3. The Schmidt decomposition & purifications

a) The Schmidt decomposition

Consider a bipartite state $|\psi\rangle_{AB}$, and let

$$\mathrm{tr}_B |\psi\rangle\langle\psi| = \rho_A = \sum_i \underbrace{p_i}_{\neq 0} |a_i\rangle\langle a_i| \quad \text{be the}$$

eigenvalue decomposition — excluding the zero eigenvalues! — i.e. $|a_i\rangle_A$ is an orthonormal set (in fact, an ONB of $\mathrm{supp}\,\rho_A$).

Let $|x_i\rangle_B$ be <u>any</u> ONB of B, and expand $|\psi\rangle_{AB}$ in $|a_i\rangle \otimes |x_j\rangle$:

$$|\psi\rangle_{AB} = \sum c_{ij} |a_i\rangle_A |x_j\rangle_B$$

$$= \sum |a_i\rangle_A |\tilde{b}_i\rangle_B$$

with $|\tilde{b}_i\rangle_B := \sum_j c_{ij} |x_j\rangle_B$.

no ONB etc. (a priori)

We have

$$\sum p_i |a_i\rangle\langle a_i| = \mathrm{tr}_B |\psi\rangle\langle\psi|$$

$$= \mathrm{tr}_B \Big[\sum_{ii'} |a_i\rangle\langle a_{i'}|_A \otimes |\tilde{b}_i\rangle\langle \tilde{b}_{i'}|_B \Big]$$

$$= \sum_{ii'} |a_i\rangle\langle a_{i'}| \; \mathrm{tr}\big[|\tilde{b}_i\rangle\langle \tilde{b}_{i'}|_B \big]$$

$$= \sum \langle \tilde{b}_{i'} | \tilde{b}_i \rangle \; |a_i\rangle\langle a_{i'}|$$

Since the $|a_i\rangle\langle a_{i'}|$ $\forall i, i'$ are lin. indep.

(in fact, H-S-orthonormal!), we must have

$$\langle \tilde{b}_{i'} | \tilde{b}_i \rangle = p_i \, \delta_{ii'} \quad !$$

$\Rightarrow$ $|b_i\rangle_B := \frac{1}{\sqrt{p_i}} |\tilde{b}_i\rangle_B$ are orthonormal!

$\neq 0$

$$\Rightarrow \quad \boxed{\begin{array}{l} |\psi\rangle_{AB} = \sum_i \sqrt{p_i}\, |a_i\rangle_A |b_i\rangle_B \\ \text{with } \{|a_i\rangle_A\},\ \{|b_i\rangle_B\} \text{ orthonormal!} \end{array}}$$

This is called the Schmidt decomposition with Schmidt coefficients $\sqrt{p_i}$ $(=\lambda_i)$.

(The number of non-zero p_i is also called the Schmidt number or Schmidt rank.)

Key point: Any bipartite state has a Schmidt decomposition, i.e. can be written in the form above for suitable ONBs $\{|a_i\rangle_A\}$ and $\{|b_i\rangle_B\}$.

Note: $\rho_B = \mathrm{tr}_A |\psi\rangle\langle\psi| = \sum_i p_i |b_i\rangle\langle b_i|$, and (by construction) $\rho_A = \sum p_i |a_i\rangle\langle a_i|$.

$\Longrightarrow$ (i) $\{|a_i\rangle_A\}$ and $\{|b_i\rangle\}$ are the eigenbases of ρ_A & ρ_B, respectively.

(ii) ρ_A & ρ_B have the same eigenvalues (!).

(iii) If the p_i are non-degenerate, the Schmidt decomp. can be found by simply pairing up the eigenvectors of ρ_A & ρ_B!

(iv) $\{|a_i\rangle_A\}$ and $\{|b_i\rangle_B\}$ are ONBs of $\operatorname{supp}\rho_A$ and $\operatorname{supp}\rho_B$, respectively.

(Note: If $\dim A = \dim B$, we can include the zero eigenvalues & extend $\{|a_i\rangle_A\}$, $\{|b_i\rangle_B\}$ to ONBs of the full space.)

Notational convention:

Often, the bases $\{|a_i\rangle_A\}$ and $\{|b_i\rangle_B\}$ are simply denoted as

$$|i\rangle_A := |a_i\rangle_A, \text{ and}$$

$$|i\rangle_B := |b_i\rangle_B.$$

These are not the computational basis, and generally different bases on A & B $\Rightarrow$ CAREFUL!!

How is the Schmidt decomposition related to expansion of $|\psi\rangle$ in a different pair of ONBs $\{|x_i\rangle_A\}$, $\{|y_j\rangle_B\}$?

We have
$$|\psi\rangle = \sum c_{ij} \, |x_i\rangle_A \, |y_j\rangle_B$$
$$= \sum \sqrt{p_k} \, |a_k\rangle_A \, |b_k\rangle_B . \qquad (*)$$

$\Rightarrow$ There exist matrices $U = (u_{ik})$, $V = (v_{jk})$ s.th.

$$|a_k\rangle_A = \sum u_{ik} \, |x_i\rangle_A , \quad |b_k\rangle_B = \sum \overline{v_{jk}} \, |y_k\rangle_B ,$$

and
$$\delta_{k\ell} = \langle a_k | a_\ell \rangle = \sum_{ij} \overline{u_{ik}} \, u_{j\ell} \underbrace{\langle x_i | x_j \rangle}_{= \delta_{ij}}$$
$$= \sum \overline{u_{ik}} \, u_{i\ell} = (U^\dagger U)_{k\ell} ,$$

and equally $(V^\dagger V)_{k\ell} = \delta_{k\ell}$

$\Rightarrow$ U, V are isometries.

If we insert this in $(*)$:

$$\sum_{ij} c_{ij} \, |x_i\rangle_A |y_j\rangle_B = \sum_{ij} \sum_k \sqrt{p_k}\, u_{ik} \overline{v_{jk}} \; \underbrace{|x_i\rangle_A |y_j\rangle_B}_{\text{lin. indep!}}$$

$$\Rightarrow \quad c_{ij} = \sum_k \underbrace{\sqrt{p_k}}_{=:\lambda_k} u_{ik} \overline{v_{jk}} \quad \forall i,j; \quad \underline{\text{or}}$$

Any matrix $C = (c_{ij})$, $i = 1, \dots, n$, $j = 1, \dots, m$, can be written in the form

$$C = U \cdot D \cdot V^{+}, \quad \text{or}$$

$$c_{ij} = \sum_{k=1}^{r} \lambda_k u_{ik} \overline{v_{jk}}$$

with $r = \text{rank}(C) \leq n, m$, $\lambda_k > 0$, and

$$U = (u_{ik}), \quad V = (v_{jk}), \quad D = \begin{pmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & & \ddots \; \lambda_k \end{pmatrix},$$

$i = 1, \dots, n$; $k = 1, \dots, r$; $j = 1, \dots, m$, and

$U^{+}U = I_k$, $V^{+}V = I_k$ isometries.

This is called the <u>singular value decomposition (SVD)</u> of C, with <u>singular values λ_i</u>.

If the λ_i are ordered descendingly, $\lambda_1 \geq \lambda_2 \geq \ldots$, U and V are unique up to permutations of degenerate singular values.

Alternatively, one can choose U and V square $n \times n$ and $m \times m$ unitaries, and

$$D = \left(\begin{array}{ccc|c} \lambda_1 & & & \\ & \ddots & & 0 \\ & & \lambda_k & \\ \hline & 0 & & 0 \end{array}\right),$$

but the additional degrees of freedom are arbitrary.

Proposition: Any two states $|\phi\rangle, |\psi\rangle$ with identical Schmidt coefficients $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r > 0$ are related by local unitaries, i.e.

$$\exists\, U, V : \quad |\phi\rangle = (U \otimes V)\,|\psi\rangle .$$

Thus: The ordered Schmidt coefficients $\lambda_1 \geq \lambda_2 \geq \dots$ encode all non-local properties.

Proof:

$$|\phi\rangle = \sum_{i=1}^{r} \lambda_i \, |\phi_i^A\rangle \otimes |\phi_i^B\rangle$$

$$|\psi\rangle = \sum_{i=1}^{r} \lambda_i \, |\psi_i^A\rangle \otimes |\psi_i^B\rangle$$

$\{|\phi_i^A\rangle\}, \{|\psi_i^A\rangle\}$ orthonormal $\Rightarrow \exists\, U : |\phi_i^A\rangle = U|\psi_i^A\rangle \;\forall i.$

$\{|\phi_i^B\rangle\}, \{|\psi_i^B\rangle\}$ orthonormal $\Rightarrow \exists\, V : |\phi_i^B\rangle = V|\psi_i^B\rangle \;\forall i.$

$\blacksquare$

b) Purifications

Reminder: Given ρ_A on A, a state $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$

s.th. $\mathrm{tr}_B |\psi\rangle\langle\psi| = \rho_A$ is called a purification of ρ_A.

Given two purifications

$$|\phi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$$

$$|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_{B'}$$

potentially different spaces

of ρ_A, what is their relation?

Write both $|\phi\rangle$ and $|\psi\rangle$ in their Schmidt form (not a basis trafo!):

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

$$|\psi\rangle = \sum \mu_i \, |\psi_i^A\rangle \, |\psi_i^{B'}\rangle$$

(wlog λ_i, μ_i descending).

We have

$$\sum \lambda_i^2 |\phi_i^A\rangle\langle\phi_i^A| = \mathrm{tr}_B |\phi\rangle\langle\phi| = \rho_A =$$

$$= \mathrm{tr}_B |\psi\rangle\langle\psi| = \sum \mu_i^2 |\psi_i^A\rangle\langle\psi_i^A|$$

$|\phi_i^A\rangle, |\psi_i^A\rangle$ orthonormal

$\Longrightarrow$ if λ_i, μ_i non-degenerate, then

$$\lambda_i = \mu_i\,, \quad |\phi_i^A\rangle = |\psi_i^A\rangle \quad \forall i$$

(If <u>degen.</u>: Schmidt decomp. can be constructed from <u>any</u> eigendecomposition $\sum \lambda_i |\phi_i\rangle\langle\phi_i|$ of ρ_A – see Sec. a) – so we can <u>construct</u> it with the same eigenvectors $|\phi_i^A\rangle = |\psi_i^A\rangle$.)

Now construct a $U: \mathcal{H}_B \longrightarrow \mathcal{H}_{B'}$

$$\text{s.th.} \quad |\phi_i^B\rangle \longmapsto |\psi_i^{B'}\rangle.$$

U is a unitary between span $\{|\phi_i^B\rangle\}$

and $\{|\psi_i^{B'}\rangle\}$. If $\dim B' > \dim B$, it can be extended to an isometry. Then:

$$|\psi\rangle = (I_A \otimes U_B)\,|\phi\rangle.$$

Theorem: All purifications of a given ρ_A are related by a unitary (or isometry) on the purifying system.

Note: This is closely linked to the unitary/isometric ambiguity of the ensemble decomposition:

not an ONB

Any ensemble $\rho = \sum p_i |\phi_i\rangle\langle\phi_i|$ is related to a purification $|\psi\rangle = \sum \sqrt{p_i}\,|\phi_i\rangle_A |i\rangle_{B'}$ from where it can be obtained by measuring B in the computational basis. ($\to$ Homework)