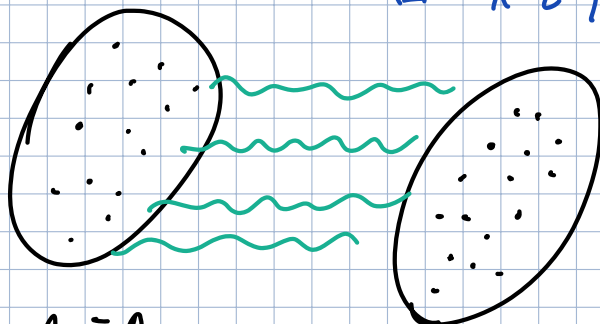


① Multi-qubit Entanglement.

(a) Recall the Bell state $|\Phi^+\rangle = \frac{1}{\sqrt{2}} \sum_{k=0}^1 |k, k\rangle \rightarrow$ Entangled state of two qubits.
 $\{ |0,0\rangle, |1,1\rangle \}$ $\xrightarrow{A_2} \frac{1}{\sqrt{2}} (|0,0\rangle + |1,1\rangle) \quad \frac{1}{\sqrt{2}} (|0,1\rangle + |1,0\rangle)$

(b) Entangled states of multiple qubits $\frac{1}{\sqrt{2}} (|0,0\rangle - |1,1\rangle) \quad \frac{1}{\sqrt{2}} (|0,1\rangle - |1,0\rangle)$
 $(\mathbb{I} \otimes X^x Z^z) |\Phi^+\rangle, x, z \in \{0,1\}$



$A_1, A_2, \dots, A_n \equiv A_{1:n}$
 (n qubits)

$B_1, B_2, \dots, B_n \equiv B_{1:n}$
 (n qubits).

$$\begin{aligned} |0\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ |1\rangle &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ |0,0\rangle &= \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \\ |0,1\rangle &= \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \end{aligned}$$

Recall: Basis for $(\mathbb{C}^2)^{\otimes n}$ is $\{ |k\rangle : k \in \{0,1\}^n \} \rightarrow 2^n$

Example: For $n=2$: $\{ |0,0\rangle, |0,1\rangle, |1,0\rangle, |1,1\rangle \}$

For $n=3$: $\{ |0,0,0\rangle, |0,0,1\rangle, |0,1,0\rangle, |0,1,1\rangle, |1,0,0\rangle, |1,0,1\rangle, |1,1,0\rangle, |1,1,1\rangle \}$

• Bell state of two n-qubit systems: $|\Phi^+\rangle_{A_{1:n} B_{1:n}} = \frac{1}{\sqrt{2^n}} \sum_{k \in \{0,1\}^n} |k, k\rangle_{A_{1:n} B_{1:n}}$

$\vec{k} = (k_1, k_2, \dots, k_n)$ Observe: $|\vec{k}, \vec{k}\rangle_{A_{1:n} B_{1:n}} = |\underline{k_1, k_2, \dots, k_n}\rangle_{A_{1:n}} \otimes |\underline{k_1, k_2, \dots, k_n}\rangle_{B_{1:n}}$
 $k_i \in \{0,1\}$

reordering $\rightarrow |\underline{k_1, k_1}\rangle_{A_1 B_1} \otimes |\underline{k_2, k_2}\rangle_{A_2 B_2} \otimes \dots \otimes |\underline{k_n, k_n}\rangle_{A_n B_n}$
 $\Rightarrow$ reordering $|\Phi^+\rangle_{A_{1:n} B_{1:n}} \rightarrow |\Phi^+\rangle_{A_1 B_1} \otimes |\Phi^+\rangle_{A_2 B_2} \otimes \dots \otimes |\Phi^+\rangle_{A_n B_n}$

$$\frac{1}{\sqrt{2^n}} \sum_{\vec{k} \in \{0,1\}^n} |\vec{k}, \vec{k}\rangle_{A_1:n B_1:n} = \frac{1}{\sqrt{2^n}} \sum_{k_1, k_2, \dots, k_n} |k_1, k_2, \dots, k_n\rangle_{A_1:n} \otimes |k_1, k_2, \dots, k_n\rangle_{B_1:n}$$

$$= \frac{1}{\sqrt{2^n}} \sum_{k_1, k_2, \dots, k_n} |k_1, k_1\rangle_{A_1 B_1} \otimes |k_2, k_2\rangle_{A_2 B_2} \otimes \dots \otimes |k_n, k_n\rangle_{A_n B_n}$$

$$= \underbrace{\left(\frac{1}{\sqrt{2}} \sum_{k_1} |k_1, k_1\rangle \right)}_{|\Phi^+\rangle_{A_1 B_1}} \otimes \underbrace{\left(\frac{1}{\sqrt{2}} \sum_{k_2} |k_2, k_2\rangle \right)}_{|\Phi^+\rangle_{A_2 B_2}} \otimes \dots \otimes \underbrace{\left(\frac{1}{\sqrt{2}} \sum_{k_n} |k_n, k_n\rangle \right)}_{|\Phi^+\rangle_{A_n B_n}}$$

- Entire Bell basis: $|\Phi_{\vec{z}, \vec{x}}\rangle_{A_{1:n} B_{1:n}} = (Z^{\vec{z}} X^{\vec{x}} \otimes \mathbb{1}) |\Phi^+\rangle_{A_{1:n} B_{1:n}}$
(of $2n$ qubits).

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\vec{z} = (z_1, z_2, \dots, z_n) \Rightarrow Z^{\vec{z}} = Z^{z_1} \otimes Z^{z_2} \otimes \dots \otimes Z^{z_n}$$

$$Z^{101} = Z \otimes \mathbb{1} \otimes Z$$

$$\vec{x} = (x_1, x_2, \dots, x_n) \Rightarrow X^{\vec{x}} = X^{x_1} \otimes X^{x_2} \otimes \dots \otimes X^{x_n}$$

(*) $\{ |\Phi_{\vec{z}, \vec{x}}\rangle : \vec{z}, \vec{x} \in \{0, 1\}^n \}$ is an ONB for $(\mathbb{C}^2)^{\otimes n} \otimes (\mathbb{C}^2)^{\otimes n}$

- GHZ states: $|\text{GHZ}_n\rangle = \frac{1}{\sqrt{2}} (|0\rangle^{\otimes n} + |1\rangle^{\otimes n}) \rightarrow n=3 \rightarrow \frac{1}{\sqrt{2}} (|0,0,0\rangle + |1,1,1\rangle)$

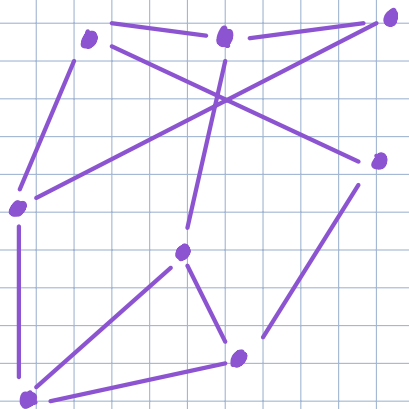
Basis for $(\mathbb{C}^2)^{\otimes n}$: $|\text{GHZ}_{\vec{z}, \vec{x}}\rangle = (Z^{\vec{z}} \otimes X^{\vec{x}}) |\text{GHZ}_n\rangle$, $\vec{z} \in \{0, 1\}$, $\vec{x} = \{0, 1\}^{n-1}$.

(*) Useful in quantum sensing and cryptography.

- Graph States: (A graph $G = (V, E)$)

(*) Useful in quantum computing!

edges.
nodes/vertices



Recipe:

- At every vertex, put the $|+\rangle$ state. ($|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$)
- For every edge, apply the controlled-Z gate

24
e

$$CZ = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix}$$

$$CZ|0,0\rangle = |0,0\rangle$$

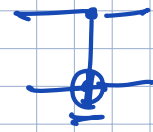
$$CZ|0,1\rangle = |0,1\rangle$$

$$CZ|1,0\rangle = |1,0\rangle$$

$$CZ|1,1\rangle = |1,1\rangle$$

$$Z|0\rangle = |0\rangle$$

$$Z|1\rangle = -|1\rangle$$



General formula: $|+\rangle^{\otimes n} = \left(\frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \right)^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{\vec{x} \in \{0,1\}^n} |\vec{x}\rangle$

$$CZ|x_1, x_2\rangle = (-1)^{x_1 x_2} |x_1, x_2\rangle$$

$n=2$:

$$\frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$$

$$\Rightarrow |G\rangle = \frac{1}{\sqrt{2^n}} \sum_{\vec{x} \in \{0,1\}^n} (-1)^{\alpha_{\vec{x}}} |\vec{x}\rangle, \quad \alpha_{\vec{x}} = \sum_{\{i,j\} \in E} x_i x_j$$

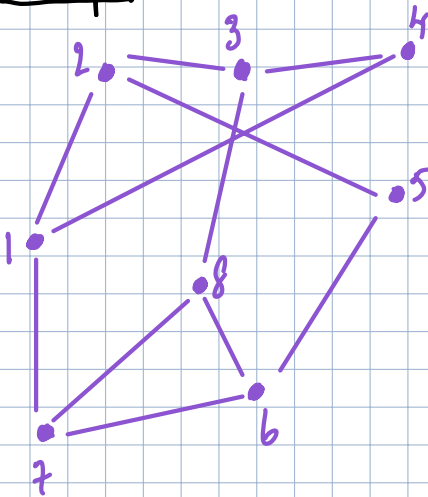


$$= \frac{1}{\sqrt{2^n}} \sum_{\vec{x} \in \{0,1\}^n} (-1)^{\frac{1}{2} \vec{x}^T A_G \vec{x}} |\vec{x}\rangle$$

Adjacency matrix of the graph

$$(A_G)_{ij} = \begin{cases} 1 & \text{if } \{i,j\} \in E \\ 0 & \text{otherwise.} \end{cases}$$

Example:



$A_G =$

	1	2	3	4	5	6	7	8
1		1		1			1	
2	1		1		1			
3		1		1				1
4	1		1					
5		1				1		
6					1		1	1
7	1					1		1
8			1			1		1

② Determining Entanglement.

⊛ Given a state vector $|\psi\rangle$, how to determine if it is entangled or not?
Precisely: $\exists |\phi_1\rangle, |\phi_2\rangle$ s.t. $|\psi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle$?

$$(a) |\psi\rangle_{AB} \in \mathbb{C}^d \otimes \mathbb{C}^d \rightarrow |\psi\rangle_{AB} = \sum_{i,j=0}^{d-1} x_{i,j} |i\rangle \otimes |j\rangle \quad (i,j|\psi\rangle = x_{i,j})$$

two-index quantity $\leftrightarrow$ matrix!

$$\text{Let } X = \sum_{i,j=0}^{d-1} x_{i,j} |i\rangle\langle j| \in L(\mathbb{C}^d) \Rightarrow \text{vec}(X) = \sum_{i,j=0}^{d-1} x_{i,j} \text{vec}(|i\rangle\langle j|) \stackrel{\text{Lemma}}{=} \sum_{i,j=0}^{d-1} x_{i,j} |i,j\rangle = |\psi\rangle!$$

$\Rightarrow$ ⊛ For every $|\psi\rangle \in \mathbb{C}^d \otimes \mathbb{C}^d$, $\exists X \in L(\mathbb{C}^d)$ such that $|\psi\rangle = \text{vec}(X) = (X \otimes \mathbb{1})|r\rangle$.

⊛ For every $|\psi\rangle \in \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2}$, $\exists X \in L(\mathbb{C}^{d_2}, \mathbb{C}^{d_1})$ s.t. $|\psi\rangle = (X \otimes \mathbb{1})|r_{d_2}\rangle$

(b) Every $X \in L(\mathbb{C}^d)$ has a Singular-value decomposition:

$$X = \underbrace{U}_{\text{unitary}} \underbrace{\Sigma}_{\substack{\text{matrix of singular values} \\ \Sigma = \begin{pmatrix} s_1 & & \\ & s_2 & \\ & & \ddots \\ & & & s_r \end{pmatrix}}} \underbrace{V^\dagger}_{\text{unitary}}$$

Singular values, $s_k > 0 \forall k$.
(unique up to ordering)

In bra-ket notation: $X = \sum_{k=1}^r s_k |e_k\rangle\langle f_k|$

rank $\equiv$ # of singular values $\rightarrow$ unique

$\{|e_k\rangle\}_k, \{|f_k\rangle\}_k$ are orthonormal (left and right singular vectors).

$$\Rightarrow |\psi\rangle = \text{vec}(X) = (\mathbb{1} \otimes X) |r\rangle = \sum_{k=1}^r S_k \text{vec}(|e_k\rangle\langle f_k|) = \sum_{k=1}^r S_k \overline{|e_k\rangle} \otimes |f_k\rangle$$

(normalisation: $\langle\psi|\psi\rangle = 1 \Rightarrow \sum_{k=1}^r S_k^2 = 1$)

↑
Schmidt coefficients.

- If $r=1$, then $|\psi\rangle = |e_1\rangle \otimes |f_1\rangle \Rightarrow$ not entangled!
- If $r>1$, then entangled! $r \equiv$ Schmidt rank.

(c) Observe: $|\psi\rangle_{AB} = \sum_{k=1}^r S_k \overline{|e_k\rangle}_A \otimes |f_k\rangle_B$

$$\begin{aligned} \langle\psi|\psi\rangle &= \left(\sum_{k=1}^r S_k \langle e_k| \otimes \langle f_k| \right) \left(\sum_{k'=1}^r S_{k'} \overline{|e_{k'}\rangle} \otimes |f_{k'}\rangle \right) \\ &= \sum_{k,k'=1}^r S_k S_{k'} \delta_{kk'} = \sum_{k=1}^r S_k^2 = 1 \end{aligned}$$

$$\Rightarrow \text{Tr}_B[|\psi\rangle\langle\psi|_{AB}] = \text{Tr}_B \left[\sum_{k,k'=1}^r S_k S_{k'} \overline{|e_k\rangle}\langle e_{k'}|_A \otimes |f_k\rangle\langle f_{k'}|_B \right]$$

$$= \sum_{k,k'=1}^r S_k S_{k'} \overline{|e_k\rangle}\langle e_{k'}|_A \underbrace{\text{Tr}[|f_k\rangle\langle f_{k'}|]}_{=\delta_{kk'}}$$

$$= \sum_{k=1}^r S_k^2 \overline{|e_k\rangle}\langle e_k|_A \rightarrow \text{Diagonal!}$$

$$\text{Also, } \text{Tr}_A[|\psi\rangle\langle\psi|_{AB}] = \sum_{k=1}^r S_k^2 |f_k\rangle\langle f_k|$$

$\Rightarrow \text{Tr}_A[|\psi\rangle\langle\psi|_{AB}]$ and $\text{Tr}_B[|\psi\rangle\langle\psi|_{AB}]$ have the same (non-zero) eigenvalues!

(d) Suppose $r=d$, $S_k = \frac{1}{\sqrt{d}} \forall k \in \{1, 2, \dots, d\}$.

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|0,0\rangle + |1,1\rangle)$$

We call $|\psi\rangle$ maximally entangled

(Note that the marginals are maximally mixed.)

(e) Observe: $\frac{1}{\sqrt{d}} \sum_{k=1}^d |e_k\rangle \otimes |\bar{e}_k\rangle = \frac{1}{\sqrt{d}} \sum_{k=1}^d \left(\sum_{j=0}^{d-1} |j\rangle \chi_{j,k} \right) |e_k\rangle \otimes \left(\sum_{l=0}^{d-1} |l\rangle \chi_{l,k} \right) |\bar{e}_k\rangle$

$$\begin{aligned}
 &= \frac{1}{\sqrt{d}} \sum_{k=1}^d \sum_{j,l=0}^{d-1} |j\rangle \otimes |l\rangle \langle j|e_k\rangle \chi_{l,k} |\bar{e}_k\rangle \\
 &= \frac{1}{\sqrt{d}} \sum_{k=1}^d \sum_{j,l=0}^{d-1} |j\rangle \otimes |l\rangle \langle j|e_k\rangle \chi_{l,k} |e_k\rangle \\
 &= \frac{1}{\sqrt{d}} \sum_{j,l=0}^{d-1} |j\rangle \otimes |l\rangle \langle j| \left(\sum_{k=1}^d |e_k\rangle \chi_{l,k} \right) |e_k\rangle \\
 &= \frac{1}{\sqrt{d}} \sum_{j,l=0}^{d-1} |j,l\rangle \langle j|l\rangle \\
 &= \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} |j,j\rangle \\
 &= \underline{\underline{|\Phi_d^+\rangle}}.
 \end{aligned}$$

$\langle \bar{e}_k | l \rangle = \langle e_k | l \rangle$
 $= \mathbb{1}_{k,l}$. b/c $\{|e_k\rangle\}$ is ONB!

(f) Vectorized unitaries are maximally entangled

$$|\gamma\rangle_{AB} = (U \otimes \mathbb{1}) |\Phi_d^+\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} \underbrace{U|k\rangle}_{\equiv |e_k\rangle} \otimes \underbrace{|k\rangle}_{\equiv |f_k\rangle}$$

U is unitary

$$\text{Tr}_B [|\gamma\rangle\langle\gamma|_{AB}] = \text{Tr}_B [(U \otimes \mathbb{1}_B) \Phi_{AB}^* (U^\dagger \otimes \mathbb{1}_B)]$$

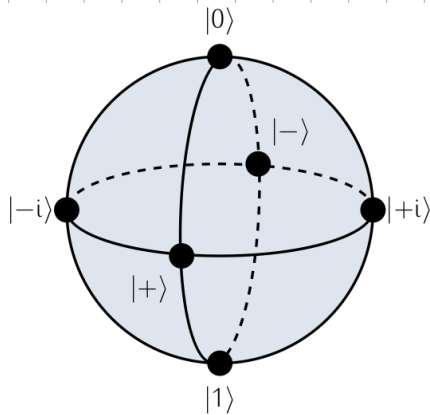
$$= \frac{1}{d} \text{tr} \left[\frac{1}{d} \text{tr} \left[\mathbf{F}_{AB}^\dagger \right] \mathbf{u}^\dagger \right] \mathbf{u}$$

$$\begin{aligned} & \text{Tr}_B [| \Phi \rangle \langle \Phi |_{AB}] \\ &= \text{Tr}_B \left[\frac{1}{d} \sum_{k, k'=0}^{d-1} |k\rangle \langle k'|_A \otimes |k\rangle \langle k'|_B \right] \\ &= \frac{1}{d} \sum_{k, k'=0}^{d-1} |k\rangle \langle k'|_A \underbrace{\text{Tr}_B [|k\rangle \langle k'|_B]}_{\langle k|k' \rangle = \delta_{k,k'}} \\ & \text{or } \text{Tr}_A [| \Psi \rangle \langle \Psi |_{AB}] \end{aligned}$$

(g) Mixed-state entanglement is much harder to characterize! (More on this later...).

③ Purification of mixed States

(a) Recall: For qubits, pure states are on the surface of the Bloch sphere; mixed states are inside.



Qubit

$|0\rangle$ or $|1\rangle$;
or *superposition*

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle,$$

$$\alpha, \beta \in \mathbb{C},$$

$$|\alpha|^2 + |\beta|^2 = 1$$

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$$

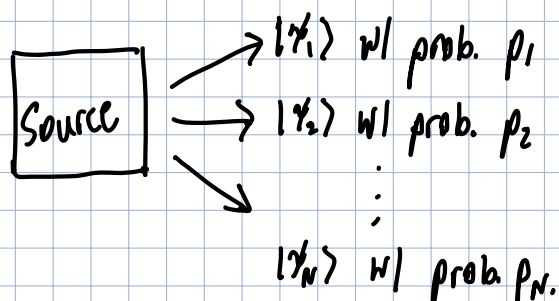
$$|\pm i\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm i|1\rangle)$$

General mixed states have the form $\rho = \sum_{k=1}^N p_k |\psi_k\rangle\langle\psi_k|$. $\text{Tr}[\rho] = \sum_k p_k = 1$ ✓

$\uparrow$
probabilities.

(b) How do mixed States arise in nature?

1. Lack of knowledge of State preparation.



⊛ Now someone uses the Source to prepare a state, but they don't tell you which one it is. How do you describe your knowledge of the system?

↳ (They don't mention the label.)

$$\rho_{XS} = \sum_{k=1}^N p_k |k\rangle_X \langle k| \otimes |x_k\rangle_S \langle x_k|$$

classical variable/register. ("which state is it?")

(This is a classical-quantum state)

($p_1 |x_1\rangle_S \langle x_1|$ $p_2 |x_2\rangle_S \langle x_2|$)

⊛ To figure out what state the system is prepared in, we measure the "classical register" X .
(wrt. POVM $\{|k\rangle_X \langle k|\}_{k=1}^N$)

$$\begin{aligned} \text{Tr}[(|k\rangle_X \langle k| \otimes \mathbb{I}_S) \rho_{XS}] &= \text{Tr}[(|k\rangle_X \langle k| \otimes \mathbb{I}_S) \sum_{k'=1}^N p_{k'} |k'\rangle_X \langle k'| \otimes |x_{k'}\rangle_S \langle x_{k'}|] \\ &= \sum_{k'=1}^N \text{Tr}[p_{k'} \underbrace{|k\rangle_X \langle k| k'\rangle_X \langle k'|}_{\delta_{k,k'}} \otimes |x_{k'}\rangle_S \langle x_{k'}|] \\ &= p_k \checkmark \quad (\text{as expected!}) \end{aligned}$$

State conditioned on outcome k (i.e., you know what the label is).

$$\downarrow \text{Tr}_X \left[\frac{(|k\rangle\langle k|_X \otimes \mathbb{I}_S) \rho_{XS} (|k\rangle\langle k|_X \otimes \mathbb{I}_S)}{p_k} \right]$$

$$= \frac{1}{p_k} \sum_{k'=1}^N \text{Tr}_X \left[(|k\rangle\langle k|_X \otimes \mathbb{I}_S) (\rho_{k'} |k'\rangle\langle k'|_X \otimes |\gamma_{k'}\rangle\langle \gamma_{k'}|_S) (|k\rangle\langle k|_X \otimes \mathbb{I}_S) \right]$$

$$\downarrow = \frac{1}{p_k} \sum_{k'=1}^N p_{k'} \underbrace{\text{Tr}_X [|k\rangle\langle k|_X |k'\rangle\langle k'|_X]}_{= \delta_{k',k}} \otimes |\gamma_{k'}\rangle\langle \gamma_{k'}|_S$$

$$\downarrow = \frac{1}{p_k} p_k |\gamma_k\rangle\langle \gamma_k|$$

$$= |\gamma_k\rangle\langle \gamma_k|$$

$$= |\gamma_k\rangle\langle \gamma_k| \quad \checkmark \quad (\text{as expected!})$$

⊗ But if you don't know the outcome/label? → Trace out the register X!

$$\text{Tr}_X (\rho_{XS}) = \text{Tr}_X \left[\sum_{k=1}^N p_k |k\rangle\langle k|_X \otimes |\gamma_k\rangle\langle \gamma_k|_S \right]$$

$$\downarrow = \sum_{k=1}^N p_k \underbrace{\text{Tr}_X [|k\rangle\langle k|_X]}_{=1} \otimes |\gamma_k\rangle\langle \gamma_k|_S$$

$$= \sum_{k=1}^N p_k |\gamma_k\rangle\langle \gamma_k|$$

$$\underline{\underline{= \sum_{k=1}^N p_k |\gamma_k\rangle\langle \gamma_k|}}$$

2. Measurement on one part of a pure state.

$$|\gamma\rangle_{AB} = \sum_{k=1}^r \sqrt{\lambda_k} |e_k\rangle_A \otimes |f_k\rangle_B \rightarrow \text{Measure A wrt POVM } \{M_A^x\}_{x \in X}$$

$$\text{Conditioned on outcome } x, \text{ state on B is } \frac{1}{p_x} \text{Tr}_A [(\sqrt{M_A^x} \otimes \mathbb{I}_B) |\gamma\rangle\langle \gamma|_{AB} (\sqrt{M_A^x} \otimes \mathbb{I}_B)]$$

$$\rho_X = \text{Tr}_B \left[(M_A^X \otimes \mathbb{I}_B) |\chi\chi\rangle_{AB} \right] = \text{Tr}_B \left[M_A^X \underbrace{\text{Tr}_B [|\chi\chi\rangle_{AB}]} \right] = \sum_{k=1}^r \lambda_k \text{Tr} [M_A^X |e_k\rangle\langle e_k|_A]$$

$$= \text{Tr}_B \left[\sum_{k,k'=1}^r \sqrt{\lambda_k \lambda_{k'}} |e_k\rangle\langle e_{k'}|_A \otimes |f_k\rangle\langle f_{k'}|_B \right]$$

$$= \sum_{k,k'=1}^r \sqrt{\lambda_k \lambda_{k'}} |e_k\rangle\langle e_{k'}|_A \underbrace{\text{Tr} [|f_k\rangle\langle f_{k'}|_B]}_{=\delta_{k,k'}}$$

$$= \sum_{k=1}^r \lambda_k |e_k\rangle\langle e_k|_A$$

$$\text{Tr}_A \left[(\sqrt{M_A^X} \otimes \mathbb{I}_B) |\chi\chi\rangle_{AB} (\sqrt{M_A^X} \otimes \mathbb{I}_B) \right] = \text{Tr}_A \left[\sum_{k,k'=1}^r \sqrt{M_A^X} |e_k\rangle\langle e_{k'}|_A \sqrt{M_A^X} \otimes |f_k\rangle\langle f_{k'}|_B \right]$$

$$= \sum_{k,k'=1}^r \text{Tr} \left[\sqrt{M_A^X} |e_k\rangle\langle e_{k'}|_A \sqrt{M_A^X} \right] |f_k\rangle\langle f_{k'}|_B$$

$$= \sum_{k,k'=1}^r \text{Tr} [M_A^X |e_k\rangle\langle e_{k'}|_A] |f_k\rangle\langle f_{k'}|_B. \rightarrow \text{Not a pure state in general.}$$

3. Entanglement with an (unknown) environment.

Consider a mixed state $\rho_S = \sum_{k=1}^r \lambda_k |\chi_k\rangle\langle\chi_k|$ (spectral decomposition).

↑
eigenvalues

↓
eigenvectors (orthonormal).

(*) Note: $\text{Tr}(\rho_S) = 1 \Rightarrow \text{Tr} \left[\sum_{k=1}^r \lambda_k \underbrace{\text{Tr} [|\chi_k\rangle\langle\chi_k|]}_{=1} \right] = \sum_{k=1}^r \lambda_k = 1$ (eigenvalues sum to one).

(*) Note: $\rho_S \geq 0 \Rightarrow \lambda_k \geq 0 \forall k. \Rightarrow 0 \leq \lambda_k \leq 1 \forall k.$

⊛ There exists a pure state $|\psi\rangle_{ES}$ such that $\text{Tr}_E[|\psi\rangle\langle\psi|_{ES}] = \rho_S$.
↑
environment

Proof: (by explicit construction) Consider $\sqrt{\rho_S} = \sum_{k=1}^r \sqrt{\lambda_k} |\chi_k\rangle\langle\chi_k|_S$

Then $|\psi\rangle_{ES} = (\eta_E \otimes \sqrt{\rho_S}) |\Gamma\rangle = (\eta_E \otimes \sum_{k=1}^r \sqrt{\lambda_k} |\chi_k\rangle\langle\chi_k|_S) |\Gamma\rangle$
↑ ↑ ↑
 $\dim(\eta_E) \geq r$ $|\Gamma\rangle = \sum_{k=1}^{d-1} |k, k\rangle$

$$= \sum_{k=1}^r \sqrt{\lambda_k} (\eta_E \otimes |\chi_k\rangle\langle\chi_k|_S) |\Gamma\rangle_{ES} = \sum_{k=1}^r \sqrt{\lambda_k} |\bar{\chi}_k\rangle_E \otimes |\chi_k\rangle_S$$

$|\bar{\chi}_k\rangle_E \otimes |\chi_k\rangle_S$

• This is a state vector: $\langle\psi|\psi\rangle = \left(\sum_{k=1}^r \sqrt{\lambda_k} \langle\bar{\chi}_k|_E \otimes \langle\chi_k|_S \right) \left(\sum_{k'=1}^r \sqrt{\lambda_{k'}} |\bar{\chi}_{k'}\rangle_E \otimes |\chi_{k'}\rangle_S \right)$

$$= \sum_{k,k'=1}^r \sqrt{\lambda_k \lambda_{k'}} \underbrace{\langle\bar{\chi}_k|\bar{\chi}_{k'}\rangle}_{\delta_{k,k'}} \underbrace{\langle\chi_k|\chi_{k'}\rangle}_{\delta_{k,k'}}$$

$$= \sum_{k=1}^r \lambda_k$$

$$= 1 \quad \checkmark$$

$$\begin{aligned} \text{Tr}_E[|\psi\rangle\langle\psi|_{ES}] &= \text{Tr}_E[(\eta_E \otimes \sqrt{\rho_S}) |\Gamma\rangle\langle\Gamma|_{ES} (\eta_E \otimes \sqrt{\rho_S})] \\ &\downarrow \\ &= \sqrt{\rho_S} \underbrace{\text{Tr}_E[|\Gamma\rangle\langle\Gamma|_{ES}]}_{\text{environment}} \sqrt{\rho_S} \end{aligned}$$

$$\begin{aligned}
& \downarrow^{d-1} \\
& = \sum_{k,k'=0}^{d-1} \text{Tr}_E [|k\rangle\langle k'|_E \otimes |k\rangle\langle k'|_S] \\
& \quad \downarrow^{d-1} \\
& = \sum_{k,k'=0}^{d-1} \delta_{k,k'} |k\rangle\langle k'|_S \\
& = \sum_{k=0}^{d-1} |k\rangle\langle k|_S = \mathbb{I}_S.
\end{aligned}$$

$\sqrt{\rho} \mathbb{I} \sqrt{\rho} = \rho$

$\downarrow$
 $= \rho_S \checkmark$