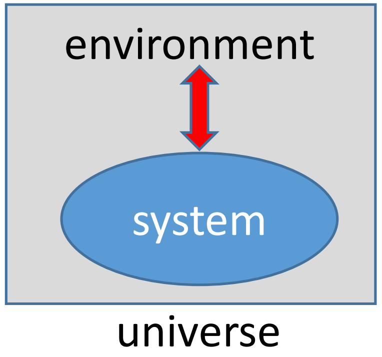
Ph/CS 219A
Quantum Computation

Lecture 2. Density Operators

This is the first of several lectures in which we will develop the theory of *open quantum systems*.



We say that a system is “open” if it can exchange energy and information with its environment.

This topic is worthy of study because all real quantum systems are open.

It is important for us because no quantum computer can be perfectly isolated from its environment.

Interactions with the environment drive decoherence, which can be controlled using quantum error correction (subject of winter term).

To study open systems, we consider a closed “universe” consisting of a system and its environment, where the environment is *unobserved.*

See Chapter 2 of the Lecture Notes.

Axioms for closed quantum systems

The axioms formulate mathematically how we model: (1) states, (2) observables, (3) measurements, (4) dynamics, (5) composition.

(1) A *state* is a *ray* in *Hilbert space.*

(Dirac notation) $|\psi\rangle \in \mathcal{H}, \quad \langle\phi|\psi\rangle = \langle\psi|\phi\rangle^* \in \mathbb{C}, \quad 1 = \quad \|\psi\| \quad = \quad \sqrt{\langle\psi|\psi\rangle}$

Identify $|\psi\rangle \equiv \lambda|\psi\rangle, \quad \lambda \in \mathbb{C}, \quad \lambda \neq 0$ E.g., $|\psi\rangle \equiv e^{i\alpha}|\psi\rangle, \quad \alpha \in \mathbb{R}$

But $a|\phi\rangle + b|\psi\rangle \not\equiv a|\phi\rangle + be^{i\alpha}|\psi\rangle$

Multiplying a state vector by an overall phase has no physical effect. But changing the phase in a superposition of two state vectors is physically meaningful.

"Dual vector" $\langle\phi|: \quad |\psi\rangle \to \langle\phi|\psi\rangle \in \mathbb{C}$ Maps vectors to complex numbers.

Axioms for closed quantum systems

(2) An observable is a self-adjoint operator on Hilbert space.

$$A: \quad \mathcal{H} \to \mathcal{H}, \quad A = A^\dagger, \quad \langle \phi | A | \psi \rangle = \langle A^\dagger \phi | \psi \rangle$$

Self-adjoint operators can be diagonalized:

$$A = \sum_n a_n E_n, \quad a_n \in \mathbb{R}, \quad E_n E_m = \delta_{nm} E_m, \quad E_n = E_n^\dagger$$

a_n is an eigenvalue of A, E_n is the corresponding orthogonal projector

(3) Probabilities of measurement outcomes are determined by the "Born rule":

$$\text{Prob}(a_n) = \quad \| E_n | \psi \rangle \|^2 \quad = \quad \langle \psi | E_n | \psi \rangle$$

Post-measurement state: $\quad | \psi \rangle \to \dfrac{E_n | \psi \rangle}{\| E_n | \psi \rangle \|}$

If we measure again right away we get the same outcome a second time.

Expectation value of the measurement outcome: $\quad \langle A \rangle = \sum_n a_n \text{Prob}(a_n) = \langle \psi | A | \psi \rangle$

Axioms for closed quantum systems

(4) Time evolution is determined by the Schroedinger equation: $\frac{d}{dt}|\psi(t)\rangle = -iH(t)|\psi(t)\rangle$

The Hamiltonian *H(t)* is a self-adjoint operator, which might depend on time.

The evolution proceeds via a sequence of infinitesimal unitary operators:

$$\psi(t+dt)\rangle = (I - iH(t)dt)|\psi(t)\rangle = e^{-iH(t)dt}|\psi(t)\rangle = U(t+dt,t)|\psi(t)\rangle$$

(5) The Hilbert space of composite system AB is the tensor product of A and B: $\mathcal{H}_{AB} = \mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}$

dimension $d_A d_B$, orthonormal basis $\{|i\rangle_A \otimes |b\rangle_B\}$

These axioms make a distinction between *evolution*, which is deterministic, and *measurement*, which is probabilistic.

Qubit

$$\dim(\mathcal{H}) = 2, \quad \mathcal{H} = \text{span}\{|0\rangle, |1\rangle\}$$

Another popular notation: $\mathcal{H} = \text{span}\{|\uparrow\rangle, |\downarrow\rangle\}$

Basis for linear operators:
("Pauli operators")

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Also known as $\{I, X, Y, Z\}$

$|\psi\rangle = a|0\rangle + b|1\rangle$ Measure $\sigma_3 \to \text{Prob}(|0\rangle) = |a|^2, \quad \text{Prob}(|1\rangle) = |b|^2, \quad |a|^2 + |b|^2 = 1$

Is a qubit any different than a flipped coin which comes up either heads or tails? Yes, because while there is only one way to look at a bit there are many different ways to look at a qubit!

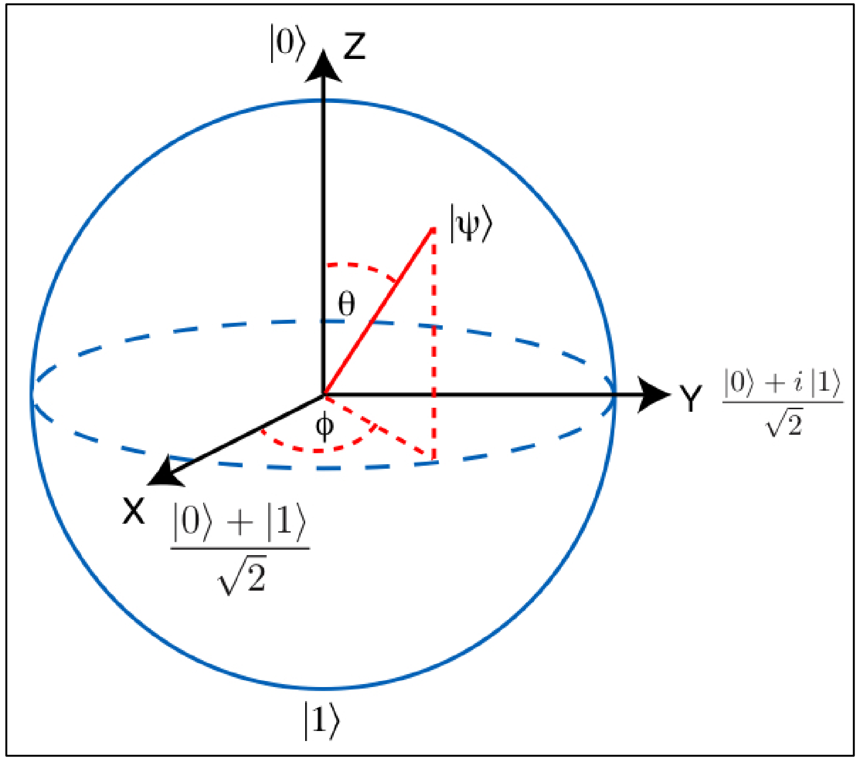
Qubit

$$|\psi(\theta,\phi)\rangle = e^{-i\phi/2}\cos(\theta/2)\,|0\rangle + e^{i\phi/2}\sin(\theta/2)\,|1\rangle$$

$$\theta \in [0,\pi], \quad \phi \in [0,2\pi)$$

$$\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

$$\hat{n}\cdot\vec{\sigma} = n_1\sigma_1 + n_2\sigma_2 + n_3\sigma_3 \rightarrow \hat{n}\cdot\vec{\sigma}\,|\psi(\theta,\phi)\rangle = |\psi(\theta,\phi)\rangle$$



Although a measurement "along the *z* axis" on the *Bloch sphere* does not yield a definite outcome, a measurement along a different appropriately chosen axis *does* yield a definite outcome.

Given a single copy of the state of a qubit, with no *a priori* knowledge about the state, we cannot determine θ and ϕ unambiguously. But given many identically prepared copies, we *can*.

$$\langle\sigma_1\rangle = \sin\theta\cos\phi, \quad \langle\sigma_2\rangle = \sin\theta\sin\phi, \quad \langle\sigma_3\rangle = \cos\theta$$

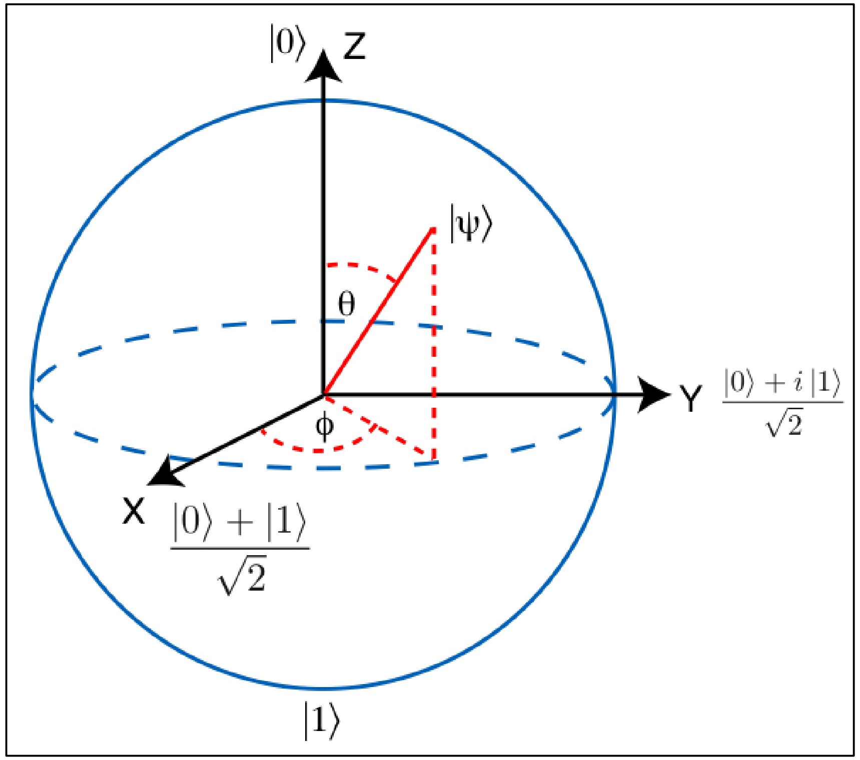
Measure enough copies to determine the expectation value of all three observables with a small error.

Quantum "Interference"

$$|\psi(\theta,\phi)\rangle = e^{-i\phi/2}\cos(\theta/2)\,|\uparrow\rangle_z + e^{i\phi/2}\sin(\theta/2)\,|\downarrow\rangle_z$$

$$\theta\in[0,\pi],\quad \phi\in[0,2\pi)$$

$$\langle\sigma_1\rangle = \sin\theta\cos\phi,\quad \langle\sigma_2\rangle = \sin\theta\sin\phi,\quad \langle\sigma_3\rangle = \cos\theta$$



Example: In the state $|\uparrow\rangle_z$, $\langle\sigma_3\rangle = 1$, in the state $|\downarrow\rangle_z$, $\langle\sigma_3\rangle = -1$
Coherently superpose these states:

$$\boxed{|\uparrow\rangle_x = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_z + |\downarrow\rangle_z\right),\quad \langle\sigma_1\rangle = 1}\qquad \boxed{|\downarrow\rangle_x = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_z - |\downarrow\rangle_z\right),\quad \langle\sigma_1\rangle = -1}$$

If we measure either of these *x* eigenstates in the *z* eigenstate basis: $\mathrm{Prob}(|\uparrow\rangle_z) = \frac{1}{2} = \mathrm{Prob}(|\downarrow\rangle_z)$

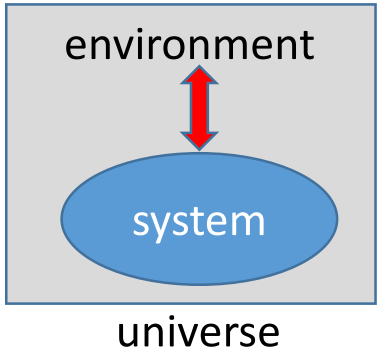
And if we measure either *z* eigenstate in the *x* eigenstate basis: $\mathrm{Prob}(|\uparrow\rangle_x) = \frac{1}{2} = \mathrm{Prob}(|\downarrow\rangle_x)$

The relative phase really matters! If we naively think of a superposition of eigenstates as a ensemble of possible states, each occurring with some probability, then we would conclude that in the state

$$\boxed{|\uparrow\rangle_z = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_x + |\downarrow\rangle_x\right)}$$

spin up and spin down along the z axis are equally probably. That's wrong --- it's always spin up. Probabilities can add in unexpected ways! Amplitudes can interfere constructively or destructively.

Open quantum systems



We have formulated the quantum rules for a closed quantum system. But we want to consider now the corresponding rules for an open quantum system --- one that interacts with its environment, where the environment is unobserved. In that case the rules are different.

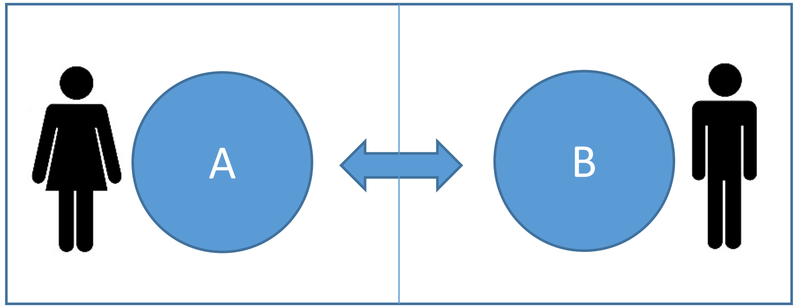
States are *not* rays in Hilbert space.
Measurements are *not* orthogonal projections.
Evolution is *not* unitary.

What are the new rules?

Recall the 5th axiom: a composite system AB is a tensor product of two Hilbert spaces, the A space and the B space.

Suppose we don't have access to B; we can observe only A. **Example**:

$$|\psi\rangle_{AB} = a\,|0\rangle_A \otimes |0\rangle_B + b\,|1\rangle_A \otimes |1\rangle_B = a\,|00\rangle + b\,|11\rangle$$

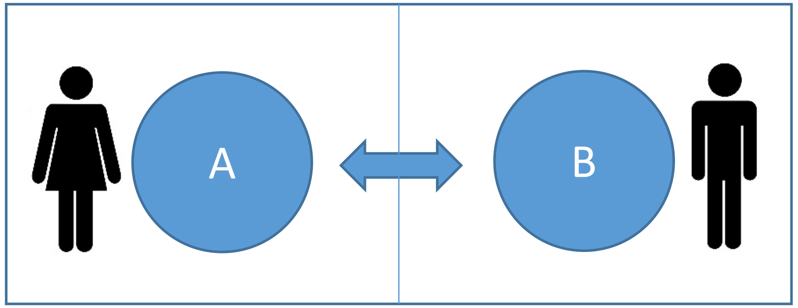


What if system B were measured in the *z* basis. That is, the measured observable is $I_A \otimes Z_B$. According to our measurement axiom, …

$$|0\rangle_A \otimes |0\rangle_B, \quad \text{Prob} = |a|^2,$$
$$|1\rangle_A \otimes |1\rangle_B, \quad \text{Prob} = |b|^2 .$$

The post-measurement state is a correlated state of A and B. If we observe only A, then $\text{Prob}(|0\rangle_A) = |a|^2, \quad \text{Prob}(|1\rangle_A) = |b|^2 .$

Open quantum systems



Consider a general Hermitian operator measured by A: $A = M_A \otimes I_B$

$$ {}_{AB}\langle \psi | M_A \otimes I_B | \psi \rangle_{AB} = \left(a^* \langle 00 | + b^* \langle 11 | \right) M_A \otimes I_B \left(a | 00 \rangle + b | 11 \rangle \right) = | a |^2 \langle 0 | M_A | 0 \rangle + | b |^2 \langle 1 | M_A | 1 \rangle $$

(because $|0\rangle$ and $|1\rangle$ are orthogonal on states of B). We may write.

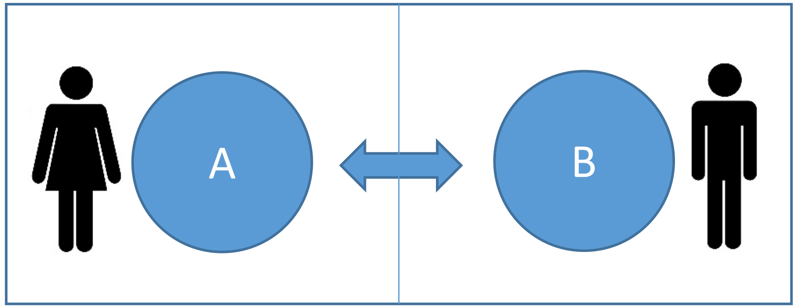
$$ {}_{AB}\langle \psi | M_A \otimes I_B | \psi \rangle_{AB} = \mathrm{tr}\left(M_A \rho_A \right), \quad \text{where} \quad \rho_A = | a |^2 | 0 \rangle\langle 0 | + | b |^2 | 1 \rangle\langle 1 | . $$

The operator ρ_A is called the "density operator" (or "density matrix") of system A.

The density operator has a natural "ensemble interpretation." We can imagine that Bob measured B in the z basis (whether he really did the measurement or not). In doing so, he prepared either $|0\rangle$ with probability $|a|^2$ or $|1\rangle$ with probability $|b|^2$.

No matter what Alice measures on system A, she can't tell the difference between measuring in the joint state $|\psi\rangle_{AB}$ of the composite system AB, and measuring in the corresponding ensemble of possible states for system A alone. The density operator encodes the probability distribution of outcomes for any conceivable measurement Alice might perform on A. In this sense, it provides a complete physical description of system A.

Open quantum systems



Consider a general Hermitian operator measured by A: $M_A \otimes I_B$

$$ {}_{AB}\langle \psi | M_A \otimes I_B | \psi \rangle_{AB} = \left(a^* \langle 00| + b^* \langle 11| \right) M_A \otimes I_B \left(a|00\rangle + b|11\rangle \right) = |a|^2 \langle 0|M_A|0\rangle + |b|^2 \langle 1|M_A|1\rangle $$

(because $|0\rangle$ and $|1\rangle$ are orthogonal on states of B). We may write.

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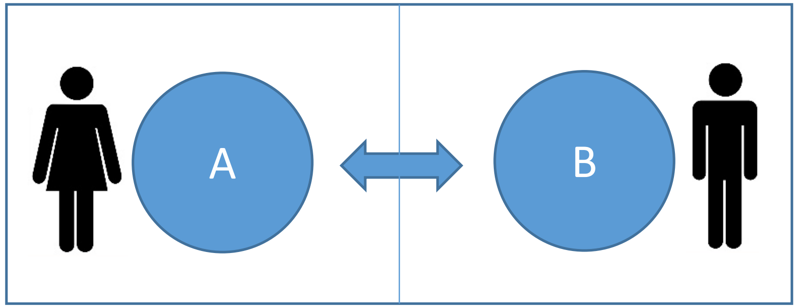
Example: $|\psi\rangle_{AB} = \frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle \right) \quad \rightarrow \quad \rho_A = \frac{1}{2}\left(|0\rangle\langle 0| + |1\rangle\langle 1| \right) = \frac{1}{2} I$

Then: $\mathrm{tr}\left(\vec{\sigma} \cdot \hat{n} \right) \rho_A = 0$ Along any axis, “spin up” and “spin down” occur with equal probability (=1/2).

Open quantum systems



Consider a general Hermitian operator measured by A: $A = M_A \otimes I_B$

Now, a more general state of AB: $|\psi\rangle_{AB} = \sum_{i,\mu} a_{i\mu} |i\rangle_A \otimes |\mu\rangle_B, \quad \sum_{i,\mu} |a_{i\mu}|^2 = 1$

$$ {}_{AB}\langle\psi| M_A \otimes I_B |\psi\rangle_{AB} = \sum_{j,\nu} a^*_{j\nu} \left({}_A\langle j| \otimes {}_B\langle \nu| \right) \left(M_A \otimes I_B \right) \sum_{i,\mu} a_{i\mu} \left(|i\rangle_A \otimes |\mu\rangle_B \right) = \sum_{i,j,\mu} a^*_{j\mu} a_{i\mu} \langle j| M_A |i\rangle $$

Write this as $\quad {}_{AB}\langle\psi| M_A \otimes I_B |\psi\rangle_{AB} = \mathrm{tr}\left(\rho_A M_A\right), \quad$ where $\quad \rho_A = \sum_{i,j,\mu} a^*_{j\mu} a_{i\mu} |i\rangle\langle j| \equiv \mathrm{tr}_B\left(|\psi\rangle\langle\psi|\right)$

The density operator of A is obtained by taking the "partial trace" over B of the projector $\left(|\psi\rangle\langle\psi|\right)_{AB}$

Think of a "dual vector"
for B as a map from AB to A.

$$ {}_B\langle\mu|: \quad \mathcal{H}_{AB} \to \mathcal{H}_A, \quad |\mu\rangle_B: \quad \mathcal{H}^*_{AB} \to \mathcal{H}^*_A $$

$$ {}_B\langle\mu|i,\nu\rangle_{AB} = \delta_{\mu\nu} |i\rangle_A, \quad {}_{AB}\langle i,\nu|\mu\rangle_B = \delta_{\mu\nu\, A}\langle i| $$

In general:

$$ \mathrm{tr}_B\left(M_{AB}\right) = \sum_\mu {}_B\langle\mu| M_{AB} |\mu\rangle_B $$

In particular:

$$ \rho_A = \sum_\mu {}_B\langle\mu|\psi\rangle\langle\psi|\mu\rangle_B $$

We can evaluate the partial trace in any basis we like.

Properties of the density operator

$$\rho_A = \sum_{i,j,\mu} a^*_{i\mu} a_{j\mu} |i\rangle\langle j| \equiv \mathrm{tr}_B\left(|\psi\rangle\langle\psi|\right), \quad \text{where} \quad |\psi\rangle_{AB} = \sum a_{i\mu} |i,\mu\rangle_{AB}$$

The density operator is Hermitian. $\rho = \rho^\dagger$

The density operator is nonnegative. $\langle\phi|\rho|\phi\rangle = \sum_{i,j,\mu} a^*_{j\mu} a_{i\mu} \langle\phi|i\rangle\langle j|\phi\rangle = \sum_\mu \left|\sum_i a_{i\mu}\langle\phi|i\rangle\right|^2 \geq 0$

The density operator has unit trace. $\mathrm{tr}\rho = \sum |a_{i\mu}|^2 = \| \, |\psi\rangle_{AB} \|^2 = 1$

Hence there is an orthonormal basis in which the density operator is diagonal. The eigenvalues are nonnegative real numbers which sum to one.

$$\rho = \sum_a p_a |a\rangle\langle a|, \quad p_a \geq 0, \quad \sum_a p_a = 1$$

In the ensemble interpretation, the eigenvalue is the probability that the corresponding basis state has been prepared in system A.

If there is just one nonzero eigenvalue, we say the state of A is “pure”. Otherwise it is “mixed”.

Schmidt decomposition of a bipartite pure state

Using the basis in which the density operator of A is diagonal, we can put the bipartite pure state in a standard form.

$$|\psi\rangle_{AB} = \sum a_{i\mu} |i\rangle_A \otimes |\mu\rangle_B, \quad \text{and suppose} \quad \rho_A = \sum_i p_i |i\rangle\langle i|$$

Let's write: $|\psi\rangle_{AB} = \sum |i\rangle_A \otimes |\tilde{i}\rangle_B$, where $|\tilde{i}\rangle = \sum_\mu a_{i\mu} |\mu\rangle_B$ (not necessarily orthogonal or normalized)

Then $\rho_A = \sum_i p_i |i\rangle\langle i| = \sum_{i,j} \left(|i\rangle\langle j|\right)_A \mathrm{tr}_B\left(|\tilde{i}\rangle\langle\tilde{j}|\right) = \sum_{i,j} \left(|i\rangle\langle j|\right)_A \langle\tilde{j}|\tilde{i}\rangle$

Hence $\langle\tilde{j}|\tilde{i}\rangle = \delta_{ij} p_i \quad \rightarrow \quad |i'\rangle_B = \dfrac{1}{\sqrt{p_i}} |\tilde{i}\rangle_B \quad (p_i > 0)$ are orthonormal vectors

and $|\psi\rangle_{AB} = \sum_i \sqrt{p_i}\, |i\rangle_A \otimes |i'\rangle_B$

This is the *Schmidt decomposition* of the bipartite state. The orthonormal bases are called *Schmidt bases* and the coefficients are called *Schmidt coefficients*.

Here we have used the freedom to perform independent unitary changes of basis in both system A and system B to do a singular value decomposition of the matrix *a*, and the Schmidt coefficients are the singular values of *a*.

Schmidt decomposition of a bipartite pure state

$$|\psi\rangle_{AB} = \sum_i \sqrt{p_i}\,|i\rangle_A \otimes |i'\rangle_B \quad \text{where} \quad \{|i\rangle_A\} \quad \text{and} \quad \{|i'\rangle_B\} \quad \text{are orthonormal bases.}$$

We can also do the partial trace over A to find the density operator for B: $\mathrm{tr}_A\left(|\psi\rangle\langle\psi|\right) = \sum_i p_i\,|i'\rangle\langle i'|$

We see that the density operators for A and B have the same nonzero eigenvalues. The two subsystems do not necessarily have the same dimension, so the number of zero eigenvalues could be different.

The number of nonzero terms in the Schmidt decomposition is called the *Schmidt rank*. This is the same as the rank (number of nonzero eigenvalues) for the density operators of A and B.

If the Schmidt rank of AB is one, the state is a *product state*. Then the “marginal state” of A or B is a pure state.

$$|\psi\rangle_{AB} = |\phi\rangle_A \otimes |\chi\rangle_B$$

If the Schmidt rank is greater than one, then we say that the state of AB is *entangled*, or *nonseparable*.

It is not possible to increase the Schmidt rank by sending classical messages between A and B, or by performing local operations (unitary transformations or measurements acting on either A or B). The only way to create entanglement of A and B is with an operation that acts jointly on A and B, or by sending quantum states between A and B.

Faster than light?

Consider $$|\psi\rangle_{AB} = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_z \otimes |\uparrow\rangle_z + |\downarrow\rangle_z \otimes |\downarrow\rangle_z\right) = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_x \otimes |\uparrow\rangle_x + |\downarrow\rangle_x \otimes |\downarrow\rangle_x\right)$$

In this case the two eigenvalues of the density operator are degenerate: $$\rho_A = \frac{1}{2} I_A$$

Therefore (in this case) the Schmidt basis is ambiguous; the bipartite state can be expressed in Schmidt form in more than one way (in fact, infinitely many ways).

Alice and Bob want to exploit their shared entanglement for communication. Alice could measure in the *z* basis, finding a uniformly random outcome. If Bob also measures in that basis, he finds the same random outcome. So Alice and Bob acquire correlated random bits. **But this conveys no information from one party to another**.

They try a different method. To send 0, Alice measures her qubit in the *z* basis; to send 1, she measures her qubit in the x basis. So she prepares for Bob a uniform mixture of spin up and down along the *z* axis in the first case, a uniform mixture of spin up and down along the x axis in the second case. **This doesn't work either. Bob has the same density operator in either case, and no measurement on his system can tell the difference between the two cases.**

When Alice and Bob share an entangled state, their two qubits are correlated. This is different than a classical correlation, in that the correlation occurs in more than one measurement basis. But the correlation cannot be used for instantaneous communication!

“Quantum eraser”

Consider $$|\psi\rangle_{AB} = \frac{1}{\sqrt{2}}(|\uparrow\rangle_z \otimes |\uparrow\rangle_z + |\downarrow\rangle_z \otimes |\downarrow\rangle_z) = \frac{1}{\sqrt{2}}(|\uparrow\rangle_x \otimes |\uparrow\rangle_x + |\downarrow\rangle_x \otimes |\downarrow\rangle_x)$$

Alice could measure her qubit in the *z* or *x* basis, and tell Bob the basis and outcome before he measures his qubit. Then he would have a known *z* eigenstate or a known *x* eigenstate. He could update his description of the qubit using this knowledge, recovering an updated pure state. But he needed a message from Alice to perform the update.

An *incoherent* mixture of spin up and down along the *z* axis is different than a *coherent* superposition of spin up and down along the *z* axis. In the latter case, but not the former, relative phases matter.

A coherent superposition of spin up and down along the *z* axis can behave like a spin pointing along the *x* axis only if **no one could possibly know** whether the spin points up of down along the *z* axis.

That’s not the situation when A and B are entangled. The two spins are correlated, so for example spin A encodes “which-way” information about spin B. I could in principle find our whether spin A points up or down along the *z* axis by measuring spin B along the *z* axis.

But **it is possible to erase the which-way information about A that is encoded in B**. For example, suppose Bob measures his spin along the *x* axis, and obtains a definite outcome, which he can report to Alice. When Alice receives this information from Bob, she has a pure state, a coherent superposition of spin up and down along the *z* axis. This is possible, because the information about whether the spin points up or down along the z axis has been permanently erased!