2. Mixed States

a) The density operator

Consider a bipartite state $|\psi\rangle_{AB} = \sum c_{ij} |i\rangle|j\rangle$.

We have access to A only.

Can we characterize the measurement outcomes for meas. on A in a simple way?

(i.e. without having to consider B, which we anyway cannot access!)

Consider measurement operator Π.
(e.g. $\Pi = E_i$ projector, or exp. value, ...)

Measurement of $\Pi \equiv \Pi_A$ on A

$\Longleftrightarrow$ measurement of $\Pi_A \otimes I_B$ on A & B.

$$\langle\psi|\Pi_A \otimes I_B|\psi\rangle = \sum_{\substack{ij\\ i'j'}} \overline{c_{i'j'}} \langle i'|\langle j'|(\Pi_A \otimes I_B)\, |i\rangle|j\rangle\, c_{ij}$$

$$= \sum \overline{c_{i'j'}}\, c_{ij}\, \langle i'|\Pi_A|i\rangle \underbrace{\langle j'|j\rangle}_{=\delta_{j'j}}$$

$$= \sum_{ii'} \Big(\sum_j \overline{c_{i'j}}\, c_{ij} \Big) \langle i' | \Pi_A | i \rangle = (*)$$

<u>Now</u>: Define ρ_A – a $d_A \times d_A$ matrix – via

$$(\rho_A)_{ii'} = \sum_j c_{ij} \overline{c_{i'j}} = (C \cdot C^\dagger)_{ii'},$$

with the matrix $C = (c_{ij})_{ij}$,

or equivalently $\rho_A = \sum_{i,i',j} c_{ij} \overline{c_{i'j}} |i\rangle\langle i'|$

and introduce the <u>trace</u>

$$\mathrm{tr}(X) = \sum_k \langle k | X | k \rangle$$

can be <u>any</u> ONB, not necessarily comp. basis.

<u>Note</u>: The trace is

- cyclic: $\mathrm{tr}(AB) = \sum_k \langle k | AB | k \rangle$

$$= \sum_k \langle k | A \Big(\sum_l |l\rangle\langle l| \Big) B | k \rangle$$

$$= \sum_{kl} \langle k | A | l \rangle \langle l | B | k \rangle$$

$$= \sum_{kl} \langle l | B | k \rangle \langle k | A | l \rangle = \mathrm{tr}(BA)$$

<u>Note</u>: A, B need <u>not</u> be square!

- and thus basis-independent:

$$\mathrm{tr}(U^\dagger X U) = \mathrm{tr}(X U U^\dagger) = \mathrm{tr}(X),$$

and thus $\mathrm{tr}(X) = \sum \langle k | X | k \rangle$

$$= \sum \underbrace{(\langle k | U^\dagger)}_{\langle v_k |} X \underbrace{(U | k \rangle)}_{| v_k \rangle}$$

$$= \sum \langle v_k | X | v_k \rangle \text{ for } \underline{\text{any}} \text{ ONB,}$$

- the sum of the eigenvalues:

$$\mathrm{tr}(X) = \mathrm{tr}(X A A^{-1}) = \mathrm{tr}(A^{-1} X A),$$

with $A^{-1} X A$ the eigenvalue decomposition.

- and of course linear:

$$\mathrm{tr}(A) + \lambda \, \mathrm{tr}(B) = \mathrm{tr}(A + \lambda B).$$

Then,

$$(*) = \sum_{ii'} \overbrace{\left(\sum_j \overline{c_{i'j}}\, c_{ij} \right)}\, \langle i' | \Pi_A | i \rangle$$

trace of a number is itself!

$$= \sum_{ii'} \left(\sum_j \overline{c_{i'j}}\, c_{ij} \right) \operatorname{tr}\left[\langle i' | \Pi_A | i \rangle \right]$$

cyclicity of trace!

$$= \sum_{ii'} \left(\sum_j c_{ij}\, \overline{c_{i'j}} \right) \operatorname{tr}\left[|i\rangle \langle i' | \Pi_A \right]$$

linearity of trace!

$$= \operatorname{tr}\Big[\underbrace{\Big(\sum_{ii'j} c_{ij}\, \overline{c_{i'j}}\, |i\rangle\langle i'| \Big)}_{=\rho_A} \Pi_A \Big]$$

$$= \operatorname{tr}\left[\rho_A \Pi_A \right].$$

<u>i.e.:</u> $\langle \psi | \Pi_A \otimes I_B | \psi \rangle = \operatorname{tr}\left[\rho_A \Pi_A \right],$

where $\rho_A = \sum_{ii'j} c_{ij}\, \overline{c_{i'j}}\, |i\rangle\langle i'|,$

or $\rho_A = C C^\dagger$, with $C = (c_{ij})_{ij}$.

ρ_A is called the density operator, density matrix, or mixed state. It characterizes systems where we only have partial knowledge, such as access to only part of the system.

In contrast, a state $|\psi\rangle \in \mathcal{H}$ is called a pure state.

Properties of ρ_A:

- $\rho_A = CC^\dagger \Rightarrow \rho_A^\dagger = (CC^\dagger)^\dagger = CC^\dagger = \rho_A$

- ρ_A is positive semidefinite:

$$\langle\phi|\rho_A|\phi\rangle = \langle\phi|CC^\dagger|\phi\rangle = (C^\dagger|\phi\rangle)^\dagger \underbrace{(C^\dagger|\phi\rangle)}_{=:|\phi'\rangle}$$

$$= \langle\phi'|\phi'\rangle \geq 0 \quad \forall \phi.$$

We write $\rho_A \geq 0$.

Note: $X \geq 0$, i.e. $\langle\phi|X|\phi\rangle \geq 0 \;\forall\, |\phi\rangle$

$\Longleftrightarrow X = X^\dagger$ & all eigenvalues of X are ≥ 0.

(In part., $X \geq 0 \Rightarrow X = X^\dagger$)

- $\mathrm{tr}(\rho_A) = \sum_i (CC^\dagger)_{ii} = \sum_{ij} c_{ij}\,\overline{c_{ij}} = \sum |c_{ij}|^2 = 1.$

Properties of density operators:

- $\rho_A \geq 0$ (implies $\rho_A = \rho_A^\dagger$)
- $\mathrm{tr}(\rho_A) = 1.$

Will see soon: This provides an alternative fundamental definition of a state – i.e., any ρ_A with the properties above can arise if we only have access to part of the system.

Note: All ρ_A with the above property form a convex set S, i.e.:

$$\rho, \sigma \in S \Rightarrow p\rho + (1-p)\sigma \in S, \quad 0 \leq p \leq 1.$$

Is there an ambiguity in ρ_A, just as the phase ambiguity for pure states?

Theorem: ρ_A is uniquely determined by all measurement outcomes $\mathrm{tr}[\rho_A \Pi]$ for $\Pi = \Pi^\dagger$.

(i.e., by all averages, though probabilities, i.e. Π orth. proj., also suffices.)

Proof: Let $V = \{ M \mid M = M^\dagger \}$. V is a vector space over $\mathbb{R}$.

$(M,N) := \mathrm{tr}[M^\dagger N]$ defines a scalar product on V

(the "Hilbert-Schmidt scalar product").

Pick an ONB $\{\Pi_i\}$ of V, $\mathrm{tr}[\Pi_i^\dagger \Pi_j] = \delta_{ij}$.

Then, the map $$X \longmapsto \sum \Pi_i \,\mathrm{tr}[\Pi_i^\dagger X]$$
$$= \sum \Pi_i \,(\Pi_i, X)$$

acts as the identity on V. Thus,

$$\rho_A = \sum \Pi_i \,\mathrm{tr}[\Pi_i \rho_A],$$

i.e., ρ_A is fully specified by all meas. outcomes (and thus, there must be a unique ρ_A for any given physical state. ∎

(Note: We didn't really use that we have hermitian matrices – the same ideas work for $V_{\mathbb{C}} = \{\Pi\}$ over $\mathbb{C}$. Then the $\cdot^\dagger$ are important – and we must show that $V_{\mathbb{C}}$ has a hermitian basis over $\mathbb{C}$ – which it does.)

In particular: No ambiguity in ρ_A
$\Rightarrow$ all numbers meaningful!

Where did the phase $|\psi_A\rangle \sim e^{i\phi}|\psi_A\rangle$ go?

Density matrix for a pure state $|\psi_A\rangle$:

number

$$\langle\psi_A|\Pi|\psi_A\rangle = \mathrm{tr}\left[\langle\psi_A|\Pi|\psi_A\rangle\right]$$

$$= \mathrm{tr}\Big[\Pi \underbrace{|\psi_A\rangle\langle\psi_A|}_{=\rho_A}\Big]$$

cycl.

$\Rightarrow$ $\rho_A = |\psi_A\rangle\langle\psi_A|$: projector onto $|\psi_A\rangle$.

(Phase naturally drops out!)

b) The partial trace

Just seen: Pure state on AB $\rightarrow$ Mixed state on A.

What if AB itself is already mixed
(e.g. from a pure ABC?)

Same approach: How to describe most general measurement on A, given a state ρ_{AB}?

$$\mathrm{tr}\left[(\Pi_A \otimes I_B)\,\rho_{AB}\right] = \sum \langle i \underbrace{j| \Pi \otimes I | i' j'}_{=\delta_{jj'}}\rangle \langle i'j'| \rho_{AB} | ij\rangle$$

$$= \sum_{ii'j} \langle i|\Pi|i'\rangle \langle i'j|\rho_{AB}|ij\rangle$$

$$= \mathrm{tr}\Big[\Pi \cdot \Big(\sum_{ii'j} |i'\rangle_A \langle i'j|\, \rho_{AB}\, |ij\rangle\langle i|_A\Big)\Big]$$

$$= \mathrm{tr}\left[\Pi \cdot \rho_A\right]$$

where we define

$$\rho_A = \sum |i'\rangle_A\langle i'j|\, \rho_{AB}\, |ij\rangle\langle i|_A$$

$$= \sum_j (I_A \otimes \langle j|_B)\, \rho_{AB}\, (I_A \otimes |j\rangle_B)$$

$$= \sum_j \langle j|_B\, \rho_{AB}\, |j\rangle_B$$

$$=: \mathrm{tr}_B(\rho_{AB})$$: the "partial trace"

In components:

$$(\mathrm{tr}_B(\rho_{AB}))_{ii'} = \langle i|_A \Big(\sum_j \langle j|_B\, \rho_{AB}\, |j\rangle_B\Big) |i'\rangle$$

$$= \sum_j (\rho_{AB})_{(ij),(i'j)}$$

(Note: The partial trace can also be seen as the canonical embedding of

$$\mathrm{tr} : B(\mathcal{H}_A) \longrightarrow \mathbb{C}$$

into $B(\mathcal{H}_A) \otimes B(\mathcal{H}_B)$)

linear ("bounded") operators on $\mathcal{H}_A$.

Note: ρ_A is also called reduced density matrix (or operator) of ρ_{AB} (or $|\psi_{AB}\rangle$).

c) Purifications

Is any density matrix ρ ($\rho \geq 0$, $\mathrm{tr}\,\rho = 1$) physical (i.e., coming from a pure state, as by our axioms)?

Purification of mixed state ρ:

Consider any decomposition $\rho = \sum \lambda_i |\phi_i\rangle\langle\phi_i|$, $\lambda_i > 0$, e.g. the eigenvalue decomposition, and define

any ONB

$$|\psi\rangle_{AB} := \sum \sqrt{\lambda_i}\, |\phi_i\rangle_A |i\rangle_B$$

Then

$$\mathrm{tr}_B\big[|\psi\rangle\langle\psi|\big] = \mathrm{tr}_B\Big[\sum_{ij} \sqrt{\lambda_i \lambda_j}\, |\phi_i\rangle\langle\phi_j| \otimes |i\rangle\langle j|\Big]$$

$$= \sum_{ij} \sqrt{\lambda_i \lambda_j}\, |\phi_i\rangle\langle\phi_j| \otimes \underbrace{\mathrm{tr}_B\big[|i\rangle\langle j|\big]}_{=\delta_{ij}}$$

$$= \sum \lambda_i |\phi_i\rangle\langle\phi_i| = \rho$$

$\Rightarrow$ Yes, every ρ is physical (in the sense above).

$\Longrightarrow$ Density operators ρ can serve as an alternative fundamental definition of a state in quantum theory.

Definition: A $|\psi\rangle_{AB}$ s.th. $\mathrm{tr}_B |\psi\rangle\langle\psi| = \rho$ is called a purification of ρ.

Note: The ambiguity of purifications – i.e., how are two purifications $|\psi\rangle, |\phi\rangle$ of ρ, $\mathrm{tr}_B(|\psi\rangle\langle\psi|) = \mathrm{tr}_B(|\phi\rangle\langle\phi|) = \rho$, related – will be addressed later.

d) Ensemble interpretation of the density matrix

Consider $|\psi\rangle = \alpha|00\rangle + \beta|11\rangle$:

$$\Rightarrow \rho_A = \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix} = |\alpha|^2 |0\rangle\langle 0| + |\beta|^2 |1\rangle\langle 1|$$

$$\Rightarrow \mathrm{tr}[\Pi \rho_A] = |\alpha|^2 \langle 0|\Pi|0\rangle + |\beta|^2 \langle 1|\Pi|1\rangle .$$

$\Rightarrow$ Can be interpreted as having the pure state $|0\rangle$ with probability $p_0 = |\alpha|^2$, and $|1\rangle$ w/ $p_1 = |\beta|^2$.

"ensemble interpretation" of density matrix

However: We have derived ρ_A from a pure state $|\psi\rangle_{AB}$ — isn't this contradictory?

Imagine B does a measurement in the Z basis:

$$|\psi\rangle = \alpha|00\rangle + \beta|11\rangle \xrightarrow{p_0 = |\alpha|^2} |\psi_0\rangle_A = |0\rangle_A$$

$$|\psi\rangle = \alpha|00\rangle + \beta|11\rangle \xrightarrow{p_1 = |\beta|^2} |\psi_1\rangle_A = |1\rangle_A$$

The post-measurement state of Alice is $|\psi_0\rangle = |0\rangle$ with $p_0 = |\alpha|^2$, and $|\psi_1\rangle = |1\rangle$ with $p_1 = |\beta|^2$.

<u>But</u>: Alice <u>does not know outcome</u> of Bob

$\Rightarrow$ meas. of B produces an <u>ensemble</u>

$$\{(p_0, |0\rangle), (p_1, |1\rangle)\} \equiv \begin{pmatrix} |\alpha|^2 & \\ & |\beta|^2 \end{pmatrix}.$$

(<u>But note</u>: Bob <u>knows</u> outcome $\Rightarrow$ his description is different: he would describe Alice's state <u>either</u> as $|0\rangle\langle 0|$ <u>or</u> as $|1\rangle\langle 1|$!

<u>I.e.</u>: <u>State assigned</u> dep. on <u>knowledge</u>!

<u>But</u>: Bob could also measure in different basis, e.g. $|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$!

$$|\psi\rangle = \alpha|00\rangle + \beta|11\rangle \xrightarrow{\text{X-meas. on } B}$$

$$p_+ = \frac{|\alpha|^2+|\beta|^2}{2} = \frac{1}{2} \longrightarrow |\psi_+\rangle_A = \frac{\alpha|0\rangle + \beta|1\rangle}{|\alpha|^2+|\beta|^2}$$

$$p_- = \frac{|\alpha|^2+|\beta|^2}{2} = \frac{1}{2} \longrightarrow |\psi_-\rangle_A = \frac{\alpha|0\rangle - \beta|1\rangle}{|\alpha|^2+|\beta|^2}$$

non-orthogonal!

Ensemble $\{(p_+, |\psi_+\rangle), (p_-, |\psi_-\rangle)\}$

Indeed, $p_+ |\psi_+\rangle\langle\psi_+| + p_- |\psi_-\rangle\langle\psi_-| = \rho_A$!

<u>Different ensemble</u> for <u>same state</u>

$\Longrightarrow$ <u>ensemble interpretation is ambiguous!</u>

(Even # of terms can vary, etc. $\rightarrow$ HW)

How are two different ensemble decompositions related?

Theorem: Let $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| = \sum_j q_j |\phi_j\rangle\langle\phi_j|$.

no need for ONBs!!

Then, there exists a unitary $\mathcal{U} = (u_{ij})_{ij}$ s.th.

$$\sqrt{p_i}\,|\psi_i\rangle = \sum_j u_{ij} \sqrt{q_j}\,|\phi_j\rangle,$$

and vice versa. (If the number of terms in the two sums is different, the smaller should be padded with $p_i = 0$ and suitable $|\psi_i\rangle$.)

Proof:

"$\Leftarrow$": Let $\sqrt{p_i}\,|\psi_i\rangle = \sum u_{ij} \sqrt{q_j}\,|\phi_j\rangle$.

Then $\sum_i p_i |\psi_i\rangle\langle\psi_i| = \sum_i \left(\sum_j u_{ij} \sqrt{q_j}\,|\phi_j\rangle\right)\left(\sum_{j'} \overline{u_{ij'}} \sqrt{q_{j'}}\langle\phi_{j'}|\right)$

$$= \sum_{jj'} \sqrt{q_j}\,|\phi_j\rangle\langle\phi_{j'}| \sqrt{q_{j'}} \underbrace{\left(\sum_i \overline{u_{ij'}}\, u_{ij}\right)}_{(\mathcal{U}^\dagger \mathcal{U})_{j'j} = \delta_{jj'}}$$

$$= \sum_j q_j |\phi_j\rangle\langle\phi_j|.$$

"$\Longrightarrow$": First, assume $|\phi_j\rangle$ is an eigenstate of ρ.

Define $u_{ij} = \langle \phi_j | \psi_i \rangle \dfrac{\sqrt{p_i}}{\sqrt{q_j}}$.

Then, $\sum_j u_{ij} \sqrt{q_j} \, |\phi_j\rangle = \sum_j \sqrt{q_j} \, |\phi_j\rangle\langle\phi_j|\psi_i\rangle \dfrac{\sqrt{p_i}}{\sqrt{q_j}}$

$= \sqrt{p_i} \, |\psi_i\rangle$,

and $\sum_i u_{ij} \overline{u_{ij'}} = \sum_i \langle \phi_j | \psi_i \rangle \langle \psi_i | \phi_{j'} \rangle \dfrac{p_i}{\sqrt{q_j q_{j'}}}$

$\sum p_i |\psi_i\rangle\langle\psi_i|$

$= \underbrace{\langle \phi_j | \overset{\shortparallel}{\rho} | \phi_{j'} \rangle}_{= q_j \delta_{jj'}} \dfrac{1}{\sqrt{q_j q_{j'}}} = \delta_{jj'}$,

$\Rightarrow (u_{ij})$ has orthogonal columns

$\Rightarrow (u_{ij})$ can be extended to a unitary

(and correspondingly padding $\sum q_j |\phi_j\rangle\langle\phi_j|$ with $q_j = 0$).

General case: Relate

$$\sum p_i |\psi_i\rangle\langle\psi_i| \xleftrightarrow{u_{ik}} \underbrace{\sum r_k |e_k\rangle\langle e_k|}_{\text{eigenbasis}} \xleftrightarrow{v_{jk}} \sum q_j |\phi_j\rangle\langle\phi_j|$$

& combine the unitaries u_{ik} & v_{jk}

→ Homework.

e) Unitary evolution & projective measurement for mixed states

How does a mixed state evolve under a unitary U?

– Can be assessed in diff. ways, e.g. through purifications (here) or ensemble interpretation (HW) –

Consider state ρ & unitary U.

Let $|\psi\rangle = |\psi\rangle_{AB}$ be a purification of ρ,

$$\mathrm{tr}_B |\psi\rangle\langle\psi| = \rho_A .$$

Then, $\quad |\psi\rangle \longmapsto (U_A \otimes I_B)|\psi\rangle$

$$\Longrightarrow \rho_A = \mathrm{tr}_B |\psi\rangle\langle\psi|$$

$$\longmapsto \mathrm{tr}_B\left[(U_A \otimes I_B)|\psi\rangle\langle\psi|(U_A^\dagger \otimes I_B)\right]$$

$$= U_A \,\mathrm{tr}_B\left[(I_A \otimes I_B)|\psi\rangle\langle\psi|(I_A \otimes I_B)\right] U_A^\dagger$$

$$= U_A \rho_A U_A^\dagger .$$

How does proj. measurement $\{E_n\}$ act on ρ_A?

By construction of ρ_A, $\quad p_n = \mathrm{tr}[E_n \rho_A]$.

Post-meas. state:

$$\rho_{A,n} = \frac{1}{p_n} \mathrm{tr}_B\left[(E_n \otimes I)|\psi\rangle\langle\psi|(E_n^\dagger \otimes I)\right]$$

$$= \frac{1}{p_n} E_n \rho_A E_n^\dagger .$$

$\boxtimes$

(Note: Both derivations indep. of chosen purification
$\rightarrow$ well-defined.)