How do we describe prob dists over quantum states?

Note about generality and deal with $|\psi\rangle \in \mathbb{C}^d$ as much as possible.

Ans: Density matrices

For $|\psi\rangle \in \mathbb{C}^d$, the corresponding d.m. is $|\psi\rangle\langle\psi|$.

Def. Let $\{(p_a, |\psi_a\rangle)\}_a$ be an ensemble of pure states

meaning p_a is a prob. dist. $p_a \geq 0$, $\sum_a p_a = 1$.

Then, the corresponding d.m. is $\rho := \sum_a p_a |\psi_a\rangle\langle\psi_a|$.

If d.m. is rank 1, $\rho = |\psi\rangle\langle\psi|$ then called pure.
If not rank 1, then called mixed.

Central thesis: d.m. formalization is necessary and sufficient.

Examples

$$|0\rangle \mapsto \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad |1\rangle \mapsto \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$|+\rangle \mapsto \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \qquad |-\rangle \mapsto \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$\text{coin-flip} = \frac{|0\rangle\langle 0| + |1\rangle\langle 1|}{2} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{|+\rangle\langle +| + |-\rangle\langle -|}{2}.$$

$$|EPR\rangle \mapsto \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

$$\text{shared randomness} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Thm (Total characterization)

① Let ρ correspond to $\{(p_a, |\psi_a\rangle)\}$.

Then $\rho \geq 0$, $\mathrm{tr}(\rho) = 1$.

② If $\rho \geq 0$, $\mathrm{tr}(\rho) = 1 \Rightarrow \exists$ corresponding ensemble yielding ρ.

Def ρ is a dm. iff $\rho \geq 0$, $\mathrm{tr}(\rho) = 1$.

Pf of ① Since each $p_a \in \mathbb{R}$, $|\psi_a\rangle\langle\psi_a|$ Hermitian $\Rightarrow \rho$ is Hermitian.

For any vector $|v\rangle$,

$$\langle v|\rho|v\rangle = \langle v|\left(\sum_a p_a |\psi_a\rangle\langle\psi_a|\right)|v\rangle$$

$$= \sum_a p_a \langle v|\psi_a\rangle\langle\psi_a|v\rangle$$

$$= \sum_a p_a |\langle v|\psi\rangle|^2 \geq 0.$$

$$\mathrm{tr}(\rho) = \mathrm{tr}\left(\sum_a p_a |\psi_a\rangle\langle\psi_a|\right)$$

$$= \sum_a p_a \,\mathrm{tr}\left(|\psi_a\rangle\langle\psi_a|\right)$$

$$= \sum_a p_a \langle\psi_a|\psi_a\rangle = \sum_a p_a = 1.$$

Pf of (2)

Spectral thm: $\rho = \sum_a \lambda_a |v_a\rangle\langle v_a|$ eigendecomposition

$\rho \geq 0 \Rightarrow \lambda_a \geq 0$ and $1 = \mathrm{tr}(\rho) = \sum_a \lambda_a$

so λ is a prob. dist.

So $\{(\lambda_a, |v_a\rangle)\}$ is a well-defined ensemble.

Updating density matrices — Derived consequences

If a state is represented by ρ and unitary U is applied.

Then, $\rho \mapsto U\rho U^\dagger$.

Pf. Consider any ensemble $\{(p_a, |\psi_a\rangle)\}$ corresponding to ρ.

New ensemble $\{(p_a, U|\psi_a\rangle)\}$. Corresponds to

$$\rho = \sum_a p_a U|\psi_a\rangle\langle\psi_a|U^\dagger = U\left(\sum_a p_a |\psi_a\rangle\langle\psi_a|\right)U^\dagger = U\rho U^\dagger. \quad \square$$

Measurements:

For bit b, define $\Pi_b = |b\rangle\langle b| \otimes \mathbb{1}$.

If first qubit measured, then

$$\Pr[b] = \mathrm{tr}(\Pi_b \rho)$$

post-measurement state is $\sigma = \dfrac{\Pi_b \rho \Pi_b}{\mathrm{tr}(\Pi_b \rho)}$

and if no measurement is recorded, then state equals

$$\Pi_0 \rho \Pi_0 + \Pi_1 \rho \Pi_1.$$

Pf. $\rho = \sum_a p_a |\psi_a\rangle\langle\psi_a|$ be any ensemble decomposition.

Observe $\Pi_0 + \Pi_1 = \mathbb{1}$ and $\Pi_0 \Pi_1 = 0$, then

$$|\psi_a\rangle = \Pi_0 |\psi_a\rangle + \Pi_1 |\psi_a\rangle$$

Then $\Pr[b \mid a] = \left\| (\langle b| \otimes \mathbb{1}) |\psi_a\rangle \right\|^2$

$= \left\| \Pi_b |\psi_a\rangle \right\|^2$

$= \langle \psi_a | \Pi_b | \psi_a \rangle$

Then $\Pr[b] = \sum_a p_a \Pr[b \mid a]$

$= \sum_a p_a \langle \psi_a | \Pi_b | \psi_a \rangle$

$= \sum_a p_a \operatorname{tr}\left(\Pi_b |\psi_a\rangle\langle\psi_a| \right)$

$= \operatorname{tr}\left(\Pi_b \sum_a p_a |\psi_a\rangle\langle\psi_a| \right)$

$= \operatorname{tr}(\Pi_b \rho)$.

If b observed, so $\Pr[b] > 0$. Then for event a, post-state is

$$\frac{\Pi_b |\psi_a\rangle}{\left\| \Pi_b |\psi_a\rangle \right\|} = \frac{\Pi_b |\psi_a\rangle}{\sqrt{\langle \psi_a | \Pi_b | \psi_a \rangle}}$$

as a dist. $\sigma_b^a := \dfrac{\Pi_b |\psi_a\rangle\langle\psi_a| \Pi_b}{\langle \psi_a | \Pi_b | \psi_a \rangle}$

If b has occurred, then $\Pr[a \mid b] = \dfrac{p_a \Pr[b \mid a]}{\Pr[b]}$.

post-measurement dim.

$$\sigma_b = \sum_a \Pr[a \mid b]\, \sigma_b^a$$

$$= \sum_a \frac{p_a \langle \psi_a | \Pi_b | \psi_a \rangle}{\Pr[b]} \cdot \frac{\Pi_b |\psi_a\rangle\langle\psi_a| \Pi_b}{\langle \psi_a | \Pi_b | \psi_a \rangle}$$

$$= \frac{\Pi_b \left(\sum_a p_a |\psi_a\rangle\langle\psi_a| \right) \Pi_b}{\mathrm{tr}(\Pi_b \rho)}$$

$$= \frac{\Pi_b \rho \Pi_b}{\mathrm{tr}(\Pi_b \rho)}.$$

Lastly, use that if measurement is not known then

$$\Pr[0]\, \sigma_0 + \Pr[1]\, \sigma_1 = \Pi_0 \rho \Pi_0 + \Pi_1 \rho \Pi_1.$$