In fact, there are infinitely many ensembles for the same density operator.

Even the number of terms can vary:

For example:

\[ |4\rangle = \frac{\alpha |00\rangle + \beta |11\rangle}{\sqrt{2}} + \frac{\alpha |02\rangle + \beta |12\rangle}{\sqrt{3}} \]

Reason in basis \( |0\rangle, |1\rangle, |2\rangle \):

\[ \frac{|2\rangle + |3\rangle}{\sqrt{2}} = |\pm\rangle \]

- Decomposition of the two previous solutions:

\[ \Rightarrow p_4 = p_0 |0\rangle |0\rangle + p_1 |1\rangle |1\rangle + p_+ |4\rangle |4\rangle + p_- |4\rangle |4\rangle \]

\[ = |1\rangle |1\rangle / 2 + 1/4 + 1/4 + 1/4 \]

How are different ensembles related?

**Theorem:** Let 
\[ q = \sum p_i |4_i\rangle |4_i\rangle = \sum q_j |\phi_j\rangle |\phi_j\rangle. \]

Then, there is a unitary \( U = (u_{ij}) \) s.t.,

\[ p_i |4_i\rangle = \sum u_{ij} q_j |\phi_j\rangle, \]

and vice versa. (If the number of \( i \)'s and \( j \)'s is different, pad the smaller one with two vectors.)
Proof:

\[ \leftarrow: \text{ det } \mathbf{T}_i \quad \text{det} \quad = \sum_{j} \sqrt{q_j} |\phi_j, 1\rangle \langle \phi_j, 1| . \]

Then

\[ \sum_{i} \mathbf{T}_{i} / \mathbf{4}_{i} \times \mathbf{4}_{i} = \sum_{i} \left( \sum_{j} \sqrt{q_j} |\phi_j, 1\rangle \langle \phi_j, 1| \right) \left( -\sum_{j} \sqrt{q_j} |\phi_j, 1\rangle \langle \phi_j, 1| \right) \]

\[ = \sum_{j} \sqrt{q_j} |\phi_j, 1\rangle \langle \phi_j, 1| \left( \sum_{j} \frac{\sqrt{q_j}}{q_j} \right) \]

\[ = \sum_{j} \sqrt{q_j} |\phi_j, 1\rangle \langle \phi_j, 1| \]

\[ \Rightarrow: \text{ First, assume } |\phi_j, 1\rangle \text{ is an eigenvector. Define} \]

\[ u_{ij} = \langle \phi_j, 1 \mid \mathbf{4}_i \rangle \cdot \frac{\sqrt{P_i}}{\sqrt{q_j}} \]

Then

\[ \sum_{j} u_{ij} \sqrt{q_j} |\phi_j, 1\rangle = \sum_{j} \sqrt{q_j} |\phi_j, 1\rangle \langle \phi_j, 1| \frac{\sqrt{P_i}}{\sqrt{q_j}} = \frac{\sqrt{P_i}}{\sqrt{q_j}} |\phi_j, 1\rangle \]

and

\[ \sum_{i} u_{ij} u_{ij}^* = \sum_{i} \langle \phi_j, 1 \mid \mathbf{4}_i \rangle \langle \mathbf{4}_i \mid \phi_j, 1 \rangle \frac{P_i}{q_j q_{j'}} \]

\[ = \langle \phi_j, 1 \mid \mathbf{4}_i \rangle \left( \frac{1}{q_j q_{j'}} \right) = \delta_{jj'} \]

\[ = g_{jj'} \]

\[ \Rightarrow u_{ij} \text{ has orthogonal columns } \Rightarrow \text{ can be extended to} \]

unitary (by padding $|\phi_i\rangle$ with zero vectors).

General case: go via eigenvectors & covariance matrices! \[ \square \]
Consider bipartite state $\ket{\psi_{AB}}$, and let

$$\tr_B \ket{\psi_{AB}} = \rho_A = \sum \rho_i \ket{i_A} \braket{i_A} = \rho_A \text{ ONB},$$

choose an ONB $\ket{a_j}_B$ for $B$, and expand

$$\ket{\psi_{AB}} = \sum c_{ij} \ket{i_A} \ket{a_j}_B$$

$$= \sum \ket{i_A} \ket{b_i}_B, \quad \ket{b_i}_B = \sum c_{ij} \ket{a_j} \text{ ONB}!$$

Now \( \sum \rho_i \ket{i} \braket{i} = \tr_B \ket{\psi_{AB}} = \tr_B \left( \sum \ket{i} \braket{i} \right) \)

$$= \sum \ket{i} \braket{i} \langle a_j | b_i \rangle \langle b_i | a_j \rangle$$

$$= \sum \langle b_i | b_i \rangle \langle i | i \rangle$$

$\ket{i} \braket{i}$ is a basis for the space of matrices (linear maps):

$$\Rightarrow \quad \langle b_i | b_i \rangle = \delta_{i i'} \delta_i$$
\[ i_B \equiv \frac{1}{\sqrt{p_i}} |i_A| \quad \text{ONB for } B \]

different from \( i_A \)!

\[ |4> = \sum_i \sqrt{p_i} |i_A> |i_B> \]

with \( |i_A>, |i_B> \) ONBs

"Schmidt decomposition" with

Schmidt coefficients \( \sqrt{p_i} \).

Note: \( s_B = \text{tr}_A |4\times4| = \sum_i p_i |i_B><i_B| \)

\[ = D |i_B> \text{ is the eigenbasis of } s_B! \]

\( p_i \) non-degenerate \( \Rightarrow \) Schmidt decomposition

obtained by pairing up eigenvectors of \( s_A \) and \( s_B \)!

Important consequence: Eigenvalues of \( s_A \) and \( s_B \) are equal!
How is the Schmidt decomposition related to other expansions?

\[ |\psi\rangle = \sum C_{ij} |x_i\rangle |y_j\rangle \]

\[ = \sum \sqrt{P_k} |k\rangle_A |k\rangle_B \]

\[ \Rightarrow \exists \text{ unitaries } u_{ik}, v_{jk} \text{ s.t.} \]

\[ |k\rangle_A = \sum u_{ik} |x_i\rangle \quad \quad |k\rangle_B = \sum v_{jk} |y_j\rangle \]

(append qubits if necessary).

Must above + lin. indep.

\[ c_{ij} = \sum_k u_{ik} \sqrt{P_k} v_{jk} \]

\[ (u_{ik})^T (v_{jk}) \]

or

\[ C = UDV^T \quad \text{with } U, V \text{ unitary, } D \text{ diagonal} \]

"Singular value decomposition" (SVD)
Recall: any two states $|\psi\rangle, |\phi\rangle$ of identical Schmidt coefficients are related by local unitaries, i.e.:

$\exists U, V \text{ s.t. } |\phi\rangle = (U \otimes V) |\psi\rangle$

I.e.: All non-local properties are encoded in the $P_i$.

**Proof:**

$|\phi\rangle = \sum \sqrt{p_i} \left| \phi_i^A \right> \otimes \left| \phi_i^B \right>$

$|\psi\rangle = \sum \sqrt{p_i} \left| \psi_i^A \right> \otimes \left| \psi_i^B \right>$

$\left| \phi_i^A \right>, \left| \psi_i^A \right> \text{ orthogonal } \Rightarrow \exists U: \left| \phi_i^A \right> = U \left| \psi_i^A \right> \forall i$

$\left| \phi_i^B \right>, \left| \psi_i^B \right> \text{ orthogonal } \Rightarrow \exists V: \left| \phi_i^B \right> = V \left| \psi_i^B \right> \forall i$

(Note: if necessary, we have to pad the $P_i$ with zeros and embed Hilbert space in larger one.)

**Purification:**

Have seen: Bipartite state $|\psi\rangle_{AB}$ with access to $A$ only

$\Rightarrow$ described by $\gamma_A$, $\gamma_A \geq 0$, $\text{tr} \gamma_A = 1$

Will now show: any such $\gamma_A$ can be seen as arising for $|\psi\rangle_{AB}$ ("purification")
Let \( s = \sum p_i \langle \phi_i | \phi_i \rangle \)

\[ \langle \phi_{\alpha} | \phi_{\beta} \rangle = \sum | p_i \rangle \langle \phi_i | A | i \rangle_{\beta} \]

Orthomomral,

Then \( \langle \phi_{\beta} | \psi | \psi \rangle = \sum_{i,j} \langle i | \phi_i | A | i \rangle_{\beta} \langle j | \phi_j | A | j \rangle_{\beta} = \delta_{ki} \delta_{kj} = \delta_{ij} \)

\[ = \sum_k p_k | \phi_k \rangle \langle \phi_k | \checkmark \]

\( | \psi \rangle \) is called a projection of \( s \).

Note: a measurement in basis \( | i \rangle_{\beta} \) prepares a state \( \{ p_i, | \phi_i \rangle \} \)

- We can always choose \( \text{dim} (H_{\beta}) \leq \text{dim} (H_A) \) by using an eigenvalue decomposition of \( s \).
  
  (In fact, \( \text{dim} H_{\beta} = \# \text{eigenvalue decompositions of } s \)).

Many different projections exist! How are they related?

Let \((H_A, | \psi \rangle) \) be projections of \( s \).

Write both in their Schmidt decomposition:
\[ |\Phi\rangle = \sum_i \lambda_i^A |\Phi_i^A\rangle |\Phi_i^B\rangle \]

\[ |\Psi\rangle = \sum_i \lambda_i |\Psi_i^A\rangle |\Psi_i^B\rangle . \]

We have \( \sum_i \lambda_i |\Phi_i^A\rangle |\Phi_i^B\rangle = \sum_i \lambda_i |\Psi_i^A\rangle |\Psi_i^B\rangle \]

\( \Rightarrow |\Phi_i^A\rangle = |\Psi_i^B\rangle \text{ if } \lambda_i \text{ are degenerate} \)

and we know from construction of Schmidt decomposition that we can choose \( |\Phi_i^A\rangle = |\Psi_i^B\rangle \) \( \forall i \).

Now choose \( U \) s.t. \( U |\Phi_i^B\rangle = |\Psi_i^B\rangle \) \( \forall i \).

\( \Rightarrow |\Psi\rangle = (U \otimes U) |\Phi\rangle . \)

All purifications are related by a unitary on the purifying system.

(Note: This can be seen as a reformulation of the unitary relation of ensemble decompositions.)
1. Unitary evolution of mixed states

How does a mixed state \( \rho_A \) evolve under a unitary \( U_A \)?

Consider purification \( 1_4 \rho_{AB} \rightarrow 1_3 1_4 \psi^+_{AB} = \rho'_{AB} \).

\[
1_4 \rightarrow (U_A \otimes U_B) 1_4 \psi_{AB}^+ \rightarrow
\]

\[
\Rightarrow \rho_A = tr_B 1_4 \psi_{AB}^+ \rightarrow tr_B \left[ (U_A \otimes U_B) 1_4 \psi_{AB}^+ (U_A^+ \otimes U_B^+) \right]
\]

\[
= U_A \cdot tr_B \left[ (U_A \otimes U_B) 1_4 \psi_{AB}^+ (U_A^+ \otimes U_B^+) \right] U_A^+
\]

\[
= U_A \rho A \bar{U}_A^+
\]

2. Measurement of mixed states

Projective measurement \( E_u \):

Have seen: \( P_u = tr [E_u \rho_A] \).

Post-measurement state:

\[
\rho_{A,u} = \frac{1}{P_u} \cdot tr_B \left( (E_u \otimes 1_4) 1_4 \psi^+_{AB} (E_u^+ \otimes 1_4) \right)
\]

\[
= \frac{1}{P_u} \cdot E_u \rho A \bar{E}_u^+
\]
Have seen: additional syste \( B \) more risk situation

What measurements can we do by adding an extra syste? 

Idea: Add "ancilla" \( B \), act \( \psi \) unitary \( \rho_{AB} \), and measure \( B \) in computational basis \( \ket{0}, \ldots, \ket{d-1} \).

Post-measurement state (approximate):

\[
\tilde{S}_u^A = \langle u |_B U (\sigma_A \otimes \ket{0}_B \langle 0 |_B) U^+ | u \rangle_B \\
= \Pi_u \sigma_A \Pi_u^+, \text{ with } \Pi_u = \langle u |_B U | 0 \rangle_B.
\]

and \( P_u = \text{tr}(\tilde{S}_u^A) = \text{tr}(\Pi_u \sigma_A \Pi_u^+) = \text{tr}(\Pi_u^f \Pi_u \sigma_A) \)

\[
S_u^A = \frac{1}{P_u} \tilde{S}_u^A \quad \text{post-meas. state.}
\]
What properties does \( \Pi_a \) have?

\[
\sum \Pi_a^+ \Pi_a = \sum_{\substack{n \in \mathbb{N} \cup \{0\} \\triangleright n}} n \left| u \right\rangle \left\langle u \right| \left| 0 \right\rangle_\mathcal{B} = \left| u \right\rangle \left( \sum_{\mathcal{A}} A_{A_0} \right) \left| 0 \right\rangle_\mathcal{B}
\]

\[
= \left| u \right\rangle A_0 \left| 0 \right\rangle_\mathcal{B}
\]

(Also follows from \( 1 = \sum \Pi_a = \sum \operatorname{tr} \left( \Pi_a^+ \Pi_a \rho \right) = \operatorname{tr} \left( \sum \Pi_a^+ \Pi_a \rho \right) \).

A set of \( \left\{ \Pi_a \right\} \) (or \( \left\{ \Pi_a^+ \Pi_a \right\} \)) with \( \sum \Pi_a^+ \Pi_a = 1 \) is called a "positive operator-valued measure" (POVM), and the corresponding measurement a POVM measurement.

Can any set \( \Pi_a \) with \( \sum \Pi_a^+ \Pi_a = 1 \) be realized by extensions and unitaries?

\[
\begin{pmatrix}
\Pi_0 \\
\vdots \\
\Pi_{d-1}
\end{pmatrix}
\]

\[
\sum \Pi_a^+ \Pi_a = 1
\]

\[\rightarrow\text{matrix of orthogonal}
\]

\[\rightarrow\text{coefficients}
\]

\[\rightarrow\text{...}\]
can be extended to unitary $U$

\[ U = \begin{bmatrix}
\langle 0 \rangle_B \\
\langle 1 \rangle_B \\
\vdots \\
\langle d-1 \rangle_B
\end{bmatrix}
\]

\[ \langle 0 \rangle_B | 0 \rangle_B = 1_U. \]

\[ \Rightarrow \text{measurement } \{ \Pi_n \} \text{ can be realized by unitary } U \text{ & projective measurement!} \]

5. General evolution - superoperators

What evolutions can we realize by evolving a larger system with a unitary?

\[ \begin{array}{c}
\text{Input} \\
| x \rangle_A \\
| 0 \rangle_B
\end{array} \rightarrow \begin{array}{c}
U \\
| x \rangle_A \\
| 0 \rangle_B
\end{array} \rightarrow \begin{array}{c}
\text{Output} \\
| x \rangle_A \\
\text{discard} = \text{trace out} \\
\end{array} \]