Lecture 3: Basic Principles in Quantum Mechanics

The Postulates, Density Matrices, and Entanglement

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Lecture Overview

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Postulate 1: State Space

- **Axiom**: Every isolated physical system is associated with a Hilbert space $\mathscr{H}$, called the *state space* of the system.
  - ◇ The system is completely described by its **state vector**: a unit vector $|\psi\rangle \in \mathscr{H}$.
  - ◇ **Normalization:** $\langle\psi|\psi\rangle = 1$.
  - ◇ **Dimension:** for n qubits, $\dim \mathscr{H} = 2^n$.
  - ◇ **Global phase:** $|\psi\rangle$ and $e^{i\theta} |\psi\rangle$ describe the same physical state.
- **Remark:** Postulate 1 is purely kinematic — it tells us *what* the state is, not how it changes. The next postulate governs dynamics.

Postulate 2: Evolution

- **Axiom**: The evolution of a *closed* quantum system is described by a **unitary transformation**.
  - ◇ The state $|\psi\rangle$ at time t_1 evolves to $|\psi'\rangle = U|\psi\rangle$ at time t_2, where $U^\dagger U = I$.
- In continuous time, evolution is governed by the **Schrödinger equation**:

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle,$$

  where H is the **Hamiltonian** (energy operator) of the system.
- For a *time-independent* Hamiltonian, the formal solution is:

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle, \qquad U = e^{-iHt/\hbar}.$$

  - ◇ Since H is Hermitian, $U = e^{-iHt/\hbar}$ is automatically unitary. (Verify!)

Why Must Evolution Be Unitary?

Unitarity is not an arbitrary choice — it is forced by two physical requirements.

- **Preservation of normalization:** a state must remain a valid state (total probability $= 1$):

$$\| U |\psi\rangle \|^2 = \langle\psi| U^\dagger U |\psi\rangle = \langle\psi|\psi\rangle = 1. \checkmark$$

- **Preservation of inner products (reversibility):** for any two states $|\psi\rangle$, $|\phi\rangle$:

$$(U|\psi\rangle)^\dagger (U|\phi\rangle) = \langle\psi| U^\dagger U |\phi\rangle = \langle\psi|\phi\rangle .$$

  - This guarantees that transition probabilities are preserved and the evolution is reversible ($U^{-1} = U^\dagger$ always exists).

Consequence: The No-Cloning Theorem

Claim: no unitary machine can copy an unknown quantum state.

- **Suppose** a unitary U and a fixed blank state $|s\rangle$ exist such that, for *any* input $|\psi\rangle$:
$$U(|\psi\rangle\,|s\rangle) = |\psi\rangle\,|\psi\rangle\,.$$
- Apply this to two different states $|\psi\rangle$ and $|\phi\rangle$:
$$U(|\psi\rangle\,|s\rangle) = |\psi\rangle\,|\psi\rangle\,, \qquad U(|\phi\rangle\,|s\rangle) = |\phi\rangle\,|\phi\rangle\,.$$
- Take the inner product of the two resulting states, using unitarity ($U^\dagger U = I$) and $\langle s|s\rangle = 1$:
$$\langle\psi|\phi\rangle = \big(\langle\psi|\phi\rangle\big)^2.$$
- This is a quadratic equation $x = x^2$, i.e. $x(x-1) = 0$, so $\langle\psi|\phi\rangle \in \{0, 1\}$.

Conclusion: a single machine can only "clone" states that are identical or perfectly orthogonal — a *general-purpose* cloning machine is impossible.

The Copenhagen Interpretation

Quantum mechanics is mathematically precise, but its *physical meaning* is debated.

- There are many ways to interpret quantum mechanics — different ways of relating the wave function to experimental results and to our fundamental picture of nature.
  - Some interpretations even conflict with each other.
- The **Copenhagen interpretation** (Bohr, Heisenberg) is the most widely taught:
  - A system does *not* have definite properties until it is measured.
  - The wave function $|\psi\rangle$ encodes *probabilities*, not hidden classical values.
  - Measurement causes an instantaneous **collapse** of the wave function.
- These principles were revolutionary: they imply nature is fundamentally probabilistic, not merely uncertain due to our ignorance.

Postulate 3: Quantum Measurement

- **Axiom**: Quantum measurements are described by a collection $\{M_m\}$ of **measurement operators** acting on the state space, satisfying the **completeness relation**:

$$\sum_m M_m^\dagger M_m = I.$$

- If the system is in state $|\psi\rangle$ just before measurement:
  - ◇ The **probability** of obtaining outcome m is

$$p(m) = \langle\psi| M_m^\dagger M_m |\psi\rangle \geq 0.$$

  - ◇ The **post-measurement state** (given outcome m) is

$$|\psi_m\rangle = \frac{M_m |\psi\rangle}{\sqrt{p(m)}}.$$

- The completeness condition guarantees $\sum_m p(m) = 1$ for *any* $|\psi\rangle$, as required of a valid probability distribution.

Projective Measurements

The most important special case of Postulate 3 uses operators $M_m = P_m$ that are **orthogonal projectors**:

$$\begin{aligned} P_m &= P_m^\dagger \quad \text{(Hermitian)}, \\ P_m^2 &= P_m \quad \text{(idempotent)}, \\ P_m P_n &= \delta_{mn} P_m \quad \text{(orthogonal)}. \end{aligned}$$

- **Repeatability:** a second measurement immediately gives the same outcome:
$$P_m\left(\frac{P_m|\psi\rangle}{\sqrt{p(m)}}\right) = \frac{P_m|\psi\rangle}{\sqrt{p(m)}}. \checkmark$$
- **Why projective measurements matter:**
  - ◇ They are directly tied to *Hermitian observables* (next slide).
  - ◇ They model the "ideal" measurement, with no information loss beyond collapse.

Observables and Expectation Values

- Every measurable physical quantity is called an **observable** and is represented by a **Hermitian operator** A on $\mathscr{H}$.
  - By the spectral theorem (Lecture 2), $A = \sum_m \lambda_m P_m$, where $\lambda_m \in \mathbb{R}$ are the eigenvalues and P_m the corresponding orthogonal eigenprojectors.
- **Measuring** the observable A on state $|\psi\rangle$:
  - Yields one eigenvalue λ_m, with probability $p(m) = \langle\psi| P_m |\psi\rangle$.
  - The state collapses into the eigenspace of λ_m.
- **Expectation value:** the average outcome over many repeated measurements is denoted $\langle A \rangle$ and computed as:

$$\langle A \rangle := \sum_m \lambda_m \, p(m) = \langle\psi| A |\psi\rangle \, .$$

  - The second equality is a convenient shortcut — it avoids computing the full spectral decomposition of A.

Positive Operator-Valued Measures (POVMs)

For some experiments we only care about *measurement statistics*, not the post-measurement state.

- Define **POVM elements** $E_m := M_m^\dagger M_m$ for each outcome m. The set $\{E_m\}$ satisfies:
  - **Positivity:** $E_m \geq 0 \quad$ (since $\langle\psi| E_m |\psi\rangle = \| M_m |\psi\rangle \|^2 \geq 0$).
  - **Completeness:** $\sum_m E_m = I$.
- The probability of outcome m is $p(m) = \langle\psi| E_m |\psi\rangle$.
- **Why POVMs matter:**
  - *Non-orthogonal state discrimination:* projective measurements cannot perfectly distinguish non-orthogonal states; POVMs allow *Unambiguous State Discrimination* — never wrong, but sometimes inconclusive.
  - *More outcomes than dimensions:* a POVM can have $n > d$ elements for a d-dimensional system.
  - *Noisy detectors:* POVM elements absorb detector inefficiency directly into the operator.

Complementarity and the Uncertainty Principle

A consequence of wave-particle duality is that certain pairs of observables are **mutually exclusive** in precision.

- **Mathematical analogue:** the Fourier transform

$$\hat{f}(\xi) = \int_{-\infty}^{\infty} f(x)\, e^{-2\pi i x \xi}\, dx$$

  shows that a function sharply localized in x must be broadly spread in ξ, and vice versa.
- **Physical version (Heisenberg):** for position $\hat{x}$ and momentum $\hat{p}$, $\Delta x \cdot \Delta p \geq \hbar/2$, where Δx, Δp are standard deviations over repeated measurements.
- **General form:** for any two observables A and B,

$$\Delta A \cdot \Delta B \ \geq \ \frac{1}{2}\left|\langle [A,B] \rangle\right|,$$

  where $[A,B] := AB - BA$ is the **commutator**. We derive this next.

Variance of an Observable

For an observable M in state $|\psi\rangle$, define the **centered operator** $\tilde{M} := M - \langle M \rangle I$, where $\langle M \rangle = \langle\psi| M |\psi\rangle$ is the expectation value defined earlier.

- The **variance** of M is

$$(\Delta M)^2 := \langle \tilde{M}^2 \rangle = \langle\psi| M^2 |\psi\rangle - \big(\langle\psi| M |\psi\rangle\big)^2.$$

- $\Delta M = \sqrt{(\Delta M)^2}$ is the **standard deviation** — the typical spread of measurement outcomes around the mean $\langle M \rangle$.
- We now derive the uncertainty relation between ΔA and ΔB for two observables A, B.

Derivation of the Uncertainty Principle

Let $\tilde{A} = A - \langle A \rangle I$ and $\tilde{B} = B - \langle B \rangle I$ as above.

1. **Cauchy-Schwarz inequality:**

$$(\Delta A)^2 (\Delta B)^2 = \langle \tilde{A}^2 \rangle \langle \tilde{B}^2 \rangle \;\geq\; \left| \langle \tilde{A}\tilde{B} \rangle \right|^2 .$$

2. **Decompose** $\tilde{A}\tilde{B}$ into Hermitian and anti-Hermitian parts:

$$\tilde{A}\tilde{B} = \underbrace{\frac{\tilde{A}\tilde{B} + \tilde{B}\tilde{A}}{2}}_{\text{Hermitian: real expectation}} + \underbrace{\frac{\tilde{A}\tilde{B} - \tilde{B}\tilde{A}}{2}}_{\text{anti-Hermitian: imaginary expectation}} .$$

3. Writing $\langle \tilde{A}\tilde{B} \rangle = x + iy$ with $x, y \in \mathbb{R}$, since $|x + iy|^2 \geq y^2$:

$$(\Delta A)^2 (\Delta B)^2 \;\geq\; \left| \frac{\langle [\tilde{A}, \tilde{B}] \rangle}{2} \right|^2 = \frac{|\langle [A, B] \rangle|^2}{4} .$$

Taking square roots: $\quad \Delta A \cdot \Delta B \;\geq\; \dfrac{1}{2} \left| \langle [A, B] \rangle \right| .$

Pure vs. Mixed States

So far we have described systems by state vectors $|\psi\rangle$. But two situations demand a more general description:

1. **Classical ignorance:** we prepare the system in state $|\psi_i\rangle$ with probability μ_i but do not know which one was actually prepared.
2. **Subsystem of an entangled pair:** (covered later) even with full knowledge of a composite pure state, a subsystem cannot in general be described by any state vector.

- A **pure state** is one we know exactly: $|\psi\rangle$.
  - ◇ It can be a superposition $|\Psi\rangle = \sum_i \alpha_i |\psi_i\rangle$, with $\sum_i |\alpha_i|^2 = 1$.
- A **mixed state** is a *statistical ensemble* $\{(\mu_i, |\psi_i\rangle)\}$: the system is in state $|\psi_i\rangle$ with probability μ_i, where $\sum_i \mu_i = 1$.

Superposition vs. Statistical Mixture

These two descriptions are *physically different* and must not be confused.

- **Example:** a 50/50 statistical mixture of $|0\rangle$ and $|1\rangle$ is *not* the same as the coherent superposition $\frac{|0\rangle+|1\rangle}{\sqrt{2}}$.
- **Superposition** is quantum "and-ness":
  - A specific, coherent state that is a linear combination of both.
  - Before measurement, the system possesses *interference terms*.
- **Statistical mixture** is classical "either-or" uncertainty:
  - Each individual system is in a definite (but unknown) pure state.
  - Measurement reveals a pre-existing reality; there is no coherence, no interference.

The next slide makes this comparison concrete using density matrices.

Density Matrices: Superposition vs. Mixture

	Superposition $\frac{\|0\rangle+\|1\rangle}{\sqrt{2}}$	**Mixture** $\{(\frac{1}{2}, \|0\rangle), (\frac{1}{2}, \|1\rangle)\}$
Density matrix	$\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$	$\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$
$\mathrm{Tr}(\rho^2)$	1 (pure)	$1/2 < 1$ (mixed)

- The off-diagonal entries (the $1/2$'s in the left matrix) are **coherences** — they encode interference and are the hallmark of a quantum superposition.
- The mixture has *zero* coherences: no interference, purely classical uncertainty about which basis state is present.
- (Density matrices are defined formally on the next slide; here we preview them to make the distinction concrete.)

The Density Operator: Definition

For a mixed state $\{(\mu_i, |\psi_i\rangle)\}$ (with $\mu_i \geq 0$, $\sum_i \mu_i = 1$), define the **density operator**:

$$\rho := \sum_i \mu_i \left|\psi_i\right\rangle \left\langle\psi_i\right| .$$

- **For a pure state** $|\psi\rangle$: $\rho = \left|\psi\right\rangle \left\langle\psi\right|$ (a rank-1 projector).
- ρ satisfies three characterizing properties:
  1. **Hermitian:** $\rho = \rho^\dagger$ (each $\left|\psi_i\right\rangle \left\langle\psi_i\right|$ is Hermitian).
  2. **Positive semi-definite:** $\left\langle\phi\right| \rho \left|\phi\right\rangle = \sum_i \mu_i \left|\langle\psi_i|\phi\rangle\right|^2 \geq 0$ for all $|\phi\rangle$.
  3. **Unit trace:** $\mathrm{Tr}(\rho) = \sum_i \mu_i \,\mathrm{Tr}\big(\left|\psi_i\right\rangle \left\langle\psi_i\right|\big) = \sum_i \mu_i = 1$.
- Conversely, *any* operator satisfying (1)–(3) is a valid density operator for some ensemble.

Density Operator: Worked Example

Example: the density operator of the pure state $|+\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}$ is

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

- This matches the left-hand entry of the comparison table on the previous slide.
- Notice the global phase of $|\psi\rangle$ disappears: $|\psi\rangle$ and $e^{i\theta}|\psi\rangle$ give the *identical* density matrix ρ, consistent with Postulate 1.

Expectation Values via the Density Operator

The density operator unifies expectation-value calculations for both pure and mixed states.

- For a mixed state $\rho = \sum_i \mu_i |\psi_i\rangle \langle\psi_i|$, the expectation value of observable A is:

$$\langle A\rangle = \sum_i \mu_i \langle\psi_i| A |\psi_i\rangle = \sum_i \mu_i \operatorname{Tr}\big(A |\psi_i\rangle \langle\psi_i|\big) = \operatorname{Tr}(A\rho).$$

  - ◇ The key step $\langle\psi| A |\psi\rangle = \operatorname{Tr}(A |\psi\rangle \langle\psi|)$ follows from the cyclic property of trace.

- **Measurement probability (POVM form):** $p(m) = \operatorname{Tr}(E_m\rho)$.
- **Unitary evolution** of the density operator:

$$\rho \longrightarrow U\rho U^\dagger.$$

Characterizing Purity

The eigenvalues of ρ reveal how "mixed" a state is. Write the spectral decomposition $\rho = \sum_i \lambda_i \left|u_i\right\rangle \left\langle u_i\right|$, where $\lambda_i \geq 0$ and $\sum_i \lambda_i = 1$.

- **Purity measure:** $\mathrm{Tr}(\rho^2) = \sum_i \lambda_i^2$.
  - ◇ **Pure state:** exactly one $\lambda_i = 1$, the rest 0 $\Rightarrow$ $\mathrm{Tr}(\rho^2) = 1$ and $\rho^2 = \rho$.
  - ◇ **Mixed state:** at least two nonzero λ_i. Since $0 < \lambda_i < 1 \Rightarrow \lambda_i^2 < \lambda_i$, we get $\mathrm{Tr}(\rho^2) < 1$.
- **Maximally mixed state** in dimension d: $\rho = I_d/d$, with all eigenvalues equal to $1/d$:

$$\mathrm{Tr}(\rho^2) = \frac{1}{d}.$$

- **Summary:** $\dfrac{1}{d} \leq \mathrm{Tr}(\rho^2) \leq 1$, with equality on the right iff ρ is pure.

Postulate 4: Composite Systems

- **Axiom**: The state space of a composite physical system is the **tensor product** of the component state spaces:

$$\mathscr{H}_{12} = \mathscr{H}_1 \otimes \mathscr{H}_2 = \text{span}\{|u_i\rangle \otimes |v_j\rangle \mid |u_i\rangle \in \mathscr{H}_1,\ |v_j\rangle \in \mathscr{H}_2\}.$$

- The inner product on $\mathscr{H}_{12}$ is defined on product vectors by

$$\langle u_1 \otimes v_1,\ u_2 \otimes v_2\rangle := \langle u_1, u_2\rangle_{\mathscr{H}_1} \cdot \langle v_1, v_2\rangle_{\mathscr{H}_2},$$

  and extended by linearity.

- If system 1 is in $|\psi\rangle$ and system 2 is in $|\phi\rangle$, the joint state is the **product state** $|\psi\rangle \otimes |\phi\rangle \equiv |\psi\phi\rangle$.
- **Crucially:** not every state in $\mathscr{H}_1 \otimes \mathscr{H}_2$ is a product state. States that cannot be written as $|\psi\rangle \otimes |\phi\rangle$ are **entangled** (next section).

Separability vs. Entanglement

- A pure state $|\Psi\rangle \in \mathscr{H}_1 \otimes \mathscr{H}_2$ is **separable** if it can be written as

$$|\Psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$$

  for some $|\psi_1\rangle \in \mathscr{H}_1$, $|\psi_2\rangle \in \mathscr{H}_2$. Otherwise it is **entangled**.
- Entanglement implies correlations that cannot be explained by any classical shared randomness.

Example: Is $|\Phi^+\rangle$ Separable?

Consider $|\Phi^+\rangle = \dfrac{|00\rangle + |11\rangle}{\sqrt{2}}$. Suppose it were separable:

$$|\Phi^+\rangle = (c_1 |0\rangle + c_2 |1\rangle) \otimes (d_1 |0\rangle + d_2 |1\rangle).$$

- Expanding the right-hand side:

$$c_1 d_1 |00\rangle + c_1 d_2 |01\rangle + c_2 d_1 |10\rangle + c_2 d_2 |11\rangle .$$

- Matching coefficients with $|\Phi^+\rangle = \frac{1}{\sqrt{2}} |00\rangle + 0 \cdot |01\rangle + 0 \cdot |10\rangle + \frac{1}{\sqrt{2}} |11\rangle$ requires:

$$c_1 d_2 = 0, \qquad c_2 d_1 = 0, \qquad c_1 d_1 = c_2 d_2 = \frac{1}{\sqrt{2}}.$$

- But $c_1 d_2 = 0$ forces $c_1 = 0$ or $d_2 = 0$ — either way, $c_1 d_1 = \frac{1}{\sqrt{2}} \neq 0$ or $c_2 d_2 = \frac{1}{\sqrt{2}} \neq 0$ becomes impossible. **Contradiction.**

Conclusion: $|\Phi^+\rangle$ is entangled.

The Bell States (EPR Pairs)

The four **Bell states** form an orthonormal basis for $\mathbb{C}^2 \otimes \mathbb{C}^2$ and are maximally entangled:

$$\left|\Phi^+\right\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}, \qquad \left|\Phi^-\right\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}},$$
$$\left|\Psi^+\right\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}, \qquad \left|\Psi^-\right\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}.$$

- **Orthonormality:** all four are mutually orthogonal and have norm 1. (Verify for one pair!)
- **"Perfectly defined, yet maximally random":** each is a pure global state, yet measuring qubit A alone gives a completely random outcome — and simultaneously determines qubit B, regardless of distance (made precise in the next section).
- **Applications:** quantum teleportation, superdense coding, quantum cryptography, quantum error correction.

The Partial Trace

Problem: if AB is in a joint state ρ^{AB}, how do we describe subsystem A alone?

- The answer is the **reduced density matrix** $\rho^A = \mathrm{Tr}_B(\rho^{AB})$, obtained by *tracing out* subsystem B.
- **Definition on product operators:**

$$\mathrm{Tr}_B\big(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|\big) := |a_1\rangle\langle a_2| \cdot \langle b_2|b_1\rangle\,.$$

  - ◇ $|a_1\rangle\langle a_2|$ remains as the operator on subsystem A.
  - ◇ $\langle b_2|b_1\rangle$ is a number coming from tracing over B.
- **Interpretation:** ρ^A captures everything that Alice (holding system A) can know, without any access to Bob's system B.

Example: Partial Trace of a Bell State

Consider the maximally entangled state $|\Phi^+\rangle = \dfrac{|00\rangle + |11\rangle}{\sqrt{2}}$.

- The joint density matrix is:

$$\rho^{AB} = \tfrac{1}{2}\big(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|\big).$$

- Tracing out B using the basis $\{|0\rangle_B, |1\rangle_B\}$, only terms with matching B-indices survive (since $\langle 1|0\rangle = \langle 0|1\rangle = 0$):

$$\rho^A = \tfrac{1}{2}\big(|0\rangle\langle 0| \underbrace{\langle 0|0\rangle}_{1} + |1\rangle\langle 1| \underbrace{\langle 1|1\rangle}_{1}\big) = \tfrac{1}{2}\big(|0\rangle\langle 0| + |1\rangle\langle 1|\big) = \frac{I}{2}.$$

Conclusion: the reduced state of A is the *maximally mixed state*. A pure global state can yield a maximally mixed local state — the defining signature of maximal entanglement.

Partial Trace: Matrix Block Formulation

For numerical computation, the partial trace has an elegant block-matrix form.

- Partition $X \in \mathbb{C}^{mn \times mn}$ as an $m \times m$ array of $n \times n$ blocks: $X = [H_{ij}]$.
- Define the two partial traces:

$$\mathrm{Tr}_A(X) := \sum_{i=1}^{m} H_{ii} \ \in \mathbb{C}^{n \times n}, \qquad \mathrm{Tr}_B(X) := [\mathrm{Tr}(H_{ij})] \ \in \mathbb{C}^{m \times m}.$$

- **Useful identities** (for $A \in \mathbb{C}^{m \times m}$, $B \in \mathbb{C}^{n \times n}$):

$$\mathrm{Tr}_A(A \otimes B) = \mathrm{Tr}(A)\, B, \qquad \mathrm{Tr}_B(A \otimes B) = \mathrm{Tr}(B)\, A.$$

Separability Test and Exercise

- **Separability test:** a matrix $X = A \otimes B$ must satisfy

$$\mathrm{Tr}(X)\, X = \mathrm{Tr}_B(X) \otimes \mathrm{Tr}_A(X).$$

- **Exercise:** Is the following matrix separable?

$$\frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

- *Hint:* compute $\mathrm{Tr}_A(X)$ and $\mathrm{Tr}_B(X)$ using the block formulas from the previous slide, then check the identity above.

Schmidt Decomposition

Theorem (Schmidt): for any pure state $|\psi\rangle \in \mathscr{H}_A \otimes \mathscr{H}_B$, there exist orthonormal sets $\{|u_i\rangle\} \subset \mathscr{H}_A$, $\{|v_i\rangle\} \subset \mathscr{H}_B$, and non-negative reals $\sqrt{\lambda_i}$ such that:

$$|\psi\rangle = \sum_{i=1}^{r} \sqrt{\lambda_i}\, |u_i\rangle |v_i\rangle\,, \qquad \sum_i \lambda_i = 1.$$

- The $\sqrt{\lambda_i}$ are the **Schmidt coefficients**; r is the **Schmidt rank**.
- **Proof idea:** write $|\psi\rangle = \sum_{ij} M_{ij} |i\rangle_A |j\rangle_B$ for some matrix M; apply the SVD $M = U\Sigma V^\dagger$. The Schmidt coefficients are the singular values, and $|u_i\rangle$, $|v_i\rangle$ the left/right singular vectors.
- **Entanglement criterion:** $|\psi\rangle$ is separable if and only if its Schmidt rank is 1.

Schmidt Coefficients and Reduced Density Matrices

The Schmidt decomposition directly determines the reduced density matrices:

$$\rho^A = \mathrm{Tr}_B\big(|\psi\rangle\langle\psi|\big) = \sum_i \lambda_i |u_i\rangle\langle u_i|,$$
$$\rho^B = \mathrm{Tr}_A\big(|\psi\rangle\langle\psi|\big) = \sum_i \lambda_i |v_i\rangle\langle v_i|.$$

- The Schmidt coefficients squared, λ_i, are precisely the *eigenvalues* of both ρ^A and ρ^B — the two reduced states share the same spectrum.
- This explains the Bell-state example: $|\Phi^+\rangle$ has Schmidt rank 2 with $\lambda_1 = \lambda_2 = \frac{1}{2}$, giving $\rho^A = \rho^B = I/2$ (maximally mixed), consistent with what we computed directly.

Purification

Problem: a mixed state ρ^A cannot be described by a single state vector. Can we always embed it as a pure state in a larger space?

- **Theorem:** for any density matrix ρ^A on $\mathscr{H}_A$, there exists a pure state $\left|\psi^{AR}\right\rangle \in \mathscr{H}_A \otimes \mathscr{H}_R$ (with reference system R) such that

$$\rho^A = \mathrm{Tr}_R\left(\left|\psi^{AR}\right\rangle \left\langle\psi^{AR}\right|\right).$$

- **Canonical construction:** use the spectral decomposition $\rho^A = \sum_i p_i \left|i\right\rangle_A \left\langle i\right|$, introduce an auxiliary system R with orthonormal basis $\{\left|i\right\rangle_R\}$, and set

$$\left|\psi^{AR}\right\rangle = \sum_i \sqrt{p_i}\, \left|i\right\rangle_A \otimes \left|i\right\rangle_R .$$

- **Physical meaning:** mixedness of ρ^A can always be interpreted as entanglement with an unobserved environment.

Verifying the Purification Construction

We check that tracing out R from $\left|\psi^{AR}\right\rangle$ recovers ρ^A.

- Form the density matrix of the purification:

$$\rho^{AR} = \left|\psi^{AR}\right\rangle \left\langle\psi^{AR}\right| = \sum_{i,j} \sqrt{p_i p_j} \; |i\rangle \langle j|_A \otimes |i\rangle \langle j|_R \, .$$

- Take the partial trace over R, using $\mathrm{Tr}\big(|i\rangle \langle j|_R\big) = \langle j|i\rangle = \delta_{ij}$:

$$\mathrm{Tr}_R(\rho^{AR}) = \sum_{i,j} \sqrt{p_i p_j} \; |i\rangle \langle j|_A \cdot \delta_{ij} = \sum_i p_i \, |i\rangle \langle i|_A = \rho^A . \checkmark$$

Non-Uniqueness of Purification

The purification $\left|\psi^{AR}\right\rangle$ is not unique — infinitely many pure states reduce to the same ρ^A.

- **Theorem:** any two purifications $\left|\psi^{AR}\right\rangle$ and $\left|\phi^{AR}\right\rangle$ of the same ρ^A are related by a **unitary** V_R acting *only* on the reference system R:

$$\left|\phi^{AR}\right\rangle = (I_A \otimes V_R)\left|\psi^{AR}\right\rangle.$$

- **Intuition:** from Alice's perspective (tracing out R), any local transformation Bob applies to R is invisible — all purifications describe the same physics on A.

Why Purification Matters

- **Practical implication:** one can always choose the most convenient purification for a proof or calculation, since all purifications are physically equivalent on the system of interest.
- Purification is used in the proofs of several central quantum information theorems:
  - The Holevo bound (limits on classical information extractable from quantum states).
  - Monotonicity of quantum entropy under partial trace.
  - The Stinespring dilation of quantum channels.
- It also gives the conceptual bridge to our final topic: general (non-unitary) evolution.

Quantum Channels and the Kraus Representation

When a quantum system interacts with its environment, the evolution is generally *not* unitary.

- **Setup:** system S and environment E begin in a product state $\rho^S \otimes |e_0\rangle\langle e_0|$ and undergo a joint unitary evolution U.
- Tracing out the environment gives the **Kraus representation** of the resulting channel:

$$\rho^S \longrightarrow \mathcal{E}(\rho^S) = \sum_k E_k \, \rho^S \, E_k^\dagger, \qquad E_k := \langle e_k| \, U \, |e_0\rangle \, ,$$

  where the **Kraus operators** E_k satisfy $\sum_k E_k^\dagger E_k = I$.
- **Special case:** ordinary unitary evolution corresponds to a single Kraus operator $E_1 = U$: $\mathcal{E}(\rho) = U\rho U^\dagger$.
- This is the most general physically allowed evolution of an open quantum system; quantum channels will be studied in depth in Lecture 11.

Summary of Lecture 3

- **Four Postulates:** (1) states are unit vectors in $\mathscr{H}$; (2) closed evolution is unitary; (3) measurements are described by $\{M_m\}$ with $\sum_m M_m^\dagger M_m = I$; (4) composite systems use tensor products.
- **No-Cloning Theorem:** unitarity forbids copying an unknown quantum state.
- **Observables and uncertainty:** Hermitian operators give real eigenvalues and expectation values $\langle A \rangle = \langle \psi | A | \psi \rangle$; non-commuting observables obey $\Delta A \, \Delta B \geq \frac{1}{2} |\langle [A, B] \rangle|$.
- **Density operator** ρ: Hermitian, PSD, unit trace; $\mathrm{Tr}(\rho^2) = 1$ iff pure.
- **Entanglement:** a pure composite state that is not a product state; Bell states are the prototypical maximally entangled states.
- **Partial trace** $\rho^A = \mathrm{Tr}_B(\rho^{AB})$ extracts the local state of a subsystem.
- **Schmidt decomposition** and **purification**: every entangled pure state factors via SVD; every mixed state arises as the reduced state of some larger pure state.

Looking Ahead: Lecture 4

With the postulates established, we move to the computational model. In Lecture 4 we will cover:

- **Single-qubit gates** as 2×2 unitary matrices: Pauli gates, Hadamard, phase gates.
- **Multi-qubit gates:** CNOT and the preparation of Bell states.
- **Quantum circuits:** the circuit model of quantum computation.
- **Universal gate sets** and the Solovay-Kitaev theorem.
- **Quantum protocols:** superdense coding and quantum teleportation.