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 $e^{j\theta}|\psi\rangle$ spans the same one-dimensional subspace of $\mathcal{H}$.

A Quantum Bit (Qubit)

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 $e^{j\theta}|\psi\rangle$ 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.

Postulate 3 – Quantum Measurements

A quantum measurement is described by a collection $\{M_m\}$ of *measurement operators*, acting on the Hilbert space associated to a quantum system being measured and satisfying the *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

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

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

$$\sum_m \mathcal{P}(m) = \sum_m \langle\psi|M_m^\dagger M_m|\psi\rangle = \langle\psi|\left(\sum_m M_m^\dagger M_m\right)|\psi\rangle = \langle\psi|\psi\rangle = 1.$$

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.
  - $\mathcal{P}(0) = \langle\psi|M_0^\dagger M_0|\psi\rangle = \langle\psi|M_0|\psi\rangle = \langle\psi|0\rangle\langle 0|\psi\rangle = |a|^2.$
  - $\mathcal{P}(1) = \langle\psi|M_1^\dagger M_1|\psi\rangle = \langle\psi|M_1|\psi\rangle = \langle\psi|1\rangle\langle 1|\psi\rangle = |b|^2.$
  - State after measurement

$$\begin{aligned} \frac{M_0|\psi\rangle}{|a|} &= \frac{a}{|a|}|0\rangle, \\ \frac{M_1|\psi\rangle}{|b|} &= \frac{b}{|b|}|1\rangle. \end{aligned}$$

Projective (von Neumann) Measurements

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

$$M = \sum_m m P_m$$

  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

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

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

$$\sum_m \mathcal{P}(m) = \sum_m \langle\psi|P_m|\psi\rangle = \langle\psi|\left(\sum_m P_m\right)|\psi\rangle = \langle\psi|\psi\rangle = 1.$$

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

$$\begin{aligned}\mathcal{E}(M) &= \sum_m m\mathcal{P}(m) = \sum_m m\langle\psi|P_m|\psi\rangle \\ &= \langle\psi|\left(\sum_m mP_m\right)|\psi\rangle = \langle\psi|M|\psi\rangle.\end{aligned}$$

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

$$\begin{aligned} \mathcal{P}(+1) &= \langle\psi|0\rangle\langle 0|\psi\rangle = 1/2 \\ \mathcal{P}(-1) &= \langle\psi|1\rangle\langle 1|\psi\rangle = 1/2 \end{aligned}$$

- $\langle Z\rangle = 0$

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.,

$$\begin{aligned} A &= \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|, \\ B &= \sum_i \mu_i |\psi_i\rangle\langle\psi_i|. \end{aligned}$$

$$|\langle\psi|[A,B]|\psi\rangle|^2 \leq 4\langle\psi|A^2|\psi\rangle\langle\psi|B^2|\psi\rangle$$

- 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

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

- 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

$$\delta^2(C)\delta^2(D) = \langle\psi|A^2|\psi\rangle\langle\psi|B^2|\psi\rangle \geq \frac{|\langle\psi|[A,B]|\psi\rangle|^2}{4} = \frac{|\langle\psi|[C,D]|\psi\rangle|^2}{4}.$$

Heisenberg Uncertainty Principle

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

- $\mathcal{Q}_i$: ith quantum system.
- $\mathcal{H}_i$: the Hilbert space associated to the quantum system $\mathcal{Q}_i$.
- $\mathcal{H} = \otimes_i \mathcal{H}_i$: the Hilbert space associated to the composite system of $\mathcal{Q}_i$'s.
- $|\psi_i\rangle$: a state of quantum system $\mathcal{Q}_i$.
- $|\psi\rangle = \otimes_i |\psi_i\rangle$: 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

$$ad = bc = 0.$$

- $a = c = 0 \Rightarrow \frac{|00\rangle+|11\rangle}{\sqrt{2}} = e^{j\theta}|11\rangle$, a contradiction.
- $b = d = 0 \Rightarrow \frac{|00\rangle+|11\rangle}{\sqrt{2}} = e^{j\theta'}|00\rangle$, 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.

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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 ρ 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.
- ρ : 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.

$$\begin{array}{rcl} |\psi_i\rangle & \xrightarrow{U} & U|\psi_i\rangle \\ \rho = \sum_i p_i|\psi_i\rangle\langle\psi_i| & \xrightarrow{U} & \rho' = \sum_i p_i U|\psi_i\rangle\langle\psi_i|U^\dagger = U\rho U^\dagger. \end{array}$$

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.
- ρ : 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

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

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

$$\begin{aligned} \mathcal{P}(m) &= \sum_i p_i \mathcal{P}(m|i) = \sum_i p_i \ \mathrm{tr}(M_m^\dagger M_m|\psi_i\rangle\langle\psi_i|) \\ &= \mathrm{tr}\left(M_m^\dagger M_m \left(\sum_i p_i|\psi_i\rangle\langle\psi_i|\right)\right) = \mathrm{tr}(M_m^\dagger M_m \rho) = \mathrm{tr}(M_m \rho M_m^\dagger). \end{aligned}$$

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

$$\begin{aligned}
\rho^{(m)} &= \sum_i \mathcal{P}(i|m)|\psi_i^{(m)}\rangle\langle\psi_i^{(m)}| = \sum_i \mathcal{P}(i|m) \frac{M_m|\psi_i\rangle\langle\psi_i|M_m^\dagger}{\langle\psi_i|M_m^\dagger M_m|\psi_i\rangle} \\
&= \frac{\sum_i p_i M_m|\psi_i\rangle\langle\psi_i|M_m^\dagger}{\mathcal{P}(m)} = \frac{M_m \rho M_m^\dagger}{\mathrm{tr}(M_m^\dagger M_m \rho)} = \frac{M_m \rho M_m^\dagger}{\mathrm{tr}(M_m \rho M_m^\dagger)}.
\end{aligned}$$

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 ρ : 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.

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Characterization of Density Operators

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

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

Proof $\Longrightarrow$

- $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$.
- $\mathrm{tr}(\rho) = \sum_i p_i \mathrm{tr}(|\psi_i\rangle\langle\psi_i|) = \sum_i p_i \langle\psi_i|\psi_i\rangle = \sum_i p_i = 1$.
- $\langle\varphi|\rho|\varphi\rangle = \sum_i p_i \langle\varphi|\psi_i\rangle\langle\psi_i|\varphi\rangle = \sum_i p_i |\langle\varphi|\psi_i\rangle|^2 \geq 0$.

Proof $\Longleftarrow$

- ρ is positive with a spectral decomposition

$$\rho = \sum_j \lambda_j |\psi_j\rangle\langle\psi_j|.$$

- λ_j : non-negative eigenvalues.
- $|\psi_j\rangle$: eigenvectors.
- $1 = \mathrm{tr}(\rho) = \sum_j \lambda_j$.
- $\{\lambda_j, |\psi_j\rangle\}$: an ensemble of pure states giving rise to the density operator ρ.

A Criterion of Pure States

A density operator ρ is in a pure state if and only if

$$\mathrm{tr}(\rho^2) = 1.$$

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

Proof

Let ρ be a density operator with spectral decomposition

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

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

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

we have

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

where equality holds if and only if only one λ_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

$$\rho = \sum_i p_i \rho_i.$$

- ρ_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 ρ_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 $\{M_m\}$

$$\rho' = \sum_m \mathcal{P}(m)\rho^{(m)} = \sum_m \mathrm{tr}(M_m \rho M_m^\dagger) \frac{M_m \rho M_m^\dagger}{\mathrm{tr}(M_m \rho M_m^\dagger)} = \sum_m M_m \rho M_m^\dagger.$$

Average for Projective Measurement

- ρ : density operator for a quantum system
- M : an observable for the quantum system with spectral decomposition
$$M = \sum_m m P_m$$
- $\mathcal{P}(m) = \mathrm{tr}(P_m \rho P_m) = \mathrm{tr}(P_m^2 \rho) = \mathrm{tr}(P_m \rho)$: the probability that outcome m occurs
- $\langle M \rangle$: the average measurement value

$$\boxed{\langle M \rangle = \sum_m m \mathcal{P}(m) = \sum_m m \ \mathrm{tr}(P_m \rho) = \mathrm{tr}(M \rho).}$$

What Class of Ensembles Gives Rise to a Particular ρ ?

- $\rho = \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1|$ (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 ρ, i.e.,

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \rho = \sum_j q_j |\varphi_j\rangle\langle\varphi_j|$$

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.

Proof $\Longleftarrow$

- $|v_i\rangle \equiv \sqrt{p_i}|\psi_i\rangle$, $|w_j\rangle \equiv \sqrt{q_j}|\varphi_j\rangle$.

Since

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

we have

$$\begin{aligned}
\sum_i p_i|\psi_i\rangle\langle\psi_i| &= \sum_i |v_i\rangle\langle v_i| = \sum_i \sum_{jk} z_{ij} z_{ik}^* |w_j\rangle\langle w_k| \\
&= \sum_{jk}\left(\sum_i z_{ij} z_{ik}^*\right)|w_j\rangle\langle w_k| \\
&= \sum_j |w_j\rangle\langle w_j| \\
&= \sum_j q_j|\varphi_j\rangle\langle\varphi_j|.
\end{aligned}$$

Proof $\Longrightarrow$

By spectral decomposition of ρ, we have

$$\rho = \sum_k \lambda_k |k\rangle\langle k| = \sum_k |k'\rangle\langle k'|,$$

where λ_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

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

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 $S = [jk]$ 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

$$
\begin{aligned}
\sum_j z_{ij}|w_j\rangle &= \sum_j \sum_k t_{ik} s^*_{jk} \sum_l s_{jl}|l'\rangle \\
&= \sum_{kl} t_{ik}|l'\rangle \sum_j s^*_{jk} s_{jl} \\
&= \sum_k t_{ik}|k'\rangle \\
&= |v_i\rangle
\end{aligned}
$$

Postulates of Quantum Mechanics

– Density Operator Version

Postulate 1 – States

Associated to an *isolated* physical system is a Hilbert space $\mathcal{H}$ (eg, 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 ρ_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 ρ of the system at time t_1 is related to the state ρ' 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.

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If the pre-measurement state of the quantum system is ρ, then the probability that result m occurs is given by

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

and the post-measurement state of the system is

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

The completeness euqation expresses the fact that probabilities sum to one

$$\begin{aligned} \sum_m \mathcal{P}(m) &= \sum_m \mathrm{tr}(M_m \rho M_m^\dagger) = \sum_m \mathrm{tr}(M_m^\dagger M_m \rho) \\ &= \mathrm{tr}\left(\left(\sum_m M_m^\dagger M_m\right) \rho\right) = \mathrm{tr}(\rho) = 1. \end{aligned}$$

Postulate 4 – Composite Systems

- $\mathcal{Q}_i$: ith quantum system.
- $\mathcal{H}_i$: the Hilbert space associated to the quantum system $\mathcal{Q}_i$.
- $\mathcal{H} = \otimes_i \mathcal{H}_i$: the Hilbert space associated to the composite system of $\mathcal{Q}_i$'s.
- ρ_i : the state in which the quantum system $\mathcal{Q}_i$ is prepared.
- $\rho = \otimes_i \rho_i$: the joint state of the composite system.

Reduced Density Operator

Definition

$$\rho^A \stackrel{\triangle}{=} \mathrm{tr}_B(\rho^{AB}).$$

- ρ^{AB} : density operators for composite quantum system AB.
- $\rho^A \stackrel{\triangle}{=} \mathrm{tr}_B(\rho^{AB})$: 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.
- $\rho^{A} = \mathrm{tr}_B(\rho^{AB}) = \rho \ \mathrm{tr}(\sigma) = \rho$: correct description of system A.
- $\rho^{B} = \mathrm{tr}_A(\rho^{AB}) = \mathrm{tr}(\rho)\sigma = \sigma$: 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

$$M = \sum_m m P_m.$$

- $M \otimes I$: 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 $B \Longleftrightarrow |m\rangle \otimes |\psi\rangle$ 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 ρ^{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

$$\mathrm{tr}(Mf(\rho^{AB})) = \langle M \rangle = \langle M \otimes I \rangle = \mathrm{tr}((M \otimes I)\rho^{AB}).$$

Existence : $f(\rho^{AB}) = \mathbf{tr}_B(\rho^{AB})$

- $\rho^{AB} = \sum_i \alpha_i T_i^A \otimes T_i^B$: a linear operator on the state space of the composite system AB.

$$
\begin{aligned}
& \operatorname{tr}((M \otimes I)\rho^{AB}) \\
= \; & \operatorname{tr}((M \otimes I)(\sum_i \alpha_i T_i^A \otimes T_i^B)) = \operatorname{tr}(\sum_i \alpha_i (M T_i^A) \otimes T_i^B) \\
= \; & \operatorname{tr}(\operatorname{tr}_B(\sum_i \alpha_i (M T_i^A) \otimes T_i^B)) = \operatorname{tr}(\sum_i \alpha_i (M T_i^A) \ \operatorname{tr}(T_i^B)) \\
= \; & \operatorname{tr}(M(\sum_i \alpha_i T_i^A \ \operatorname{tr}(T_i^B))) = \operatorname{tr}(M \ \operatorname{tr}_B(\sum_i \alpha_i T_i^A \otimes T_i^B)) \\
= \; & \operatorname{tr}(M \ \operatorname{tr}_B(\rho^{AB})).
\end{aligned}
$$

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 $L^H(\mathcal{H})$.
- $f(\rho^{AB}) = \sum_i M_i \operatorname{tr}(M_i f(\rho^{AB}))$: the expansion of $f(\rho^{AB})$ by the orthonormal basis $\{M_i\}$.

Since

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

we have

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

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

$$\begin{aligned}\rho^{12} &= \left(\frac{|00\rangle + |11\rangle}{\sqrt{2}}\right)\left(\frac{\langle 00| + \langle 11|}{\sqrt{2}}\right) \\ &= \frac{|00\rangle\langle 00| + |11\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 11|}{2}.\end{aligned}$$

- ρ^1 : the reduced density operator of the first qubit

$$
\begin{aligned}
\rho^1 &= \mathrm{tr}_2(\rho^{12}) \\
&= \frac{\mathrm{tr}_2(|00\rangle\langle 00|) + \mathrm{tr}_2(|11\rangle\langle 00|) + \mathrm{tr}_2(|00\rangle\langle 11|) + \mathrm{tr}_2(|11\rangle\langle 11|)}{2} \\
&= \frac{|0\rangle\langle 0|\langle 0|0\rangle + |1\rangle\langle 0|\langle 0|1\rangle + |0\rangle\langle 1|\langle 1|0\rangle + |1\rangle\langle 1|\langle 1|1\rangle}{2} \\
&= \frac{|0\rangle\langle 0| + |1\rangle\langle 1|}{2} = \frac{I}{2}.
\end{aligned}
$$

- Reduced density operator ρ^1 for the first qubit is in a *mixed* state while the two-qubit system is in a *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 λ_i are non-negative real numbers with

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

- λ_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 λ_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.

$$
\begin{aligned}
|\psi\rangle &= \sum_{jk}\sum_i u_{ji} d_{ii} v_{ik} |j\rangle|k\rangle \\
&= \sum_i d_{ii}\left(\sum_j u_{ji}|j\rangle\right)\left(\sum_k v_{ik}|k\rangle\right) = \sum_i \lambda_i |i_A\rangle|i_B\rangle.
\end{aligned}
$$

- $|i_A\rangle = \sum_j u_{ji}|j\rangle$: orthonormal states of subsystem A

$$\langle i_A|i'_A\rangle = \sum_{jj'} u^*_{ji} u_{j'i'} \langle j|j'\rangle = \sum_j u^*_{ji} u_{ji'} = \delta_{ii'}.$$

- $|i_B\rangle = \sum_k v_{ik}|k\rangle$: 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.

$$(U \otimes I)|\psi\rangle = \sum_i \lambda_i (U \otimes I)(|i_A\rangle \otimes |i_B\rangle) = \sum_i \lambda_i U|i_A\rangle |i_B\rangle.$$

Purification

- ρ_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

$$|AR\rangle \stackrel{\triangle}{=} \sum_i \sqrt{p_i}|i_A\rangle|i_R\rangle.$$

$$
\begin{aligned}
\mathrm{tr}_R(|AR\rangle\langle AR|) &= \sum_{ij}\sqrt{p_i p_j}\,\mathrm{tr}_R(|i_A\rangle\langle j_A| \otimes |i_R\rangle\langle j_R|) \\
&= \sum_{ij}\sqrt{p_i p_j}\,|i_A\rangle\langle j_A|\mathrm{tr}(|i_R\rangle\langle j_R|) \\
&= \sum_{i} p_i |i_A\rangle\langle i_A| = \rho_A.
\end{aligned}
$$

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