

Understanding quantum information and computation

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Lesson 12

Purifications and fidelity



Purifications

Definition

A *purification* of a state (represented by a density matrix) is a pure state of a larger, compound system that leaves the original state when the rest of the compound system is traced out.

In mathematical terms: if X is a system in a state ρ , and $|\psi\rangle$ is a quantum state vector of a pair (X, Y) such that

$$\rho = \text{Tr}_Y(|\psi\rangle\langle\psi|)$$

then $|\psi\rangle$ is a purification of ρ .

Fact

Every density matrix ρ has a purification like this provided that Y has at least as many classical states as X .

This is a critically important notion in quantum information theory.

Existence of purifications

Suppose X is a system and ρ is a density matrix representing a state of X . Consider any expression of ρ as a convex combination of pure states.

$$\rho = \sum_{a=0}^{n-1} p_a |\phi_a\rangle\langle\phi_a|$$

In this expression (p_0, \dots, p_{n-1}) is a probability vector and $|\phi_0\rangle, \dots, |\phi_{n-1}\rangle$ are quantum state vectors.

Here's a purification of ρ :

$$|\psi\rangle = \sum_{a=0}^{n-1} \sqrt{p_a} |\phi_a\rangle \otimes |a\rangle$$

(We're assume for simplicity that the classical states of Y include $0, \dots, n-1$.)

$$\text{Tr}_Y(|\psi\rangle\langle\psi|) = \sum_{a,b=0}^{n-1} \sqrt{p_a}\sqrt{p_b} |\phi_a\rangle\langle\phi_b| \text{Tr}(|a\rangle\langle b|) = \sum_{a=0}^{n-1} p_a |\phi_a\rangle\langle\phi_a| = \rho$$

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Example

$$\rho = \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{pmatrix} = \frac{1}{2} |0\rangle\langle 0| + \frac{1}{2} |+\rangle\langle +|$$

$$|\psi\rangle = \frac{1}{\sqrt{2}} |0\rangle \otimes |0\rangle + \frac{1}{\sqrt{2}} |+\rangle \otimes |1\rangle$$

Schmidt decompositions

Every quantum state vector $|\psi\rangle$ of a pair of systems (X, Y) can be expressed in a special form known as a *Schmidt decomposition*:

$$|\psi\rangle = \sum_{a=0}^{r-1} \sqrt{p_a} |x_a\rangle \otimes |y_a\rangle \quad (p_0, \dots, p_{r-1} > 0)$$

Both of the sets $\{|x_0\rangle, \dots, |x_{r-1}\rangle\}$ and $\{|y_0\rangle, \dots, |y_{r-1}\rangle\}$ must be *orthonormal*.

Finding a Schmidt decomposition

1. Compute a spectral decomposition of the reduced state $\rho = \text{Tr}_Y(|\psi\rangle\langle\psi|)$:

$$\rho = \sum_{a=0}^{r-1} p_a |x_a\rangle\langle x_a| \quad (p_0, \dots, p_{r-1} > 0)$$

2. For each $a = 0, \dots, r-1$ define $|y_a\rangle$ as follows:

$$|y_a\rangle = \frac{(\langle x_a| \otimes \mathbb{1})|\psi\rangle}{\sqrt{p_a}}$$

Schmidt decompositions

Example

Consider this state of a pair of qubits (X, Y):

$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle \otimes |0\rangle + \frac{1}{\sqrt{2}}|+\rangle \otimes |1\rangle$$

First compute a spectral decomposition of the reduced state of X:

$$\rho = \cos^2(\pi/8) |\psi_{\pi/8}\rangle\langle\psi_{\pi/8}| + \sin^2(\pi/8) |\psi_{5\pi/8}\rangle\langle\psi_{5\pi/8}|$$

We will make these selections:

$$p_0 = \cos^2(\pi/8), \quad p_1 = \sin^2(\pi/8), \quad |x_0\rangle = |\psi_{\pi/8}\rangle, \quad |x_1\rangle = |\psi_{5\pi/8}\rangle.$$

It remains to compute $|y_0\rangle$ and $|y_1\rangle$:

$$|y_0\rangle = \frac{(\langle x_0| \otimes \mathbb{1})|\psi\rangle}{\sqrt{p_0}} = |+\rangle \quad |y_1\rangle = \frac{(\langle x_1| \otimes \mathbb{1})|\psi\rangle}{\sqrt{p_1}} = -|-\rangle$$

Schmidt decompositions

Example

Consider this state of a pair of qubits (X, Y):

$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle \otimes |0\rangle + \frac{1}{\sqrt{2}}|+\rangle \otimes |1\rangle$$

$$p_0 = \cos^2(\pi/8), \quad p_1 = \sin^2(\pi/8), \quad |x_0\rangle = |\psi_{\pi/8}\rangle, \quad |x_1\rangle = |\psi_{5\pi/8}\rangle.$$

$$|y_0\rangle = \frac{(\langle x_0| \otimes \mathbb{1})|\psi\rangle}{\sqrt{p_0}} = |+\rangle \quad |y_1\rangle = \frac{(\langle x_1| \otimes \mathbb{1})|\psi\rangle}{\sqrt{p_1}} = -|-\rangle$$

We obtain the following Schmidt decomposition of $|\psi\rangle$:

$$|\psi\rangle = \cos(\pi/8) |\psi_{\pi/8}\rangle \otimes |+\rangle - \sin(\pi/8) |\psi_{5\pi/8}\rangle \otimes |-\rangle$$

Unitary equivalence of purifications

Unitary equivalence of purifications

Suppose that $|\psi\rangle$ and $|\phi\rangle$ are pure states of a pair of systems (X, Y) that satisfy

$$\text{Tr}_Y(|\psi\rangle\langle\psi|) = \rho = \text{Tr}_Y(|\phi\rangle\langle\phi|)$$

There exists a unitary operation U on Y alone that transforms $|\psi\rangle$ into $|\phi\rangle$:

$$(\mathbb{1}_X \otimes U)|\psi\rangle = |\phi\rangle$$

Consider a spectral decomposition of ρ .

$$\rho = \sum_{a=0}^{r-1} p_a |x_a\rangle\langle x_a|$$

Compute Schmidt decompositions for both $|\psi\rangle$ and $|\phi\rangle$:

$$|\psi\rangle = \sum_{a=0}^{r-1} \sqrt{p_a} |x_a\rangle \otimes |y_a\rangle \quad |\phi\rangle = \sum_{a=0}^{r-1} \sqrt{p_a} |x_a\rangle \otimes |z_a\rangle$$

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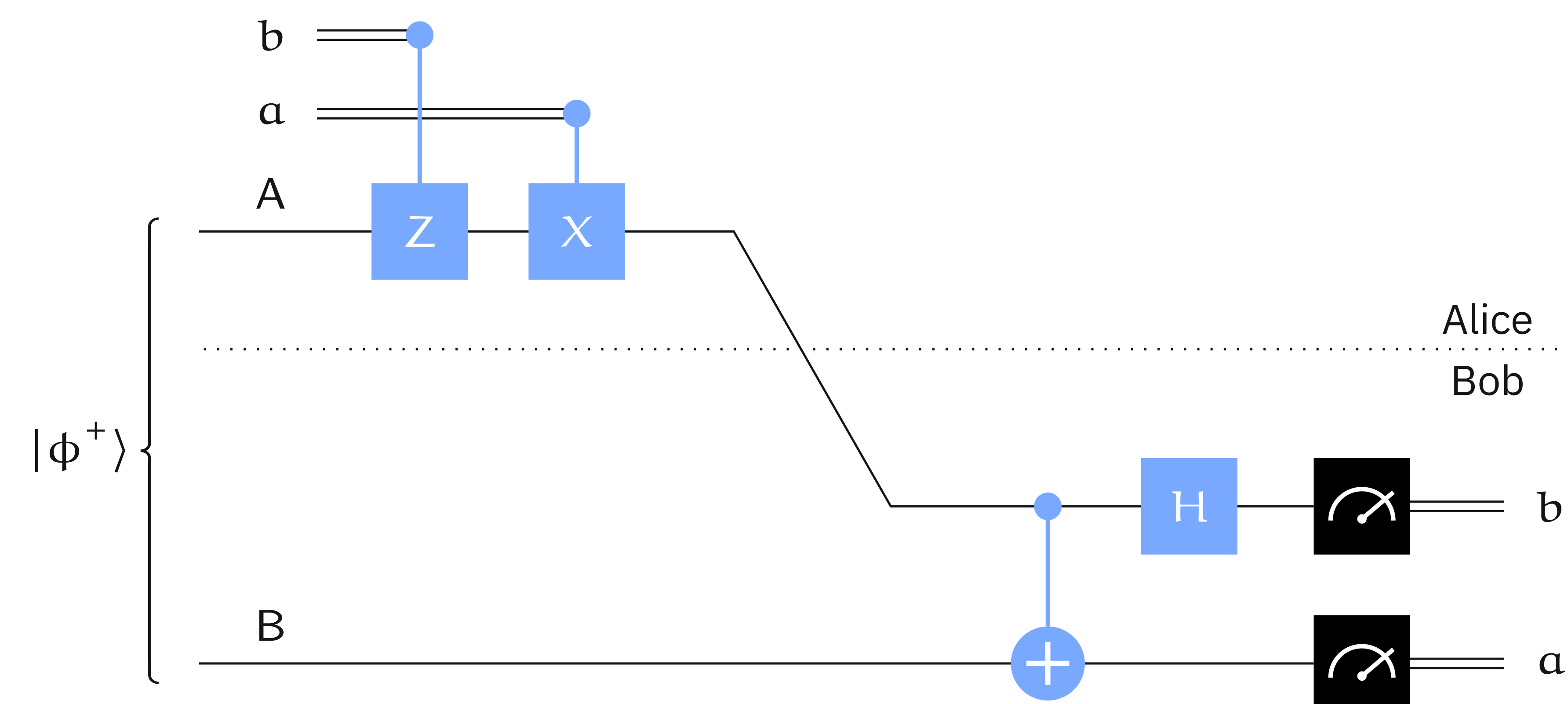
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Compute Schmidt decompositions for both $|\psi\rangle$ and $|\phi\rangle$:

$$|\psi\rangle = \sum_{\alpha=0}^{r-1} \sqrt{p_\alpha} |x_\alpha\rangle \otimes |y_\alpha\rangle \quad |\phi\rangle = \sum_{\alpha=0}^{r-1} \sqrt{p_\alpha} |x_\alpha\rangle \otimes |z_\alpha\rangle$$

Choose U to be any unitary matrix satisfying $U|y_\alpha\rangle = |z_\alpha\rangle$ for $\alpha = 0, \dots, r-1$.

Example: superdense coding



$$|\phi^+\rangle = \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$$

$$|\phi^-\rangle = \frac{1}{\sqrt{2}}|00\rangle - \frac{1}{\sqrt{2}}|11\rangle$$

$$|\psi^+\rangle = \frac{1}{\sqrt{2}}|01\rangle + \frac{1}{\sqrt{2}}|10\rangle$$

$$|\psi^-\rangle = \frac{1}{\sqrt{2}}|01\rangle - \frac{1}{\sqrt{2}}|10\rangle$$

The reduced state of B for all four Bell states is the completely mixed state.

$$\text{Tr}_A(|\phi^+\rangle\langle\phi^+|) = \text{Tr}_A(|\phi^-\rangle\langle\phi^-|) = \text{Tr}_A(|\psi^+\rangle\langle\psi^+|) = \text{Tr}_A(|\psi^-\rangle\langle\psi^-|) = \frac{1}{2}$$

By the *unitary equivalence of purifications*, we conclude that Alice can transform $|\phi^+\rangle$ to any of the four Bell states by applying a unitary operation to A alone.

Cryptographic implications

The unitary equivalence of purifications has implications to *quantum cryptography*.
For instance, it rules out an unconditionally secure quantum protocol for *bit commitment*.

Bit commitment

Bit commitment is a cryptographic primitive allowing Alice to *commit* to a selection of a bit $b \in \{0, 1\}$, which remains hidden until she chooses to *reveal* it to Bob.

- Binding property: Alice cannot change her mind once she's committed to b .
- Concealing property: Bob cannot determine b until Alice chooses to reveal it.

Let A and B be Alice's and Bob's systems in a *purified* version of a hypothetical protocol and let $|\psi_0\rangle$ and $|\psi_1\rangle$ be the states of (A, B) after Alice commits but before she reveals.

If the protocol is perfectly concealing, then

$$\text{Tr}_A(|\psi_0\rangle\langle\psi_0|) = \text{Tr}_A(|\psi_1\rangle\langle\psi_1|)$$

This implies that the protocol is not binding: Alice can change her commitment by performing a unitary operation on A alone.

HJW theorem

Hughston-Jozsa-Wootters theorem

Suppose X and Y are systems and $|\phi\rangle$ is a quantum state vector of (X, Y) .

Let N be a positive integer, let (p_0, \dots, p_{N-1}) be a probability vector, and let $|\psi_0\rangle, \dots, |\psi_{N-1}\rangle$ be quantum state vectors of X such that

$$\text{Tr}_Y(|\phi\rangle\langle\phi|) = \sum_{\alpha=0}^{N-1} p_{\alpha} |\psi_{\alpha}\rangle\langle\psi_{\alpha}|$$

There exists a measurement $\{P_0, \dots, P_{N-1}\}$ of Y such that these statements are true when Y is measured when (X, Y) is in the state $|\phi\rangle$:

- Each measurement outcome $\alpha \in \{0, \dots, N-1\}$ appears with probability p_{α} .
- Conditioned on obtaining the outcome α , the state of X becomes $|\psi_{\alpha}\rangle$.

HJW theorem

Proof sketch. We have the following relationship:

$$\sum_{a=0}^{N-1} p_a |\psi_a\rangle\langle\psi_a| = \rho = \text{Tr}_Y(|\phi\rangle\langle\phi|)$$

Introduce a new system Z having classical states $\{0, \dots, N-1\}$. These two state vectors of (X, Y, Z) are both purifications of ρ :

$$\begin{aligned} |\gamma_0\rangle &= |\phi\rangle_{XY} \otimes |0\rangle_Z \\ |\gamma_1\rangle &= \sum_{a=0}^{N-1} \sqrt{p_a} |\psi_a\rangle_X \otimes |0\rangle_Y \otimes |a\rangle_Z \end{aligned}$$

By the unitary equivalence of purifications, there is a unitary operation on (Y, Z) that transforms $|\gamma_0\rangle$ into $|\gamma_1\rangle$:

$$(\mathbb{1}_X \otimes U)|\gamma_0\rangle = |\gamma_1\rangle$$

HJW theorem

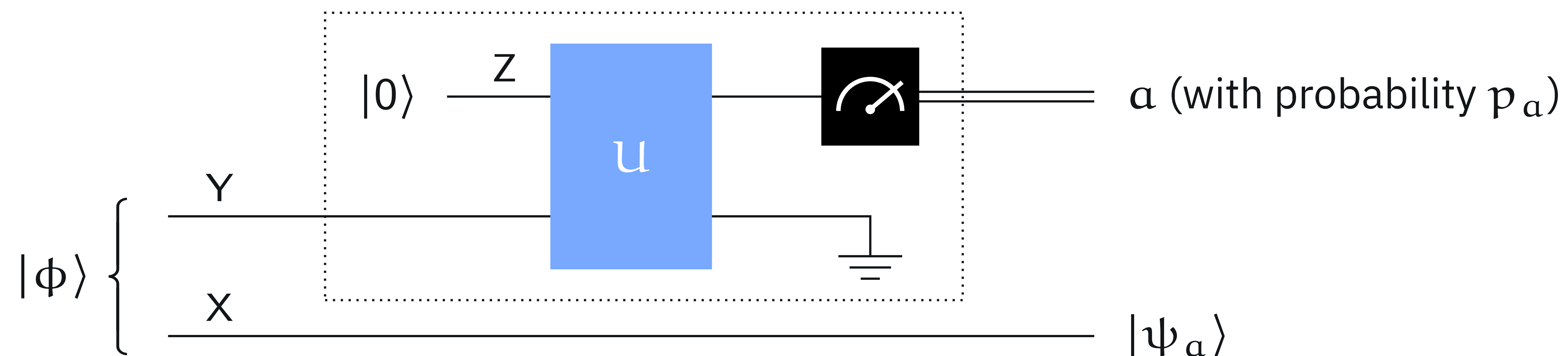
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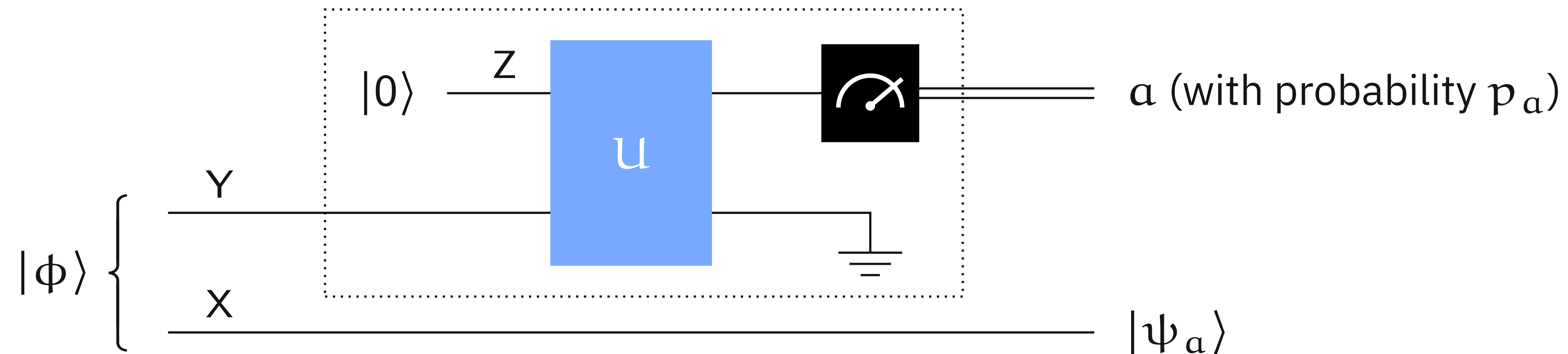
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This measurement is described by matrices $\{P_0, \dots, P_{N-1}\}$ defined as follows:

$$P_a = (\mathbb{1}_Y \otimes \langle 0|)U^\dagger(\mathbb{1}_Y \otimes |a\rangle\langle a|)U(\mathbb{1}_Y \otimes |0\rangle)$$

Definition of fidelity

The fidelity between two quantum states measures their *similarity* or *overlap*.

For two states represented by density matrices ρ and σ it is defined as follows:

$$F(\rho, \sigma) = \text{Tr} \sqrt{\sqrt{\rho} \sigma \sqrt{\rho}}$$

The matrix $\sqrt{\rho} \sigma \sqrt{\rho}$ is positive semidefinite: $\sqrt{\rho} \sigma \sqrt{\rho} = M^\dagger M$ for $M = \sqrt{\sigma} \sqrt{\rho}$. We can therefore take the square root of this matrix:

$$\sqrt{\rho} \sigma \sqrt{\rho} = \sum_{k=0}^{n-1} \lambda_k |\phi_k\rangle \langle \phi_k| \quad \Rightarrow \quad \sqrt{\sqrt{\rho} \sigma \sqrt{\rho}} = \sum_{k=0}^{n-1} \sqrt{\lambda_k} |\phi_k\rangle \langle \phi_k|$$

$$F(\rho, \sigma) = \sum_{k=0}^{n-1} \sqrt{\lambda_k}$$

An equivalent formula in terms of the trace norm $\|M\|_1 = \text{Tr} \sqrt{M M^\dagger} = \text{Tr} \sqrt{M^\dagger M}$:

$$F(\rho, \sigma) = \|\sqrt{\rho} \sqrt{\sigma}\|_1 = \|\sqrt{\sigma} \sqrt{\rho}\|_1$$

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The trace norm can also be defined as $\|M\|_1 = \max_{\mathcal{U}} |\text{Tr}(M\mathcal{U})|$ (maximum over all unitary \mathcal{U}).

$$F(\rho, \sigma) = \max_{\mathcal{U} \text{ unitary}} |\text{Tr}(\sqrt{\rho} \sqrt{\sigma} \mathcal{U})|$$

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$$F(\rho, \sigma) = \max_{\mathcal{U} \text{ unitary}} |\text{Tr}(\sqrt{\rho} \sqrt{\sigma} \mathcal{U})|$$

There are simpler formulas when at least one of the states is pure:

$$F(|\phi\rangle\langle\phi|, |\psi\rangle\langle\psi|) = |\langle\phi|\psi\rangle|$$

$$F(|\phi\rangle\langle\phi|, \sigma) = \sqrt{\langle\phi|\sigma|\phi\rangle}$$

Properties of fidelity

1. For any two density matrices ρ and σ we have $0 \leq F(\rho, \sigma) \leq 1$.
 - $F(\rho, \sigma) = 0$ if and only if ρ and σ have orthogonal images.
 - $F(\rho, \sigma) = 1$ if and only if $\rho = \sigma$.
2. The fidelity is symmetric: $F(\rho, \sigma) = F(\sigma, \rho)$.
3. The fidelity is multiplicative for product states:

$$F(\rho_1 \otimes \cdots \otimes \rho_m, \sigma_1 \otimes \cdots \otimes \sigma_m) = F(\rho_1, \sigma_1) \cdots F(\rho_m, \sigma_m)$$

4. For any two density matrices ρ and σ and any channel Φ we have

$$F(\rho, \sigma) \leq F(\Phi(\rho), \Phi(\sigma))$$

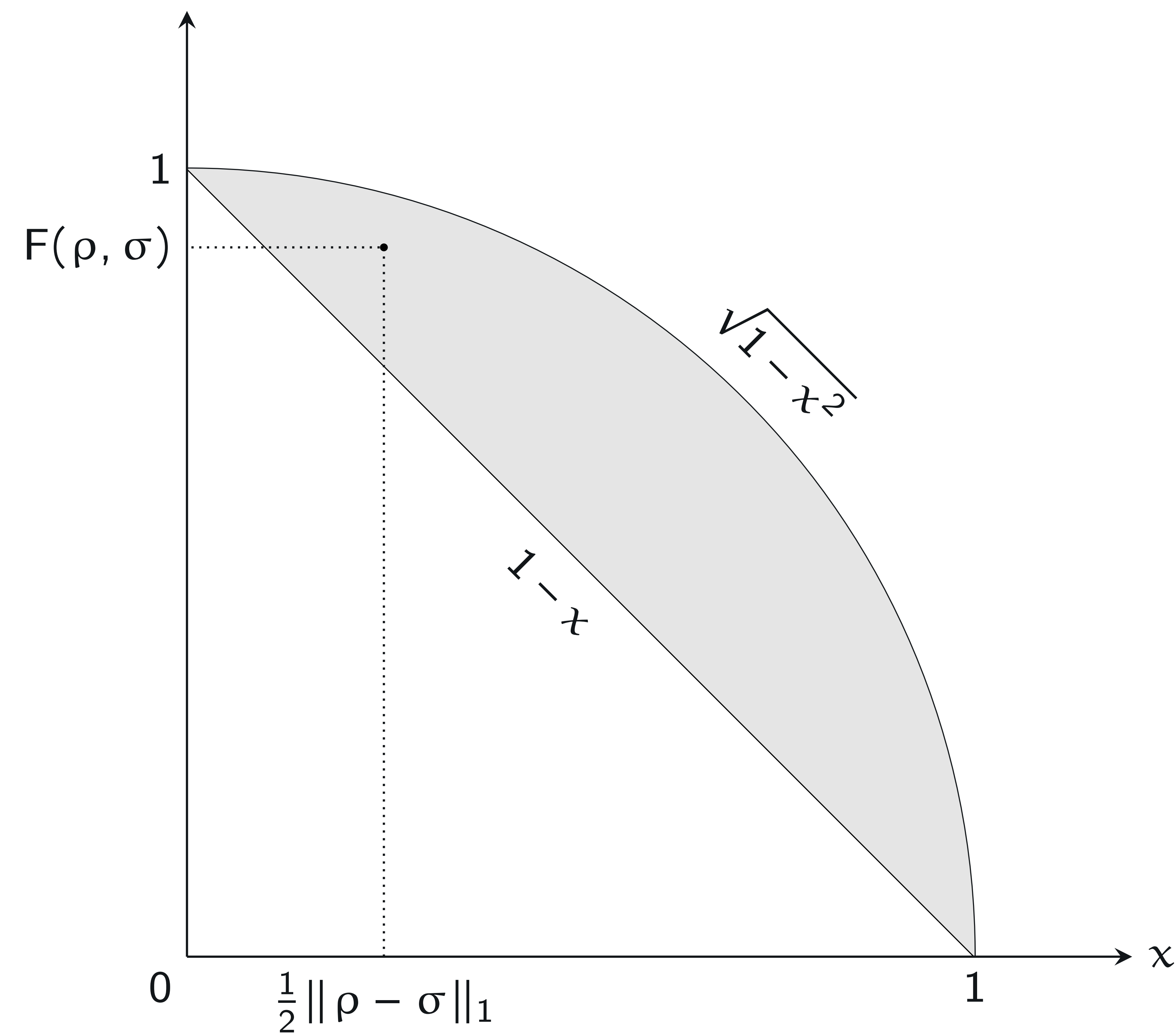
5. There is a close relationship between fidelity and trace distance:

$$1 - \frac{1}{2} \|\rho - \sigma\|_1 \leq F(\rho, \sigma) \leq \sqrt{1 - \frac{1}{4} \|\rho - \sigma\|_1^2}$$

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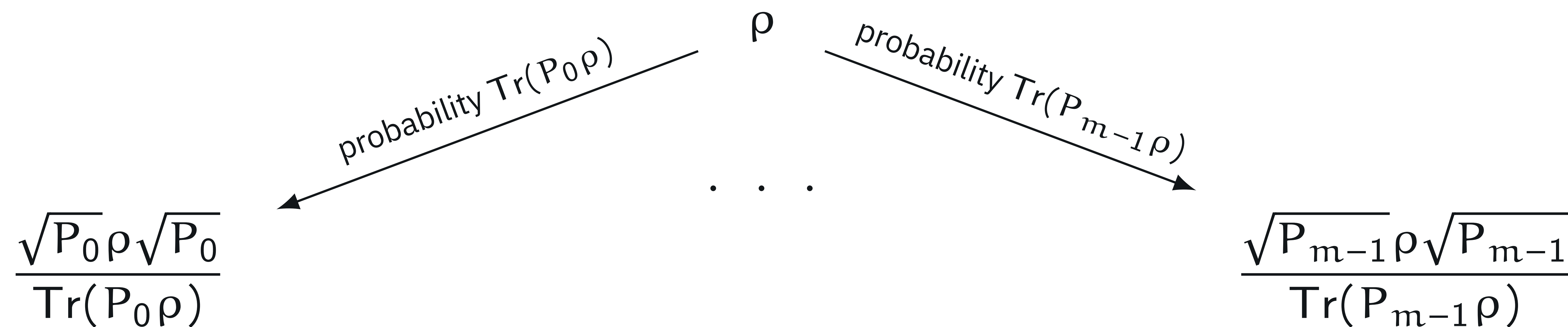


Gentle measurement lemma

Let X be a system, let ρ be a state of X , and let $\{P_0, \dots, P_{m-1}\}$ be a measurement. Suppose that one of the measurement outcomes is very likely to appear.

$$\text{Tr}(P_0 \rho) > 1 - \varepsilon$$

A *non-destructive* implementation of this measurements (through Naimark's theorem) works like this:



The gentle measurement lemma implies that only a *small disturbance* occurs when the likely measurement outcome appears.

$$F\left(\rho, \frac{\sqrt{P_0} \rho \sqrt{P_0}}{\text{Tr}(P_0 \rho)}\right)^2 > 1 - \varepsilon$$

Gentle measurement lemma

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We can evaluate the fidelity between the pre- and post-measurement states:

$$\begin{aligned} F\left(\rho, \frac{\sqrt{P_0} \rho \sqrt{P_0}}{\text{Tr}(P_0 \rho)}\right) &= \text{Tr} \sqrt{\frac{\sqrt{\rho} \sqrt{P_0} \rho \sqrt{P_0} \sqrt{\rho}}{\text{Tr}(P_0 \rho)}} = \text{Tr} \sqrt{\left(\frac{\sqrt{\rho} \sqrt{P_0} \sqrt{\rho}}{\sqrt{\text{Tr}(P_0 \rho)}}\right)^2} \\ &= \text{Tr}\left(\frac{\sqrt{\rho} \sqrt{P_0} \sqrt{\rho}}{\sqrt{\text{Tr}(P_0 \rho)}}\right) = \frac{\text{Tr}(\sqrt{P_0} \rho)}{\sqrt{\text{Tr}(P_0 \rho)}} \geq \frac{\text{Tr}(P_0 \rho)}{\sqrt{\text{Tr}(P_0 \rho)}} \end{aligned}$$

$$P_0 = \sum_{k=0}^{n-1} \lambda_k |\psi_k\rangle\langle\psi_k|$$

$$\text{Tr}(\sqrt{P_0} \rho) = \sum_{k=0}^{n-1} \sqrt{\lambda_k} \langle\psi_k|\rho|\psi_k\rangle \geq \sum_{k=0}^{n-1} \lambda_k \langle\psi_k|\rho|\psi_k\rangle = \text{Tr}(P_0 \rho)$$

Gentle measurement lemma

Let X be a system, let ρ be a state of X , and let $\{P_0, \dots, P_{m-1}\}$ be a measurement. Suppose that one of the measurement outcomes is very likely to appear.

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We can evaluate the fidelity between the pre- and post-measurement states:

$$\begin{aligned} F\left(\rho, \frac{\sqrt{P_0} \rho \sqrt{P_0}}{\text{Tr}(P_0 \rho)}\right) &= \text{Tr} \sqrt{\frac{\sqrt{\rho} \sqrt{P_0} \rho \sqrt{P_0} \sqrt{\rho}}{\text{Tr}(P_0 \rho)}} = \text{Tr} \sqrt{\left(\frac{\sqrt{\rho} \sqrt{P_0} \sqrt{\rho}}{\sqrt{\text{Tr}(P_0 \rho)}}\right)^2} \\ &= \text{Tr} \left(\frac{\sqrt{\rho} \sqrt{P_0} \sqrt{\rho}}{\sqrt{\text{Tr}(P_0 \rho)}}\right) = \frac{\text{Tr}(\sqrt{P_0} \rho)}{\sqrt{\text{Tr}(P_0 \rho)}} \geq \frac{\text{Tr}(P_0 \rho)}{\sqrt{\text{Tr}(P_0 \rho)}} = \sqrt{\text{Tr}(P_0 \rho)} \end{aligned}$$

$$F\left(\rho, \frac{\sqrt{P_0} \rho \sqrt{P_0}}{\text{Tr}(P_0 \rho)}\right)^2 \geq \text{Tr}(P_0 \rho) > 1 - \varepsilon$$

Uhlmann's theorem

Uhlmann's theorem is a fundamentally important fact connecting fidelity with purifications.

Uhlmann's theorem

The fidelity between two quantum states equals the *maximum inner product* (in absolute value) between two purifications of these states.

In greater detail...

Suppose ρ and σ are density matrices representing states of a system X , and let Y be a system with at least as many classical states as X .

$$F(\rho, \sigma) = \max \left\{ |\langle \phi | \psi \rangle| : \text{Tr}_Y(|\phi\rangle\langle\phi|) = \rho, \text{Tr}_Y(|\psi\rangle\langle\psi|) = \sigma \right\}$$

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Consider spectral decompositions of ρ and σ :

$$\rho = \sum_{a=0}^{n-1} p_a |u_a\rangle\langle u_a| \quad \text{and} \quad \sigma = \sum_{b=0}^{n-1} q_b |v_b\rangle\langle v_b|$$

These state vectors purify ρ and σ :

$$\sum_{a=0}^{n-1} \sqrt{p_a} |u_a\rangle \otimes |\overline{u_a}\rangle \quad \text{and} \quad \sum_{b=0}^{n-1} \sqrt{q_b} |v_b\rangle \otimes |\overline{v_b}\rangle$$

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By the unitary equivalence of purifications, all purifications of ρ and σ to (X, Y) take these forms (for U and V unitary):

$$|\phi\rangle = \sum_{a=0}^{n-1} \sqrt{p_a} |u_a\rangle \otimes U |\overline{u_a}\rangle \quad \text{and} \quad |\psi\rangle = \sum_{b=0}^{n-1} \sqrt{q_b} |v_b\rangle \otimes V |\overline{v_b}\rangle$$

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$$\max \left\{ |\langle \phi | \psi \rangle| : \text{Tr}_Y(|\phi\rangle\langle\phi|) = \rho, \text{Tr}_Y(|\psi\rangle\langle\psi|) = \sigma \right\}$$

$$= \max_{U, V \text{ unitary}} \left| \sum_{a,b=0}^{n-1} \sqrt{p_a} \sqrt{q_b} \langle u_a | v_b \rangle \langle v_b | V^T \bar{U} | u_a \rangle \right|$$

$$= \max_{U, V \text{ unitary}} \left| \text{Tr} \left(\sqrt{\rho} \sqrt{\sigma} V^T \bar{U} \right) \right| = \left\| \sqrt{\rho} \sqrt{\sigma} \right\|_1 = F(\rho, \sigma)$$