Vocabulary

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1 Quantum state tomography

- **What is QST?** Reconstruct an unknown quantum state based on measures on several copies of the state

- **Why?** Verify quantum algorithms, study decoherence, validate communication protocols, ...

- **How?** Linear inversion, Bayes estimation, Maximum likelihood estimation, ...

2 Definitions

2.1 Basic vocabulary

- **Entanglement:** Quantum entanglement is a special connection between two or more particles where their states are linked, no matter how far apart they are. If you measure one particle, you instantly know the result for the other — even if it's on the other side of the universe. This happens because the particles share a single combined quantum state, not separate ones.

- **Decoherence:** Decoherence is the process where a quantum system loses its "quantum behavior" because it interacts with its environment. When that happens, the system stops being in a superposition of states and starts behaving like a normal, classical object. It's basically what makes quantum effects disappear in the real world.

- **Transmittance:** Transmittance means how much light passes through something. If a material or an optical component has high transmittance, it lets most of the light through. If it has low transmittance, some of the light is absorbed, scattered, or reflected — so less light gets to the other side. A photonic computer uses light (photons) instead of electricity to process information.
  When light travels through optical components — like waveguides, beam splitters, or interferometers — not all photons make it to the end. Some are:

  - Absorbed by the material,
  - Scattered in unwanted directions

– reflected at imperfect surfaces.

This means the transmittance is less than 1, and part of the signal is lost. In photonic computing, imperfect transmittance = photon loss = noise, which reduces signal clarity and fidelity in quantum or optical operations.

- **Indistinguishability:** Indistinguishability means that two or more photons are completely identical in every measurable property — such as their wavelength (color), polarization, arrival time, and spatial mode. In other words, there is no way to tell them apart, even in principle.
  When you measure the probability of a quantum state in a photonic computer, you don't measure just once — you repeat the experiment many times with identically prepared photons. Each photon (or group of photons) acts as a new "copy" of the same quantum state. You collect statistics — how often each outcome happens — to estimate the probability distribution. Perfect indistinguishability is never achieved. Even with excellent control, photons might be:

  – off by a few picoseconds in arrival time,

  – have slightly different spectral widths,

  – pass through components with tiny temperature or fabrication variations.

  Indistinguishability less than 100% means your "identical" photons aren't perfectly identical — so quantum interference isn't perfect, and that shows up as noise in the measured state probabilities.

2.2   Spin

In quantum mechanics, **spin** is an **intrinsic form of angular momentum** carried by elementary particles, atoms, and nuclei. It does not come from a physical rotation—particles such as electrons are not literally spinning spheres—but it behaves mathematically as if they had an internal angular momentum. Spin is a fundamental quantum property, just like mass or charge. It characterizes how a particle responds to **rotations** and **magnetic fields**. A particule has a predefined constant spin.

For example, an electron, proton, or neutron has a spin value of $\frac{1}{2}$, meaning that when you measure its spin along any direction, you can only obtain two possible results: "up" or "down". A photon, on the other hand, has spin 1, meaning it has three possible orientations $(-1, 0, +1)$, although only two are physically observable (left and right circular polarizations).

- **Spin and Measurement** When you measure a spin-$\frac{1}{2}$ particle along an axis (say the z-axis), it can only be found in one of two states:

$$|\uparrow\rangle_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |\downarrow\rangle_z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

These correspond to spin "up" and "down" along that axis. If you measure along another axis (like x or y), the same particle's spin states become superpositions of $|\!\uparrow\rangle_z$ and $|\!\downarrow\rangle_z$:

$$|\psi\rangle = \alpha|\!\uparrow\rangle_z + \beta|\!\downarrow\rangle_z, \quad \text{with } |\alpha|^2 + |\beta|^2 = 1.$$

- **Mathematical Representation**

  For spin-$\frac{1}{2}$ systems, spin observables are represented by the **Pauli matrices**:

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

  Each Pauli matrix corresponds to a spin measurement along one of the three spatial axes (x, y, or z). Measuring σ_z checks whether the spin is aligned ($+1$) or anti-aligned (-1) with the z-axis.

- **Spin on the Bloch Sphere**

  A qubit's spin state can be visualized as a vector on the **Bloch sphere**, where:

  - The north pole represents $|0\rangle = |\!\uparrow\rangle_z$,
  - The south pole represents $|1\rangle = |\!\downarrow\rangle_z$,
  - Any point on the sphere corresponds to a superposition of these two states.

  The direction of the Bloch vector corresponds to the mean spin direction:

  $$\vec{r} = \langle \psi | \vec{\sigma} | \psi \rangle.$$

2.3   Bloch sphere

- **General qubit state:**
  A qubit is a normalized vector in a 2D complex Hilbert space:

  $$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad \alpha, \beta \in \mathbb{C}, \quad |\alpha|^2 + |\beta|^2 = 1$$

  As α and β are both complex numbers, we have a total of 4 missing values (both the real and imaginary number of α and β). With the probability condition of $|\alpha|^2 + |\beta|^2 = 1$, we can remove one degree of freedom, and as the **global phase** has no physical meaning (multiplying the entire state by a complex phase $e^{i\gamma}$ doesn't change the physical state, i.e. the probabilities), we can remove another degree of freedom.

- **Parameterization of the qubit state:**
  As we have removes 2 degrees of freedom, we can always express α and β using only 2 variables as:
  $$\alpha = \cos\left(\frac{\theta}{2}\right), \quad \beta = e^{i\phi} \sin\left(\frac{\theta}{2}\right)$$

  where $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi)$. Thus:

  $$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi} \sin\left(\frac{\theta}{2}\right)|1\rangle$$

This form corresponds exactly to a **point on a unit sphere** with spherical coordinates (θ, ϕ). Note that removing the normalization condition gives us the 3 necessary variables needed in spherical coordinates in 3 dimensions.

- **From qubit state to Bloch vector:**
  We define the **Bloch vector** $\vec{r}$ as the expectation value of the **Pauli vector operator**:
  $$\vec{r} = \langle\psi|\vec{\sigma}|\psi\rangle$$
  where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, and the Pauli matrices are:
  $$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

  Computing this gives:
  $$\vec{r} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}$$

  Hence, $|\vec{r}| = 1$ for a pure state — i.e., the qubit lies **on the surface of the unit sphere**.

- **Density matrix representation:**
  The qubit density matrix can be written as:
  $$\rho = |\psi\rangle\langle\psi| = \frac{1}{2}\left(I + \vec{r}\cdot\vec{\sigma}\right)$$

  For mixed states, $|\vec{r}| < 1$, and the vector lies **inside** the Bloch sphere.

2.4 Pure state

A **pure state** in quantum mechanics is a state that contains **complete information** about a quantum system — it is described by a **single state vector** (or wavefunction) $|\psi\rangle$ in a Hilbert space.

$$|\psi\rangle = \sum_i c_i|i\rangle, \quad c_i \in \mathbb{C}, \quad \sum_i |c_i|^2 = 1$$

- **Density matrix form**

  A pure state can be written as:
  $$\rho = |\psi\rangle\langle\psi|$$

  It satisfies:
  $$\rho^2 = \rho \quad \text{and} \quad \text{Tr}(\rho^2) = 1$$

  This distinguishes it from a **mixed state**, where $\text{Tr}(\rho^2) < 1$.
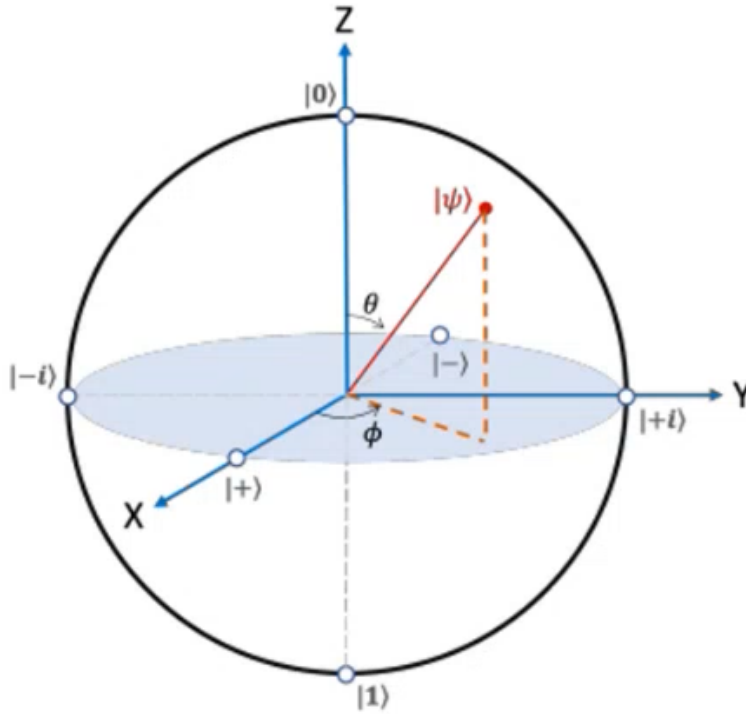
- **Physical meaning**

Figure 1: Qubit representation

 – A pure state represents **maximal knowledge** of the system.
 – Measurement probabilities are **deterministically** derived from $|\psi\rangle$ via Born's rule:
$$P(a_i) = |\langle a_i|\psi\rangle|^2$$
 – In contrast, a **mixed state** represents **statistical uncertainty** over several possible pure states.

- **Example:**

  For a qubit:
$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle$$
  is a **pure state**, lying **on the surface** of the Bloch sphere.

2.5 Mixed state

A **mixed state** is a **statistical ensemble of pure states** — it represents **incomplete information** about the quantum system.

Mathematically, a mixed state is described by a **density matrix** ρ that is **not a projector** (i.e. $\rho^2 \neq \rho$).

- **Formal definition**

A mixed state is given by:
$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

where:

- $|\psi_i\rangle$ are **pure states** (normalized vectors in Hilbert space),
- $p_i \geq 0$ and $\sum_i p_i = 1$,
- ρ is **Hermitian**, **positive semidefinite**, and has **unit trace**.

This represents a **classical probability distribution** over quantum states: we do not know *which* pure state the system is in, only the probabilities p_i.

A common misconception about mixed state is the difference between pure state and superposition. A particle in superposition is in several different states at the same time and has a *complex probability* of being measured in one of those state. We have $\sum |c_i|^2 = 1$. On the other hand, mixed state is a *classical probability* of being in a pure state, with $\sum p_i = 1$. We can have both mixed state and superposition at the same time.

- **Mathematical properties**

  - $\rho^2 \neq \rho$
  - $\mathrm{Tr}(\rho) = 1$
  - $0 < \mathrm{Tr}(\rho^2) < 1$

  The value of $\mathrm{Tr}(\rho^2)$ quantifies the **purity** of the state. Pure states satisfy $\mathrm{Tr}(\rho^2) = 1$; mixed states satisfy $\mathrm{Tr}(\rho^2) < 1$.

- **Physical interpretation**

  A mixed state arises when:

  - The system is in a **probabilistic mixture** of several possible pure states.
  - The system is **entangled** with another system and we **trace out** the environment.
  - There is **decoherence** due to noise or measurement.

- **Example (qubit)**

  Pure state:
  $$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \Rightarrow \rho = |\psi\rangle\langle\psi| = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

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

  Mixed state:
  $$\rho = \frac{1}{2}|0\rangle\langle0| + \frac{1}{2}|1\rangle\langle1| = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

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

This mixed state represents **classical uncertainty** — the qubit is either $|0\rangle$ or $|1\rangle$ with 50% probability, but not in a coherent superposition.

- **On the Bloch sphere**

    - **Pure states:** points **on the surface** ($|\vec{r}| = 1$).
    - **Mixed states:** points **inside the sphere** ($|\vec{r}| < 1$).
    - The **maximally mixed state** $\rho = \frac{I}{2}$ lies at the **center**.

2.6 Density matrix

The **density matrix**, usually denoted by ρ, is a mathematical object that provides a complete description of a quantum system, whether it is in a **pure state** or a **mixed state**. Unlike the ket notation $|\psi\rangle$, which only describes pure states, the density matrix can represent statistical mixtures of different quantum states. It plays a central role in quantum computing, quantum machine learning, and quantum state tomography.

- **Definition:** The density matrix ρ is defined as

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

    where p_i are probabilities ($p_i \geq 0$, $\sum_i p_i = 1$) and $|\psi_i\rangle$ are the possible quantum states of the system.

- **Pure state case:** If the system is in a single well-defined state $|\psi\rangle$, then $\rho = |\psi\rangle \, \langle\psi|$. In this case, $\rho^2 = \rho$ and $\mathrm{Tr}(\rho^2) = 1$.

- **Mixed state case:** When the system is in a statistical mixture of several states, $\rho^2 \neq \rho$ and $\mathrm{Tr}(\rho^2) < 1$. Mixed states arise from incomplete knowledge or interactions with an environment (decoherence).

- **Properties:** The density matrix always satisfies:

    - $\rho = \rho^\dagger$ (Hermitian)
    - $\rho \geq 0$ (positive semi-definite)
    - $\mathrm{Tr}(\rho) = 1$ (normalized)

- **Dimension:** For a system of n qubits, the density matrix ρ has size $2^n \times 2^n$, since the Hilbert space dimension is $d = 2^n$.

- **Physical meaning:** Each element ρ_{ij} represents the probability amplitudes and coherences between the basis states $|i\rangle$ and $|j\rangle$. The diagonal terms represent population probabilities, while the off-diagonal terms encode quantum coherences.

- **Measurement probabilities:** The probability of measuring an outcome corresponding to a projector M is given by

$$P(M) = \text{Tr}(M\rho).$$

- **Role in quantum tomography and QML:** In quantum state tomography, the goal is to reconstruct ρ from experimental measurements. In quantum machine learning, ρ can encode the data or the state of a quantum model, and methods such as **Maximum Likelihood Estimation (MLE)** are used to estimate it from observed results.

3 Maximum Likelihood estimation