3. Mixed states

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

We have only access to A.

$\rightarrow$ How can we characterize measurement on A?

Meas. M on A $\Longleftrightarrow$ meas. $M_A \otimes \mathbb{1}_B$ on $A+B$.

$$\langle\psi| M_A \otimes \mathbb{1}_B |\psi\rangle = \sum c^*_{i'j'} \langle i'|\langle j'| (M_A \otimes \mathbb{1}_B) |i\rangle|j\rangle c_{ij}$$

$$= \sum c^*_{i'j'} c_{ij} \langle i'|M_A|i\rangle \underbrace{\langle j'|j\rangle}_{=\delta_{jj'}}$$

$$= \sum_{ii'} \Big(\sum_j c^*_{i'j} c_{ij} \Big) \langle i'|M_A|i\rangle = (*)$$

Define ρ_A ($d_A \times d_A$ matrix) via $(\rho_A)_{ii'} = \sum_j c^*_{i'j} c_{ij} = CC^\dagger$

(with $C = (c_{ij})_{ij}$), or equiv. $\rho_A = \sum_{ii'j} c^*_{i'j} c_{ij} |i\rangle\langle i'|$

... $(*) = \mathrm{tr}[\rho_A M]$,

with the <u>trace</u> $\mathrm{tr}(X) = \sum \langle k|X|k\rangle$. ONB!

<u>Note</u>: The trace is cyclic: $\mathrm{tr}(AB) = \sum_k \langle k|AB|k\rangle$

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

$$= \sum \langle l|BA|l\rangle = \mathrm{tr}(BA).$$

and thus basis-indep: $tr(X) = tr(U^\dagger U X) = tr(U X U^\dagger)$. (19)

ρ_A is called <u>density operator</u> or <u>density matrix</u>, or <u>mixed state</u>.
It characterizes systems where we only have <u>partial knowledge</u>.

<u>Properties of ρ_A:</u>

- $\rho_A = CC^\dagger \Rightarrow \rho_A^\dagger = (CC^\dagger)^\dagger = CC^\dagger = \rho_A$
- ρ_A is positive semi-definite (= all eigenvalues ≥ 0), $\rho_A \geq 0$

$$\langle\phi|\rho_A|\phi\rangle = \langle\phi|CC^\dagger|\phi\rangle = (C^\dagger|\phi\rangle)^\dagger (C^\dagger|\phi\rangle) \geq 0 \quad \forall|\phi\rangle.$$

- $tr(\rho_A) = \sum_i (CC^\dagger)_{ii} = \sum_{ij} c_{ij} c_{ij}^* = \langle\psi|\psi\rangle = 1.$

<u>Properties of density operators:</u>

- $\rho_A^\dagger = \rho_A$
- $\rho_A \geq 0$
- $tr(\rho_A) = 1$

<u>Note:</u> Consequence: For $0 < p < 1$, ρ, ρ' density ops, $p\rho + (1-p)\rho'$ is also density op $\Rightarrow$ density ops form <u>convex set</u>!

Is ρ_A uniquely determined by

$$\mathrm{tr}[M\rho_A] = \langle\psi|_{AB}\ M\otimes 1\ |\psi\rangle_{AB}\ ?$$

<u>Yes</u>: $\mathrm{tr}[X^\dagger Y]$ is scalar product, & overlap of ρ_A w/ all herm. M determines herm. part of ρ_A <u>entirely</u>!

(<u>Consequence</u>: All numbers in ρ_A meaningful → no phase ambiguity!)

What <u>is</u> ρ_A for pure state $|\phi\rangle_A$?

$$\langle\phi|M|\phi\rangle = \mathrm{tr}[\langle\phi|M|\phi\rangle] = \mathrm{tr}[M\,|\phi\rangle\langle\phi|]$$

$$\Rightarrow \rho = |\phi\rangle\langle\phi| \quad \text{(projector onto } |\phi\rangle\text{)}.$$

<u>Partial trace</u>:

Given <u>general</u> state ρ_{AB} on $A+B$ (e.g. $\rho_{AB}=|\psi\rangle\langle\psi|$), what is descr. of meas M_A on A?

$$\mathrm{tr}[(M\otimes I)\,\rho_{AB}] = \sum_{ij\,i'j'} \langle i\underbrace{j|M\otimes I|i'j'}_{\delta_{jj'}}\rangle\langle i'j'|\rho_{AB}|ij\rangle$$

$$= \sum \langle i|M|i'\rangle\langle i'j|\rho_{AB}|ij\rangle = \mathrm{tr}[M\cdot\rho_A],$$

Where we def. the <u>partial trace</u>

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

$$= \sum \left(\mathbb{1}_A \otimes \langle j'|_B\right)\left(\rho_{AB}\right)\left(\mathbb{1}_A \otimes |j\rangle_B\right)$$

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

$$=: \underline{\underline{\mathrm{tr}_B\, \rho_{AB}}}$$

(In components: $\left(\mathrm{tr}_B\, \rho_{AB}\right)_{ii'} = \sum_j \left(\rho_{AB}\right)_{(ij)(i'j)}$)

Is any density matrix ρ <u>physical</u>?

Take $\rho = \sum \lambda_i |\phi_i\rangle\langle\phi_i|$ eigenval. decomp.; and

def $|\psi\rangle_{AB} = \sum_i \sqrt{\lambda_i}\, |\phi_i\rangle_A |i\rangle_B$ ("purification" of ρ)

$\Rightarrow \mathrm{tr}_B\left[|\psi\rangle_{AB}\langle\psi|_{AB}\right] = \mathrm{tr}_B\left[\sum \sqrt{\lambda_i \lambda_j}\, |\phi_i\rangle\langle\phi_j| \otimes |i\rangle\langle j|\right]$

$= \sum \lambda_i |\phi_i\rangle\langle\phi_i| = \rho \Rightarrow$ <u>yes</u> ✓

Density matrix can serve as <u>alternative definition</u> of state.

Ensemble interpretation of density matrix

Consider $|\psi\rangle_{AB} = \alpha|00\rangle + \beta|11\rangle$

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

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

$\Rightarrow$ Can be interpreted as having $|0\rangle$ w/ prob. $p_0 = |\alpha|^2$ & $|1\rangle$ w/ prob. $p_1 = |\beta|^2$. "<u>ensemble interpretation</u>"

$\Rightarrow$ Is this consistent w/ <u>pure</u> state $|\psi\rangle_{AB}$?

Let B do proj. meas. in Z basis:

$$|\psi\rangle = \alpha|00\rangle + \beta|11\rangle \quad \begin{array}{l} \xrightarrow{p_0 = |\alpha|^2} |\psi_0\rangle_A = |0\rangle_A \\ \text{Z meas. on B} \\ \xrightarrow{p_1 = |\beta|^2} |\psi_1\rangle_A = |1\rangle_A \end{array}$$

$\Rightarrow$ Alice doesn't know outcome $\Rightarrow$ <u>ensemble</u>

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

(<u>Note</u>: Bob's description is different: he knows outcome and would describe his state as <u>either</u> $|0\rangle\langle 0|$ <u>or</u> $|1\rangle\langle 1|$)

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

$$|\psi\rangle = \alpha|00\rangle + \beta|11\rangle \xrightarrow{X \text{ meas.}} \quad p_+ = \frac{|\alpha|^2+|\beta|^2}{2} = \frac{1}{2} \qquad |\psi_+\rangle_A = \frac{\alpha|0\rangle + \beta|1\rangle}{|\alpha|^2+|\beta|^2}$$

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

<u>not</u> orthogonal!

<u>Different ensemble</u> $\quad \rho_A = p_+ |\psi_+\rangle\langle\psi_+| + p_- |\psi_-\rangle\langle\psi_-|$

for same state $\Longrightarrow$ <u>ens. interpretation ambiguous!</u>

(Number of terms can vary ($\to$ HW!), non-orth. states as $|\psi_\pm\rangle$, ...)

<u>How are diff. ensembles related?</u>

Note: <u>Not</u> orthogonal, just $\langle\psi_i|\psi_i\rangle = 1$

<u>Theorem:</u> Let $\rho = \sum p_i |\psi_i\rangle\langle\psi_i| = \sum q_j |\phi_j\rangle\langle\phi_j|$.

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

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

and vice versa. (If there are less j's than i's, pad with zeros, and vice versa.)

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

Then
$$\sum_i p_i |\psi_i\rangle\langle\psi_i| = \sum_i \Big(\sum_j u_{ij}\sqrt{q_j}|\phi_j\rangle\Big)\Big(\sum_{j'} u^*_{ij'}\sqrt{q_{j'}}\langle\phi_{j'}|\Big)$$
$$= \sum_{jj'} \sqrt{q_j q_{j'}}\,|\phi_j\rangle\langle\phi_{j'}| \underbrace{\Big(\sum_i u^*_{ij'} u_{ij}\Big)}_{=\delta_{jj'}}$$
$$= \sum q_j |\phi_j\rangle\langle\phi_j| .$$

"$\Rightarrow$": Homework / see later (equiv. of purifications).

4. Schmidt decomposition and purifications

Given $|\psi\rangle_{AB}$ bipartite, let

$$\mathrm{tr}_B|\psi\rangle\langle\psi| = \rho_A = \sum p_i |i\rangle_A\langle i|_A$$

with $|i\rangle_A$ eigenbasis (ONB) ("abuse" of notation...)

Choose <u>some</u> ONB $|a_j\rangle_B$ of B, expand

$$|\psi\rangle_{AB} = \sum_{ij} c_{ij}\,|i\rangle_A |a_j\rangle_B$$
$$= \sum_i |i\rangle_A \Big(\sum_j c_{ij}|a_j\rangle_B\Big) \quad =: |b_i\rangle : \text{ no ONB}$$

$$\dots = \sum |i\rangle_A |b_i\rangle_B$$

We have $\sum_i p_i |i\rangle\langle i| = tr_B |\psi\rangle\langle\psi| = tr_B \left(\sum_{ii'} |i\rangle\langle i'|_A \otimes |b_i\rangle\langle b_{i'}|_B \right)$

$$= \sum_{ii'} |i\rangle\langle i'|_A \otimes tr\left(|b_i\rangle\langle b_{i'}|_B \right)$$

$$= \sum_{ii'} \langle b_{i'} | b_i \rangle \cdot |i\rangle\langle i'|$$

Since $|i\rangle\langle i'|$ is basis (lin. indep.) in space of matrices:

$$\Longrightarrow \langle b_{i'} | b_i \rangle = \delta_{i'i}\, p_i$$

$$\Longrightarrow |i\rangle_B := \frac{1}{\sqrt{p_i}} |b_i\rangle \text{ is } \underline{\text{ONB for B}}$$

different basis than $|i\rangle_A$ (→ notation!)

<u>Schmidt decomposition</u>:

Any $|\psi\rangle_{AB}$ can be written as

$$|\psi\rangle_{AB} = \sum_i \lambda_i |i\rangle_A |i\rangle_B ,$$

with ONBs $|i\rangle_A$ & $|i\rangle_B$. The $\lambda_i = \sqrt{p_i} \geq 0$ are called Schmidt coefficients.

Note: $\rho_B = tr_A |\psi\rangle\langle\psi| = \sum_i \lambda_i^2 |i\rangle_B \langle i|_B$

$\Rightarrow |i\rangle_B$ eigenbasis of ρ_B!

$\Rightarrow$ If p_i non-degen.: Schmidt decomp. obtained by pairing eigenvectors of ρ_A & ρ_B.

<u>Important consequence:</u> For pure states $|\psi\rangle_{AB}$, ρ_A and ρ_B have the <u>same eigenvalues</u>!

How is <u>Schmidt dec.</u> related to <u>other expansions</u>?

$$|\psi\rangle = \sum c_{ij} |x_i\rangle_A |y_j\rangle_B$$

some ONBs

$$= \sum \lambda_k |k\rangle_A |k\rangle_B .$$

$|x_i\rangle_A, |y_j\rangle_B, |k\rangle_A, |k\rangle_B$ ONBs

$\Rightarrow \exists$ unitaries u_{ik}, v_{jk} s.th.

$$|k\rangle_A = \sum u_{ik} |x_i\rangle_A \; ; \; |k\rangle_B = \sum v_{jk}^* |y_j\rangle_B$$

(pad w/ zeros if necessary...)

$$\Rightarrow \sum c_{ij} |x_i\rangle_A |y_j\rangle_B = \sum \lambda_k u_{ik} v_{jk}^* |x_i\rangle_A |y_j\rangle_B$$

$$\xRightarrow{\text{lin. indep. of } |x_i\rangle_A |y_j\rangle_B} \quad c_{ij} = \sum_k u_{ik} \lambda_k v_{jk}^*,$$

$$\text{or} \quad C = U \cdot D \cdot V^\dagger \qquad (C \equiv (c_{ij}))$$

with U, V unitary, and $D = \begin{pmatrix} \lambda_1 & & & 0 \\ & \ddots & & \\ & & \lambda_k & \\ 0 & & & 0 \end{pmatrix}$

$\boxed{\text{"Singular value decomposition" (SVD) of } C}$

(Derivation of SVD ($\to$ HW): U diagonalizes $CC^\dagger$, V $C^\dagger C$
$\Leftrightarrow$ derivation of Schmidt decomp.!)

<u>Remark:</u> Any two states $|\phi\rangle, |\psi\rangle$ w/ ident. Schmidt coeffs are related by local unitaries, i.e.

$$\exists U, V: \; |\phi\rangle = U \otimes V |\psi\rangle.$$

$\Rightarrow$ the λ_i contain <u>all</u> non-local properties,

$\lambda_1 \geq \lambda_2 \geq \ldots$

Proof: $|\phi\rangle = \sum \lambda_i |\phi_i^A\rangle \otimes |\phi_i^B\rangle$ (ONBs)

$|\psi\rangle = \sum \lambda_i |\psi_i^A\rangle \otimes |\psi_i^A\rangle$ (ONBs)

$|\phi_i^A\rangle, |\psi_i^A\rangle$ ONB $\Rightarrow \exists U : |\phi_i^A\rangle = U|\psi_i^A\rangle \ \forall i$

& same for B : $\exists V : |\phi_i^B\rangle = V|\psi_i^B\rangle \ \forall i$ $\square$

(Again: Pad w/ 0 if necessary.)

Purification:

Any $|\psi\rangle_{AB}$ s.th. $\mathrm{tr}_B |\psi\rangle\langle\psi|_{AB} = \rho_A$ is called a <u>purification</u> of ρ_A.

need not be orthogonal!

(E.g. $\rho_A = \sum p_i |\psi_i\rangle\langle\psi_i| \Rightarrow \sum \sqrt{p_i} |\psi_i\rangle|i\rangle$ is purif.)

Given two purifications $|\phi\rangle$ & $|\psi\rangle$ of ρ_A, what is their relation?

Write $|\phi\rangle, |\psi\rangle$ in <u>Schmidt form</u>:

$$|\phi\rangle = \sum \lambda_i |\phi_i^A\rangle |\phi_i^B\rangle$$

(all ONBs)

$$|\psi\rangle = \sum \mu_i |\psi_i^A\rangle |\psi_i^B\rangle$$

λ_i, μ_i wlog descending.

We have

$$\sum \lambda_i |\phi_i^A\rangle\langle\phi_i^A| = tr_B |\phi\rangle\langle\phi| = tr_B |\psi\rangle\langle\psi| = \sum \mu_i |\psi_i^A\rangle\langle\psi_i^A|$$

$\Rightarrow \lambda_i = \mu_i$, $|\phi_i^A\rangle = |\psi_i^A\rangle$ (up to phase)

if λ_i non-degen. (degen. $\to$ HW)

Now choose U s.th. $U|\phi_i^B\rangle = |\psi_i^B\rangle$ $\forall i$ ($\Rightarrow U$ unitary)

$$\Rightarrow \quad |\psi\rangle = (\mathbb{1} \otimes U)|\phi\rangle.$$

$\boxed{\text{All purifications are related by a unitary on the purifying system.}}$

(Note: Closely related to unitary equivalence of ensemble decompositions $\to$ HW!)

36. Mixed states – unitary evolution + projective measurement

Unitary evolution of mixed state

How does a mixed state ρ_A evolve under a unitary U_A?

Consider purification $|\psi\rangle_{AB}$, $tr_B |\psi\rangle\langle\psi| = \rho_A$.

$$|\psi\rangle \longmapsto (U_A \otimes \mathbb{1}_B)|\psi\rangle$$