Learners' Space

Introduction to Quantum Computing

"Quantum computation will be the first technology that allows useful tasks to be performed in collaboration between parallel universes."

— David Deutsch

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Week 1

1. Basics of Quantum Mechanics

Quantum Mechanics is based on two important objects—Wave Functions and Operators.

- **Wave Function:** A wave function is a vector in a complex Hilbert space that represents the state of a quantum system, encoding all its measurable properties.
- **Operators:** In quantum mechanics, operators are linear transformations that represent measurable quantities like position, momentum, or energy.

1.1 Linear Algebra

Linear algebra takes the notion of ordinary vectors to an abstract form. Consequently, the fundamental objects of linear algebra are vector spaces.

1.1.1 Vectors

A vector space consists of :

- a set of abstract objects or vectors - $(|\alpha\rangle, |\beta\rangle, |\gamma\rangle, ...)$
- a set of scalars taken from the field of complex numbers - $(a, b, c, ...)$

They are closed under vector addition and scalar multiplication.

- **Vector Addition :**

$$\text{Addition}: \ |\alpha\rangle + |\beta\rangle = |\gamma\rangle$$

$$\text{Commutative}: \ |\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle$$

$$\text{Associative}: \ |\alpha\rangle + (|\beta\rangle + |\gamma\rangle) = (|\alpha\rangle + |\beta\rangle) + |\gamma\rangle$$

$$\text{Null Vector}: \ |\alpha\rangle + 0 = |\alpha\rangle$$

$$\text{Inverse Vector}: \ |\alpha\rangle + |-\alpha\rangle = 0$$

- **Scalar Multiplication :**

$$\text{Multiplication}: \ a\,|\alpha\rangle = |\gamma\rangle$$

Distributive :

$$a(|\alpha\rangle + |\beta\rangle = a\,|\alpha\rangle + a\,|\beta\rangle$$
$$(a+b)\,|\alpha\rangle = a\,|\alpha\rangle + b\,|\alpha\rangle$$

Associative : $a(b|\alpha\rangle = (ab)|\alpha\rangle$

Null and Identity : $0|\alpha\rangle = 0$ and $1|\alpha\rangle = |\alpha\rangle$

Inverse Vector : $|-\alpha\rangle = (-1)|\alpha\rangle = -|\alpha\rangle$

1.1.2 Linear Combination of Vectors

A linear combination of vectors is given by,

$$a|\alpha\rangle + b|\beta\rangle + c|\gamma\rangle + ...$$

A set of vectors $\{|v_i\rangle\} = \{|v_1\rangle, |v_2\rangle, |v_3\rangle, ..., |v_n\rangle\}$ is said to span a vector space if all vectors in the space can be obtained by linear combination of the spanning set $\{|v_i\rangle\}$;

$$|\alpha\rangle = a_1|v_1\rangle + a_2|v_2\rangle + a_3|v_3\rangle + ... + a_n|v_n\rangle$$

The spanning set $\{|v_i\rangle\}$ is said to be linearly independent if its elements cannot be written as a linear combination of the remaining elements, i.e.,

$$a_1|v_1\rangle + a_2|v_2\rangle + ... + a_n|v_n\rangle = 0, \forall\, a_i = 0$$

This implies that : $|v_k\rangle \neq \sum_{i\neq k} -\frac{a_i}{a_k}|v_k\rangle$.

1.1.3 Basis Vectors

Any spanning set $\{|v_i\rangle\}$ that is linearly independent forms a **basis** for the vector space. For any vector $|\alpha\rangle$:

$$|\alpha\rangle = a_1|v_1\rangle + a_2|v_2\rangle + a_3|v_3\rangle + ... + a_n|v_n\rangle$$

$$|\alpha\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

Exercise: How would you represent the basis vectors in the notation? Can you use this to work out the axioms of a vector space?

1.1.4 Inner Product

The inner product is a generalization of the notion of dot products to vector spaces.

$$\underbrace{(|\alpha\rangle, |\beta\rangle)}_{\text{two vectors from the space } V} = \underbrace{c}_{\text{complex number from the field } C}$$

- **Dual Vector**: One can also use the dual vector space $\{\langle\alpha|\}$, which is a vector space of all linear transformations of the space $V \to C$, together with vector addition and scalar multiplication.

  $$\langle\alpha|(|\beta\rangle) \equiv \langle\alpha|\beta\rangle \equiv (|\alpha\rangle, |\beta\rangle)$$

  We call $\langle\alpha|$ the dual vector.

- **Properties of Inner Products**:
  - $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*$
  - $\langle\alpha|\alpha\rangle \geq 0$ with $\langle\alpha|\alpha\rangle = 0$ if and only if $|\alpha\rangle = 0$
  - Linearity in the original vector space,

$$\langle\alpha|\left(b\,|\beta\rangle + c\,|\gamma\rangle\right) = b\,\langle\alpha|\beta\rangle + c\,\langle\alpha|\gamma\rangle$$

  A vector space equipped with an inner product is called an inner product space.

1.1.5 Orthonormal Basis

The norm of a vector in the vector space V is given by the relation

$$||V|| \to \mathbb{R}$$

*Note the scalar field associated with V can be complex in general. For inner product spaces, the inner product naturally allows one to define a norm such that

$$||\alpha|| = \sqrt{\langle\alpha|\alpha\rangle} \in \mathbb{R},\ \therefore\ \langle\alpha|\alpha\rangle \geq 0$$

The norm generalizes the notion of length. It is positive definite, homogeneous, and sub-additive. Allows for the definition of a metric $||\alpha - \beta||$ between vectors.

- A vector $|\alpha\rangle$ with unit norm is "normalized".
- Two vectors that satisfy $\langle\alpha|\beta\rangle = 0$ are said to be "orthogonal".

Consider the basis $\{|v_i\rangle\}$ that satisfies $\langle v_i|v_j\rangle = \delta_{ij}$ and therefore forms an orthonormal basis. Now if,

$$|\alpha\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} \text{ and } |\beta\rangle = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

$$\langle\alpha|\beta\rangle = a_1^* b_1 + a_2^* b_2 + ... + a_n^* b_n$$

Also, $\langle\alpha| = \begin{pmatrix} a_1^* & a_2^* & \cdots & a_n^* \end{pmatrix}$ is the row vector whose components and conjugate of $|\alpha\rangle$.

Exercise : Show that, $||\alpha||^2 = \langle\alpha|\alpha\rangle = \sum_i |a_i|^2$.

One can generalize the notion of an angle through the relation;

$$cos\theta = \frac{|\,\langle\alpha|\beta\rangle\,|}{\sqrt{\langle\alpha|\alpha\rangle\,\langle\beta|\beta\rangle}}$$

The absolute value of $cos\theta$ is less than 1 as,

$$|\,\langle\alpha|\beta\rangle\,|^2 \leq \langle\alpha|\alpha\rangle\,\langle\beta|\beta\rangle \ \text{(Cauchy - Shwarz Inequality)}$$

Exercise : Suppose $\{|w_i\rangle\}$ is a basis set for an inner product space. Show that one can find an orthonormal basis $\{|v_i\rangle\}$ by the iterative method :

$$\text{Set } |v_1\rangle = \frac{|w_1\rangle}{\sqrt{\langle w_1|w_1\rangle}} = \frac{|w_1\rangle}{||\,|w_1\rangle\,||}$$

$$\text{For } 1 \leq k \leq d-1;\ |v_{k+1}\rangle = \frac{|w_{k+1}\rangle - \sum_{i=1}^{k} \langle v_i|w_{k+1}\rangle\,|v_i\rangle}{||\ |w_{k+1}\rangle - \sum_{i=1}^{k} \langle v_i|w_{k+1}\rangle\,|v_i\rangle\,||}$$

This is called the **Gram-Schmidt procedure**. Prove that $\{|v_i\rangle\}$ is indeed orthonormal.

Note:

- A **Banach Space** is a vector space over $\mathbb{R}$ and $\mathbb{C}$ equipped with a norm, and it is complete with respect to that norm.
- A **Hilbert Space** is a vector space equipped with an inner product and it is complete with respect to the norm induced by that inner product.

1.1.6 Linear Operators and Matrices

A linear operator takes every vector in a vector space and "transforms" into another vector, keeping the linear structure intact,

$$T : V \to W \text{ such that } T(a\,|\alpha\rangle + b\,|\beta\rangle) = aT\,|\alpha\rangle + bT\,|\beta\rangle$$

Another example:

$$T\,|\alpha\rangle = T(\sum_i a_i\,|v_i\rangle) = \sum_i a_i T\,|v_i\rangle$$

For instance the identity operator and the null operator,

$$I\,|\alpha\rangle = |\alpha\rangle\,;\ 0\,|\alpha\rangle = 0$$

Matrices provide the most convenient way to represent linear operators and can be easily integrated with the row and column matrices for the vector and dual-vector space. Let $\{|v_i\rangle\}$ be the basis for V and $\{|w_i\rangle\}$ be the basis for W, and $T : V \to W$

$$T\,|v_1\rangle = \sum_{i=1}^{m} t_{i1}\,|w_i\rangle$$

$$T\,|v_2\rangle = \sum_{i=1}^{m} t_{i2}\,|w_i\rangle$$

$$\vdots$$

$$T\,|v_n\rangle = \sum_{i=1}^{m} t_{in}\,|w_i\rangle$$

So, if

$$|\alpha\rangle = \sum_{j=1}^{n} a_j |v_j\rangle \,;\, T|\alpha\rangle = \sum_{j=1}^{n} a_j T |v_j\rangle$$

$$T|\alpha\rangle = \sum_{j=1}^{n} a_j \sum_{i=1}^{m} t_{ij} |w_i\rangle = \sum_{i=1}^{m}\sum_{j=1}^{n} t_{ij} a_j |w_i\rangle$$

Therefore the linear operator T transforms the components,

$$T|\alpha\rangle = |\beta\rangle \,;\, |\beta\rangle = \sum_{i=1}^{m} b_i |w_i\rangle \,;\, b_i = \sum_{j=1}^{n} t_{ij} a_j$$

$$T = \begin{pmatrix} t_{11} & t_{12} & t_{13} & \cdots & t_{1n} \\ t_{21} & t_{22} & t_{23} & \cdots & t_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t_{m1} & t_{m2} & t_{m3} & \cdots & t_{mn} \end{pmatrix} \quad \big\} \text{ Operator Matrix}$$

- **Outer Product**: One can use the relations of inner products and linear operators to represent T using the "outer product". Let us say $T : V \to W$ such that $T|\alpha\rangle = |\beta\rangle$. Define, $T = |\beta\rangle\langle\alpha|$, such that

  $$T|\alpha'\rangle = |\beta\rangle\langle\alpha|\alpha'\rangle = \langle\alpha|\alpha'\rangle|\beta\rangle$$

  If $\{|w_i\rangle\}$ and $\{|v_j\rangle\}$ are both orthonormal, then

  $$T = \sum_{ij} t_{ij} |w_i\rangle\langle v_j| \,;\, t_{ij} = \langle w_i|T|v_j\rangle$$

  An important result that comes up is the "completeness relation" for orthonormal vectors. Let $\{|v_i\rangle\}$ be an orthonormal basis set;

  $$|v\rangle = \sum_i a_i |v_i\rangle \text{ such that } \langle v_i|v\rangle = a_i, \text{ which then gives us,}$$

  $$|v\rangle = \sum_i |v_i\rangle\langle v_i|v\rangle = (\sum_i |v_i\rangle\langle v_i|)|v\rangle$$

  $$\sum_i |v_i\rangle\langle v_i| = I \quad \text{(Identity)}$$

1.1.7 Some properties of linear operators and matrices

It is now quite evident that the study of linear operators simply reduces to the study of matrices.
So, if you have two linear operators A and B, then
The sum:

$$(A + B)|\alpha\rangle = A|\alpha\rangle + B|\alpha\rangle$$

The product:

$$A(B|\alpha\rangle) = AB|\alpha\rangle$$

Similarly,

$$|\alpha'\rangle = A|\alpha\rangle\,,\; a'_i = \sum_j A_{ij}a_j$$

- The transpose of an operator A^T, interchanges the rows and columns.
- For a symmetric operator: $A = A^T$
- The complex conjugate of an operator A^*, is when all elements are replaced by their complex conjugates.
- The Hermitian conjugate or adjoint $A^\dagger$ is defined as,

$$A^\dagger = (A^*)^T$$

- A square matrix is hermitian if $A^\dagger = A$
- Matrix multiplication is not commutative in general.

$$\text{(Commutator) } [A, B] = AB - BA$$

$$\text{(Anti-Commutator) } \{A, B\} = AB + BA$$

- $(AB)^T = B^T A^T$ and $(AB)^\dagger = B^\dagger A^\dagger$
- $A^{-1}A = AA^{-1} = I,$ for a square, non-singular matrix A
- A matrix is non-singular iff $det(A) \neq 0$.
- A matrix is unitary if its inverse is equal to its adjoint.

$$A^{-1} = A^\dagger \implies AA^\dagger = A^\dagger A = I$$

Exercise :

1. Show that every real symmetric operator is also Hermitian.
2. Find the properties of the determinant and the trace of a matrix.

1.1.8 Changing the basis of the space

Now we know that a vector space can be spanned by multiple basis states. Consider $\{|v_i\rangle\}$ and $\{|w_i\rangle\}$.

$$|v_1\rangle = s_{11}|w_1\rangle + s_{21}|w_2\rangle + \cdots + s_{n1}|w_n\rangle\,, \quad \{|w_i\rangle\} \text{ forms a basis}$$

$$\therefore |v_j\rangle = \sum_i S_{ij}|w_i\rangle$$

Now,

$$|\alpha\rangle = \sum_i \bar{a}_i |w_i\rangle = \sum_j a_j |v_j\rangle = \sum_j a_j \sum_i S_{ij} |w_i\rangle = \sum_i (\sum_j S_{ij} a_j) |w_i\rangle$$

$$\therefore \tilde{a}_i = \sum_j S_{ij} a_j$$

$\implies |\alpha\rangle_{\{|w_i\rangle\}} = S |\alpha\rangle_{\{|v_j\rangle\}}$ (Representation of the same vector changes via multiplication by S.)

$$\implies |\tilde{\alpha}\rangle = S |\alpha\rangle$$

*Note $|\tilde{\alpha}\rangle$ and $|\alpha\rangle$ are the same vector but written in different bases.

So, how does an arbitrary linear operator (T) change due to the change in basis?

$$|\beta\rangle = T |\alpha\rangle, \quad \text{where both } |\beta\rangle \text{ and } |\alpha\rangle \text{ use basis } \{|v_j\rangle\}$$

Now, for the change of basis from $\{|v_j\rangle\}$ to $\{|w_i\rangle\}$, we have

$$|\tilde{\alpha}\rangle = S |\alpha\rangle, \quad \text{where the tilde refers to use of basis } \{|v_j\rangle\}$$

So, we have $|\alpha\rangle = S^{-1} |\tilde{\alpha}\rangle$.

$$S |\beta\rangle = ST |\alpha\rangle \Rightarrow |\tilde{\beta}\rangle = STS^{-1} |\tilde{\alpha}\rangle \Rightarrow |\tilde{\beta}\rangle = \tilde{T} |\tilde{\alpha}\rangle$$

Hence, we have the basis transformation for a linear operator:

$$\tilde{T} = STS^{-1}$$

Two matrices T_1 and T_2 are similar if $T_1 = ST_2S^{-1}$, for any non-singular matrix S.

1.1.9 Eigenvectors and Eigenvalues

An eigenvector of operator A satisfies

$$A |v\rangle = \lambda |v\rangle, \quad |v\rangle \neq 0$$

Eigenvectors $|v\rangle$ and eigenvalues λ are obtained by solving the characteristic equation:

$$c(\lambda) = \det (A - \lambda I) = 0,$$

with the solutions being the eigenvalues.

The collection of all eigenvalues is called the *spectrum*.
If the eigenvectors span the space, they can form a basis, and in this basis, the operator A is a diagonal matrix with eigenvalues as the diagonal elements.

For transformation from an arbitrary basis to the eigenbasis, the similarity transformation S is constructed by using the eigenvectors $\{|v_i\rangle\}$ as the columns of S^{-1}.

So if A has a basis of eigenvectors $\{|v_i\rangle\}$, then there exists a similarity transformation

$$(S^{-1})_{ij} = (\langle v_i|)_j$$

such that

$$A_{\text{diag}} = SAS^{-1}$$

where the diagonal elements are the eigenvalues $\{\nu_i\}$.

- Every **normal matrix**, i.e., $A^\dagger A = AA^\dagger$ is diagonalizable.
- Diagonal representation:

$$A = \sum_i \lambda_i \left|i\right\rangle \left\langle i\right|, \quad \langle i|j\rangle = \delta_{ij}$$

  where λ_i are the eigenvalues.

- Any two matrices A and B that commute can be diagonalized with the same similarity transformation. $\implies$ A and B can be **simultaneously diagonalized**.
- **Adjoint Operators** — The Hermitian adjoint of a linear operator A is defined by the following:

$$\langle A^\dagger \alpha|\beta\rangle = \langle \alpha|A|\beta\rangle \quad \forall \left|\alpha\right\rangle, \left|\beta\right\rangle \in V$$

  In the language of dual vector space, we see:

$$\langle \alpha|A|\beta\rangle = \alpha^\dagger A b = (A^\dagger \alpha)^\dagger b = \langle A^\dagger \alpha|\, \beta$$

  Adjoint corresponds to vector in the dual space.

- Properties of **Hermitian Operators**, i.e., $A^\dagger = A$
  1. A has real eigenvalues.
  2. The eigenvectors of A with distinct eigenvalues are orthogonal.
  3. Eigenvectors of A spans the space and therefore is diagonalizable.

1.1.10 Tensor Product

A tensor product is a general method for constructing larger vector spaces from smaller constituent vector spaces. It plays a crucial role in understanding various aspects of quantum mechanics, ranging from entanglement to strongly correlated many-body quantum systems. Say, V and W are vector spaces of dimension m and n, then

$$V \otimes W \text{ is a vector space of dimension } m \times n$$

If $\{\left|v_i\right\rangle\}_{i=1}^m$ and $\{\left|w_j\right\rangle\}_{j=1}^n$ are the orthonormal basis, then the new vector space is spanned by the basis

$$\{\left|z_k\right\rangle\}_{k=1}^{mn} = \{\left|v_i\right\rangle\}_{i=1}^m \otimes \{\left|w\right\rangle_j\}_{j=1}^n$$

Consider the famous **Bell state** or the singlet state:

$$\left|\psi\right\rangle = \frac{1}{\sqrt{2}}\{\left|01\right\rangle - \left|10\right\rangle\} = \frac{1}{\sqrt{2}}\{\left|0\right\rangle_A \otimes \left|1\right\rangle_B - \left|1\right\rangle_A \otimes \left|0\right\rangle_B\}$$

$$\{\left|0\right\rangle, \left|1\right\rangle\} \in V \otimes V$$

Properties of tensor product

1. $z(|v\rangle \otimes |w\rangle) = z\,|v\rangle \otimes |w\rangle = |v\rangle \otimes z\,|w\rangle$
2. $(|v_1\rangle + |v_2\rangle) \otimes |w\rangle = |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle$
3. $(A \otimes B)(|v\rangle \otimes |w\rangle) = A\,|v\rangle \otimes B\,|w\rangle$

Some examples of tensor product: Let $|v\rangle \in V$ and $|w\rangle \in W$, such that

$$|v\rangle = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \text{ and } |w\rangle = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$$

$$|v\rangle \otimes |w\rangle = \begin{pmatrix} v_1 \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} \\ v_2 \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} v_1 w_1 \\ v_1 w_2 \\ v_2 w_1 \\ v_2 w_2 \end{pmatrix}$$

Again, let A and B be to linear operators acting on V and W respectively, such that

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \text{ and } B = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}$$

Similarly, tensor products can be applied to higher dimensional vector spaces.

2. Quantum State, Evolution and Measurements

In the previous section, we established that quantum mechanical states and operators are naturally associated with a certain type of vector space. This raises a question: **What are the defining properties of a quantum system?**

2.1 Axioms : Quantum State, Observables, Evolution, and Measurement

- The state space of an isolated quantum system is associated with a Hilbert space. The state of the system is represented by a **unit vector** in this Hilbert space.

Hilbert Space:

- Complex vector space
- Equipped with an inner product
- Normed and complete

Note: We assume that the relevant Hilbert space is finite-dimensional.

A quantum state, denoted as $|\psi\rangle$, is a vector (more precisely, a ray) in Hilbert space $\mathcal{H}$:

$$|\psi\rangle \in \mathcal{H}$$

The inner product between two states $|\psi\rangle$ and $|\phi\rangle$ is written as:

$$\langle\psi|\phi\rangle \in \mathbb{C}, \qquad \langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$$

The norm of a state (unit norm condition) is given by:

$$\| \, |\psi\rangle \, \|^2 = \langle\psi| \, |\psi\rangle = 1$$

Principle of superposition : any linear combination of valid states is also a valid state:

$$a\,|\psi\rangle + be^{i\phi}\,|\phi\rangle \qquad (a, b \in \mathbb{C},\ \phi \in \mathbb{R})$$

The dual vector space consists of linear functionals:

$$\langle\phi| : |\psi\rangle \mapsto \langle\phi|\psi\rangle \in \mathbb{C}$$

Remark: Global phases do not affect the physical state. Therefore, a quantum state $|\psi\rangle$ is actually represented by the set of vectors $\{e^{i\chi}\,|\psi\rangle \mid \chi \in \mathbb{R}\}$, which is referred to as a *ray*.

2.1.1 Comparison with the Wavefunction Representation

How does this formalism compare to the familiar quantum state $\Psi(x)$?

$$\begin{aligned}
|\psi\rangle &\longrightarrow \Psi(x) && \text{(function as vectors in } \mathcal{H}) \\
\langle\phi|\psi\rangle &\longrightarrow \int \phi^*(x)\,\psi(x)\,dx && \text{(inner product)} \\
\langle\psi|\phi\rangle &\longrightarrow \int \psi^*(x)\,\phi(x)\,dx \\
\|\,|\psi\rangle\,\| = 1 &\longrightarrow \int |\psi(x)|^2 dx = 1 && \text{(normalized)} \\
|\psi\rangle = \sum_n c_n\,|\phi_n\rangle &\longrightarrow \Psi(x) = \sum_n c_n\,\phi_n(x)
\end{aligned}$$

For infinite-dimensional spaces, we assume the space is complete.

2.1.2 Hermitian Operators and Quantum Measurement

All observables are self-adjoint (Hermitian) operators on the Hilbert space.

The adjoint of a quantum operator A is denoted $A^\dagger$ and is defined by

$$\langle\phi|\,A\,|\psi\rangle = \langle A^\dagger\phi|\psi\rangle$$

For any observable A, $A^\dagger = A$: all observables are Hermitian. Diagonalizable Hermitian operators can be written as (a_n are real eigenvalues, $|\phi_n\rangle$ are orthonormal eigenstates) :

$$A = \sum_n a_n\;|\phi_n\rangle\,\langle\phi_n|$$

Hermitian operators have a **discrete spectrum** ($\{|\phi_n\rangle\}$ forms an orthonormal basis and $a_n \in \mathbb{R}$, the projector $|\phi_n\rangle\,\langle\phi_n|$ projects to the eigenspace of a_n.) :

$$A = \sum_n a_n\;|\phi_n\rangle\,\langle\phi_n|$$

Quantum measurements use linear operators $\{M_i\}$ with outcomes m_i. For $|\psi\rangle$:

$$p(m_i) = \langle\psi|\,M_i^\dagger M_i\,|\psi\rangle$$

Post-measurement state: $|\psi_f\rangle = \dfrac{M_i\,|\psi\rangle}{\sqrt{\langle\psi|\,M_i^\dagger M_i\,|\psi\rangle}}$

Measurement operators satisfy the completeness relation: $\sum_i M_i^\dagger M_i = I$

Example: $|\psi\rangle = a|0\rangle + b|1\rangle$, $M_0 = |0\rangle\langle 0|$ and $M_1 = |1\rangle\langle 1|$

$$M_0^\dagger M_0 + M_1^\dagger M_1 = I$$

Born's rule :

$$p(m_0 = 0) = \langle\psi| M_0^\dagger M_0 |\psi\rangle = \langle\psi| 0\rangle\langle 0 |\psi\rangle = |a|^2$$
$$p(m_1 = 1) = \langle\psi| M_1^\dagger M_1 |\psi\rangle = \langle\psi| 1\rangle\langle 1 |\psi\rangle = |b|^2$$

Exercise:
i) Prove that $\sum_i M_i^\dagger M_i = I$
ii) Calculate the post-measurement state in the above example.

2.1.3 Time Evolution of a Closed Quantum System

The time evolution of a closed quantum system is determined by a unitary operator. Given an initial state $|\psi_i\rangle$, U is a unitary operator satisfying $U^\dagger U = UU^\dagger = \mathbb{I}$, the evolution is described by

$$|\psi_i\rangle \longrightarrow U|\psi_i\rangle = |\psi_f\rangle$$

At this stage, quantum mechanics does not specify which particular U describes the actual dynamics of the system.

Restatement: The time evolution of a closed system is determined by the Schrödinger equation:

$$\frac{d}{dt}|\psi(t)\rangle = -iH|\psi(t)\rangle$$

Here, H is the Hamiltonian of the system and, in general, can be time-dependent. Importantly, H is a Hermitian operator.

For infinitesimal time intervals Δt, $U(t+\Delta t, t)$ represents the unitary operator for evolution from t to $t+\Delta t$, the evolution proceeds via:

$$\begin{aligned}|\psi(t+\Delta t)\rangle &= (\mathbb{I} - iH(t)\,\Delta t)\,|\psi(t)\rangle \\ &= \underbrace{e^{-iH(t)\,\Delta t}}_{U(t+\Delta t,\, t)}|\psi(t)\rangle\,,\end{aligned}$$

Importantly, the evolution of the closed system is a linear transformation in the Hilbert space $\mathcal{H}$, which contains the states of the physical system. The complexity of the system lies in its complex description.

The Hamiltonian has a **spectral decomposition**, where E_n and $|E_n\rangle$ are the energy eigenvalues and eigenstates respectively.

$$H = \sum_n E_n |E_n\rangle \langle E_n| ,$$

In the energy eigenbasis, using $c_n = \langle E_n|\psi\rangle$ as expansion coefficients, any state $|\psi\rangle$ can be written as :

$$|\psi\rangle = \sum_n c_n |E_n\rangle ,$$

Therefore, the infinitesimal time evolution gives:

$$|\psi(t+\Delta t)\rangle = e^{-iH\Delta t} |\psi(t)\rangle$$

$$= e^{-iH\Delta t} \sum_n c_n(t) |E_n\rangle$$

$$= \sum_n e^{-iE_n\Delta t} c_n(t) |E_n\rangle \qquad \text{(assuming } H \text{ is constant for } \Delta t\text{)}$$

For Hermitian H: $e^{-iH\Delta t} |E_n\rangle = e^{\text{const}} |E_n\rangle$ since $H |E_n\rangle = E_n |E_n\rangle$

Composite System Structure and Hamiltonian Action

The Hilbert space of the composite system is:

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \quad \text{with basis } \{|i_A\rangle \otimes |j_B\rangle\}$$

where $\{|i_A\rangle\}$ and $\{|j_B\rangle\}$ are orthonormal bases for $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. The dimension of the composite system is:

$$d = d_A \times d_B.$$

2.2 Measurement: Projective vs. POVM

In our discussion of the axioms/postulates, we focused on a very special form of measurement: **Operators $\{M_i\}$ with outcomes $\{m_i\}$:**

$$M_i |\psi\rangle , \qquad \text{with probability } p(m_i) = \langle\psi| M_i^\dagger M_i |\psi\rangle .$$

Most discussions in quantum mechanics are focused on **projective measurements**.

Suppose we want to measure an observable P (a Hermitian operator) with real eigenvalues $\{p_i\}$ and eigenstates $\{|p_i\rangle\}$ (spectral representation):

$$P = \sum_i p_i |p_i\rangle \langle p_i| \,.$$

For projective measurement: $M_i = |p_i\rangle \langle p_i| \,, P = \sum_i p_i M_i$.

The outcome p_i is obtained with probability $|\langle p_i|\psi\rangle|^2$, and the post-measurement state is $|p_i\rangle$.

Expectation/average value of an observable:

$$E(P) = \sum_i p_i \, \mathrm{prob}(m_i) = \sum_i p_i \langle\psi| M_i^\dagger M_i |\psi\rangle = \langle\psi| P |\psi\rangle \,.$$

Exercise: Calculate the standard deviation of P.

Example of a projective measurement: $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Eigenvalues: $+1, -1$ and projectors $|0\rangle \langle 0|$, $|1\rangle \langle 1|$.

For a quantum state $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$:

$$M_1 = |0\rangle \langle 0| \,, \qquad M_2 = |1\rangle \langle 1|$$

$$\text{Expectation value:} \quad \langle\psi| \sigma_z |\psi\rangle = (|\alpha|^2 - |\beta|^2)$$

$$\langle\psi| M_1 |\psi\rangle = |\alpha|^2, \qquad \langle\psi| M_2 |\psi\rangle = |\beta|^2$$

Note: It is quite common to associate projective measurements with a Hermitian operator, but not all measurements are projective.

Generalizing: In principle, one can extend the notion of measurement to any "general" positive valued operator.

Operators: $\{M_i\}$ with outcomes $\{m_i\}$ and $\sum_i M_i^\dagger M_i = I$

One can define a positive semi-definite operator, $E_i = M_i^\dagger M_i$

The set of operators $\{E_i\}$ is called a POVM (positive operator valued measurement) with outcome probability:

$$p(m_i) = \langle\psi| E_i |\psi\rangle \,, \qquad \sum_i E_i = I$$

Note that a POVM does not give you a well-defined post-measurement state.

2.3 Distinguishing Quantum States

Consider two parties: Alice and Bob. Alice prepares a state $|\psi_i\rangle$ where $i = 1, \ldots, n$. Bob performs a measurement with operators $\{M_j\}$ (e.g., $M_1 = |1\rangle\langle 1|$, $M_2 = |0\rangle\langle 0|$).

If the set $\{|\psi_i\rangle\}$ is orthonormal, Bob can reliably distinguish the states, always getting the correct answer.

For $M_j = |\psi_j\rangle\langle\psi_j|$, the probability of outcome j is

$$p_j = |\langle\psi_j| M_j |\psi_j\rangle|^2 = 1.$$

But what happens if $\{|\psi_i\rangle\}$ is not orthonormal?

For simplicity, assume Alice sends either $|\psi_1\rangle$ or $|\psi_2\rangle$, where $\langle\psi_1|\psi_2\rangle \neq 0$, and since $\langle\psi_1|\phi\rangle = 0$ and $\langle\phi|\phi\rangle = 1$:

$$|\psi_2\rangle = \alpha|\psi_1\rangle + \beta|\phi\rangle, \qquad |\alpha|^2 + |\beta|^2 = 1, \quad |\beta| < 1,$$

Suppose Bob's measurement satisfies the following :

$$\langle\psi_1| M_1^\dagger M_1 |\psi_1\rangle = 1 \qquad \text{and} \qquad \langle\psi_2| M_2^\dagger M_2 |\psi_2\rangle = 1 \tag{϶}$$

From the completeness relation $\sum_i M_i^\dagger M_i = \mathbb{I}$, it follows that

$$\sum_i \langle\psi_1| M_i^\dagger M_i |\psi_1\rangle = 1 \quad \Rightarrow \quad \langle\psi_1| M_2^\dagger M_2 |\psi_1\rangle = 0 \quad \Rightarrow \quad M_2|\psi_1\rangle = 0$$

Now, as $M_2|\psi_2\rangle = \alpha M_2|\psi_1\rangle + \beta M_2|\phi\rangle = \beta M_2|\phi\rangle$, $|\beta| < 1$, $\langle\phi| M_2^\dagger M_2 |\phi\rangle \leq 1$. We get :

$$\langle\psi_2| M_2^\dagger M_2 |\psi_2\rangle = |\beta|^2 \langle\phi| M_2^\dagger M_2 |\phi\rangle < 1 \tag{ϖ}$$

Also, since $\sum_i M_i^\dagger M_i = \mathbb{I}$:

$$\langle\phi| M_2^\dagger M_2 |\phi\rangle \leq \sum_i \langle\phi| M_i^\dagger M_i |\phi\rangle = 1,$$

The assumptions in (϶) and (ϖ) are contradictory: perfect discrimination of non-orthogonal states is impossible.

What can be done if Bob chooses to use a POVM?

Let us assume Alice sends $|\psi_1\rangle = |0\rangle$ and $|\psi_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$.

In this instance, Bob uses a POVM $\{E_1, E_2, E_3\}$:

$$E_1 = \frac{\sqrt{2}}{1+\sqrt{2}} \left|1\right\rangle \left\langle 1\right|$$

$$E_2 = \frac{\sqrt{2}}{1+\sqrt{2}} \cdot \frac{1}{2}(\left|0\right\rangle \left\langle 0\right| - \left|0\right\rangle \left\langle 1\right| - \left|1\right\rangle \left\langle 0\right| + \left|1\right\rangle \left\langle 1\right|)$$

$$E_3 = \mathbb{I} - E_1 - E_2$$

Now if Alice sends the state $\left|\psi_1\right\rangle = \left|0\right\rangle$ and Bob measures E_1, then

$$\left\langle \psi_1\right| E_1 \left|\psi_1\right\rangle = 0 \Rightarrow \text{if } E_1 \neq 0,\ \left|\psi_2\right\rangle \text{ is detected.}$$

Similarly, $E_2 \neq 0 \Rightarrow$ that the state is $\left|\psi_1\right\rangle$.

For other outcomes, Bob is unable to give an answer.

Importantly, Bob does not make a mistake using POVM.

2.4 Measurement in a composite system

From the axiom, a composite system has a combined state space given by the tensor product:

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$$

$$\text{Quantum states:} \quad \left|i\right\rangle_{AB} = \left|i\right\rangle_A \otimes \left|j\right\rangle_B$$

$$\text{Quantum operators:} \quad (M_A \otimes M_B) \left|\psi\right\rangle_{AB}$$

$$\left|\psi\right\rangle_{AB} = \sum_{i,j} a_{ij} \left|i\right\rangle_A \otimes \left|j\right\rangle_B$$

Consider a quantum system Q and we want to use measurement operators $\{M_i\}$. We consider an "ancilla" system M with an orthonormal basis $\{\left|m_i\right\rangle\}$ that corresponds to the possible outcomes of M.

Let us define an operator U that gives us:

$$U \left|\psi\right\rangle \otimes \left|0\right\rangle = \sum_i M_i \left|\psi\right\rangle \otimes \left|m_i\right\rangle$$

$$\left\langle \phi\right| \left\langle 0\right| U^\dagger U \left|\psi\right\rangle \left|0\right\rangle = \sum_{i,i'} \left\langle \phi\right| M_i^\dagger M_{i'} \left|\psi\right\rangle \left\langle m_{i'}|m_i\right\rangle$$

$$= \sum_i \left\langle \phi|M_i^\dagger M_i|\psi\right\rangle = \left\langle \phi|\psi\right\rangle$$

($U^\dagger U = I$ preserves inner product and can be generalized to a unitary.)

Make a joint projective measurement $\{P_i\}$:

$$P_i = \mathbb{I}_Q \otimes |m_i\rangle \langle m_i|$$

$$\begin{aligned} p(m_i) &= \langle\psi| \langle 0| U^\dagger (\mathbb{I}_Q \otimes |m_i\rangle \langle m_i|) U |\psi\rangle |0\rangle \\ &= \sum_{j,j'} \langle\psi| M_j^\dagger \langle m_j|m_i\rangle \langle m_i|m_{j'}\rangle M_j |\psi\rangle \\ &= \langle\psi| M_i^\dagger M_i |\psi\rangle \end{aligned}$$

Joint quantum state of the system after P_i:

$$(\mathbb{I}_Q \otimes |m_i\rangle \langle m_i|) U |\psi\rangle |0\rangle / \sqrt{p(m_i)}$$

$$= (\mathbb{I}_Q \otimes |m_i\rangle \langle m_i|) \sum_j M_j |\psi\rangle \otimes |m_j\rangle / \sqrt{p(m_i)}$$

$$= M_i |\psi\rangle \otimes |m_i\rangle / \sqrt{\langle\psi| M_i^\dagger M_i |\psi\rangle}$$

So, POVM is an operator U and projective measurement in a composite system.

2.4.1 Projective Realization of POVMs

- Measure the state $|\psi\rangle$ in system Q with a POVM $\{E_i\}$, where $E_i = M_i^\dagger M_i$ and $\{M_i\}$ is a set of linear operators on Q.
- We couple Q with an ancilla A (think of this as a measuring apparatus coupled to Q). The ancilla A has an orthonormal basis $\{|m_i\rangle\}$.

So, how does POVM work?

$$\{E_i = M_i^\dagger M_i\} \text{ acts on } Q \qquad \xrightarrow{\text{Probability}} \qquad p(m_i) = \langle\psi| E_i |\psi\rangle$$

Now think of the composite state in $Q + A$, say the state is $|\psi\rangle \otimes |0\rangle$, where $|0\rangle$ is some fixed state in A and the POVM $\{E_i\} = \{M_i^\dagger M_i\}$ acts on Q.

We can always find an operator $U = \sum_i M_i \otimes |m_i\rangle \langle 0|$ such that:

$$U |\psi\rangle \otimes |0\rangle = \sum_i M_i |\psi\rangle \otimes |m_i\rangle$$

Now, let's see how this works:

$$U |\psi\rangle |0\rangle = \sum_i M_i |\psi\rangle |m_i\rangle$$

$$\langle 0| \langle\psi| U^\dagger U |\psi\rangle |0\rangle = \sum_{i,i'} \langle m_i| \langle\psi| M_i^\dagger M_{i'} |\psi\rangle |m_{i'}\rangle$$

$$= \sum_{i,i'} \langle\psi|M_i^\dagger M_{i'}|\psi\rangle \langle m_i|m_i'\rangle$$

$$= \sum_i \langle\psi| M_i^\dagger M_i |\psi\rangle = \langle\psi| \left(\sum_i E_i\right) |\psi\rangle$$

$$= \langle\psi| I |\psi\rangle = 1 \qquad (\text{since } \sum_i E_i = I)$$

Exercise: U can be extended to be unitary, i.e., $U^\dagger U = I$.

So the joint state in $Q + A$ is $|\Phi\rangle = U|\psi\rangle|0\rangle$ and we use the projective measurement $\{\mathbb{I}_Q \otimes |m_i\rangle\langle m_i|\}$.

Probability:

$$p(m_i) = \langle\phi| (\mathbb{I}_A \otimes |m_i\rangle\langle m_i|) |\phi\rangle = \langle 0| \langle\psi| U^\dagger (\mathbb{I}_A \otimes |m_i\rangle\langle m_i|) U |\psi\rangle |0\rangle$$

$$= \sum_{j,j'} \langle m_j| \langle\psi| M_j^\dagger (\mathbb{I}_A \otimes |m_i\rangle\langle M_i|) M_{j'} |\psi\rangle |m_j'\rangle$$

$$= \sum_{j,j'} \langle\psi|M_j^\dagger \mathbb{I}_A M_{j'}|\psi\rangle \otimes \langle m_j|m_i\rangle \langle m_i|m_{j'}\rangle$$

$$= \langle\psi| M_i^\dagger M_i |\psi\rangle = \langle\psi| E_i |\psi\rangle$$

Thus, any POVM can be realized as a projective measurement on a larger Hilbert space.

2.5 A Quantum Bit - Qubit

The analogue to a classical computational bit is the qubit (a quantum bit).

What is a qubit? State in a 2D Hilbert space:

$$\{|0\rangle, |1\rangle\} \qquad \Longleftrightarrow \qquad \{|+\rangle, |-\rangle\} \qquad \Longleftrightarrow \qquad \{|H\rangle, |V\rangle\}$$

Linear operators in the qubit space are spanned by the Pauli operators and the identity:

$$\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

A qubit state in the σ_z basis:

$$|\psi\rangle = a|0\rangle + b|1\rangle$$

Measurement in σ_z basis gives:

$$p(|0\rangle) = |a|^2, \quad p(|1\rangle) = |b|^2, \quad |a|^2 + |b|^2 = 1$$

But a qubit is more than just probabilities - it contains information about all observables. Using spherical coordinates:

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle, \quad \theta \in [0,\pi],\ \phi \in [0,2\pi]$$

This parameterization allows visualization in a 3D unit sphere - the Bloch sphere. Constraints: Normalization ($|\alpha|^2 + |\beta|^2 = 1$) and global phase irrelevance leave two real parameters.

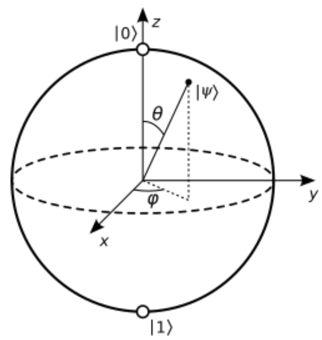

Figure 1: Bloch sphere

Bloch vector representation:

$$\hat{n} = (\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta) \quad \leftrightarrow \quad |\psi(\theta,\phi)\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$

Any spin component operator in space - $\hat{n}\cdot\vec{\sigma} = n_1\sigma_x + n_2\sigma_y + n_3\sigma_z$ satisfies :

$$\hat{n}\cdot\vec{\sigma}\,|\psi(\theta,\phi)\rangle = |\psi(\theta,\phi)\rangle$$

Even though measuring in the σ_z basis gives two outcomes ($|0\rangle$ or $|1\rangle$), there always exists an operator (like $\hat{n}\cdot\vec{\sigma}$) for which $|\psi(\theta,\phi)\rangle$ is an eigenstate. This reflects the qubit's ability to encode information about any observable.

Example: $|\psi(\pi/2,0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |+\rangle$

- In σ_z basis: $p(|0\rangle) = p(|1\rangle) = 1/2$
- In σ_x basis: $\sigma_x|+\rangle = |+\rangle \Rightarrow p(|+\rangle) = 1$

Exercises:

1. Find the other eigenstate of σ_x
2. Calculate $\langle\sigma_x\rangle$, $\langle\sigma_y\rangle$, and $\langle\sigma_z\rangle$ for $|\psi(\theta,\phi)\rangle$

3. Open Quantum Systems

Sometimes our system of interest S is not isolated. Rather, it interacts with or is embedded inside a larger space. Suppose there exists an environment $\mathcal{E}$ such that $S + \mathcal{E}$ forms the larger combined system.

The combined state of the system and environment is still described by a state vector:

$$|\Psi\rangle_{S+\mathcal{E}}$$

which follows the postulates of standard quantum mechanics for isolated systems.

However, the system S alone is no longer described by a single pure state $|\psi\rangle$. Instead, it is described by a statistical ensemble of states $\{|\psi_i\rangle\}$ with associated probabilities p_i. This is captured by the **density matrix**:

$$\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i|$$

As such, we must define a new set of rules to describe the unisolated or open system, governed by the density matrix ρ. These rules must be consistent with all the axioms that apply to the larger Hilbert space.

Why is this necessary?

- No quantum physical system of interest is truly isolated. To understand the interactions and dynamics, an "open system" description is essential.
- It allows for robust error correction in realistic systems.
- It provides a bridge between quantum mechanics and statistical physics.

Now,

$$\underbrace{|\Psi\rangle_{S+\mathcal{E}}}_{\text{contains all the knowledge of the larger } S+\mathcal{E} \text{ Hilbert space ("Closed")}} \Rightarrow \underbrace{\rho_S}_{\text{contains the knowledge of only the system } S \text{ ("Open")}}$$

Why does ρ_S only contain partial information or some ignorance?

An intuitive answer is because a lot of the information in $S+\mathcal{E}$ could be in the correlations between S and $\mathcal{E}$, which cannot be captured while defining ρ_S. On the other hand, if no correlation exists between S and $\mathcal{E}$, then ρ_S contains all the information about S i.e.,

$$\rho_S = |\psi\rangle \langle\psi|_S$$

So, one can connect $|\psi\rangle$ with complete information about a quantum system or a "pure state" and $\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i|$, with probabilistic or "mixed" state of a system.

3.1 The Density Matrix

Also called the "density operator"—it is an equivalent description of quantum states that take into account the fact that the relevant system is not isolated or closed.

3.1.1 Imperfect State Preparation - Ensemble of States

Imagine a quantum experiment that outputs the quantum state $|\psi\rangle$ - but each time there is a certain error, say due to fluctuations in the laser or some magnetic field. Say, we actually end up with the state $|\psi_i\rangle$ with probability p_i—an ensemble of pure states $\{p_i, |\psi_i\rangle\}$.
Expectation value of some observable A : $\langle\psi_i|A|\psi_i\rangle$ But instead of just $\langle\psi_i|A|\psi_i\rangle$ we have to deal with an ensemble of $\{|\psi_i\rangle\}$ with some probability $\{p_i\}$,

$$\langle A\rangle = \sum_i p_i \langle\psi_i|A|\psi_i\rangle$$

$$= \sum_{i,j} p_i \langle\psi_i|A|j\rangle \langle j|\psi_i\rangle$$

$\{|j\rangle\}$ is some complete orthonormal basis,

$$= \sum_{j,i} p_i \langle j|A|\psi_i\rangle \langle\psi_i|j\rangle$$

$$= \sum_j \langle j|A \sum_i p_i |\psi_i\rangle \langle\psi_i|\, j\rangle$$

So, the density matrix of the ensemble $\{p_i, |\psi_i\rangle\}$ is

$$\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i|$$

and

$$\langle A\rangle = Tr(A\rho)$$

It is easy to see that the density matrix of a quantum state $|\psi\rangle$ is nothing but $|\psi\rangle\langle\psi|$. Many texts refer to ρ as the state of a system.
A state $|\psi\rangle$ $(\rho = |\psi\rangle\langle\psi|)$ is called a "pure state", as opposed to an ensemble $\{p_i, |\psi_i\rangle\}$ $(\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|)$ which is called a "mixed state", implying it is a classical mixture of pure quantum states.

3.1.2 Properties of the Density Matrix ρ

- It is Hermitian :

$$\rho^\dagger = \sum_i p_i^* (|\psi_i\rangle\langle\psi_i|)^\dagger$$

$$= \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

$$= \rho$$

- It has unit trace:

$$Tr(\rho) = Tr(\sum_i p_i |\psi_i\rangle\langle\psi_i|)$$

$$\sum_i p_i Tr(|\psi_i\rangle\langle\psi_i|)^* = 1 \quad (\text{as } \sum_i p_i = 1 \text{ by definition})$$

- ρ is **positive semidefinite:**
  Any hermitian linear operator $M \in \mathcal{L}(\mathcal{H})$ is positive semidefinite if $\langle\phi|M|\phi\rangle \geq 0, \forall \ |\phi\rangle \in \mathcal{H}$.
  $$\langle\phi|\rho|\phi\rangle = \sum_i p_i \langle\phi|\psi_i\rangle \langle\psi_i|\phi\rangle$$
  $$\sum_i p_i |\langle\phi|\psi_i\rangle|^2 \geq 0, \text{ as } p_i \geq 0 \ \forall \ i$$
  If we diagonalize ρ and write its eigen decomposition or its spectral decomposition, then by extension of the above arguments we need all its eigenvalues to be positive.
  $$\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i|$$
  $$\sum_i \lambda_i |e_i\rangle \langle e_i| \,; \text{ where } \{\lambda_i, |e_i\rangle\} \text{ is the eigenvalues and eigenstates of } \rho$$
  Then ρ is positive semidefinite if $\lambda_i \geq 0 \ \forall \ i$. This holds true for all positive semidefinite matrices or operators.

- Measurements: Again we begin with set of operators $\{M_k\}$ with outcomes $\{m_k\}$. Let ρ correspond to some ensemble $\{p_i, |\psi_i\rangle\}$. Please note that $\sum_k M_k^\dagger M_k = I$. Probability of outcome m_k, subject to the state being $|\psi_i\rangle$ with probability p_i
  $$p(m_k|p_i) = \langle\psi_i|M_k^\dagger M_k|\psi_i\rangle$$
  So, the probability of getting the outcome m_k is
  $$p(m_k) = \sum_i p(m_k|p_i)p_i$$
  $$= \sum_i p_i \langle\psi_i|M_k^\dagger M_k|\psi_i\rangle$$
  $$= Tr(p_i M_k^\dagger M_k |\psi_i\rangle \langle\psi_i|)$$
  $$= Tr(M_k^\dagger M_k \rho)$$
  Similarly, for the post measurement state :-
  $$|\psi_i^k\rangle = M_k |\psi_i\rangle / \sqrt{p(m_k|p_i)}$$
  $$\therefore \rho_k = \sum_i p_i |\psi_i^k\rangle \langle\psi_i^k|$$
  $$= \sum_i p_i M_k |\psi_i^k\rangle \langle\psi_i^k| M_k^\dagger / p(m_k|p_i)$$
  $$= \frac{M_k \rho M_k^\dagger}{Tr(M_k^\dagger M_k \rho)}.$$

- Quantum Evolution: For closed system the evolution is straight forward,

$$\rho \xrightarrow{u} \sum_i p_i u |\psi_i\rangle \langle\psi_i| u^\dagger = u_\rho u^\dagger$$

In general, any quantum evolution is described a linear operator, $\rho \to \mathcal{E}(\rho)$, such that $\rho(t) = \mathcal{E}\rho(0)$ is also a valid density matrix.

- Composite System : Again similar to the axioms of quantum mechanics, the Hilbert Space is a tensor product and since density matrices are linear operators,

$$\rho \to \rho_1 \otimes \rho_2 \otimes \rho_3 \otimes ... \otimes \rho_N$$

Exercise:

1. Prove that $Tr(|\psi\rangle \langle\psi|) = 1$ in words.
2. Show that one can define $\rho = \sum_i p_i\rho_i$, where ρ_i is a set of mixed state density matrices i.e., $\rho_i \neq |\psi_i\rangle \langle\psi_i|$.
3. Prove that $\langle\phi|M|\phi\rangle \in \mathbb{R}$ if M is Hermitian.

3.1.3 The Density Matrix of a Qubit

Let us consider an operational definition of a density matrix in the qubit Hilbert space. Therefore, φ for a qubit is a 2×2 Hermitian matrix that satisfies:

$$\text{eig}(\varphi) \geq 0 \quad \text{and} \quad \text{Tr}(\varphi) = 1.$$

$$\varphi = \begin{pmatrix} a & c \\ c^* & b \end{pmatrix}, \quad a + b = 1.$$

Now, we know that all linear operators in the qubit space are spanned by the Pauli matrices and the identity:

$$\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

So any Hermitian φ can be written as:

$$\varphi = \alpha \left[I + x\sigma_x + y\sigma_y + z\sigma_z\right].$$

Now, $\text{Tr}(\sigma_i) = 0$ for $i = x, y, z$, therefore $\alpha = \frac{1}{2}$, and we have:

$$\varphi = \frac{1}{2}\left(I + \vec{r} \cdot \vec{\sigma}\right),$$

where $\vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$ and $\vec{r} = \{x, y, z\}$. For positivity condition, $\text{eig}(\varphi) \geq 0$.

$$\text{eig}(\varphi) = \frac{1}{2}\left(1 \pm \sqrt{x^2 + y^2 + z^2}\right) \geq 0.$$

So for $\text{eig}(\varphi) \geq 0$, we need:

$$\vec{r} \cdot \vec{r} = x^2 + y^2 + z^2 \leq 1.$$

Therefore, the length of the Bloch vector $\vec{r}$ is less than or equal to unity. For $|\vec{r}| = 1$, $\text{eig}(\varphi) = 1, 0$, and $\varphi = |\psi\rangle\langle\psi|$ and is therefore pure.

Importantly, if we consider a Bloch sphere, all vectors that lie on the surface of the sphere are pure quantum states.

3.1.4 The Classical Notion of Ensembles — Coherent vs. Incoherent

In a previous section we discussed the importance of the superposition by looking at the state

$$|+\rangle = \frac{1}{\sqrt{2}} \{|0\rangle + |1\rangle\} \quad \text{in the } \sigma_z \text{ basis.}$$

While the state gives $|0\rangle$ and $|1\rangle$ with probability $\frac{1}{2}$ when measured in the σ_z basis, there is always a preferred basis (σ_x in this case), where we get $|+\rangle$ with probability 1. However, for the state

$$\varphi = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|, \quad \text{again in } \sigma_z \text{ basis,}$$

measurement in any basis will always give probability $\frac{1}{2}$:

$$\langle\psi(\theta,\phi)|\varphi|\psi(\theta,\phi)\rangle = \frac{1}{2}.$$

This distinguishes the coherent superposition in $|+\rangle$ with the incoherent mixing in φ.

Exercise:

1. Find out where does the state $\varphi = \frac{1}{2}\mathbb{I}$ lie on the Bloch sphere.
2. Using the ensemble definition of φ, show that $\text{Tr}(\varphi^2) \leq 1$. When is $\text{Tr}(\varphi^2) = 1$?

3.1.5 Composite quantum systems and the partial trace

We finally make the connection between density operators and composite quantum systems. For example, consider a bipartite system AB with the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. A density matrix φ_{AB} in this space is a positive semi-definite Hermitian matrix with unit trace.

For two qubits:

$$\varphi_{AB} = \varphi_A \otimes \varphi_B \qquad \text{(product state)}$$

Density matrix for each qubit can be written in the Bloch sphere form as $\varphi_A = \frac{1}{2}(\mathbb{I} + \vec{a} \cdot \vec{\sigma})$ and $\varphi_B = \frac{1}{2}(\mathbb{I} + \vec{b} \cdot \vec{\sigma})$

Examples:

$$\varphi_{AB} = |0\rangle\langle 0|_A \otimes |1\rangle\langle 1|_B \qquad \text{(pure product state)}$$

$$\varphi_{AB} = \frac{\mathbb{I}}{2} \otimes \frac{\mathbb{I}}{2} \qquad \text{(maximally mixed state)}$$

$$\varphi_{AB} = |\Psi^-\rangle\langle\Psi^-|, \quad |\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \quad \text{(singlet state)}$$

To determine the state of subsystem A within a composite quantum system, we perform a partial trace over subsystem B. This operation is formally defined as a linear map

$$\mathrm{Tr}_B : \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B) \to \mathcal{L}(\mathcal{H}_A)$$

It acts on density operators as follows :

$$\varphi_A = \mathrm{Tr}_B(\varphi_{AB}) = \sum_k (\mathbb{I}_A \otimes \langle k|_B)\, \varphi_{AB}\, (|k\rangle_B \otimes \mathbb{I}_A)$$

Here, $\{|k\rangle_B\}$ denotes any orthonormal basis for the Hilbert space $\mathcal{H}_B$. Intuitively, we are tracing out all degrees of freedom not belonging to subsystem A.

Special case : When the composite system is in a product state, the partial trace operation is particularly simple. For $\varphi_{AB} = \varphi_A \otimes \varphi_B$, we have

$$\mathrm{Tr}_B(\varphi_{AB}) = \varphi_A \otimes \mathrm{Tr}(\varphi_B) = \varphi_A$$

Similarly, tracing out subsystem A yields the reduced state of B, again, it amounts to tracing out all degrees of freedom not belonging to B :

$$\varphi_B = \mathrm{Tr}_A(\varphi_{AB})$$

Let us now consider the singlet state,

$$\varphi_{AB} = |\Psi^-\rangle\langle\Psi^-| = \frac{1}{2}\{|01\rangle\langle 01| - |01\rangle\langle 10| - |10\rangle\langle 01| + |10\rangle\langle 10|\}$$

To find the reduced state on A, we use the basis $\{|0\rangle_B, |1\rangle_B\}$ and compute :

$$\varphi_A = \mathbb{I}_A \otimes \langle 0|_B \varphi_{AB} |0\rangle_B \otimes \mathbb{I}_A + \mathbb{I}_A \otimes \langle 1|_B \varphi_{AB} |1\rangle_B \otimes \mathbb{I}_A$$

$$= \frac{1}{2}\{\mathbb{I}_A \otimes \langle 0|10\rangle\langle 10|0\rangle \otimes \mathbb{I}_A + \mathbb{I}_A \otimes \langle 1|01\rangle\langle 01|1\rangle \otimes \mathbb{I}_A\}$$

$$\therefore \varphi_A = \frac{1}{2}\{|1\rangle\langle 1| + |0\rangle\langle 0|\} = \frac{1}{2}\mathbb{I}_A$$

Exercise : Compute the reduced state φ_B for the same singlet state.

Now why does partial trace work?

From the axioms of quantum mechanics, we know that any pure state in a composite system can be written in a joint basis. If $\{|i\rangle_A\}$ is a basis in $\mathcal{H}_A$ and $\{|j\rangle_B\}$ is a basis in $\mathcal{H}_B$, then $\{|i\rangle_A \otimes |j\rangle_B\}$ forms a basis in $\mathcal{H}_A \otimes \mathcal{H}_B$.

Thus, any pure state of the composite system can be written as:

$$|\Psi\rangle_{AB} = \sum_{ij} \alpha_{ij} |i\rangle_A \otimes |j\rangle_B = \sum_{ij} \alpha_{ij} |i\rangle_A |j\rangle_B$$

If we wish to find the expectation value of an observable M_A that acts only on $\mathcal{H}_A$:

$$\langle M_A \rangle = \langle \Psi_{AB}|(M_A \otimes \mathbb{I}_B)|\Psi_{AB}\rangle$$

$$= \sum_{i,j} \alpha^*_{ij} \langle j|_B \langle i|_A (M_A \otimes \mathbb{I}_B) \sum_{i',j'} \alpha_{i'j'} |i'\rangle_A |j'\rangle_B$$

$$= \sum_{i,j,i',j'} \alpha^*_{ij}\alpha_{i'j'} \langle i|_A M_A |i'\rangle_A \otimes \langle j|_B \mathbb{I}_B |j'\rangle_B$$

$$= \sum_{i,j,i'} \alpha^*_{ij}\alpha_{i'j} \langle i|_A M_A |i'\rangle_A$$

$$= \mathrm{Tr}(M_A \varphi_A)$$

Now, let us explicitly compute the reduced density matrix $\varphi_A = \mathrm{Tr}_B(|\Psi\rangle\langle\Psi|_{AB})$:

$$\mathrm{Tr}_B(|\Psi\rangle\langle\Psi|_{AB}) = \sum_k \langle k|_B \sum_{i,j,i',j'} \alpha^*_{ij}\alpha_{i'j'} |i'\rangle_A |j'\rangle_B \langle i|_A \langle j|_B |k\rangle_B$$

$$= \sum_{i,j,i',j'} \alpha^*_{ij}\alpha_{i'j'} |i'\rangle\langle i|_A \otimes \langle k_B|j'\rangle_B \langle j|k\rangle_B$$

$$= \sum_{i,i',j} \alpha^*_{ij}\alpha_{i'j} |i'\rangle_A \langle i|_A = \varphi_A$$

Thus, the expectation value can be written as:

$$\mathrm{Tr}(M_A \varphi_A) = \sum_k \langle k|_A M_A \varphi_A |k_A\rangle$$

$$= \sum_{i,i',j,k} \langle k|_A \alpha^*_{ij}\alpha_{i'j} M_A |i'\rangle \langle i| |k\rangle_A = \sum_{i,i',j} \alpha^*_{ij}\alpha_{i'j} \langle i|M_A |i'\rangle$$

Expectation Value via Reduced State

Performing a measurement or calculating the expectation value of a subsystem in a composite system is equivalent to doing the measurement directly on the reduced state.

Show that : $\boxed{\mathrm{Tr}\left[(M_A \otimes I_B)\Psi_{AB}\right] = \mathrm{Tr}_A\left[M_A \varphi_A\right]}$

3.1.6 Purification of a mixed quantum state

All quantum states fall under what is often termed the "Church of the Larger Hilbert Space," which asserts that every state can be regarded as part of a larger quantum system that is pure and deterministic. For mixed states, this concept is quite straightforward:

Since φ is a Hermitian operator, it admits a spectral decomposition:

$$\varphi = \sum_k \lambda_k \left|k\right\rangle \left\langle k\right|$$

Each $\lambda_k \geq 0$, the set $\{|k\rangle\}$ is orthonormal, and $\sum_k \lambda_k = 1$. That is, φ is positive semi-definite and normalized so that $\mathrm{Tr}(\varphi) = 1$, ensuring the coefficients λ_k form a probability distribution.

Note : You can also establish the spectral decomposition without reference to any particular orthonormal set of states for φ.

A **purification** of φ is a pure state $|\Psi\rangle_{AB}$ in a larger Hilbert space, such that :

$$\varphi_A = \mathrm{Tr}\left(|\Psi\rangle \langle\Psi|_{AB}\right)$$

Given the spectral decomposition, one purification is

$$|\Psi\rangle_{AB} = \sum_k \sqrt{\lambda_k}\ |k\rangle_A \otimes |e_k\rangle_B\,.$$

Thus, every mixed state φ can always be viewed as arising from a global pure state $|\Psi\rangle_{AB}$, and the mixedness now arises due to the **correlations** in $|\Psi\rangle_{AB}$ between A and B.

This perspective connects the randomness in ensemble preparation, and the ambiguity of mixed states, to nonclassical correlations that exist because φ_A is part of a larger quantum system.

Purifications are not unique:

$$|\Phi\rangle_{AB} = \left(\mathbb{I}_A \otimes U_B\right)|\Psi\rangle_{AB}$$

Above expression is also a valid purification for any unitary U_B (i.e., $U_B^\dagger U_B = \mathbb{I}$), and yields

$$\varphi_A = \mathrm{Tr}_B\left(|\Phi\rangle \langle\Phi|_{AB}\right)$$

3.1.7 Pure state decompositions of a quantum state

For an n-dimensional quantum system A, the state φ_A is given by

$$\varphi_A = \sum_{i=1}^{n} \lambda_i |i\rangle \langle i|$$

$\{\lambda_i, |i\rangle\}$ is the eigen-decomposition of φ_A. There also exist other pure state decompositions, such that :

$$\varphi_A = \sum_{k=1}^{m} p_k |\phi_k\rangle \langle \phi_k|$$

$\{p_k\}$ form a probability distribution ($p_k \geq 0$, $\sum_k p_k = 1$), and each $|\phi_k\rangle$ is a pure state.

Then, we have the relation

$$\sqrt{p_k} |\phi_k\rangle = \sum_{i=1}^{n} u_{ki} \sqrt{\lambda_i} |i\rangle$$

(u_{ki} being the elements of some unitary matrix U.)

Proof:

Consider the purification of φ_A :

$$|\Psi\rangle_{AB} = \sum_i \sqrt{\lambda_i} |i\rangle_A \otimes |i\rangle_B$$

and an alternative purification :

$$|\Phi\rangle_{AC} = \sum_k \sqrt{p_k} |\phi_k\rangle_A \otimes |k\rangle_C$$

We know that for some unitary matrix U :

$$|\Phi\rangle_{AC} = (\mathbb{I} \otimes U) |\Psi\rangle_{AB}$$

Projecting onto the C basis :

$$(\mathbb{I}_A \otimes_C \langle k|) |\Phi\rangle_{AC} = \mathbb{I}_A \otimes_C \langle k| U |\Psi\rangle_{AB}$$

it yields

$$\sqrt{p_k} |\phi_k\rangle_A = \sum_i u_{ki} \sqrt{\lambda_i} |i\rangle_A$$

where $u_{ki} = {}_c\langle k|U|i\rangle_B$.

Note: Here, $\{|i\rangle\}$ is the eigen-decomposition of φ_A, but the second decomposition is arbitrary, so the above relation will hold for all pure state decompositions.

3.1.8 The Schmidt decomposition

Any bipartite pure state $|\Psi\rangle_{AB}$ can be written as:

$$|\Psi\rangle_{AB} = \sum_{i=1}^{r} \lambda_i \, |i\rangle_A \otimes |i\rangle_B$$

where $\{|i\rangle_A\}$ and $\{|i\rangle_B\}$ are sets of orthonormal basis vectors in A and B respectively, λ_i are the Schmidt coefficients, and r is the Schmidt rank.

The Schmidt decomposition has an important property :
The reduced density matrices φ_A and φ_B have identical eigenvalues.

$$\varphi_A = \sum_i \lambda_i^2 \, |i\rangle \langle i|_A \, , \qquad \varphi_B = \sum_i \lambda_i^2 \, |i\rangle \langle i|_B$$

and $\{|i\rangle_A\}$ and $\{|i\rangle_B\}$ are the eigenbases for φ_A and φ_B. Also,

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

Proof:

Let $|\Psi\rangle_{AB} = \sum_{i,j} a_{ij} \, |i\rangle_A \otimes |j\rangle_B$, $\{|i\rangle_A\}$ and $\{|j\rangle_B\}$ are orthonormal bases for A and B.

Define

$$|i\rangle_B = \sum_j a_{ij} \, |j\rangle_B$$

so that in general,

$$\varphi_A = \sum_i \lambda_i^2 \, |i\rangle \langle i|_A$$

Also, from

$$\varphi_A = \mathrm{Tr}_B(|\Psi\rangle \langle\Psi|_{AB}) = \mathrm{Tr}_B\left(\sum_{i,j} |i\rangle \langle i|_A \otimes |i\rangle \langle j|_B\right)$$

$$= \sum_{i,j} |i\rangle\langle j|_A \otimes \sum_k \langle k|i\rangle_B \langle j|k\rangle_B = \sum_{i,j} |i\rangle\langle j|_A \otimes \sum_k \langle j|k\rangle\langle k|i\rangle_B, \ \text{(where } \sum_k |k\rangle\langle k| = I\text{)}$$

$$= \sum_{i,j} \langle j|i\rangle_B |i\rangle\langle j|_A$$

Comparing with $\varphi_A = \sum_i \lambda_i^2 \, |i\rangle \langle i|_A$, we see $\{\lambda_i \, |i\rangle_B\}$ forms an orthonormal basis in B, and the Schmidt decomposition gives :

$$|\Psi\rangle_{AB} = \sum_i \lambda_i \, |i\rangle_A \otimes |i\rangle_B$$

Thus, the Schmidt decomposition not only provides a canonical form for bipartite pure states, but also reveals the structure of entanglement and the spectra of the reduced density matrices.

3.1.9 The ambiguity of an ensemble

A linear combination of two density matrices is also a density matrix (ensemble interpretation):

$$\varphi = p\,\varphi_1 + (1-p)\,\varphi_2, \qquad 0 \le p \le 1.$$

Exercise: Check that φ satisfies the criteria for a density matrix if φ_1 and φ_2 do.

Thus, density matrices are a convex subset of the real vector space of Hermitian operators.

Importantly, no *pure* quantum state, i.e., $\varphi = |\psi\rangle\langle\psi|$, can be expressed as a convex combination of density matrices.

Let us now consider the density matrix:

$\varphi_1 = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{1}{2}I_2$, $\frac{1}{2}I_2$ is the maximally mixed state (identity matrix).

But consider the states:

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \qquad |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

$$\varphi_2 = \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -| = \frac{1}{2}I_2$$

So, $\varphi_1 = \varphi_2$ regardless of the underlying ensemble of states, which is a bit weird. Let us say that we have a cat, which is either alive ($|0\rangle$) or dead ($|1\rangle$) with probability 1/2. But, now if the cat is in the more complicated Schrödinger state ($|+\rangle$, $|-\rangle$), with superpositions, we still get the same density matrix.

There is no operation that can distinguish the two, and this feature has no classical analogue.