EE641000 Quantum Information and Computation

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Unit Two – Principles of Quantum Mechanics
Postulates of Quantum Mechanics
Postulate 1 – States

Associated to an isolated physical system is a Hilbert space $\mathcal{H}$ (eg, a finite-dimensional complex inner product space). The system is completely described by its state, which is represented by a one-dimensional subspace of the Hilbert space $\mathcal{H}$.

- A one-dimensional subspace of $\mathcal{H}$ can be represented by a unit vector $|\psi\rangle$ in it.

- A state of the system can be represented by a unit vector $|\psi\rangle$ in the Hilbert space $\mathcal{H}$, where $|\psi\rangle$ is called a state vector.
  - This unit vector representation of a state is not unique since each of $|\psi\rangle$ and $e^{i\theta}|\psi\rangle$ spans the same one-dimensional subspace of $\mathcal{H}$. 

A quantum bit (qubit) is the state represented by unit vectors of a two-dimensional Hilbert space $\mathcal{H}$ associated with a physical system.

- $\{ |0\rangle, |1\rangle \}$ : an orthonormal basis of $\mathcal{H}$.
- $|\psi\rangle = a|0\rangle + b|1\rangle$ : a unit vector in $\mathcal{H}$ where $|a|^2 + |b|^2 = 1$.

- The unit vector $|\psi\rangle$ and each of $e^{i\theta}|\psi\rangle$ represent the same state of a qubit.
Postulate 2 - Time Evolution

The evolution of a closed quantum system is described by a unitary operator. That is, the state $|\psi\rangle$ of the system at time $t_1$ is related to the state $|\psi'\rangle$ of the system at time $t_2$ by a unitary operator $U$ which depends only on the times $t_1$ and $t_2$,\

$$|\psi'\rangle = U|\psi\rangle.$$
Postulate 2’ – Time Evolution Revisited

The time evolution of the state of a closed quantum system is described by the Schrödinger equation,

$$i\hbar \frac{d|\psi\rangle}{dt} = H|\psi\rangle.$$

where

- $\hbar$ : the Planck’s constant
- $H$ : a Hermitian operator known as the Hamiltonian of the closed system
Solution of Schrödinger Equation

\[ |\psi(t)\rangle = e^{-i \frac{H}{\hbar} (t - t_0)} |\psi(t_0)\rangle = U(t; t_0) |\psi(t_0)\rangle \]

- \( H \) : a Hermitian operator
- \( U(t; t_0) = e^{-i \frac{H}{\hbar} (t - t_0)} \) : a unitary operator for given \( t \) and \( t_0 \).
A quantum measurement is described by a collection \( \{M_m\} \) of
\textit{measurement operators}, acting on the Hilbert space associated to a
quantum system being measured and satisfying the \textit{completeness}
equation

\[
\sum_m M_m^{\dagger} M_m = I.
\]

\( m \) : the index which represents possible measurement outcomes.
If the pre-measurement state of the quantum system is $|\psi\rangle$, then the probability that a measurement result $m$ occurs is given by

$$P(m) = \langle \psi | M_m^\dagger M_m | \psi \rangle,$$

and the post-measurement state of the system is

$$\frac{M_m | \psi \rangle}{\sqrt{\langle \psi | M_m^\dagger M_m | \psi \rangle}}.$$

The completeness equation expresses the fact that probabilities sum to one

$$\sum_m P(m) = \sum_m \langle \psi | M_m^\dagger M_m | \psi \rangle = \langle \psi | \left( \sum_m M_m^\dagger M_m \right) | \psi \rangle = \langle \psi | \psi \rangle = 1.$$
Measurement of a Qubit

- $\mathcal{H}$: a two-dimensional Hilbert space associated to a quantum system.
- $\{|0\rangle, |1\rangle\}$: an orthonormal basis of $\mathcal{H}$.
- $M_0 = |0\rangle\langle 0|$, $M_1 = |1\rangle\langle 1|$: measurement operators.
  - Hermitian operators.
  - $M_0^2 = M_0$ and $M_1^2 = M_1$.
  - Completeness equation is satisfied

$$M_0^\dagger M_0 + M_1^\dagger M_1 = M_0^2 + M_1^2 = M_0 + M_1 = I.$$
• $|\psi\rangle = a|0\rangle + b|1\rangle$: a qubit being measured.
  
  $- \mathcal{P}(0) = \langle \psi \vert M_0^\dagger M_0 \vert \psi \rangle = \langle \psi \vert M_0 \vert \psi \rangle = \langle 0 \vert \langle 0 \vert \psi \rangle = |a|^2$.
  
  $- \mathcal{P}(1) = \langle \psi \vert M_1^\dagger M_1 \vert \psi \rangle = \langle \psi \vert M_1 \vert \psi \rangle = \langle 1 \vert \langle 1 \vert \psi \rangle = |b|^2$.

  $- \text{State after measurement}$

  \[
  \frac{M_0 \vert \psi \rangle}{|a|} = \frac{a}{|a|} \vert 0 \rangle, \\
  \frac{M_1 \vert \psi \rangle}{|b|} = \frac{b}{|b|} \vert 1 \rangle. 
  \]
Projective (von Neumann) Measurements

- $M$: a Hermitian operator on the Hilbert space, called an *observable*, with the spectral decomposition

$$M = \sum_{m} mP_m$$

where $P_m$ is the projector onto the eigenspace of $M$ associated with eigenvalue $m$.

- The projectors $\{P_m\}$ are measurement operators.
  
  * $P_m^\dagger = P_m$ and $P_m^2 = P_m$.

- Completeness equation:

$$\sum_m P_m^\dagger P_m = \sum_m P_m^2 = \sum_m P_m = I.$$  

- $m$: possible outcomes of the measurement.
If the pre-measurement state of the quantum system is $|\psi\rangle$, then the probability that an outcome $m$ occurs is given by

$$P(m) = \langle \psi | P_m^\dagger P_m | \psi \rangle = \langle \psi | P_m | \psi \rangle,$$

and the post-measurement state of the system is

$$\frac{P_m | \psi \rangle}{\sqrt{\langle \psi | P_m | \psi \rangle}}.$$

The completeness relation expresses the fact that probabilities sum to one

$$\sum_m P(m) = \sum_m \langle \psi | P_m | \psi \rangle = \langle \psi | \left( \sum_m P_m \right) | \psi \rangle = \langle \psi | \psi \rangle = 1.$$
Repeatability of a Projective Measurement $M$

- $|\psi\rangle$: pre-measurement state.

- $|\psi_m\rangle = P_m|\psi\rangle/\sqrt{\langle\psi|P_m|\psi\rangle}$: post-measurement state once the outcome $m$ is measured, which occurs with probability $\langle\psi|P_m|\psi\rangle$.

- $P_m|\psi_m\rangle = P_m|\psi\rangle/\sqrt{\langle\psi|P_m|\psi\rangle}$: post-measurement state after repeating the same projective measurement $M$, which occurs with probability

$$\langle\psi_m|P_m|\psi_m\rangle = \frac{\langle\psi|P_m^\dagger P_m|\psi\rangle}{\langle\psi|P_m|\psi\rangle} = \frac{\langle\psi|P_m|\psi\rangle}{\langle\psi|P_m|\psi\rangle} = 1.$$
Not every measurement is a projective measurement!
Average Value of an Observable $M$

$$\mathcal{E}(M) = \sum_m m\mathcal{P}(m) = \sum_m m\langle\psi|P_m|\psi\rangle$$

$$= \langle\psi\rvert \left( \sum_m mP_m \right) \rvert \psi\rangle = \langle\psi\rvert M \rvert \psi\rangle.$$  

- $\langle M \rangle \equiv \langle\psi\rvert M \rvert \psi\rangle$.

- Variance of observable $M$

$$\sigma^2(M) = \langle (M - \langle M \rangle)^2 \rangle = \langle M^2 \rangle - \langle M \rangle^2.$$
Two Descriptions of Projective Measurements

- A complete set of orthogonal projectors \( \{P_m\} \)
  \[
  \sum_m P_m = I \quad \text{and} \quad P_m P_{m'} = \delta_{mm'} P_m
  \]
  - Observable: \( M = \sum_m m P_m \)
  - \( m \): real numbers

- An orthonormal basis \( \{|m\rangle\} \)
  \[
  P_m = |m\rangle \langle m|
  \]
  - Observable: \( M = \sum_m m |m\rangle \langle m| \)
  - \( m \): real numbers
Observable $Z$ on a Qubit

- The observable $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ has eigenvalues +1 and -1
  with eigenvectors $|0\rangle$ and $|1\rangle$ respectively
- $Z = |0\rangle\langle 0| - |1\rangle\langle 1|$ : spectral decomposition
- $|\psi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ : a qubit.

\[
P(+1) = \langle \psi | 0 \rangle \langle 0 | \psi \rangle = 1/2
\]
\[
P(-1) = \langle \psi | 1 \rangle \langle 1 | \psi \rangle = 1/2
\]
- $\langle Z \rangle = 0$
Heisenberg Uncertainty Principle
Commutator and Anti-commutator

- $A$ and $B$ : two operators.
- Commutator : $[A, B] \equiv AB - BA$
  - $[A, B] = 0 : A$ commutes with $B$.
- Anti-commutator : $\{A, B\} \equiv AB + BA$.
  - $\{A, B\} = 0 : A$ anti-commutes with $B$. 
**Pauli Matrices (Pauli Operators)**

\[
X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.
\]

- Hermitian and unitary.
- \([X, Y] = 2iZ, [Y, Z] = 2iX\) and \([Z, X] = 2iY\).
Simultaneous Diagonalization of Two Normal Operators

Let $A$ and $B$ be two normal operators. Then $[A, B] = 0$ if and only if there exists an orthonormal basis $\{|\psi_i\rangle\}$ such that $A$ and $B$ are diagonalizable with respective to that basis, i.e.,

\begin{align*}
A &= \sum_i \lambda_i |\psi_i\rangle\langle \psi_i|, \\
B &= \sum_i \mu_i |\psi_i\rangle\langle \psi_i|.
\end{align*}
\[ |\langle \psi | [A, B] | \psi \rangle|^2 \leq 4\langle \psi | A^2 | \psi \rangle \langle \psi | B^2 | \psi \rangle \]

- \(A \) and \(B\) : two Hermitian operators.
- With \(\langle \psi | AB | \psi \rangle = x + iy\) where \(x, y\) real numbers, we have \(\langle \psi | BA | \psi \rangle = (\langle \psi | AB | \psi \rangle)^\dagger = x - iy\) and then
  \[ \langle \psi | [A, B] | \psi \rangle = 2iy \quad \text{and} \quad \langle \psi | \{A, B\} | \psi \rangle = 2x. \]
- \(|\langle \psi | [A, B] | \psi \rangle|^2 + |\langle \psi | \{A, B\} | \psi \rangle|^2 = 4|\langle \psi | AB | \psi \rangle|^2.\]
- Schwarz inequality :
  \[ |\langle \psi | AB | \psi \rangle|^2 \leq \langle \psi | A^2 | \psi \rangle \langle \psi | B^2 | \psi \rangle.\]

Thus we have
\[ |\langle \psi | [A, B] | \psi \rangle|^2 \leq 4|\langle \psi | AB | \psi \rangle|^2 \leq 4\langle \psi | A^2 | \psi \rangle \langle \psi | B^2 | \psi \rangle.\]
Heisenberg Uncertainty Principle

\[ \delta(C)\delta(D) \geq \frac{|\langle \psi | [C, D] | \psi \rangle|^2}{2}. \]

- \( C \) and \( D \): two observables.
- With \( A = C - \langle C \rangle \) and \( B = D - \langle D \rangle \), we have
  \[ [A, B] = [C, D]. \]
- \( \delta^2(C) = \langle (C - \langle C \rangle)^2 \rangle = \langle A^2 \rangle = \langle \psi | A^2 | \psi \rangle. \)
- \( \delta^2(D) = \langle (D - \langle D \rangle)^2 \rangle = \langle B^2 \rangle = \langle \psi | B^2 | \psi \rangle. \)

Now we have
\[ \delta^2(C)\delta^2(D) = \langle \psi | A^2 | \psi \rangle \langle \psi | B^2 | \psi \rangle \geq \frac{|\langle \psi | [A, B] | \psi \rangle|^2}{4} = \frac{|\langle \psi | [C, D] | \psi \rangle|^2}{4}. \]
If we prepare a large number of quantum systems in identical states, $|\psi\rangle$, and then perform measurements of $C$ on some of those systems, and of $D$ on others, then the standard deviation $\delta(C)$ of all measurement results of $C$ times the standard deviation $\delta(D)$ of all measurement results of $D$ will satisfy the inequality

$$\delta(C)\delta(D) \geq \frac{|\langle \psi | [C, D]|\psi\rangle|}{2}.$$
An Example

- $X$ and $Y$: Pauli observables.
- $[X, Y] = 2iZ$.
- $|\psi\rangle = |0\rangle$: quantum system state.
- $\delta(X)\delta(Y) \geq \langle 0|Z|0 \rangle = 1$. 
Positive Operator-Valued Measure (POVM) Measurements

- \( \{M_m\} \): a collection of measurement operators with
  \[
  \sum_m M_m^\dagger M_m = I.
  \]
- \( \mathcal{P}(m) = \langle \psi | M_m^\dagger M_m | \psi \rangle \).
- \( E_m \equiv M_m^\dagger M_m \): positive operators, called POVM elements
  \[
  \sum_m E_m = I \quad \text{and} \quad \mathcal{P}(m) = \langle \psi | E_m | \psi \rangle.
  \]
- \( \{E_m\} \): a POVM.
- Useful when only the measurement statistics matter.
For a projective measurement \( \{P_m\} \), all the POVM elements are the same as the measurement operators since

\[
E_m = P_m^\dagger P_m = P_m^2 = P_m.
\]
What Are POVMs?

- A collection of positive operators \( \{E_m\} \).
- Satisfying the completeness relation

\[
\sum_m E_m = I.
\]

The corresponding measurement operators can be chosen as \( \{\sqrt{E_m}\} \).
Postulate 4 – Composite Systems

- $Q_i$ : $i$th quantum system.
- $\mathcal{H}_i$ : the Hilbert space associated to the quantum system $Q_i$.
- $\mathcal{H} = \bigotimes_i \mathcal{H}_i$ : the Hilbert space associated to the composite system of $Q_i$’s.
- $|\psi_i\rangle$ : a state of quantum system $Q_i$.
- $|\psi\rangle = \bigotimes_i |\psi_i\rangle$ : the joint state of the composite system.
Entangled States

- States in a composite quantum system.
- Not a direct product of states of component systems.
- \((|00\rangle + |01\rangle)/\sqrt{2}\) is not an entangled state since
  \[
  \frac{|00\rangle + |01\rangle}{\sqrt{2}} = |0\rangle \left( \frac{|0\rangle + |1\rangle}{\sqrt{2}} \right).
  \]
- Bell states in a two-qubit system are entangled states
  \[
  \frac{|00\rangle + |11\rangle}{\sqrt{2}}, \quad \frac{|00\rangle - |11\rangle}{\sqrt{2}}, \quad \frac{|01\rangle + |10\rangle}{\sqrt{2}}, \quad \frac{|01\rangle - |10\rangle}{\sqrt{2}}.
  \]
A Proof

Suppose that

$$\frac{|00\rangle + |11\rangle}{\sqrt{2}} = (a|0\rangle + b|1\rangle) \otimes (c|0\rangle + d|1\rangle)$$

$$= ac|00\rangle + ad|01\rangle + bc|10\rangle + bd|11\rangle,$$

where $|a|^2 + |b|^2 = |c|^2 + |d|^2 = 1$. Then we have

$$ad = bc = 0.$$

- $a = c = 0 \Rightarrow \frac{|00\rangle + |11\rangle}{\sqrt{2}} = e^{i\theta}|11\rangle$, a contradiction.
- $b = d = 0 \Rightarrow \frac{|00\rangle + |11\rangle}{\sqrt{2}} = e^{i\theta'}|00\rangle$, a contradiction.
The Density Operator Formulation of Quantum Mechanics

- A convenient means for describing quantum systems whose states is not completely known.
- A convenient tool for the description of individual subsystems of a composite quantum system.
An Ensemble of Quantum Pure States \( \{p_i, |\psi_i\rangle\} \)

- \( |\psi_i\rangle \): states of a quantum system, called pure states.
- \( p_i \): the probability that the quantum system is in pure state \( |\psi_i\rangle \),

\[
\sum_i p_i = 1.
\]

- The density operator or density matrix which represents this ensemble is

\[
\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|.
\]

- Not necessary a spectral decomposition of \( \rho \) since \( \{|\psi_i\rangle\} \) may not be an orthonormal set.
Evolution of a Density Operator

- $U$: a unitary operator, describing the evolution of a closed quantum system during a time interval.

- $\rho$: a density operator, representing an ensemble $\{p_i, |\psi_i\rangle\}$ of pure states, which describes the initial state of the system.

- $U\rho U^\dagger$: density operator, describing the final state of the system.

$$
|\psi_i\rangle \xrightarrow{U} U|\psi_i\rangle \\
\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \xrightarrow{U} \rho' = \sum_i p_i U|\psi_i\rangle\langle\psi_i| U^\dagger = U\rho U^\dagger.
$$
Measurement Effect on a Density Operator

- \( \{M_m\} \) : a collection of measurement operators, acting on the Hilbert space associated to the system being measured and satisfying the completeness equation

\[
\sum_{m} M_m^\dagger M_m = I.
\]

- \( m \) : index which represents possible measurement outcomes.

- \( \rho \) : a density operator, representing an ensemble \( \{p_i, |\psi_i\rangle\} \) of pure states.
If the pre-measurement state of the quantum system is $|\psi_i\rangle$, then the probability of getting result $m$ is

$$P(m|i) = \langle \psi_i | M_m^\dagger M_m | \psi_i \rangle = \text{tr}(M_m^\dagger M_m | \psi_i \rangle \langle \psi_i |),$$

and the post-measurement state of the system is

$$|\psi_i^{(m)}\rangle = \frac{M_m | \psi_i \rangle}{\sqrt{\langle \psi_i | M_m^\dagger M_m | \psi_i \rangle}}.$$

The total probability of getting result $m$ is

$$P(m) = \sum_i p_i P(m|i) = \sum_i p_i \text{tr}(M_m^\dagger M_m | \psi_i \rangle \langle \psi_i |)$$

$$= \text{tr} \left( M_m^\dagger M_m \left( \sum_i p_i | \psi_i \rangle \langle \psi_i | \right) \right) = \text{tr}(M_m^\dagger M_m \rho) = \text{tr}(M_m \rho M_m^\dagger).$$
After a measurement which yields the result \( m \), we have

- \( \{ \mathcal{P}(i|m), |\psi_i^{(m)}\rangle \} \) : an ensemble of pure states

- \( \mathcal{P}(i|m) \) : the probability that the quantum system is in pure state \( |\psi_i^{(m)}\rangle \) given that outcome \( m \) is measured

\[
\mathcal{P}(i|m) = \frac{p_i \mathcal{P}(m|i)}{\mathcal{P}(m)}
\]

- \( \rho^{(m)} \) : density operator, describing the state of the quantum system after the outcome \( m \) is measured

\[
\rho^{(m)} = \sum_i \mathcal{P}(i|m)|\psi_i^{(m)}\rangle \langle \psi_i^{(m)}| = \sum_i \mathcal{P}(i|m) \frac{M_m |\psi_i\rangle \langle \psi_i| M_m^\dagger}{\langle \psi_i| M_m^\dagger M_m |\psi_i\rangle} = \sum_i p_i M_m |\psi_i\rangle \langle \psi_i| M_m^\dagger = \frac{M_m \rho M_m^\dagger}{\text{tr}(M_m^\dagger M_m \rho)} = \frac{M_m \rho M_m^\dagger}{\text{tr}(M_m \rho M_m^\dagger)}.
\]
Pure States vs Mixed States

- Pure state $|\psi\rangle$: a quantum system whose state is exactly known as $|\psi\rangle$ and can be described by the density operator

\[ \rho = |\psi\rangle\langle\psi|. \]

- Mixed state $\rho$: a quantum system whose state is not completely known and is described by the density operator

\[ \rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|. \]

- A pure state can be regarded as a very special mixed state.
Characterization of Density Operators

$\rho$ is a density operator associated with an ensemble \( \{ p_i, |\psi_i\rangle \} \) if and only if

- Unit trace condition : \( \text{tr}(\rho) = 1 \).
- Positivity condition : \( \rho \) is a positive operator.
Proof

- $\rho = \sum_i p_i |\psi_i \rangle \langle \psi_i|.$
- $\text{tr}(\rho) = \sum_i p_i \text{tr}(|\psi_i \rangle \langle \psi_i|) = \sum_i p_i \langle \psi_i | \psi_i \rangle = \sum_i p_i = 1.$
- $\langle \varphi | \rho | \varphi \rangle = \sum_i p_i \langle \varphi | \psi_i \rangle \langle \psi_i | \varphi \rangle = \sum_i p_i |\langle \varphi | \psi_i \rangle|^2 \geq 0.$
\[ \rho = \sum_j \lambda_j |\psi_j\rangle \langle \psi_j|, \]

- \( \rho \) is positive with a spectral decomposition
- \( \lambda_j \) : non-negative eigenvalues.
- \( |\psi_j\rangle \) : eigenvectors.
- \( 1 = \text{tr}(\rho) = \sum_j \lambda_j \).
- \( \{\lambda_j, |\psi_j\rangle\} \) : an ensemble of pure states giving rise to the density operator \( \rho \).
A Criterion of Pure States

A density operator \( \rho \) is in a pure state if and only if

\[
\text{tr}(\rho^2) = 1.
\]

- For a mixed (not a pure) state \( \rho \), we have \( \text{tr}(\rho^2) < 1 \).
Proof

Let $\rho$ be a density operator with spectral decomposition

$$\rho = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|,$$

where $\lambda_i \geq 0$ and $\text{tr}(\rho) = \sum_i \lambda_i = 1$. Since

$$\rho^2 = \sum_i \lambda_i^2 |\psi_i\rangle\langle\psi_i|,$$

we have

$$\text{tr}(\rho^2) = \sum_i \lambda_i^2 \leq \sum_i \lambda_i^2 + 2 \sum_{i<j} \lambda_i \lambda_j = (\sum_i \lambda_i)^2 = 1,$$

where equality holds if and only if only one $\lambda_i$ is non-zero and is equal to one, i.e., $\rho = |\psi_i\rangle\langle\psi_i|$, a pure state.
Mixture of Mixed States

\[ \rho = \sum_i p_i \rho_i. \]

- \( \rho_i \) : density operator corresponding to an ensemble \( \{ p_{ij}, |\psi_{ij}\rangle\} \)
  \[ \rho_i = \sum_j p_{ij} |\psi_{ij}\rangle \langle \psi_{ij}|. \]

- \( p_i \) : probability that the state of the quantum system is prepared in \( \rho_i \).

The probability of being in the pure state \( |\psi_{ij}\rangle \) is \( p_i p_{ij} \) and the overall density operator to describe the state of the quantum system is

\[ \rho = \sum_{ij} p_i p_{ij} |\psi_{ij}\rangle \langle \psi_{ij}| = \sum_i p_i \sum_j p_{ij} |\psi_{ij}\rangle \langle \psi_{ij}| = \sum_i p_i \rho_i. \]
Density Operator After Unspecified Measurement $\{M_m\}$

\[
\rho' = \sum_m \mathcal{P}(m) \rho^{(m)} = \sum_m \text{tr}(M_m \rho M_m^\dagger) \frac{M_m \rho M_m^\dagger}{\text{tr}(M_m \rho M_m^\dagger)} = \sum_m M_m \rho M_m^\dagger.
\]
• \( \rho \): density operator for a quantum system

• \( M \): an observable for the quantum system with spectral decomposition

\[
M = \sum_{m} m P_{m}
\]

• \( \mathcal{P}(m) = \text{tr}(P_{m} \rho P_{m}) = \text{tr}(P_{m}^{2} \rho) = \text{tr}(P_{m} \rho) \): the probability that outcome \( m \) occurs

• \( \langle M \rangle \): the average measurement value

\[
\langle M \rangle = \sum_{m} m \mathcal{P}(m) = \sum_{m} m \text{tr}(P_{m} \rho) = \text{tr}(M \rho).
\]
What Class of Ensembles Gives Rise to a Particular $\rho$?

- $\rho = \frac{3}{4} |0\rangle\langle 0| + \frac{1}{4} |1\rangle\langle 1| $ (spectral decomposition).
- $|a\rangle = \sqrt{\frac{3}{4}} |0\rangle + \sqrt{\frac{1}{4}} |1\rangle$, $|b\rangle = \sqrt{\frac{3}{4}} |0\rangle - \sqrt{\frac{1}{4}} |1\rangle$.

$$\frac{1}{2} |a\rangle\langle a| + \frac{1}{2} |b\rangle\langle b| = \frac{3}{4} |0\rangle\langle 0| + \frac{1}{4} |1\rangle\langle 1| = \rho.$$ 

- A lesson: the collection of eigenstates of a density operator is not an especially privileged ensemble.
Unitary Freedom in the Ensemble for Density Operators

Two ensembles \( \{p_i, |\psi_i\rangle\} \) and \( \{q_i, |\varphi_j\rangle\} \) give rise to the same density operator \( \rho \), i.e.,

\[
\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|, \quad \rho = \sum_j q_j |\varphi_j\rangle \langle \varphi_j|
\]

if and only if

\[
\sqrt{p_i} |\psi_i\rangle = \sum_j z_{ij} \sqrt{q_j} |\varphi_j\rangle
\]

where \( z_{ij} \) is a unitary matrix of complex numbers and pure states with zero probability are padded to the smaller ensemble to have the same size as the larger one.
\textbf{Proof} \leftarrow

- \ket{v_i} = \sqrt{p_i} \ket{\psi_i}, \ket{w_j} = \sqrt{q_j} \ket{\varphi_j}.

Since

\[ |v_i\rangle = \sum_j z_{ij} |w_j\rangle, \]

we have

\[
\sum_i p_i |\psi_i\rangle \langle \psi_i| = \sum_i |v_i\rangle \langle v_i| = \sum_i \sum_{jk} z_{ij} z^*_{ik} |w_j\rangle \langle w_k|
\]

\[ = \sum_{jk} \left( \sum_i z_{ij} z^*_{ik} \right) |w_j\rangle \langle w_k|
\]

\[ = \sum_j |w_j\rangle \langle w_j|
\]

\[ = \sum_j q_j |\varphi_j\rangle \langle \varphi_j|. \]
Proof

By spectral decomposition of $\rho$, we have

$$\rho = \sum_{k} \lambda_k |k\rangle \langle k| = \sum_{k} |k'\rangle \langle k'|,$$

where $\lambda_k$ are positive, $|k\rangle$ are orthonormal and $|k'\rangle = \sqrt{\lambda_k} |k\rangle$.

- $|u\rangle$: a vector in the orthogonal complement $\text{Span}\{|k'\rangle\}^\perp$ of $\text{Span}\{|k'\rangle\}$.

Then

$$0 = \sum_{k} \langle u|k'\rangle \langle k'|u\rangle = \langle u|\rho|u\rangle = \sum_{i} \langle u|v_i\rangle \langle v_i|u\rangle = \sum_{i} |\langle u|v_i\rangle|^2$$

which implies that

$$|u\rangle \in \text{Span}\{|v_i\rangle\}^\perp.$$
Thus

\[ \text{Span}\{|k'\rangle\}^\perp \subseteq \text{Span}\{|v_i\rangle\}^\perp \text{ and then Span}\{|v_i\rangle\} \subseteq \text{Span}\{|k'\rangle\}. \]

For each \(|v_i\rangle\), we have

\[ |v_i\rangle = \sum_k c_{ik} |k'\rangle \]

Then

\[ \rho = \sum_k |k'\rangle \langle k'| = \sum_i |v_i\rangle \langle v_i| = \sum_{kl} \left( \sum_i c_{ik} c_{il}^* \right) |k'\rangle \langle l'| \]

Since the operators \(|k'\rangle \langle l'|\) are linearly independent, we have

\[ \sum_i c_{ik} c_{il}^* = \delta_{kl} \]

By appending more columns to the matrix \(C = [c_{ik}]\), we obtain a
unitary matrix $T = [t_{ik}]$ such that

$$|v_i\rangle = \sum_k t_{ik} |k'\rangle$$

where some zero vectors are padded into the list of $|k'\rangle$. Similarly, there is a unitary matrix $S = [j_k]$ such that

$$|w_j\rangle = \sum_k s_{jk} |k'\rangle$$

Then with $Z = TS^\dagger$ a unitary matrix and $Z = [z_{ij}]$, we have

$$|v_i\rangle = \sum_j z_{ij} |w_j\rangle$$

since
\[ \sum_j z_{ij} |w_j\rangle = \sum_j \sum_k t_{ik} s_{jk}^* \sum_l s_{jl} |l'\rangle \]
\[ = \sum_{kl} t_{ik} |l'\rangle \sum_j s_{jk}^* s_{jl} \]
\[ = \sum_k t_{ik} |k'\rangle \]
\[ = |v_i\rangle \]
Postulates of Quantum Mechanics

- Density Operator Version
**Postulate 1 – States**

Associated to an *isolated* physical system is a Hilbert space $\mathcal{H}$ (e.g., a finite-dimensional complex inner product space). The state of the system is completely described by its *density operator*, which is a positive operator with trace one acting on the Hilbert space $\mathcal{H}$. If the quantum system is in the state $\rho_i$ with probability $p_i$, then the density operator for this system is

$$\rho = \sum_i p_i \rho_i.$$
Postulate 2 - Time Evolution

The evolution of a *closed* quantum system is described by a *unitary operator*. That is, the state $\rho$ of the system at time $t_1$ is related to the state $\rho'$ of the system at time $t_2$ by a unitary operator $U$ which depends only on the times $t_1$ and $t_2$,

$$\rho' = U \rho U^\dagger.$$
Postulate 3 – Quantum Measurements

• \( \{M_m\} \) : a collection of measurement operators, acting on the Hilbert space associated to the system being measured and satisfying the completeness equation

\[
\sum_m M_m^\dagger M_m = I.
\]

• \( m \) : measurement outcomes that may occur in the experiment.
If the pre-measurement state of the quantum system is $\rho$, then the probability that result $m$ occurs is given by

$$P(m) = \text{tr}(M_m \rho M_m^\dagger),$$

and the post-measurement state of the system is

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

The completeness equation expresses the fact that probabilities sum to one

$$\sum_m \mathcal{P}(m) = \sum_m \text{tr}(M_m \rho M_m^\dagger) = \sum_m \text{tr}(M_m^\dagger M_m \rho)$$

$$= \text{tr} \left( \left( \sum_m M_m^\dagger M_m \right) \rho \right) = \text{tr}(\rho) = 1.$$
Postulate 4 – Composite Systems

- $Q_i$: $i$th quantum system.
- $H_i$: the Hilbert space associated to the quantum system $Q_i$.
- $\mathcal{H} = \bigotimes_i H_i$: the Hilbert space associated to the composite system of $Q_i$’s.
- $\rho_i$: the state in which the quantum system $Q_i$ is prepared.
- $\rho = \bigotimes_i \rho_i$: the joint state of the composite system.
Reduced Density Operator
Definition

\[ \rho^A \triangleq \text{tr}_B(\rho^{AB}). \]

- \( \rho^{AB} \): density operators for composite quantum system \( AB \).
- \( \rho^A \triangleq \text{tr}_B(\rho^{AB}) \): reduced density operator for subsystem \( A \).
  - A description for the state of subsystem \( A \): justification needed.
A Simple Justification

- $\rho^{AB} = \rho \otimes \sigma$: a direct product density operator for composite quantum system $AB$.
- $\rho^A = \text{tr}_B(\rho^{AB}) = \rho \text{ tr}(\sigma) = \rho$: correct description of system $A$.
- $\rho^B = \text{tr}_A(\rho^{AB}) = \text{tr}(\rho)\sigma = \sigma$: correct description of system $B$. 
A Further Justification
Local and Global Observables

- $M$: the observable on subsystem $A$ for a measurement carrying out on subsystem $A$, a Hermitian operator with spectral decomposition

$$M = \sum_m mP_m.$$  

- $M \otimes I$: the corresponding observable on the composite system $AB$ for the same measurement carrying out on subsystem $A$, a Hermitian operator with spectral decomposition

$$M \otimes I = \sum_m m(P_m \otimes I).$$  

- $|m\rangle$ is an eigenstate of the observable $M$ and $|\psi\rangle$ is any state of subsystem $B \leftrightarrow |m\rangle \otimes |\psi\rangle$ is an eigenstate of $M \otimes I$.  

When System $AB$ Is Prepared With State $|m\rangle \otimes |\psi\rangle$

- $m$: the outcome which occurs with probability one by the observable $M$ on subsystem $A$.
- $m$: the outcome which occurs with probability one by the observable $M \otimes I$ on the composite system $AB$.
- Consistency.
When System $AB$ Is in a Mixed State $\rho^{AB}$

- $f(\rho^{AB})$: a density operator on subsystem $A$ as a function of the density operator on system $AB$, serving as an appropriate description of the state of subsystem $A$.

- Measurement statistics must be consistent between the local observable $M$ on subsystem $A$ and the global observable $M \otimes I$ on system $AB$

$$\text{tr}(M f(\rho^{AB})) = \langle M \rangle = \langle M \otimes I \rangle = \text{tr}((M \otimes I)\rho^{AB}).$$
Existence: \( f(\rho^{AB}) = \text{tr}_B(\rho^{AB}) \)

- \( \rho^{AB} = \sum_i \alpha_i T^A_i \otimes T^B_i \): a linear operator on the state space of the composite system \( AB \).

\[
\begin{align*}
\text{tr}((M \otimes I)\rho^{AB}) &= \text{tr}((M \otimes I)(\sum_i \alpha_i T^A_i \otimes T^B_i)) = \text{tr}(\sum_i \alpha_i (MT^A_i) \otimes T^B_i) \\
&= \text{tr}(\text{tr}_B(\sum_i \alpha_i (MT^A_i) \otimes T^B_i)) = \text{tr}(\sum_i \alpha_i (MT^A_i) \text{tr}(T^B_i)) \\
&= \text{tr}(M(\sum_i \alpha_i T^A_i \text{tr}(T^B_i))) = \text{tr}(M \text{tr}_B(\sum_i \alpha_i T^A_i \otimes T^B_i)) \\
&= \text{tr}(M \text{tr}_B(\rho^{AB})).
\end{align*}
\]
Uniqueness

- $\mathcal{H}$: the Hilbert space associated to the quantum system $A$.
- $L^H(\mathcal{H})$: the real inner product space of all Hermitian operators on $\mathcal{H}$ with trace inner product.
- $\{M_i\}$: an orthonormal basis of $L^H(\mathcal{H})$.
- $f(\rho^{AB}) = \sum_i M_i \text{tr}(M_i f(\rho^{AB}))$: the expansion of $f(\rho^{AB})$ by the orthonormal basis $\{M_i\}$.

Since

$$\text{tr}(M_i f(\rho^{AB})) = \text{tr}((M_i \otimes I)\rho^{AB}) \forall i,$$

we have

$$f(\rho^{AB}) = \sum_i M_i \text{tr}((M_i \otimes I)\rho^{AB})$$

which uniquely specifies the function $f$. 
An Example

- Suppose a two-qubit system is in a pure Bell state \( \frac{|00\rangle + |11\rangle}{\sqrt{2}} \) with density operator

\[
\rho^{12} = \left( \frac{|00\rangle + |11\rangle}{\sqrt{2}} \right) \left( \frac{\langle 00| + \langle 11|}{\sqrt{2}} \right) = \frac{|00\rangle\langle 00| + |11\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 11|}{2}.
\]
\[ \rho_1 : \text{the reduced density operator of the first qubit} \]

\[
\rho_1 = \text{tr}_2 (\rho^{12}) \\
= \frac{\text{tr}_2 (|00\rangle\langle 00|) + \text{tr}_2 (|11\rangle\langle 00|) + \text{tr}_2 (|00\rangle\langle 11|) + \text{tr}_2 (|11\rangle\langle 11|)}{2} \\
= \frac{|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1|}{2} \\
= \frac{|0\rangle\langle 0| + |1\rangle\langle 1|}{2} = \frac{I}{2}. 
\]

- Reduced density operator \( \rho_1 \) for the first qubit is in a \emph{mixed} state while the two-qubit system is in a \emph{pure} state.
Schmidt Decomposition and Purification
Schmidt Decomposition

For each pure state $|\psi\rangle$ in a composite quantum system $AB$, there exist a set $\{|i_A\rangle\}$ of orthonormal states for subsystem $A$ and a set $\{|i_B\rangle\}$ of orthonormal states for subsystem $B$ of the same size such that

$$|\psi\rangle = \sum_i \lambda_i |i_A\rangle|i_B\rangle$$

where $\lambda_i$ are non-negative real numbers with

$$\sum_i \lambda_i^2 = 1.$$

- $\lambda_i$ : Schmidt coefficients.
- $\{|i_A\rangle\}$ and $\{|i_B\rangle\}$ : Schmidt “bases” for $A$ and $B$ respectively.
  - Dependent on $|\psi\rangle$.
- # of non-zero values $\lambda_i$ : Schmidt number for $|\psi\rangle$. 
Proof

• \{ |j\rangle \}, \{ |k\rangle \} : given orthonormal bases of the Hilbert spaces of subsystems \( A \) and \( B \) respectively

\[ |\psi\rangle = \sum_{jk} c_{jk} |j\rangle |k\rangle. \]

• \( C = UDV \) : singular value decomposition

\[ C = [c_{jk}], U = [u_{ji}], D = \text{diag}(d_{ii}), V = [v_{ik}], \]

\[ c_{jk} = \sum_i u_{ji} d_{ii} v_{ik}. \]

– \( U \) and \( V \) : unitary matrices.
– \( D \) : a diagonal matrix, not necessarily square.
\[
|\psi\rangle = \sum_{j} \sum_{k} \sum_{i} u_{ji} d_{ii} v_{ik} |j\rangle |k\rangle
\]

\[
= \sum_{i} d_{ii} \left( \sum_{j} u_{ji} |j\rangle \right) \left( \sum_{k} v_{ik} |k\rangle \right) = \sum_{i} \lambda_i |i_A\rangle |i_B\rangle.
\]

- \(|i_A\rangle = \sum_{j} u_{ji} |j\rangle\): orthonormal states of subsystem A

\[
\langle i_A | i_A' \rangle = \sum_{jj'} u_{ji}^* u_{j'i'} \langle j | j' \rangle = \sum_{j} u_{ji}^* u_{j'i'} = \delta_{ii'}.
\]

- \(|i_B\rangle = \sum_{k} v_{ik} |k\rangle\): orthonormal states of subsystem B

\[
\langle i_B | i_B' \rangle = \sum_{kk'} v_{ik}^* v_{i'k'} \langle k | k' \rangle = \sum_{k} v_{ik}^* v_{i'k} = \delta_{ii'}.
\]

- \(\lambda_i = d_{ii}\): non-negative real numbers

\[
1 = \langle \psi | \psi \rangle = \sum_{ii'} \lambda_i \lambda_{i'} \langle i_A | i_A' \rangle \langle i_B | i_B' \rangle = \sum_{i} \lambda_i^2.
\]
Schmidt Number for State \( |\psi\rangle = \sum_i \lambda_i |i_A\rangle |i_B\rangle \)

- "Amount" of entanglement between systems A and B when the composite system \( AB \) is in state \( |\psi\rangle \).
- Invariance under unitary transformations on subsystem A or subsystem B alone.
  - \( U \): a unitary operator on subsystem A.
  - \( U|i_A\rangle \): orthonormal states of subsystem A.

\[
(U \otimes I)|\psi\rangle = \sum_i \lambda_i (U \otimes I)(|i_A\rangle \otimes |i_B\rangle) = \sum_i \lambda_i U|i_A\rangle |i_B\rangle.
\]
• $\rho_A$ : a density operator for system $A$ with ensemble $\{p_i, |i_A\rangle\}$

$$\rho_A = \sum_{i} p_i |i_A\rangle\langle i_A|.$$  

• $R$ : a reference system.

• $\{|i_R\rangle\}$ : an orthonormal basis of the Hilbert space associated to system $R$, having the same cardinality as that of $\{|i_A\rangle\}$.

• $|AR\rangle$ : a pure state of the composite system $AR$ with

$$|AR\rangle \triangleq \sum_{i} \sqrt{p_i} |i_A\rangle |i_R\rangle.$$  

• Purification
\begin{align*}
\text{tr}_R(|AR\rangle\langle AR|) &= \sum_{ij} \sqrt{p_ip_j} \text{tr}_R(|i_A\rangle\langle j_A| \otimes |i_R\rangle\langle j_R|) \\
&= \sum_{ij} \sqrt{p_ip_j} |i_A\rangle\langle j_A| \text{tr}(|i_R\rangle\langle j_R|) \\
&= \sum_i p_i |i_A\rangle\langle i_A| = \rho_A.
\end{align*}

- A mixed state of a local system is a local view of a pure state in a global composite system.