the surface of the Bloch ball.

Proof: $g \geq 0 \Rightarrow \|\vec{a}\| = 1$

$\text{Tr } g = 1 \Rightarrow$ I have 2 eigenvalues (?)

$$\begin{cases} \lambda_0 + \lambda_1 = 1 \\ \lambda_0, \lambda_1 \geq 0 \end{cases} \quad (\text{semi definite})$$

$$\boxed{\lambda_0 \lambda_1 = \det g \geq 0}$$

$$\det \left[\frac{I}{2} + \frac{1}{2} \vec{a} \cdot \vec{\sigma} \right] = \frac{1}{4} \det \begin{bmatrix} \frac{1+a_1}{2} & \frac{a_1 + i a_2}{2} \\ \frac{a_1 - i a_2}{2} & \frac{1-a_3}{2} \end{bmatrix} \geq 0$$

↓ yields

$$\|\vec{a}\| \geq 1$$