L4 Quantum information and computing (QIC) 2020-21

Lecture 3: The Pauli matrices and the density matrix

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Aims of Lecture 3: The aims of this lecture is to introduce the Pauli matrices, write an expression for the density matrix of a qubit, introduce the concept of decoherence.

Pauli operators: The Pauli matrices form a complete set of basis vectors of 2×2 Hermitian matrices.

Figure 1: Wolfgang Pauli photographed by Roy Glauber. From Roy J. Glauber at NobelPrize.org.

This means that any operator acting on a qubit and the density matrix can be written as a linear sum of Pauli matrices with real coefficients. In the z-basis the Pauli matrices are[1]

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

and the identity matrix

$$I_2 \equiv \sigma_0 \;=\; \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \, ,$$

where the subscript 2 indicates a 2×2 identity matrix.[2] In quantum computing, it is common to define the Pauli spin matrices as

$$\mathsf{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \, , \; \mathsf{Y} = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \, , \; \mathsf{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \, .$$

[1] The Pauli matrices will be given in the Exam.

[2] Note that some books include a spin$-1/2$ angular factor $\hbar/2$ in the definition of the spin matrices, i.e. the spin$-1/2$ angular momentum operator is

$$\boldsymbol{J} = (\hbar/2)\boldsymbol{\sigma} \, .$$

These matrices represent particular examples of **single-qubit gates** called the **Pauli-X**, **Pauli-Y** and **Pauli-Z**.

In terms of the Pauli matrices, the density matrix of a qubit is

$$\begin{aligned} \rho &= \tfrac{1}{2}\left(\sigma_0 + u\sigma_x + v\sigma_y + w\sigma_z\right) \, , \\ &= \tfrac{1}{2}\left(\sigma_0 + \boldsymbol{b}\cdot\hat{\boldsymbol{\sigma}}\right) \, , \end{aligned} \tag{1}$$

where $\boldsymbol{b} = (u, v, w)$ is the Bloch vector and $\hat{\boldsymbol{\sigma}} = (\sigma_x, \sigma_y, \sigma_z)$. As ρ is Hermitian, u, v and w are all real.

Also useful to remember is that for a general qubit state vector, $|\psi\rangle$, the expectation values of Pauli-X, Y and Z matrices are equal to the x, y and z components of the Bloch vector,

$$\langle\psi|\sigma_x|\psi\rangle = (a^* \;\; b^*)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = a^*b + b^*a = u \, ,$$

$$\langle\psi|\sigma_z|\psi\rangle = (a^* \;\; b^*)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = |a|^2 - |b^2| = w \, .$$

The density matrix Why do we need it? Although a state vector is sufficient to describe a pure state, real world qubits exist in a mixed state.[3] The density matrix allows us to describe both pure and mixed states. For a pure state described by the state vector $|\psi\rangle$, the density matrix in the $\{|0\rangle, |1\rangle\}$ basis is defined as

$$\rho \;=\; |\psi\rangle\langle\psi| \, . \tag{2}$$

For the qubit state vector given by eqn (1) in Lecture 1, the density matrix is

$$\rho \;=\; \begin{pmatrix} a \\ b \end{pmatrix}(a^* \;\; b^*) = \begin{pmatrix} |a|^2 & ab^* \\ ba^* & |b|^2 \end{pmatrix} \, . \tag{3}$$

Interpretation: The diagonal terms of the density matrix are the probabilities of detection the qubit in state $|0\rangle$ or $|1\rangle$.[4] The off-diagonal terms are only non-zero if both

[3] They might be 99.99% pure but never 100%.

[4] For N identical qubits, they correspond to the **populations** of states $|0\rangle$ and $|1\rangle$.

a and b are non-zero, i.e. the qubit much be in a superposition of $|0\rangle$ and $|1\rangle$. The off-diagonal terms are referred to as **coherences** because they depend on the relative phase between $|0\rangle$ and $|1\rangle$. If there is a random time-varying relative phase, $\delta(t)$, i.e. the state vector as $|\psi\rangle = a|0\rangle + \mathrm{e}^{-\mathrm{i}\delta(t)}b|1\rangle$, then the density matrix is

$$\rho = \begin{pmatrix} |a|^2 & \mathrm{e}^{\mathrm{i}\delta(t)}ab^* \\ \mathrm{e}^{-\mathrm{i}\delta(t)}ba^* & |b|^2 \end{pmatrix} ,$$

and the time average is a statistical mixture or **mixed state**,

$$\langle\rho\rangle = \begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix} = |a|^2|0\rangle\langle 0| + |b|^2|1\rangle\langle 1| \ .$$

The decay of the off-diagonal terms due to phase fluctuations induced by the environment is known as **decoherence**. Whether the populations (diagonal terms) or coherence (off-diagonal terms) decay faster depends on how the qubit interacts with the environment. We shall discuss this again when we introduce the optical Bloch equations in Lecture 6.

Written in spherical polar coordinates, the qubit density matrix for a pure state is

$$\begin{aligned} \rho &= \begin{pmatrix} \cos\frac{\theta}{2} \\ \mathrm{e}^{\mathrm{i}\phi}\sin\frac{\theta}{2} \end{pmatrix} \left(\cos\tfrac{\theta}{2} \quad \mathrm{e}^{-\mathrm{i}\phi}\sin\tfrac{\theta}{2}\right) , \\ &= \begin{pmatrix} \cos^2\frac{\theta}{2} & \sin\frac{\theta}{2}\cos\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\phi} \\ \sin\frac{\theta}{2}\cos\frac{\theta}{2}\mathrm{e}^{\mathrm{i}\phi} & \sin^2\frac{\theta}{2} \end{pmatrix} . \end{aligned}$$

Using the half-angle formulas, $\sin^2\frac{\theta}{2} = \frac{1}{2}(1-\cos\theta)$, $\cos^2\frac{\theta}{2} = \frac{1}{2}(1+\cos\theta)$ and $\sin\frac{\theta}{2}\cos\frac{\theta}{2} = \frac{1}{2}\sin\theta$, and expanding the exponential, we find

$$\rho = \tfrac{1}{2}\begin{pmatrix} 1+\cos\theta & \sin\theta\cos\phi - \mathrm{i}\sin\theta\sin\phi \\ \sin\theta\cos\phi + \mathrm{i}\sin\theta\sin\phi & 1-\cos\theta \end{pmatrix} .$$

Using the cartesian components of the Bloch vector,

$$\begin{aligned} u &= \sin\theta\cos\phi \ , \\ v &= \sin\theta\sin\phi \ , \\ w &= \cos\theta \ , \end{aligned}$$

where $(u^2+v^2+w^2)^{1/2} = 1$.

$$\rho = \frac{1}{2}\begin{pmatrix} 1+w & u-\mathrm{i}v \\ u+\mathrm{i}v & 1-w \end{pmatrix} . \tag{4}$$

Comparing to the (a,b) form in eqn (2), we can also write that[5]

$$\begin{aligned} u &= ab^* + ba^* \ , \\ v &= \frac{1}{\mathrm{i}}(a^*b - ab^*) \ , \\ w &= |a|^2 - |b|^2 \ , \end{aligned}$$

The z-component of the Bloch vector is equal to the 'population' difference between the $|0\rangle$ and $|1\rangle$ states. The x and y-component are real and imaginary parts of the coherence.[6] Later we shall find that the real and imaginary parts oscillate in-phase or in-quadrature ($\pi/2$ out of phase) with the external driving field.

Summary:

What do you need to be able to do?

1. Explain the importance of the Pauli spin matrices.
2. Show that the expectation values of the Pauli spin operators correspond to the cartesian coordinates of the Bloch vector.
3. Write an expression for the density matrix of a qubit in terms of a and b, (θ,ϕ) or (u,v,w).
4. Explain the significance of the diagonal and off-diagonal terms in the density matrix.
5. Explain decoherence—how interactions with the environment lead to the decay of the off-diagonal terms in the density matrix.
6. Explain the difference between a pure state and a mixed state.

[5] Note that

$$\begin{aligned} ab^* + ba^* &= (a_\mathrm{r} + \mathrm{i}a_\mathrm{i})(b_\mathrm{r} - \mathrm{i}b_\mathrm{i}) + (b_\mathrm{r} + \mathrm{i}b_\mathrm{i})(a_\mathrm{r} - \mathrm{i}a_\mathrm{i}) \\ &= a_\mathrm{r}b_\mathrm{r} + a_\mathrm{i}b_\mathrm{i} + \mathrm{i}(a_\mathrm{i}b_\mathrm{r} - a_\mathrm{r}b_\mathrm{i}) + a_\mathrm{r}b_\mathrm{r} + a_\mathrm{i}b_\mathrm{i} - \mathrm{i}(a_\mathrm{i}b_\mathrm{r} - a_\mathrm{r}b_\mathrm{i}) \\ &= 2(a_\mathrm{r}b_\mathrm{r} + a_\mathrm{i}b_\mathrm{i}) = 2\Re[ab^*] \end{aligned}$$

$$a^*b - ab^* = -2\mathrm{i}(a_\mathrm{i}b_\mathrm{r} - a_\mathrm{r}b_\mathrm{i}) = -2\mathrm{i}\Im[ab^*]$$

[6] Note that as the Bloch vector pre-dates quantum computing some books use a different definition. In some cases, a factor of $\frac{1}{2}$ is absorbed into the definition of u and v, and the sphere is flipped such that $|1\rangle$ is at the North pole which changes the sign of w and v. However the definitions used here are standard in the quantum computing literature.