

Bloch Sphere Properties

PHYS161 Project1.a

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1 Background

1.1 Introduction to density matrices

When we build a quantum computer, or actually any quantum device, the states we prepare are not perfectly clean! In mathematical language, they are not *pure states*; rather, they form what we call **mixed states**.

The *mixed states* are central in quantum information science for several reasons. First, they provide a realistic description of how quantum states interact with the environment. According to [BP07], they are the language of noise and decoherence, formalized by GKSL/Lindblad dynamics and quantum channels (CPTP maps). Moreover, many phenomena are constrained by mixed states. For instance, [HHHH09] use them to describe entanglement in noisy settings.

To assess how well the device behaves, we resort to quantum tomography. It's like taking a scan of the system to figure out what is produced in the lab. In fact, this is the experimental method used to construct what is called a **density matrix**, which is a mathematical representation of mixed states.

The density operator is a mathematical object that summarizes all the observable predictions of any ensemble of pure states that lead to it—classical randomness between different pure states, with no coherence between them. Now, let's discuss the mathematical equations as described in [NC10].

The density operator describes the statistical state of a quantum system as a weighted sum over pure states:

$$\rho \equiv \sum_i p_i |\psi_i\rangle\langle\psi_i| \quad (1)$$

where p_i are the probabilities associated with the pure states $|\psi_i\rangle$. The postulates of quantum mechanics can be reconstructed in the language of the density operator. Postulate 2 will be discussed here:

The density operator transforms under a unitary operator U , which represents the unitary time evolution of the quantum system:

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \xrightarrow{U} \sum_i p_i U|\psi_i\rangle\langle\psi_i|U^\dagger = U\rho U^\dagger. \quad (2)$$

Finally, I will present some intrinsic properties of the density operator. **Theorem 2.5 (Characterization of Density Operators)**. An operator ρ represents a valid density operator if and only if it satisfies:

1. $\text{tr}(\rho) = 1$ (normalization),
2. $\rho \geq 0$ (positivity).

Idea of the proof. Any ensemble $\{p_i, |\psi_i\rangle\}$ leads to an operator $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$, which clearly has unit trace and yields non-negative expectation values, ensuring positivity. Conversely, any operator with these two properties can always be interpreted as the density operator of some ensemble.

1.2 Bloch sphere for mixed states

The Bloch sphere is a geometrical representation of a single qubit, a two-level system. Following the conditions of the density operator, we may construct a matrix that is Hermitian and has trace equal to 1:

$$\rho = \begin{pmatrix} a & b + ic \\ b - ic & 1 - a \end{pmatrix} \quad (3)$$

We begin by noting that the set

$$\{I, X, Y, Z\}$$

forms a basis for the vector space of 2×2 linear operators. Hence, for any operator ρ (not necessarily a density operator), we can write

$$\rho = a_1 I + a_2 X + a_3 Y + a_4 Z, \quad (4)$$

for some coefficients $a_1, a_2, a_3, a_4 \in \mathbb{C}$.

Since ρ is Hermitian, we must have $\rho = \rho^\dagger$. Because I, X, Y, Z are all Hermitian, this implies

$$a_j = a_j^*, \quad \text{for } j = 1, 2, 3, 4,$$

so the coefficients a_j are all real.

Next, a density operator satisfies the trace condition $\text{tr}(\rho) = 1$. Using linearity of the trace,

$$\text{tr}(\rho) = a_1 \text{tr}(I) + a_2 \text{tr}(X) + a_3 \text{tr}(Y) + a_4 \text{tr}(Z) \quad (5)$$

$$= 2a_1, \quad (6)$$

since $\text{tr}(I) = 2$ and $\text{tr}(X) = \text{tr}(Y) = \text{tr}(Z) = 0$. Thus,

$$a_1 = \frac{1}{2}. \quad (7)$$

So we may rewrite

$$\rho = \frac{1}{2}I + a_2 X + a_3 Y + a_4 Z. \quad (8)$$

To analyze the remaining coefficients, consider

$$\rho^2 = \left(\frac{1}{2}I + a_2 X + a_3 Y + a_4 Z \right)^2. \quad (9)$$

Using the Pauli matrix identities

$$X^2 = Y^2 = Z^2 = I, \quad \{\sigma_i, \sigma_j\} = 0 \quad (i \neq j),$$

the expression simplifies to

$$\rho^2 = \left(\frac{1}{4} + a_2^2 + a_3^2 + a_4^2 \right) I + a_2 X + a_3 Y + a_4 Z. \quad (10)$$

Taking the trace,

$$\text{tr}(\rho^2) = \left(\frac{1}{4} + a_2^2 + a_3^2 + a_4^2 \right) \text{tr}(I) \quad (11)$$

$$= 2 \left(\frac{1}{4} + a_2^2 + a_3^2 + a_4^2 \right). \quad (12)$$

Since $\text{tr}(\rho^2) \leq 1$ for any density operator, we obtain the constraint

$$a_2^2 + a_3^2 + a_4^2 \leq \frac{1}{4}. \quad (13)$$

Now define the *Bloch vector*

$$\vec{r} = (r_x, r_y, r_z), \quad r_x = 2a_2, \quad r_y = 2a_3, \quad r_z = 2a_4.$$

With this definition,

$$\rho = \frac{1}{2}(I + r_x X + r_y Y + r_z Z) = \frac{1}{2}(I + \vec{r} \cdot \vec{\sigma}), \quad (14)$$

with the constraint

$$\|\vec{r}\|^2 = r_x^2 + r_y^2 + r_z^2 \leq 1.$$

Thus, any single-qubit density operator can be written in the *Bloch representation*.

This Bloch vector is also called the polarization vector according to [Qui25], because the Bloch vector encodes the mean polarization (or spin orientation) of the qubit ensemble. In quantum optics, a two-level atom or a photon's polarization state can be represented by a qubit:

$$\begin{aligned} |\vec{r}| = 1 & \quad \text{Fully polarized state (pure state),} \\ |\vec{r}| < 1 & \quad \text{Partially polarized beam (mixed state),} \\ |\vec{r}| = 0 & \quad \text{Unpolarized beam (maximally mixed state).} \end{aligned}$$

1.3 Applying a single-qubit gate on a density matrix

The transformation of a single qubit is not restricted to unitary quantum gates. In fact, only *pure states* undergo quantum gates. On the other hand, *mixed states* undergo what are called **quantum operations**. Quantum operations can cause more general transformations, where the Bloch sphere may be distorted, translated, or shrunk.

In contrast, rotation of the Bloch sphere is a special case of the Bloch vector, being in a pure state [NC10]. I will show below two things. **First**, I will write the Bloch vector in spherical coordinates starting from the density matrix. **Second**, I will prove that any quantum gate is in fact a rotational matrix.

The pure state of a qubit can be written as

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right) |0\rangle + e^{i\phi} \sin\left(\frac{\theta}{2}\right) |1\rangle, \quad \theta \in [0, \pi], \quad \phi \in [0, 2\pi]. \quad (15)$$

The corresponding density matrix is

$$\rho = |\psi\rangle\langle\psi|. \quad (16)$$

The components of the Bloch vector $\vec{r} = (r_x, r_y, r_z)$ are obtained from

$$r_i = \text{Tr}(\rho \sigma_i), \quad (17)$$

which gives

$$\vec{r} = (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta). \quad (18)$$

A single-qubit unitary operator U preserves norms since $U^\dagger U = I$, implying $\langle\psi|U^\dagger U|\psi\rangle = \langle\psi|\psi\rangle$ for any state $|\psi\rangle$. Geometrically, this means U corresponds to a rotation of the Bloch sphere (up to a global phase). More precisely, any 2×2 unitary can be written as

$$U = e^{i\phi} \exp(-i\frac{\theta}{2} \hat{n} \cdot \vec{\sigma}),$$

where ϕ is a global phase, \hat{n} is a unit vector (the rotation axis), θ is the rotation angle, and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices. **Thus, every single-qubit unitary is just a rotation on the Bloch sphere combined with an irrelevant global phase.**

2 Applicable Code

For the mathematical wrap-up, the proposed implementation language is **Python**, since it offers strong libraries for numerical linear algebra (**NumPy**) and visualization (**Matplotlib/Plotly**) that are well suited to quantum information tasks. The project can be organized into four modular explorations:

1. **Density Matrix Validator & Explorer.** *Input:* an arbitrary 2×2 complex matrix. *Task:* check if it is a valid density matrix by testing $\text{tr}(\rho) = 1$ and positivity (eigenvalues ≥ 0). *Output:* a diagnostic report including trace, eigenvalues, and purity. *Stretch:* randomly generate matrices and filter those that qualify as valid states.
2. **Bloch Sphere Playground.** *Input:* a valid density matrix. *Task:* convert the matrix into a Bloch vector and back, then classify states as pure, mixed, or maximally mixed based on the norm of the vector. *Output:* visualization of the Bloch vector's position and its classification. *Stretch:* build an interactive 3D Bloch sphere plot where the effect of varying the density matrix can be observed dynamically.
3. **Unitary Rotations on the Bloch Sphere.** *Input:* a density matrix and a single-qubit unitary operator (user-selected axis and angle). *Task:* apply the unitary, show that the Bloch vector rotates rigidly, and visualize the trajectory. *Output:* updated Bloch vector location. *Stretch:* add a random unitary generator to explore arbitrary rotations.
4. **Purity vs Bloch Vector Length.** *Input:* sets of random density matrices. *Task:* compute purity $\text{Tr}(\rho^2)$ and compare with the theoretical relation $\frac{1+\|r\|^2}{2}$. *Output:* plots of purity versus Bloch vector length. *Stretch:* visualize statistical distributions of purity for ensembles of random states.

Possible challenges include the fact that many repositories are more focused on pure states or state vectors rather than mixed states. I will need to check how easy it is to plug in density matrices or channels, handle complex matrix manipulations cleanly, and build intuitive yet non-trivial visualizations (especially interactive Bloch sphere graphics). Additionally, generating ensembles of random valid states isn't entirely trivial, so I'll need to read about or experiment with different methods (e.g., random Haar states vs. ad-hoc construction) to avoid bias.

References

- [BP07] Heinz-Peter Breuer and Francesco Petruccione. *The Theory of Open Quantum Systems*. Oxford University Press, Oxford, 2007.
- [HHHH09] Ryszard Horodecki, Paweł Horodecki, Michał Horodecki, and Karol Horodecki. Quantum entanglement. *Reviews of Modern Physics*, 81(2):865–942, 2009.
- [NC10] Michael A. Nielsen and Isaac L. Chuang. *Quantum Computation and Quantum Information*. Cambridge University Press, Cambridge, 10th anniversary edition edition, 2010.
- [Qui25] A C Quillen. Phy265 lecture notes: Introducing quantum information. Technical report, 2025.