

LECTURE 3

DENSITY OPERATOR AND PARTIAL TRACE

INF587 Quantum computer science and applications

Thomas Debris-Alazard

Inria, École Polytechnique

To answer the following questions:

- How can we model the quantum state **after a measurement**?
ex: $|0\rangle$ with prob. $1/2$ and $|1\rangle$ with prob. $1/2$.
- How can we describe the quantum state relative to a **subsystem**?
ex: the first qubit of the EPR-pair $\frac{|00\rangle+|11\rangle}{\sqrt{2}}$.

→ Density operator/matrix and partial trace!

1. General properties of density operators
2. The reduced density operator, partial trace and application to the teleportation
3. Schmidt decomposition and purification

→ This course gives the basis of **quantum information theory!**

DENSITY OPERATOR

Observable: an equivalent description of projective measurements

- Observable: \mathbf{M} an Hermitian operator (*i.e.*, $\mathbf{M}^\dagger = \mathbf{M}$),
- \mathbf{M} is diagonalizable in an orthonormal basis: orthogonal projectors \mathbf{P}_m onto the eigenspaces define the measurement.
- Given $|\psi\rangle$, average outcome value:

$$\langle \mathbf{M} \rangle = \langle \psi | \mathbf{M} | \psi \rangle = \text{tr}(\mathbf{M} |\psi\rangle\langle\psi|).$$

An example:

X defines a measurement with outcome ± 1 :

$$X = |+\rangle\langle+| + (-1)|-\rangle\langle-|$$

Given $|0\rangle$ (*resp.* $|1\rangle$), the average outcome value is 0:

$$\langle 0 | X | 0 \rangle = \langle 0 | + \rangle \langle + | 0 \rangle - \langle 0 | - \rangle \langle - | 0 \rangle = \frac{1}{2} - \frac{1}{2} = 0.$$

$$\langle 1 | X | 1 \rangle = \langle 1 | + \rangle \langle + | 1 \rangle - \langle 1 | - \rangle \langle - | 1 \rangle = \frac{1}{2} - \frac{1}{2} = 0.$$

Suppose that ρ is a probabilistic mixture of quantum states:

$$\rho : |\psi_j\rangle \text{ with prob. } p_j.$$

What is the average outcome value given ρ and an observable \mathbf{M} ?

By linearity of the expectation it is given by:

$$\begin{aligned} \sum_j p_j \langle \psi_j | \mathbf{M} | \psi_j \rangle &= \sum_j p_j \text{tr} (\mathbf{M} |\psi_j\rangle\langle\psi_j|) \\ &= \text{tr} \left(\mathbf{M} \sum_j p_j |\psi_j\rangle\langle\psi_j| \right) \end{aligned}$$

Define the probabilistic mixture ρ as:

$$\rho = \sum_j p_j |\psi_j\rangle\langle\psi_j|$$

The density matrix

The density matrix ρ corresponding to a probabilistic mixture of states $(|\psi_j\rangle)_j$, the corresponding quantum state being equal to $|\psi_j\rangle$ with probability p_j , is given by

$$\rho \stackrel{\text{def}}{=} \sum_j p_j |\psi_j\rangle\langle\psi_j|$$

→ $\{p_i, |\psi_i\rangle\}$ is a set of states generating a density matrix ρ

The density matrix of a qubit

$$|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad \langle\psi| = (\bar{\alpha} \quad \bar{\beta})$$

$$|\psi\rangle\langle\psi| = \begin{pmatrix} |\alpha|^2 & \alpha\bar{\beta} \\ \bar{\alpha}\beta & |\beta|^2 \end{pmatrix}$$

- Density matrix of $|0\rangle$ (resp. $|1\rangle$) is

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \left(\text{resp.} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\right)$$

- Density matrix of $|+\rangle$ (resp. $|-\rangle$) is

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \quad \left(\text{resp.} \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}\right)$$

Exercise

- Compute the density matrix of:
 1. the probabilistic mixture of $|0\rangle$ with prob. $\frac{1}{2}$ and $|1\rangle$ with prob. $\frac{1}{2}$,
 2. the probabilistic mixture of $|+\rangle$ with prob. $\frac{1}{2}$ and $|-\rangle$ with prob. $\frac{1}{2}$,
 3. what can you conclude?
- Compare the density matrix of $|\psi\rangle$ with $e^{i\theta} |\psi\rangle$. What can you conclude?

- We have:

1. Probabilistic mixture of $|0\rangle$ with prob. $\frac{1}{2}$ and $|1\rangle$ with prob. $\frac{1}{2}$:

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

2. Probabilistic mixture of $|+\rangle$ with prob. $\frac{1}{2}$ and $|-\rangle$ with prob. $\frac{1}{2}$:

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

3. These probabilistic mixtures have the same density operator: **they are indistinguishable**

- $|\psi\rangle$ and $e^{i\theta} |\psi\rangle$ have the same density operator: **they are indistinguishable**

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→ We could have stated quantum mechanics **using density operators as the primary model of states!**

In particular: postulates of quantum mechanics given with density matrix point of view

Let \mathbf{U} be a unitary. Suppose that $|\psi\rangle$ is in the state $|\psi_i\rangle$ with probability p_i

→ After applying \mathbf{U} : $|\psi\rangle$ will be in the state $\mathbf{U}|\psi_i\rangle$ with probability p_i .

$$\left(|\psi_i\rangle\langle\psi_i| \xrightarrow{\mathbf{U}} \mathbf{U}|\psi_i\rangle\langle\psi_i|\mathbf{U}^\dagger \right)$$

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$$\left(|\psi_i\rangle\langle\psi_i| \xrightarrow{\mathbf{U}} \mathbf{U}|\psi_i\rangle\langle\psi_i|\mathbf{U}^\dagger \right)$$

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \xrightarrow{\mathbf{U}} \sum_i p_i \mathbf{U}|\psi_i\rangle\langle\psi_i|\mathbf{U}^\dagger = \mathbf{U}\rho\mathbf{U}^\dagger$$

Let $(\mathbf{M}_m)_m$ be a quantum measurement. Suppose that $|\psi\rangle$ is in the state $|\psi_i\rangle$ with probability p_i .

- If the initial state is $|\psi_i\rangle$, the probability to measure m is:

$$p(m|i) = \langle \psi_i | \mathbf{M}_m^\dagger \mathbf{M}_m | \psi_i \rangle = \text{tr} \left(\mathbf{M}_m^\dagger \mathbf{M}_m |\psi_i\rangle \langle \psi_i| \right)$$

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- Using the law of total probability, we measure m with probability:

$$p(m) = \sum_i p(m|i)p_i = \sum_i \text{tr} \left(\mathbf{M}_m^\dagger \mathbf{M}_m |\psi_i\rangle\langle\psi_i| \right) p_i = \text{tr} \left(\mathbf{M}_m^\dagger \mathbf{M}_m \rho \right).$$

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- If the initial state is $|\psi_i\rangle$ and we have measured m , the state becomes:

$$|\psi_i^m\rangle = \frac{\mathbf{M}_m |\psi_i\rangle}{\sqrt{\text{tr} \left(\mathbf{M}_m^\dagger \mathbf{M}_m |\psi_i\rangle\langle\psi_i| \right)}} = \frac{\mathbf{M}_m |\psi_i\rangle}{\sqrt{p(m|i)}}$$

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The corresponding density operator ρ_m is:

$$\rho_m = \sum_i p(i|m) |\psi_i^m\rangle\langle\psi_i^m| = \sum_i p(i|m) \frac{\mathbf{M}_m |\psi_i\rangle\langle\psi_i| \mathbf{M}_m^\dagger}{p(m|i)} = \sum_i \frac{p_i}{p(m)} \mathbf{M}_m |\psi_i\rangle\langle\psi_i| \mathbf{M}_m^\dagger$$

Let $(\mathbf{M}_m)_m$ be a quantum measurement. Suppose that $|\psi\rangle$ is in the state $|\psi_i\rangle$ with probability p_i .

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$$\rho_m = \frac{\mathbf{M}_m \rho \mathbf{M}_m^\dagger}{\text{tr} \left(\mathbf{M}_m^\dagger \mathbf{M}_m \rho \right)}$$

- Unitary Evolution U :

$$\rho \xrightarrow{U} U\rho U^\dagger$$

- Measurement $(M_m)_m$:

1. Probability to measure m :

$$\text{tr} \left(M_m^\dagger M_m \rho \right)$$

2. After measuring m :

$$\frac{M_m \rho M_m^\dagger}{\text{tr} \left(M_m^\dagger M_m \rho \right)}$$

Theorem

An operator ρ acting on an Hilbert space is a density operator if and only if

1. ρ is positive,
2. $\text{tr}(\rho) = 1$.

→ This characterization **does not rely on a set interpretation!**

In particular: give a description of quantum mechanics with density operators **that does not take as its foundation the state vector.**

\Rightarrow : Suppose $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$. Then

$$\text{tr}(\rho) = \sum_i p_i \text{tr}(|\psi_i\rangle\langle\psi_i|) = \sum_i p_i \text{tr}(\langle\psi_i|\psi_i\rangle) = \sum_i p_i = 1.$$

as $(p_i)_i$ defines a distribution. Let $|\psi\rangle$ be an arbitrary vector in the state space

$$\langle\psi|\rho|\psi\rangle = \sum_i p_i \langle\psi|\psi_i\rangle \langle\psi_i|\psi\rangle = \sum_i p_i |\langle\psi|\psi_i\rangle|^2 \geq 0.$$

\Leftarrow : Suppose ρ positive operator with trace one.

By the **spectral decomposition theorem**, there exists an orthonormal basis $(|i\rangle)_i$ (in particular the $|i\rangle$'s have norm 1) with associated positive eigenvalue $(\lambda_i)_i$ s.t

$$\rho = \sum_i \lambda_i |i\rangle\langle i|$$

But,

$$\text{tr}(\rho) = \sum_i \lambda_i = 1.$$

Therefore ρ is a $(\lambda_i)_i$ -probabilistic mixture of the quantum states $(|i\rangle)_i$.

Pure state

A state is called pure if it cannot be represented as a mixture (convex combination) of other states.

This is equivalent to the density matrix being a one dimensional projector, *i.e.*, $\rho = |\psi\rangle\langle\psi|$ where $|\psi\rangle$ is a state (a unit vector).

Mixed States

A quantum system which is not in pure state is said to be in mixed states.

Example

1. $|0\rangle$, $\frac{|0\rangle+|1\rangle}{\sqrt{2}}$, $|01\rangle$ and $\frac{|00\rangle+|11\rangle}{\sqrt{2}}$ are pure states,
2. The probabilistic state “ $|0\rangle$ with prob. $\frac{1}{2}$ and $|1\rangle$ with prob. $\frac{1}{2}$ ” is a mixed state.

Theorem

Any density operator ρ verifies

$$\text{tr}(\rho^2) \leq 1.$$

Furthermore,

$$\text{tr}(\rho^2) = 1 \iff \rho \text{ is a pure state.}$$

First: any density operator ρ can be written as $\sum_i \lambda_i |i\rangle\langle i|$ where $(|i\rangle)_i$ orthonormal basis, $\lambda_i \geq 0$ and $\sum_i \lambda_i = 1$.

→ Consequence of the fact that ρ positive operator and $\text{tr}(\rho) = 1$.

Therefore,

$$\rho^2 = \sum_i \lambda_i^2 |i\rangle\langle i|$$

Using that $(\lambda_i)_i$ is a distribution concludes the proof.

It may be tempting to interpret: $\rho \stackrel{\text{def}}{=} \frac{1}{2} |0\rangle\langle 0| + \frac{1}{2} |1\rangle\langle 1|$ as “ $|0\rangle$ with prob. $\frac{1}{2}$ and $|1\rangle$ with prob. $\frac{1}{2}$ ”.

But, ρ also verifies: $\rho = \frac{1}{2} |+\rangle\langle +| + \frac{1}{2} |-\rangle\langle -| \dots$

Eigenvectors and eigenvalues of a density operator just indicates **one of many possible** sets that may give rise to a specific density matrix

→ What class of states does give rise to a particular density operator?

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Theorem (admitted)

$\rho = \sum_i p_i |\psi_i\rangle\langle \psi_i| = \sum_i q_i |\varphi_i\rangle\langle \varphi_i|$ for quantum states $(|\psi_i\rangle)_i$ and $(|\varphi_i\rangle)_i$ and distributions $(p_i)_i$ and $(q_i)_i$ if and only if

$$\forall i, \quad \sqrt{p_i} |\psi_i\rangle = \sum_j u_{i,j} \sqrt{q_j} |\varphi_j\rangle \quad \text{where } \mathbf{U} = (u_{i,j})_{i,j} \text{ be a unitary.}$$

THE REDUCED DENSITY OPERATOR, PARTIAL TRACE

PARTIAL TRACE: REDUCTION TO A SUBSYSTEM

Problem

Given $\rho^{AB} \in A \otimes B$,^a what is the quantum state with respect to A ?

^a Abuse of notation, ρ density operator over $A \otimes B$

→ Answer: $\rho^A \stackrel{\text{def}}{=} \text{tr}_B (\rho^{AB})$ where: $\begin{cases} \rho^A & \text{the reduced density operator for } A, \\ \text{tr}_B & \text{partial trace over } B. \end{cases}$

Definition: partial trace

Given $|a_1\rangle\langle a_2| \in A$ and $|b_1\rangle\langle b_2| \in B$, define

$$\text{tr}_B (|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) = |a_1\rangle\langle a_2| \text{tr} (|b_1\rangle\langle b_2|) = \langle b_1|b_2\rangle |a_1\rangle\langle a_2| \in A.$$

then extend tr_B by linearity.

We could have defined tr_B directly as:

$$\text{tr}_B (\rho^{AB}) = \sum_i (\mathbf{1} \otimes \langle i|) \rho^{AB} (\mathbf{1} \otimes |i\rangle) \quad \text{where } (|i\rangle)_i \text{ orthonormal basis of } B$$

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→ But why this definition?

“Reduced density operator provides the correct measurement statistics for measurements made on system A ”

JUSTIFICATION OF THE PARTIAL TRACE

Given an observable \mathbf{M} on a A :

→ We want average measurements be the same when computed via ρ^A or ρ^{AB} , namely:

$$\text{tr}(\mathbf{M}\rho^A) = \text{tr}((\mathbf{M} \otimes \mathbf{I})\rho^{AB}) \quad (1)$$

→ Equation that is verified by $\rho^A = \text{tr}_B(\rho^{AB})$ (little exercise using $\text{tr}(\mathbf{A} \otimes \mathbf{B}) = \text{tr}(\mathbf{A})\text{tr}(\mathbf{B})$)

tr_B is the unique operator which verifies Equation (1)

Let f be a linear map of density operators on $A \otimes B$ to density operators on A which verifies the “average measurements”

$$\text{tr}(\mathbf{M}f(\rho^{AB})) = \text{tr}((\mathbf{M} \otimes \mathbf{I})\rho^{AB})$$

Let \mathbf{M}_i be an orthonormal basis to the space of Hermitian operators on A with respect to the inner-product $\langle \mathbf{X}, \mathbf{Y} \rangle = \text{tr}(\mathbf{X}\mathbf{Y})$:

$$f(\rho^{AB}) = \sum_i \mathbf{M}_i \text{tr}(\mathbf{M}_i f(\rho^{AB})) = \sum_i \mathbf{M}_i \text{tr}((\mathbf{M}_i \otimes \mathbf{I})\rho^{AB}) = \sum_i \mathbf{M}_i \text{tr}(\mathbf{M}_i \rho^A) = \rho^A$$

Therefore: any operator which verifies the “average measurements” is the partial trace!

Proposition

Given two density operators ρ^A and ρ^B on a A and B :

$$\text{tr}_B \left(\rho^A \otimes \rho^B \right) = \rho^A \quad \text{and} \quad \text{tr}_A \left(\rho^A \otimes \rho^B \right) = \rho^B$$

tr_B : "trace out B " ; tr_A : "trace out A ".

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tr_B : “trace out B ” ; tr_A : “trace out A ”.

Proof:

Write $\rho_A = \sum_i \lambda_i |i\rangle\langle i|$ and $\rho_B = \sum_j \mu_j |j\rangle\langle j|$ (for orthonormal bases). By definition

$$\begin{aligned} \text{tr}_B \left(\rho^A \otimes \rho^B \right) &= \sum_{i,j} \lambda_i \mu_j \text{tr}_B \left(|i\rangle\langle i| \otimes |j\rangle\langle j| \right) \\ &= \sum_{i,j} \lambda_i |i\rangle\langle i| \left(\sum_j \mu_j \langle j|j\rangle \right) \\ &= \rho^A \end{aligned}$$

where in the last line we used $1 = \text{tr}(\rho^B) = \sum_j \mu_j$.

Consider the EPR-pair: $\frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$

1. Compute the density matrix ρ^{12} (1 and 2: first and second qubit) of the EPR-pair,
2. Compute the reduced density matrices ρ^1 and ρ^2 with respect to the first and second qubit, respectively. What can you conclude?
3. Is $\rho^{12} = \rho^1 \otimes \rho^2$?

1. We have

$$\rho^{12} = \frac{1}{2} (|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|),$$

therefore (basis is ordered as $(|00\rangle, |01\rangle, |10\rangle, |11\rangle)$)

$$\rho^{12} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

2. Rewrite ρ^{12} as

$$\rho^{12} = \frac{1}{2} (|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |0\rangle\langle 1| \otimes |0\rangle\langle 1| + |1\rangle\langle 0| \otimes |1\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1|)$$

Therefore,

$$\rho^1 = \text{tr}_2(\rho^{12}) = \frac{1}{2} (|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{\mathbb{I}_2}{2} \quad \text{and} \quad \rho^2 = \text{tr}_1(\rho^{12}) = \frac{1}{2} (|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{\mathbb{I}_2}{2}$$

Although the original system was prepared as a pure state (complete knowledge), the first and the second qubit are **a uniform mixture of qubits...**

3. No: $\rho^{12} \neq \rho^1 \otimes \rho^2 = \frac{\mathbb{I}_4}{4}$.

If Alice and Bob share an EPR-pair:

- ▶ Alice's qubit is a mixed state for which she has **strictly no information/knowledge**,
- ▶ Bob's qubit is a mixed state for which he has **strictly no information/knowledge**

The joint state of the EPR pair is known **exactly** while both its first and second qubit is completely unknown (maximal uncertainty)!

Teleportation

1. Recall that after Alice's measurement, the quantum state that Alice and Bob share is with probability $\frac{1}{4}$ the three-qubits state $|a, b\rangle |\psi_{ab}\rangle$:

$$|\psi_{ab}\rangle \stackrel{\text{def}}{=} \alpha |b\rangle + (-1)^a \beta |1 - b\rangle .$$

where $a, b \in \{0, 1\}$.

Compute the reduced density operator ρ_B of Bob's system (by tracing out the first two qubits) once Alice has performed her measurement but before Bob has learned a, b .

2. What can you conclude?

1. We have the following computation:

$$\begin{aligned} \rho^{ab} &= |ab\rangle\langle ab| \otimes |\psi_{ab}\rangle\langle\psi_{ab}| \\ &= |ab\rangle\langle ab| \otimes \left(|\alpha|^2 |b\rangle\langle b| + (-1)^a \alpha \bar{\beta} |b\rangle\langle 1-b| + \right. \\ &\quad \left. (-1)^a \bar{\alpha} \beta |1-b\rangle\langle b| + |\beta|^2 |1-b\rangle\langle 1-b| \right) \end{aligned}$$

The density operator of the shared quantum state is:

$$\rho = \frac{1}{4} \left(\sum_{a,b \in \{0,1\}} \rho^{ab} \right)$$

By tracing out the first two qubits we get

$$\begin{aligned} \rho_B &= \frac{1}{4} \left((2|\alpha|^2 + 2|\beta|^2) |0\rangle\langle 0| + (2|\alpha|^2 + 2|\beta|^2) |1\rangle\langle 1| \right) \\ &= \frac{1}{2} (|0\rangle\langle 0| + |1\rangle\langle 1|) \\ &= \frac{I_2}{2} \end{aligned}$$

2. Bob's state has no dependence upon the state $|\psi\rangle$ being teleported: **any measurements performed by Bob will contain no information about $|\psi\rangle$**

→ It prevents Alice to transmit information to Bob faster than light!

SCHMIDT DECOMPOSITION AND PURIFICATION

Density operators and partial trace:

→ Useful for **studying composite quantum systems!**

Two new useful tools:

- ▶ Schmidt decomposition,
- ▶ Purification.

Theorem: Schmidt decomposition (that we admit)

For any (pure) $|\psi\rangle \in A \otimes B$, there exists

- a **unique integer d** ,
- an orthonormal set $|a_1\rangle, \dots, |a_d\rangle \in A$,
- an orthonormal set $|b_1\rangle, \dots, |b_d\rangle \in B$,
- $\lambda_1, \dots, \lambda_d > 0$

such that

$$|\psi\rangle = \sum_{i=1}^d \lambda_i |a_i\rangle |b_i\rangle$$

First Consequence:

Given (pure) $|\psi\rangle \in A \otimes B$, then

$$\rho^A = \text{tr}_B(|\psi\rangle\langle\psi|) = \sum_{i=1}^d \lambda_i^2 |a_i\rangle\langle a_i| \quad \text{and} \quad \rho^B = \text{tr}_A(|\psi\rangle\langle\psi|) = \sum_{i=1}^d \lambda_i^2 |b_i\rangle\langle b_i|$$

Therefore:

ρ^A and ρ^B have the same eigenvalues: the λ_i^2 's and possibly 0!

Definition: Schmidt's number

Given (pure) $|\psi\rangle \in A \otimes B$ with Schmidt decomposition

$$|\psi\rangle = \sum_{i=1}^d \lambda_i |a_i\rangle |b_i\rangle$$

The integer d is called **Schmidt number**. This number does not depend on the decomposition and it depends only on $|\psi\rangle$.

Theorem: a useful characterization of entanglement

A pure state $|\psi\rangle \in A \otimes B$ is entangled if and only if its Schmidt's number is > 1 if and only if ρ_A and ρ_B are mixed states (where $\rho = |\psi\rangle\langle\psi|$)

→ Proof in exercise session!

Question:

Given a mixed state ρ of A : is it possible to introduce another system R and a pure state $|\psi\rangle \in A \otimes R$ such that

$$\rho = \text{tr}_R (|\psi\rangle\langle\psi|)$$

Yes!

Spectral decomposition in an orthonormal basis of ρ :

$$\rho = \sum_{i=1}^n \lambda_i |i\rangle\langle i| \quad (\text{the } \lambda_i\text{'s are } \geq 0)$$

It is enough (exercise!) to define $|\psi\rangle$ as:

$$|\psi\rangle = \sum_{i=1}^n \sqrt{\lambda_i} |i\rangle |i\rangle .$$

→ This process is known as **purification**!

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Relation between Schmidt decomposition and purification

Purifying a mixed state: define a pure state whose Schmidt basis is just the basis in which the mixed state is diagonal!

EXERCISE SESSION
