Mixed states

Let us consider $|\psi_1\rangle$ with probability p_1 and $|\psi_2\rangle$ with probability p_2.

We claim that an accurate representation of the combined state in a matrix form is obtained by

$$\rho = \frac{1}{2}|\psi_1\rangle\langle\psi_1| + \frac{1}{2}|\psi_2\rangle\langle\psi_2|.$$

More generally, if the state $|\psi_x\rangle$ is produced with probability p_x, the density matrix representation of the resulting state is

$$\rho = \sum_x p_x |\psi_x\rangle\langle\psi_x| .$$

Verify if this is an accurate representation.

Probability of obtaining outcome '$|b\rangle$' is

$$q_{b|x} = |\langle b|\psi\rangle|^2 = \langle b|\psi_x\rangle\langle\psi_x|b\rangle .$$

$\because$ the state $|\psi_x\rangle$ is prepared (or has) probability p_x, we expect the overall probability of the outcome '$|b\rangle$' to be

$$q_b = \sum_x p_x q_{b|x}$$

Now,

$$q_b = \sum_x p_x \, q_{b|x} = \sum_x p_x \langle b | \psi_x \rangle \langle \psi_x | b \rangle$$

$$= \langle b | \underbrace{\left(\sum_x p_x | \psi_x \rangle \langle \psi_x | \right)} | b \rangle$$

$$= \langle b | \rho | b \rangle$$

which is exactly the same expression we had for the pure state.

<u>Example</u>: Suppose the density matrices for the quantum states $|0\rangle$ and $|+\rangle$ (a Hadamard basis state) are prepared with probabilities $1/2$ for each state. Find the resulting density matrix.

$$\rho = \frac{1}{2} |0\rangle\langle 0| + \frac{1}{2} |+\rangle\langle +|$$

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

(Recall: $|+\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle + |1\rangle \right)$)

$$= \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \frac{1}{4} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} = \frac{1}{4} \begin{bmatrix} 3 & 1 \\ 1 & 1 \end{bmatrix}.$$

Careful! Superposition is not the same as probabilistic combination (also called mixture). They produce different results.

Note: Different ensembles $\{(\psi_x, p_x)\}$ can produce same density matrix.

Verify: $\frac{I}{2} = \frac{1}{2}\left(|0\rangle\langle 0| + |1\rangle\langle 1|\right) = \frac{1}{2}\left(|+\rangle\langle +| + |-\rangle\langle -|\right)$.

Trace of a matrix

Trace of a $d \times d$ matrix is

$$tr(M) = \sum_{i=0}^{d-1} \langle i|M|i\rangle,$$

where $|i\rangle$ is any orthonormal basis in $\mathbb{C}^d$.

Example:

Consider the matrix $M = \begin{pmatrix} 1 & 2 \\ 2 & 2 \end{pmatrix}$. Find the trace using the computational (or standard) basis.

Solution: M is 2×2.

$\therefore$ the computational basis in $\mathbb{C}^2$ are $|0\rangle$ and $|1\rangle$.

$$\therefore tr(M) = \sum_{i=0}^{1} \langle i|M|i\rangle = \langle 0|M|0\rangle + \langle 1|M|1\rangle$$

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

$$= \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} + \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 2 \end{bmatrix} = 1 + 2 = 3$$

Verify: Clasically trace of a matrix is the sum of all diagonal terms.

Exercise: Show that for any matrices M, N we have

$$tr(MN) = tr(N^T M).$$

This produces the result

$$\langle i|A|i\rangle = tr(|i\rangle A |i\rangle) = tr(A|i\rangle\langle i|),$$

which can be used with density matrix for probability calculation.

Example:

If $\{|u_i\rangle\}_i$ is any orthonormal basis in $\mathbb{C}^d$ then we know that there is a unitary transformation U such that

$$U|i\rangle = |u_i\rangle \quad \text{for all } i = 0, 1, \ldots, d-1.$$

So, given a $d \times d$ matrix M show that

$$\mathrm{tr}(M) = \sum_i \langle u_i | M | u_i \rangle.$$

Solution:

$$\sum_i \langle u_i | M | u_i \rangle = \sum_i \langle i | U^* M U | i \rangle$$
$$= \mathrm{tr}(U^\dagger M U) = \mathrm{tr}(M U^\dagger U)$$
$$= \mathrm{tr}(M) \quad [\because U^\dagger U = I].$$

Partial trace

Consider a general matrix

$$M_{AB} = \sum_{ijkl} \gamma_{ij}^{kl} |i\rangle\langle j|_A \otimes |k\rangle\langle l|_B$$

where $|i\rangle_A, |j\rangle_A$ and $|k\rangle_B, |l\rangle_B$ are the orthonormal bases of A and B respectively.

Then partial trace over B is defined as

$$M_A = \mathrm{tr}_B(M_{AB}) = \sum_{ijkl} \gamma_{ij}^{kl} |i\rangle\langle j|_A \,\mathrm{tr}(|k\rangle\langle l|_B).$$

Problem: Let us consider the EPR pair

$$|EPR\rangle_{AB} = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

where $|0\rangle_A, |1\rangle_A$ and $|0\rangle_B, |1\rangle_B$ are the orthonormal basis of A and B used to generate the EPR state.

Calculate the partial trace operator over B.

Solution: The associated density matrix

$$\rho_{AB} = |EPR\rangle\langle EPR|_{AB}$$

$$= \frac{1}{2}\left(|0\rangle\langle 0|_A \otimes |0\rangle\langle 0|_B + |0\rangle\langle 1|_A \otimes |0\rangle\langle 1|_B + |1\rangle\langle 0|_A \otimes |1\rangle\langle 0|_B + |1\rangle\langle 1|_A \otimes |1\rangle\langle 1|_B\right).$$

$$\therefore \; tr_B(\rho_{AB}) = \frac{1}{2}\big(|0\rangle\langle 0|_A \otimes tr(|0\rangle\langle 0|_B) + |0\rangle\langle 1|_A \otimes tr(|0\rangle\langle 1|_B) + |1\rangle\langle 0|_A \otimes tr(|1\rangle\langle 0|_B) + |1\rangle\langle 1|_A \, tr(|1\rangle\langle 1|_B)\big).$$

$\because$ $tr(|0\rangle\langle 1|) = \langle 1|0\rangle = 0$; $tr(|1\rangle\langle 0|) = 0$

(i.e. trace is cyclic) but $tr(|0\rangle\langle 0|) = tr(|1\rangle\langle 1|) = 1$,

hence,

$$tr_B(\rho_{AB}) = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{I}{2}$$

(This is Alice's state)

Exercise: Find out that state which Bob has.

(Calculate partial trace operation over A, $tr_A(\rho_{AB})$).

Exercise 2: Verify that the partial traces

$\rho_A = tr_B(\rho_{AB})$ and $\rho_B = tr_A(\rho_{AB})$ are again

density matrices.

How to differentiate between two quantum states?

Trace distance

The trace distance between two quantum states ρ_0 and ρ_1 is given by

$$D(\rho_0, \rho_1) = \max_{0 \le M \le I} tr(M(\rho_0 - \rho_1)).$$

ρ_0 and ρ_1 must of same dimension.

Note: The definition expresses the trace distance as an optimization problem.

For practical calculation:

$$D(\rho_0, \rho_1) = \frac{1}{2} \| A \|_1 = \frac{1}{2} tr(\sqrt{A^\dagger A})$$

where $A = \rho_0 - \rho_1$ and $\| A \|_1$ is the Schatten 1-norm of the matrix A, i.e. sum of the singular values (which is the sum of the absolute values of its eigenvalues).

Problem: Consider $\rho_1 = |0\rangle\langle 0|$ and $\rho_2 = |+\rangle\langle +|$. Evaluate $D(\rho_1, \rho_2)$.

Solution:

$$\rho_1 - \rho_2 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} - \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \end{pmatrix}$$

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

Trace distance

$$D(\rho_1, \rho_2) = \frac{1}{2} \operatorname{tr} \sqrt{\frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix} \cdot \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix}}$$

$$= \frac{1}{2} \cdot \frac{1}{2} \operatorname{tr} \sqrt{\begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix}^2} = \frac{1}{2} \cdot \frac{1}{2} \operatorname{tr} \sqrt{\begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix} \cdot \begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix}}$$

$$= \frac{1}{2} \cdot \frac{1}{2} \operatorname{tr} \sqrt{\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}} = \frac{1}{2} \cdot \frac{1}{2} \operatorname{tr} \begin{pmatrix} \sqrt{2} & 0 \\ 0 & \sqrt{2} \end{pmatrix}$$

$$= \frac{1}{2} \cdot \frac{1}{2} \cdot 2\sqrt{2} = \frac{1}{\sqrt{2}},$$

Alternatively, find the eigenvalues

$$\operatorname{Det}[(\rho_1 - \rho_2) - \lambda I] = 0 \Rightarrow \operatorname{Det} \begin{pmatrix} \frac{1}{2} - \lambda & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} - \lambda \end{pmatrix} = 0$$

$$\Rightarrow -\left(\frac{1}{2} - \lambda\right)\left(\frac{1}{2} + \lambda\right) - \left(\frac{1}{2}\right)^2 = 0$$

$$\Rightarrow -\left(\frac{1}{2}\right)^2 + \lambda^2 - \left(\frac{1}{2}\right)^2 = 0 \Rightarrow \lambda = \pm \sqrt{2} \cdot \left(\frac{1}{2}\right) = \pm \frac{1}{\sqrt{2}}$$

$$\therefore \|A\|_1 = \left|\frac{1}{\sqrt{2}}\right| + \left|-\frac{1}{\sqrt{2}}\right| = 2 \cdot \frac{1}{\sqrt{2}} = \sqrt{2}$$

$$\therefore D(\rho_1, \rho_2) = \frac{1}{2} \|A\|_1 = \frac{1}{2} \cdot \sqrt{2} = \frac{1}{\sqrt{2}}.$$