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Learning objectives:

- Formulate axioms of QM using density operator
- Quantify entanglement of a quantum state
- Relate density matrices ρ to ensembles of pure states $\{p_a, |\psi_a\rangle\}$

Review of the density operator ρ (N2.4; P2.3; W4.1; CT. EIII):

A general state of a quantum system is described by the **density operator**

$$\boxed{\rho = \sum_i p_i \, |\psi_i\rangle\langle\psi_i|}$$

- p_i = probability to find system in pure state $|\psi_i\rangle$
- $|\psi_i\rangle$ do <u>not</u> need to be orthogonal (but are normalized)
- Ensemble of pure states $\mathcal{E} = \{p_i, |\psi_i\rangle\}$

more precisely (W4.1): $\mathcal{E} = \{p_X(x) \,|\, |\psi_x\rangle\}_{x\in\mathcal{X}}$

alphabet, e.g. eigenvalues of CSCO

X: random variable

$p_X(x)$: prob. distribution of random variable

From the ensemble definition of the density operator ρ, we can show that an operator ρ is the density operator of ensemble $\{p_i | |\psi_i\rangle\}$ iff

(i) **$\mathrm{Tr}\,\rho = 1$**

(ii) ρ is a **positive operator**: $\langle\psi|\rho|\psi\rangle \geq 0 \quad \forall |\psi\rangle$

Proof:

First direction ($\rightarrow$): Suppose $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ is a density operator.
Then:

(i) $\rightarrow$ $$\mathrm{Tr}\,\rho = \sum_i p_i \underbrace{\mathrm{Tr}(|\psi_i\rangle\langle\psi_i|)}_{=\langle\psi_i|\psi_i\rangle = 1} = \sum_i p_i = 1.$$

p_i's are probabilities

(ii) $\rightarrow$ Consider general vector $|\varphi\rangle$, then

$$\langle\varphi|\rho|\varphi\rangle = \sum_i p_i \langle\varphi|\psi_i\rangle\langle\psi_i|\varphi\rangle =$$

$$= \sum_i p_i |\langle\varphi|\psi_i\rangle|^2 \geq 0.$$

Now, the reverse direction: Suppose ρ is a positive operator with trace of one. Then, by the spectral theorem for normal operators [recall: positive operators $(A \geq 0)$ are hermitian $(A^\dagger = A)$ and hermitian operators are also normal $(AA^\dagger = A^\dagger A)$, N.2.1.6]:

$$\rho = \sum_i \lambda_i |i\rangle\langle i| \quad \text{with } \lambda_i \geq 0 \text{ \& orthonormal vectors } |i\rangle.$$

Due to $\mathrm{Tr}\,\rho = 1 \Rightarrow \sum_i \lambda_i = 1$ & λ_i's can be interpreted as probabilities.

This ρ thus corresponds to an ensemble of states

$$\mathcal{E} = \{\lambda_i \mid |i\rangle\}. \quad \square$$

Note that $\rho^\dagger = \rho$ (hermitian), which follows from the fact that ρ is positive. Also explicitly

$$\rho^\dagger = \sum_i \underbrace{p_i^*}_{=p_i \in \mathbb{R}} |\psi_i\rangle\langle\psi_i| = \rho.$$

Purity: A density operator ρ obeys $\mathrm{Tr}\,\rho^2 = 1$ iff ρ describes a pure state, i.e., $\rho = |\psi\rangle\langle\psi|$.
(N. Ex. 2.71)

$\underline{\Rightarrow}$: $\rho = |\psi\rangle\langle\psi| \Rightarrow \rho^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| =$

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

$\Rightarrow \mathrm{Tr}\,\rho^2 = \mathrm{Tr}\,\rho = 1$.

$\Leftarrow$: A general density operator ρ can be written as (using spectral decomposition):

$$\rho = \sum_i p_i \underbrace{|i\rangle\langle i|}$$

orthonormal eigenbasis of ρ

$$\Rightarrow \quad \mathrm{Tr}\,\rho^2 = \sum_{i,j,k} p_i \, p_j \, \langle k | i \rangle \langle i | j \rangle \langle j | k \rangle =$$

$$= \sum_i p_i^2$$

If ρ describes a pure state $p_1 = 1$ and all other $p_{i \neq 1} = 0$.

$\Rightarrow \quad \mathrm{Tr}\,\rho^2 = 1$ for a pure state

Otherwise, if ρ describes a mixed state with at least two $p_i \neq 0$:

From $\sum_i p_i = 1 \Rightarrow \left(\sum_i p_i \right)^2 = 1$

$$\Leftrightarrow \sum_i p_i^2 + \underbrace{\sum_{i \neq j} p_i p_j}_{> 0 \text{ as all } p_i \geq 0 \text{ and two } p_i \neq 0} = 1$$

$\Rightarrow \sum_i p_i^2 < 1$ if ρ is a mixed state. $\square$

Basis $\{I, X, Y, Z\}^{\otimes n}$ $\mathrm{Tr}\,\rho = 1$

Density operators form a convex set

(convex subset of all $4^n - 1$ $2^n \times 2^n$-dim. hermitian operators).

Given two density operators ρ_1 and ρ_2, the convex linear combination of the two is also a density operator

$$\rho = \lambda \rho_1 + (1-\lambda) \rho_2 \quad , \; 0 \leq \lambda \leq 1 .$$

Proof:

(i) $\mathrm{Tr}\,\rho = \lambda\, \mathrm{Tr} \underbrace{\rho_1}_{=1} + (1-\lambda)\, \mathrm{Tr} \underbrace{\rho_2}_{=1} = 1$ ✓

(ii) $\langle \varphi | \rho | \varphi \rangle = \lambda \underbrace{\langle \varphi | \rho_1 | \varphi \rangle}_{\geq 0} + (1-\lambda) \underbrace{\langle \varphi | \rho_2 | \varphi \rangle}_{\geq 0}$

$\geq 0 .$

$\Rightarrow \rho$ obeys both properties of a density operator. $\square$

Such a state ρ is called a mixture of the states ρ_i.

States in a convex set can be expressed as a convex linear combination of its extremal states (or extremal points of the set): Here, the extremal states are the pure states $|\psi_i\rangle\langle\psi_i|$ as we can always write:

$$\rho = \sum_{p_i} |\psi_i\rangle\langle\psi_i| \, .$$

Pure states are extremal points as they cannot be expressed as a sum of other states.

Proof:

Consider $\rho = |\psi\rangle\langle\psi|$ and let $|\psi_\perp\rangle$ denote a vector perpendicular to $|\psi\rangle$, i.e., $\langle\psi_\perp|\psi\rangle = 0$.

Assume $\rho = \lambda \rho_1 + (1-\lambda)\rho_2$, then

$$\langle\psi_\perp|\rho|\psi_\perp\rangle = 0 = \lambda \langle\psi_\perp|\rho_1|\psi_\perp\rangle + (1-\lambda)\langle\psi_\perp|\rho_2|\psi_\perp\rangle \, .$$

Since the RHS is a sum of two non-negative terms, the sum can only vanish if either

(i) both $\langle\psi_\perp|\rho_1|\psi_\perp\rangle = 0$ and $\langle\psi_\perp|\rho_2|\psi_\perp\rangle = 0$.

or (ii) $\lambda = 0, 1$.

In case (ii), we find $\rho = \rho_1$ or $\rho = \rho_2$.

In case (i), we find:

As $|\psi_\perp\rangle$ can be any vector $\perp$ to $|\psi\rangle$.

$\Rightarrow \rho_1 = \rho_2 = \rho$. $\square$

$\Rightarrow$ The pure states are the extremal points in the convex set of density matrices (ρ with $\mathrm{Tr}\rho = 1$, $\rho \geq 0$).

Only the pure states are extremal as any other ρ can be written as $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$.

<u>Boundary states of convex set:</u>

Note that the states ρ at the boundary of the convex set are density operators with at least one zero eigenvalue, since there are nearby states with negative eigenvalues. These are pure states only in single qubit case.

<u>Example:</u> Single qubit

$$\rho = \frac{1}{2}(I + \vec{r}\cdot\vec{\sigma}) \quad , |\vec{r}| = 1 \; , \; \vec{\sigma} = (X, Y, Z)$$

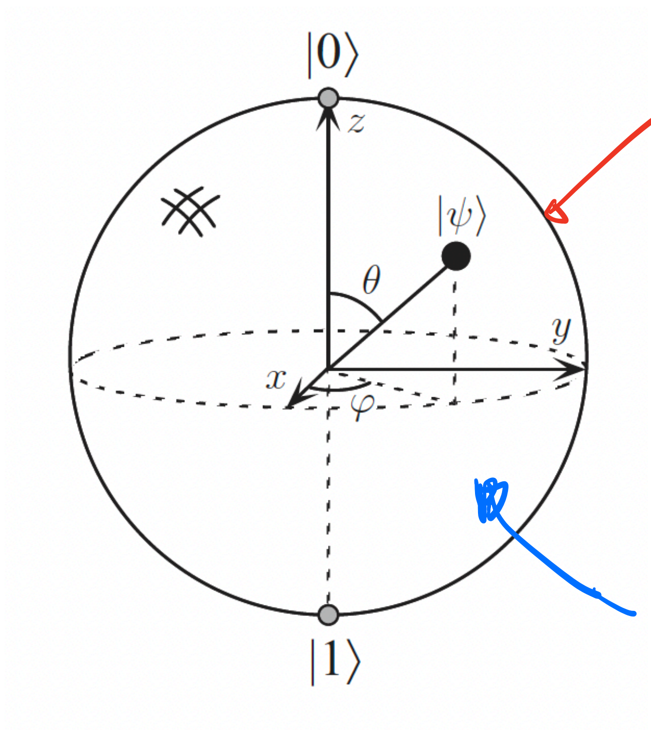


Figure 1.3. Bloch sphere representation of a qubit.

Pure states are at the surface for $|\vec{r}| = 1$:

$$\rho = |\psi\rangle\langle\psi| \hat{=} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

eigenbasis of ρ

mixed states for $|\vec{r}| < 1$.

Later discuss more properties of density matrices. But let us first review the postulates of QM using the density operator ρ.

Review of the postulates of QM (N 2.4.2):

Postulate 1: Associated to any isolated quantum system is a Hilbert space (complex vector space with inner product) – known as the state space. System is completely characterized by a density operator ρ ($\mathrm{Tr}\,\rho = 1$, $\rho \geq 0$).

If a system is in state ρ_i with probability p_i, the density operator is (convex linear combination):

$$\rho = \sum_i p_i \rho_i \quad , \quad \sum_i p_i = 1 .$$

Postulate 2: The time evolution of a closed quantum system is described by a unitary transformation U as

$$\rho(t_2) = U(t_1, t_2)\, \rho(t_1)\, U^\dagger(t_1, t_2)$$

$$U(t_1, t_2) = T \exp\left[-i \int_{t_1}^{t_2} ds\, H(s)\right]$$

time ordering operator

Hamiltonian H, $H^\dagger = H$ of the system

Postulate 3:

Measurements are described by a collection $\{M_m\}$ of measurement operators. These act on the state space of the system being measured. The index m refers to the possible measurement outcomes.
If system is in state ρ immediately before the measurement, the probability to observe result m is

$$p(m) = \mathrm{Tr}\left(M_m^{\dagger} M_m \rho \right)$$

and the state after the measurement is

$$\rho \longmapsto \frac{M_m \rho M_m^{\dagger}}{\mathrm{Tr}\left(M_m^{\dagger} M_m \rho\right)} .$$

The measurement operators fulfill the completeness relation $\sum_m M_m^{\dagger} M_m = I$.

Special case of projection measurements: $P_m = |m\rangle\langle m|$

$$M_m = P_m^{\checkmark\,\text{hermitic}} \quad \text{with} \quad P_m^2 = P_m,\; P_m^+ = P_m$$

being hermitian orthogonal projectors.

are orthogonal projectors: $M_m M_{m'} = M_m \delta_{mm'}$

$$\Rightarrow \sum_m M_m^+ M_m = \sum_m P_m = I$$

Observable (= hermitic operator)

$$M = \sum_m m P_m$$

(spectral decomposition)

- $p(m) = \mathrm{Tr}(P_m \rho)$

- State after measurement:

$$\rho \longmapsto \frac{P_m \rho P_m}{\mathrm{Tr}(P_m \rho)} \equiv \rho_m$$

$\Rightarrow$ repeated measurements yield m with $p(m) = 1$.

POVM: (positive operator-valued measure)

POVM $\{E_m\}$: $E_m = M_m^+ M_m$ are positive operators $E_m \geq 0$.
that obey completeness relation

$$\sum_m E_m = I \quad , \quad p(m) = \mathrm{Tr}(E_m \rho)$$

For any POVM $\{E_m\}$, we can define $M_m = \sqrt{E_m}$ (measurement operators) that describe a measurement with POVM $\{E_m\}$.

Since $E_m \geq 0 \Rightarrow E_m^\dagger = E_m$ and thus allow a spectral decomposition. However, the E_m do not need to be orthogonal projectors, i.e., $E_m E_{m'} \neq E_m \delta_{mm'}$ necessarily.

Generalized measurements from projective measurements on extended system:

Note that projective measurements together with unitary $\mathcal{U}$ on an enlarged system $S \otimes R$:

ancillary system with orthogonal basis $|m\rangle$ enumerating measurement outcomes of M_m.

$$\mathcal{U}\,|\psi\rangle|0\rangle = \sum_m \underbrace{M_m}_{\text{act on } S} |\psi\rangle |m\rangle$$

$\mathcal{U}$ entangles $|\psi\rangle \in S$ with ancilla system R,

is equivalent to generalized measurement as described in postulate 3 via

$$P_m = I_S \otimes |m\rangle\langle m|$$

Unitarity of $\mathcal{U}$ demands that

$$1 = \langle 0|\langle\psi|\,\mathcal{U}^\dagger\,\mathcal{U}\,|\psi\rangle|0\rangle =$$
$$= \sum_{m,n} \langle m|\langle\psi|\,M_m^\dagger M_n\,|\psi\rangle|n\rangle =$$
$$= \sum_m \langle\psi|\,M_m^\dagger M_m\,|\psi\rangle \quad \text{for any } |\psi\rangle$$
$$\Downarrow$$
$$\sum_m M_m^\dagger M_m = \mathbb{1}$$

$$\Rightarrow p(m) = \langle\psi|\langle 0|\,\mathcal{U}^\dagger P_m\,\mathcal{U}\,|\psi\rangle|0\rangle =$$

$$= \sum_{m_1, m_2} \langle\psi|\langle m_1|\,M_{m_1}^\dagger (I_S \otimes P_m) M_{m_2}\,|\psi\rangle|m_2\rangle =$$

$$= \langle \psi | M_m^\dagger M_m | \psi \rangle \quad \text{(as in postulate 3).}$$

$$\langle m_1 | P_m | m_2 \rangle = \langle m_1 | m \rangle \langle m | m_2 \rangle =$$
$$= \delta_{m_1, m} \, \delta_{m_2, m}$$

State after measurement:

$$|\psi_m\rangle = \frac{1}{N} (I_S \otimes P_m) U |\psi\rangle |0\rangle =$$

$$= \frac{1}{N} (I_S \otimes P_m) \sum_{m_1} M_m |\psi\rangle |m_1\rangle =$$

$$= \frac{M_m |\psi\rangle |m\rangle}{\sqrt{\langle \psi | M_m^\dagger M_m | \psi \rangle}} \quad \text{(as in postulate 3).}$$

Postulate 4:

The state space of a composite system is the tensor product of the state spaces of the component physical systems $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_n$.

If the system i is in state ρ_i, the density operator of the composite system reads

$$\rho = \rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_n .$$

Reduced density operator (N2.4.3, P2.3.1):

Let ρ be a density operator of a composite system $\mathcal{H}_1 \otimes \mathcal{H}_2$. Let $|i\rangle_1$ and $|i\rangle_2$ be orthonormal bases in $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively.

Hilbert space 1   Hilbert space 2

We can define reduced density operators ρ_1 and ρ_2 for the two subsystems 1 and 2 as:

$$\rho_1 = \mathrm{Tr}_2\, \rho = \sum_i \left(I_1 \otimes \langle i|_2 \right) \rho \left(I_1 \otimes |i\rangle_2 \right)$$

$$\rho_2 = \mathrm{Tr}_1\, \rho = \text{accordingly.}$$

Properties of the reduced density operator:

- $\mathrm{Tr}\, \rho_1 = 1 \quad , \quad \mathrm{Tr}\, \rho_2 = 1$

- $\rho_1 \geq 0$, $\rho_2 \geq 0$

- If $\rho = \underbrace{\sigma_1 \otimes \sigma_2}_{\text{product state}} \Rightarrow \rho_1 = \mathrm{Tr}_2\, \rho = \sigma_1$.

Examples:

① • Bell state $|\Phi^+\rangle = \frac{1}{\sqrt{2}}\left[|00\rangle + |11\rangle\right]$

$$\Rightarrow \rho = \frac{1}{2}\left[|00\rangle + |11\rangle\right]\left[\langle 00| + \langle 11|\right] =$$

$$= \begin{pmatrix} 1/2 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 \end{pmatrix}.$$

Basis $i \in \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$.

$\rho_{ij} = \langle \underset{\text{row}}{i} | \rho | \underset{\text{column}}{j} \rangle$

$$\text{Note } \mathrm{Tr}\,\rho^2 = \mathrm{Tr} \begin{array}{c|c} & \begin{array}{cccc} |00\rangle & |01\rangle & |10\rangle & |11\rangle \end{array} \\ \begin{array}{c} \langle 00| \\ \langle 01| \\ \langle 10| \\ \langle 11| \end{array} & \begin{pmatrix} 1/2 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 \end{pmatrix} \end{array} = 1$$

$\Rightarrow$ indeed ρ describes a pure state.

However,

$$\rho_1 = \mathrm{Tr}_2\, \rho = \sum_i \langle i|_2\, \rho\, |i\rangle_2 =$$

$$= \begin{array}{c|cc} & |0\rangle_1 & |1\rangle_1 \\ \hline \langle 0|_1 & \tfrac{1}{2} & 0 \\ \langle 1|_1 & 0 & \tfrac{1}{2} \end{array} \;=\; \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} = \frac{I}{2}$$

Thus, the purity equals

$$\mathrm{Tr}\, \rho_1^2 = \mathrm{Tr} \begin{pmatrix} 1/4 & 0 \\ 0 & 1/4 \end{pmatrix} = \frac{1}{2} < 1$$

$\Rightarrow$ ρ_1 describes mixed state (fully mixed state).

Can compute von-Neumann entanglement entropy:

eigenvalues of ρ

$$S_{VN} \equiv S = -\mathrm{Tr}\, \rho \ln \rho = -\sum_i p_i \ln p_i$$

go to eigenbasis of ρ

$\Rightarrow$ for the full system: $p_1 = 1$, $p_{2,3,4} = 0$

$\Rightarrow$ $S = 0$ (pure state carries no entropy)

$\Rightarrow$ for subsystem 1: $p_1 = p_2 = 1/2$:

$$S_1 = -2 \cdot \left(\frac{1}{2} \ln \frac{1}{2} \right) = \ln 2$$

(maximal entropy of a single qubit $\rightarrow$ fully mixed state)

② • Werner state

Separable fully mixed state $\frac{I_1}{2} \otimes \frac{I_2}{2}$

$$\rho(\lambda) = \lambda \frac{I}{4} + (1-\lambda) |\psi^-\rangle\langle\psi^-|$$

max. entangled state

with Bell state $|\psi^-\rangle = \frac{1}{\sqrt{2}}\left[|01\rangle - |10\rangle\right]$.

Convex combination of separable state $\frac{I}{4}$ and entangled state $|\psi^-\rangle\langle\psi^-|$.

Matrix form in Z basis (computational product basis):

$$\rho(\lambda) = \begin{pmatrix} \frac{\lambda}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{2}\left(1-\frac{\lambda}{2}\right) & \frac{\lambda-1}{2} & 0 \\ 0 & \frac{\lambda-1}{2} & \frac{1}{2}\left(1-\frac{\lambda}{2}\right) & 0 \\ 0 & 0 & 0 & \lambda/4 \end{pmatrix}$$

$$\frac{1}{4}\lambda + \frac{1-\lambda}{2} = \frac{1}{2} + \lambda \underbrace{\left(\frac{1}{4} - \frac{1}{2}\right)}_{= -\frac{1}{4}} = \frac{1}{2}\left(1 - \frac{\lambda}{2}\right)$$

Eigenvalues:

$$p_i \in \left\{ \frac{\lambda}{4}, \frac{\lambda}{4}, \frac{\lambda}{4}, 1 - \frac{3}{4}\lambda \right\} \Rightarrow \lambda \in \left[0, \frac{4}{3}\right]$$

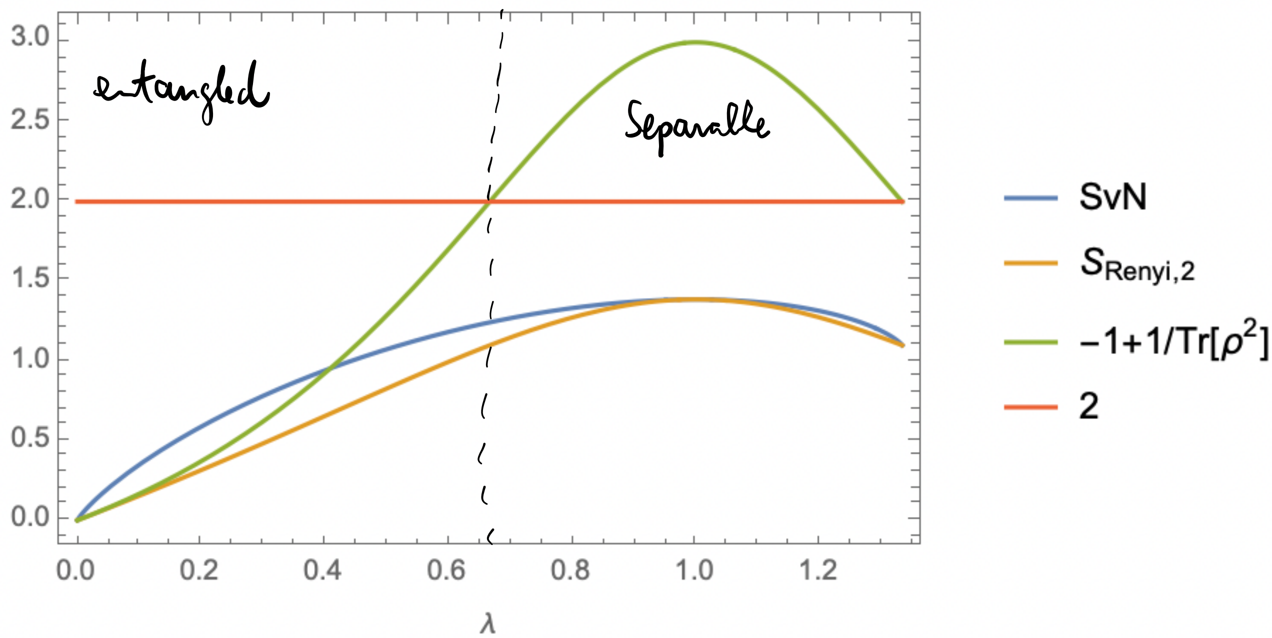
such that $\rho \geq 0$.

$\lambda = 0$: $p_i \in \{1, 0, 0, 0\}$, pure state $|\psi^-\rangle\langle\psi^-|$ $\quad S(\lambda=0) = 0$

$\lambda = \frac{2}{3}$: $p_i \in \{\frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{2}\}$, $S(\lambda = \frac{2}{3}) \approx 1.24 =$
$= \frac{1}{2}\ln 6 + \frac{1}{2}\ln 2$.

$\lambda = 1$: $p_i \in \{\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\}$: fully mixed state $\frac{I}{4}$.
$S(\lambda=1) = \ln 4 = 2\ln 2$.

$\lambda = \frac{4}{3}$: $p_i \in \{\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0\}$: $S(\lambda = \frac{4}{3}) = \ln 3$



Reduced density operator :

$$\rho_1 = Tr_2\, \rho = \begin{array}{c c} & \begin{array}{cc} |0\rangle & |1\rangle \end{array} \\ \begin{array}{c} \langle 0| \\ \langle 1| \end{array} & \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \end{array}$$

Always fully mixed state $\Rightarrow$ can get the same density matrix in many different ways.

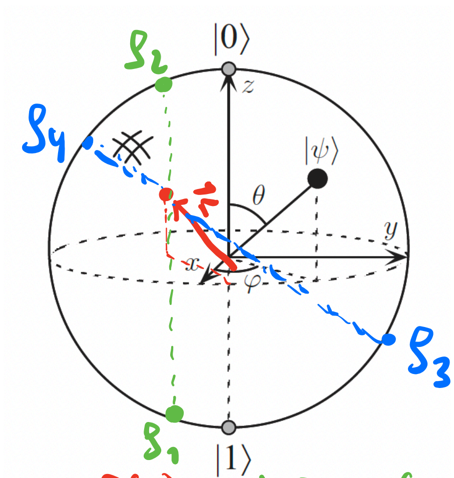
<u>General question</u>: what class of ensembles $\{p_i, |\psi_i\rangle\}$ give rise to the same density matrix ρ.

In other words: in how many ways can ρ be written as a sum of extremal states (i.e. pure states)?

<u>First</u>: let's look at a single qubit.

$$\rho(\vec{r}) = \frac{1}{2}(I + \vec{r}\cdot\vec{\sigma}) = \lambda\,\rho(\hat{m}_1) + (1-\lambda)\,\rho(\hat{m}_2)$$

with $\vec{r} = \lambda \hat{m}_1 + (1-\lambda)\,\hat{m}$.



All such chords comprise a two parameter family [i.e., the first vector $\hat{m}_1$ can be arbitrary (θ_1, ϕ_1)]

$$\rho(\vec{r}) = \lambda\rho_1 + (1-\lambda)\rho_2 = \lambda\rho_3 + (1-\lambda)\rho_4 = \dots$$

Figure 1.3. Bloch sphere representation of a qubit.

In general:

Theorem N2.6 (unitary freedom in the ensemble for density matrices): Ensemble defined by $\mathcal{E} = \{p_i \,|\, |\psi_i\rangle\}$.
Introduce the unnormalized states $|\tilde{\psi}_i\rangle = \sqrt{p_i}\,|\psi_i\rangle$, such that

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| = \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| .$$

The sets $|\tilde{\psi}_i\rangle$ and $|\tilde{\varphi}_i\rangle$ generate the same density operator iff (if and only if)

$$|\tilde{\psi}_i\rangle = \sum_j u_{ij} |\tilde{\varphi}_j\rangle$$

where u_{ij} is a unitary matrix, and we pad whichever set of vectors $|\tilde{\psi}_i\rangle$ or $|\tilde{\varphi}_i\rangle$ is smaller with additional vectors 0 so that the two sets have the same number of elements.

$\Rightarrow$ for normalized states:

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| = \sum_i q_i |\varphi_i\rangle\langle\varphi_i|$$

requires $\sqrt{p_i}\,|\psi_i\rangle = \sum_j U_{ij} \sqrt{q_j}\,|\varphi_j\rangle$

Again, pad the smaller ensemble with entries having $p_j = 0$ to make both ensembles have the same size.

Proof:

$\Rightarrow$: Suppose $|\tilde{\psi}_i\rangle = \sum_j U_{ij} |\tilde{\varphi}_j\rangle$ for unitary U_{ij}.

Then,

$$\sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| = \sum_{j,k} \underbrace{\sum_i U_{ij}\, U^*_{ik}}_{= \sum_i U_{ij} (U^\dagger)_{ki} = \delta_{jk}} |\tilde{\varphi}_j\rangle\langle\tilde{\varphi}_k| =$$

$$= \sum_j |\tilde{\varphi}_j\rangle\langle\tilde{\varphi}_j| \,. \quad \square$$

$\Leftarrow$: Conversely, suppose $\rho = \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| = \sum_j |\tilde{\varphi}_j\rangle\langle\tilde{\varphi}_j|$.

Since $\rho^\dagger = \rho \Rightarrow$ allows for a spectral decomposition

$$\rho = \sum_k \underbrace{\lambda_k}_{>0} |k\rangle\langle k|$$

orthonormal

Let's relate both $|\tilde{\psi}_i\rangle$ and $|\tilde{\varphi}_j\rangle$ to the states $|\tilde{k}\rangle = \sqrt{\lambda_k}\,|k\rangle$.

Let $|\psi\rangle$ be any vector orthonormal to the state spanned by $\{|\tilde{k}\rangle\} \Rightarrow \langle\psi|\tilde{k}\rangle\langle\tilde{k}|\psi\rangle = 0 \quad \forall\, \tilde{k}$.

$$\Rightarrow \langle\psi|\rho|\psi\rangle = 0 = \sum_i \langle\psi|\tilde{\psi}_i\rangle\langle\tilde{\psi}_i|\psi\rangle =$$

$$= \sum_i \underbrace{|\langle\psi|\tilde{\psi}_i\rangle|^2}_{\geq 0 \ \forall i}.$$

$\Rightarrow \langle\psi|\tilde{\psi}_i\rangle = 0 \ \forall i$ and all $|\psi\rangle \perp$ to space spanned by $\{|\tilde{k}\rangle\}$.

Thus, $|\tilde{\psi}_i\rangle$ can be expanded in terms of the $|\tilde{r}\rangle$:

$$|\tilde{\psi}_i\rangle = \sum_r c_{ir} |\tilde{r}\rangle .$$

Since

$$\rho = \sum_r |\tilde{r}\rangle\langle\tilde{r}| = \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| =$$

$$= \sum_{r,l} \sum_i c_{ir} c_{il}^* \underbrace{|\tilde{r}\rangle\langle\tilde{l}|}$$

these operators are linearly independent as $|\tilde{r}\rangle$ are orthonormal.

$$\sum_i c_{ir} c_{il}^* = \delta_{rl} \Longleftarrow$$

$$\langle\tilde{r}_1|\tilde{r}\rangle\langle\tilde{l}|\tilde{l}_1\rangle = \delta_{\tilde{r}\tilde{r}_1}\delta_{\tilde{l}\tilde{l}_1}$$

Assume $|\tilde{r}\rangle\langle\tilde{l}| = \sum_{\substack{r_1 \neq \tilde{r} \\ l_1 \neq \tilde{l}}} A_{r_1 l_1} |\tilde{r}_1\rangle\langle\tilde{l}_1|$

Now, $\langle\tilde{r}|\tilde{r}\rangle\langle\tilde{l}|\tilde{l}\rangle = 1 = 0$

$\Rightarrow$ cannot express this operator $|\tilde{r}\rangle\langle\tilde{l}|$ as linear combination of $|\tilde{r}_1\rangle\langle\tilde{l}_1|$ with $r_1 \neq r$, $l_1 = l$.

Since

$$\sum_i C_{ir} C^*_{il} = \delta_{rl},$$ we may append

extra columns to C to obtain a unitary matrix V

that fulfills $$|\tilde{\psi}_i\rangle = \sum_r V_{ir} |\tilde{r}\rangle.$$

We have appended zero vectors to $|\tilde{r}\rangle$.

Similarly, we find unitary matrix W such that

$$|\tilde{\varphi}_j\rangle = \sum_r W_{jr} |\tilde{r}\rangle.$$

Thus, $$|\tilde{\psi}_i\rangle = \sum_j U_{ij} |\tilde{\varphi}_j\rangle$$

with unitary $U = V W^\dagger$. □

Note that a minimal ensemble $\mathcal{E} = \{p_i \,|\, |\psi_i\rangle\}$

contains as many elements as the rank of ρ, i.e. the number of months $p_i > 0$.