

# Quantum Computing

## Chapter 02: Quantum Logic Gates

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Prachya Boonkwan

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Sirindhorn International Institute of Technology  
Thammasat University, Thailand

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# Who? Me?

- Nickname: Arm (P'N' Arm, etc.)
- Born: Aug 1981
- Work
  - Researcher at NECTEC 2005-2024
  - Lecturer at SIIT, Thammasat University 2025-now
- Education
  - B.Eng & M.Eng in Computer Engineering, Kasetsart University, Thailand
  - Obtained Ministry of Science and Technology Scholarship of Thailand in early 2008
  - Did a PhD in Informatics (AI & Computational Linguistics) at University of Edinburgh, UK from 2008 to 2013



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## Quantum Bits

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# Quantum Bit as Probability Distribution

- In quantum computing, we enable parallelism by:
  1. Converting a bitstring into a sequence of binary distributions
  2. Manipulating these distributions with complex matrix operations
  3. Sharing data structures via quantum entanglement and lazy evaluation
- Quantum state for binary distribution

$$\mathbf{u} = \begin{bmatrix} \alpha & \beta \end{bmatrix}^T$$

where  $\alpha, \beta$  are complex coefficients, and

$$P(0|\mathbf{u}) = |\alpha|^2 \quad P(1|\mathbf{u}) = |\beta|^2$$

- Discrete binary values 0 and 1 can be represented as pure quantum states

$$\begin{aligned} |0\rangle &= \begin{bmatrix} 1 & 0 \end{bmatrix}^T \\ |1\rangle &= \begin{bmatrix} 0 & 1 \end{bmatrix}^T \end{aligned}$$

This notation is called 'ket'; e.g.  $|0\rangle$  reads 'ket-zero' and  $|1\rangle$  reads 'ket-one'

- Meaning:  $|n\rangle$  is a one-hot column vector on the  $n$ -th position, where the index starts with 0, and  $n$  is a binary number

# Dirac's Notation

- The adjoint of these vectors are

$$\langle 0| = |0\rangle^* = \begin{bmatrix} 1 & 0 \end{bmatrix}$$

$$\langle 1| = |1\rangle^* = \begin{bmatrix} 0 & 1 \end{bmatrix}$$

This notation is called 'bra'

- Meaning:  $\langle n|$  is a one-hot row vector on the  $n$ -th position
- Dirac's notation:  $|n\rangle$  and  $\langle n|$ , where

$$\langle 0|0\rangle = |0\rangle \vee |0\rangle = 1$$

$$\langle 0|1\rangle = |0\rangle \vee |1\rangle = 0$$

- Mixed state: a mixture of pure states

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix} \alpha & \beta \end{bmatrix}^\top$$

$$\text{where } |\alpha|^2 + |\beta|^2 = 1$$

- Mixed state can also be seen as a superposition

$$|\psi\rangle = r_1 \text{cis}\theta_1 |0\rangle + r_2 \text{cis}\theta_2 |1\rangle$$

- Adjoint of mixed state

$$\langle\psi| = |\psi\rangle^*$$

$$= r_1 \text{cis}(-\theta_1) \langle 0| + r_2 \text{cis}(-\theta_2) \langle 1|$$

- How about  $\langle 1|1\rangle$  and  $\langle 1|0\rangle$ ?

## Exercise 2.1: Quantum State

Normalize the following vectors and rewrite them as mixed states in Dirac's notation.

$$1. \begin{bmatrix} 1 & 0 \end{bmatrix}^T$$

$$2. \begin{bmatrix} 1 & 1 \end{bmatrix}^T$$

$$3. \begin{bmatrix} \text{cis } \frac{\pi}{4} & 1 \end{bmatrix}^T$$

$$4. \begin{bmatrix} \text{cis } \frac{\pi}{6} & \text{cis}(-\frac{\pi}{6}) \end{bmatrix}$$

$$5. \begin{bmatrix} i/4 & -i/6 \end{bmatrix}$$

$$6. \begin{bmatrix} 1 & i \end{bmatrix}^T$$

$$7. \begin{bmatrix} 0 & -1+i \end{bmatrix}$$

Answer the following questions.

8. Compute the adjoints of all quantum states in Ex 1-7 and write them down in Dirac's notation.

9. Suppose  $|\psi\rangle = r_1 \text{cis}\theta_1 |0\rangle + r_2 \text{cis}\theta_2 |1\rangle$ . Show that

$$\langle\psi| = r_1 \text{cis}(-\theta_1) \langle 0| + r_2 \text{cis}(-\theta_2) \langle 1|$$

10. Show that for any complex vector  $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ ,

$$\langle\psi|\psi\rangle = |\alpha|^2 + |\beta|^2$$

[Hint:  $\mathbf{u} \vee \mathbf{v} = \sum_{k=1}^M u_k \bar{v}_k$ ]

## Exercise 2.1 (cont'd): Quantum State

Compute the inner product  $\langle \phi | \psi \rangle$  of the following state pairs.

11.  $\phi = |0\rangle$  and  $\psi = |0\rangle$

12.  $\phi = |0\rangle$  and  $\psi = -|0\rangle$

13.  $\phi = |1\rangle$  and  $\psi = |0\rangle$

14.  $\phi = |0\rangle$  and  $\psi = i|0\rangle$

15.  $\phi = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$  and  $\psi = |0\rangle$

16.  $\phi = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$  and  $\psi = \text{cis} \frac{\pi}{4} |0\rangle$

17.  $\phi = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$  and  $\psi = -\text{cis} \frac{\pi}{4} |1\rangle$

18.  $\phi = \frac{1}{\sqrt{2}}(i|0\rangle - i|1\rangle)$  and  $\psi = -\text{cis} \frac{\pi}{4} |1\rangle$

19.  $\phi = \frac{1}{\sqrt{2}}(\text{cis} \frac{\pi}{3} |0\rangle + \text{cis} \frac{2\pi}{3} |1\rangle)$  and  
 $\psi = \frac{1}{\sqrt{2}}(\text{cis}(-\frac{\pi}{3}) |0\rangle + \text{cis} \frac{\pi}{3} |1\rangle)$

Answer the following questions.

20. Compute  $\langle \phi | \psi \rangle$ , where

$$|\phi\rangle = r_1 \text{cis} \theta |0\rangle + r_2 |1\rangle$$

$$|\psi\rangle = r_1 |0\rangle + r_2 \text{cis}(-\theta) |1\rangle$$

21. Compute  $\langle \phi | \psi \rangle$ , where

$$|\phi\rangle = r_1 \text{cis} \theta_1 |0\rangle + r_2 \text{cis} \theta_2 |1\rangle$$

$$|\psi\rangle = s_1 \text{cis} \lambda_1 |0\rangle + s_2 \text{cis} \lambda_2 |1\rangle$$

22. Show that for any quantum state  $|\psi\rangle$  and phase  $\theta$ ,

$$\langle \text{cis} \theta | \psi \rangle | \text{cis} \theta | \psi \rangle \rangle = \langle \psi | \psi \rangle$$

## Quantum Operators

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# Quantum Operators

- Inner product: phase synchronicity, which implies state similarity

$$\langle \phi | \psi \rangle = |\phi\rangle \vee |\psi\rangle = |\phi\rangle^\top \overline{|\psi\rangle}$$

- How does it work?

$$\begin{aligned} \mathbf{U} |q\rangle &= \left( \sum_{k=1}^K |\phi_k\rangle \langle \psi_k| \right) |q\rangle \\ &= \sum_{k=1}^K |\phi_k\rangle (\langle \psi_k | |q\rangle) \\ &= \sum_{k=1}^K |\phi_k\rangle \langle \psi_k | q \rangle \end{aligned}$$

- Outer product: pairwise synchronicity, which implies state mapping  $|\psi\rangle \mapsto |\phi\rangle$

$$|\phi\rangle \langle \psi| = |\phi\rangle \wedge |\psi\rangle = |\phi\rangle |\psi\rangle^*$$

- Quantum operator: is a unitary matrix

$$\mathbf{U} = \sum_{k=1}^K |\phi_k\rangle \langle \psi_k|$$

where each  $(\psi_k, \phi_k)$  is a pair of input and output states

- Interpretation:

1. Input state  $|q\rangle$  is compared against each input basis  $|\psi_k\rangle$
2. Each output basis  $\phi_k$  is multiplied by input state similarity  $\langle \psi_k | q \rangle$

## Example: Quantum Operator/1

- Suppose we want to construct a quantum operator from the following state mapping

$$\begin{aligned} |0\rangle &\mapsto \frac{|0\rangle + |1\rangle}{\sqrt{2}} \\ |1\rangle &\mapsto \frac{|0\rangle - |1\rangle}{\sqrt{2}} \end{aligned}$$

- Our quantum operator is

$$\begin{aligned} \mathbf{U} &= \frac{|0\rangle + |1\rangle}{\sqrt{2}} |0\rangle^* + \frac{|0\rangle - |1\rangle}{\sqrt{2}} |1\rangle^* \\ &= \frac{|0\rangle + |1\rangle}{\sqrt{2}} \langle 0| + \frac{|0\rangle - |1\rangle}{\sqrt{2}} \langle 1| \end{aligned}$$

- Trick 1: Each  $|j\rangle \langle k|$  represents the value at position (row  $j$ , column  $k$ )

- We put  $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$  into column 0
- We put  $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$  into column 1

- Therefore, our quantum operator  $\mathbf{U}$  is:

$$\begin{aligned} \mathbf{U} &= \left[ \begin{array}{cc} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{array} \right] \\ &= \frac{1}{\sqrt{2}} \left[ \begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array} \right] \end{aligned}$$

- Beware: You always have to compute the adjoint of each input basis  $\langle \psi_k |$

## Example: Quantum Operator/2

- Now let's construct a quantum operator from the following state mapping

$$\text{cis} \frac{\pi}{4} |0\rangle \mapsto |1\rangle$$

$$\text{cis}(-\frac{\pi}{4}) |1\rangle \mapsto |0\rangle$$

- Remember:** Always compute the adjoint of the input bases

$$\begin{aligned} \mathbf{U} &= |1\rangle \left( \text{cis} \frac{\pi}{4} |0\rangle \right)^* + |0\rangle \left( \text{cis}(-\frac{\pi}{4}) |1\rangle \right)^* \\ &= |1\rangle \left( \text{cis}(-\frac{\pi}{4}) \langle 0| \right) + |0\rangle \left( \text{cis} \frac{\pi}{4} \langle 1| \right) \\ &= \text{cis}(-\frac{\pi}{4}) |1\rangle \langle 0| + \text{cis} \frac{\pi}{4} |0\rangle \langle 1| \end{aligned}$$

- Trick 1:** Each  $|j\rangle \langle k|$  represents the value at position (row  $j$ , column  $k$ )

- We put  $0|0\rangle + \text{cis}(-\frac{\pi}{4})|1\rangle$  into column 0
- We put  $\text{cis} \frac{\pi}{4} |0\rangle + 0|1\rangle$  into column 1

- Therefore, our quantum operator  $\mathbf{U}$  is:

$$\mathbf{U} = \begin{bmatrix} 0 & \text{cis} \frac{\pi}{4} \\ \text{cis}(-\frac{\pi}{4}) & 0 \end{bmatrix}$$

- Trick 2:** It is recommended to have unit input and output bases, because we want to avoid stretching
- Trick 3:** In most cases, the input bases are  $|0\rangle$  and  $|1\rangle$  for ease of understanding

## Exercise 2.2: Quantum Operator

Compute a quantum operator for the following state mappings.

1.  $|0\rangle \mapsto |1\rangle$  and  $|1\rangle \mapsto |0\rangle$
2.  $|0\rangle \mapsto i|1\rangle$  and  $|1\rangle \mapsto -i|0\rangle$
3.  $|0\rangle \mapsto |0\rangle$  and  $|1\rangle \mapsto -|1\rangle$
4.  $|0\rangle \mapsto |0\rangle$  and  $|1\rangle \mapsto i|1\rangle$
5.  $|0\rangle \mapsto |0\rangle$  and  $|1\rangle \mapsto \text{cis}(-\frac{\pi}{4})|1\rangle$
6.  $|0\rangle \mapsto \frac{|0\rangle+|1\rangle}{\sqrt{2}}$  and  $|1\rangle \mapsto \frac{|0\rangle-|1\rangle}{\sqrt{2}}$
7.  $\frac{|0\rangle+|1\rangle}{\sqrt{2}} \mapsto |0\rangle$  and  $\frac{|0\rangle-|1\rangle}{\sqrt{2}} \mapsto |1\rangle$
8.  $\text{cis}\frac{\pi}{4}|0\rangle \mapsto \text{cis}\frac{\pi}{4}|1\rangle$  and  $\text{cis}\frac{\pi}{4}|1\rangle \mapsto \text{cis}\frac{\pi}{4}|0\rangle$
9.  $\frac{\text{cis}(-\pi/4)|0\rangle+\text{cis}(-\pi/4)|1\rangle}{\sqrt{2}} \mapsto |0\rangle$  and  $\frac{\text{cis}(\pi/4)|0\rangle-\text{cis}(\pi/4)|1\rangle}{\sqrt{2}} \mapsto |1\rangle$

Answer the following questions.

10. Show that for any quantum operator  $\mathbf{U}$ , applying it twice on any quantum state yields the same state.

$$\mathbf{U}\mathbf{U}|\psi\rangle = |\psi\rangle$$

11. Show that if there exists phase  $\theta$  such that all  $k$ -th input-output pairs are in the form  $\text{cis}\theta|\psi_k\rangle \mapsto \text{cis}\theta|\phi_k\rangle$ , then the quantum operator is

$$\mathbf{U} = \sum_{k=1}^K |\phi_k\rangle \langle \psi_k|$$

$\theta$  is called a global phase.

## Exercise 2.2 (cont'd): Quantum Operator

Extract a state mapping out of each quantum operator as follows.

$$12. \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$13. \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$14. \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$15. \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$16. \frac{1}{\sqrt{2}} \begin{bmatrix} \text{cis } \frac{\pi}{4} & \text{cis } \frac{\pi}{4} \\ \text{cis } (-\frac{\pi}{4}) & -\text{cis } (-\frac{\pi}{4}) \end{bmatrix}$$

Answer the following questions.

17. Show that any quantum operator

$$\mathbf{U} = \begin{bmatrix} a & c \\ b & d \end{bmatrix}$$

can always be rewritten as

$$\mathbf{U}(\theta) = \begin{bmatrix} a & -\bar{b} \text{cis } \lambda \\ b & \bar{a} \text{cis } \lambda \end{bmatrix}$$

for some phase  $\lambda$ . [Hint:  $\mathbf{U}$  is a unitary matrix; i.e.  $\mathbf{U}^{-1} = \mathbf{U}^*$  and  $\det(\mathbf{U}) = 1$ . Note that  $\mathbf{U}^{-1} = \frac{1}{\det(\mathbf{U})} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$ ].

## Universal Rotation

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# Bloch Sphere

- Motivation: How can we represent such probability distribution with a particle's spin in a unit sphere?
- Spin coordinate is a vector function of polar angle  $\theta$  and azimuthal angle  $\phi$

$$\sigma(\theta, \phi) = \begin{bmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{bmatrix}$$

- Quantum state is like a Rubik's cube
  - Axis Z:  $|0\rangle$  = up and  $|1\rangle$  = down
  - Axis X:  $+1$  = front and  $-1$  = back
  - Axis Y:  $+i$  = right and  $-i$  = left

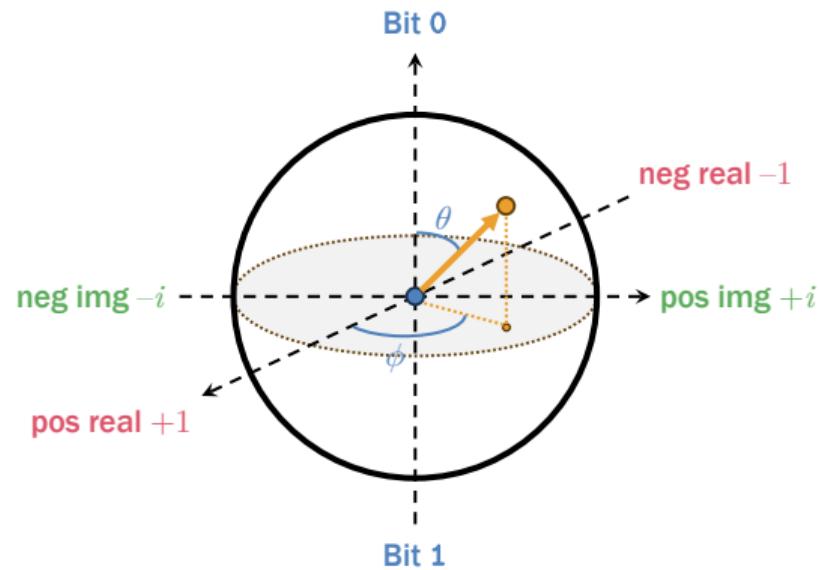


Figure 1: Bloch sphere

# Spinor

- Spinor (pronounced ‘spinner’) is a complex vector that represents a spinning object
  - Non-spinning objects take a  $360^\circ$  full rotation:  $\pi$  to flip the sign and  $2\pi$  to return to the original sign
  - Spinning objects take a  $720^\circ$  full rotation:  $2\pi$  to flip the sign and  $4\pi$  to return to the original sign
- Activity: Let’s make a one-twist Möbius strip and observe a full rotation on it
- The notion of spinor is applied only on the phase  $\theta$  to reflect the spin direction

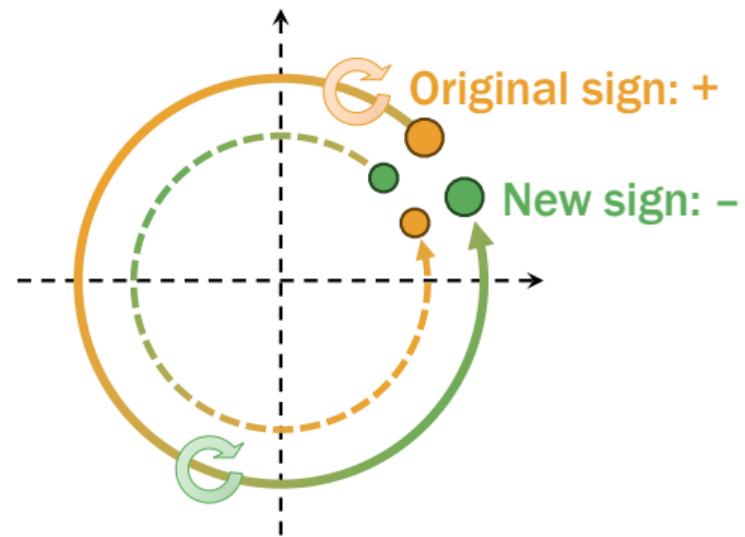


Figure 2: Rotation on a one-twist Möbius strip

# 3-Step Universal Rotation

- Any quantum operator is decomposed into 3-step rotation:  $\omega \rightarrow \frac{\theta}{2} \rightarrow \phi$

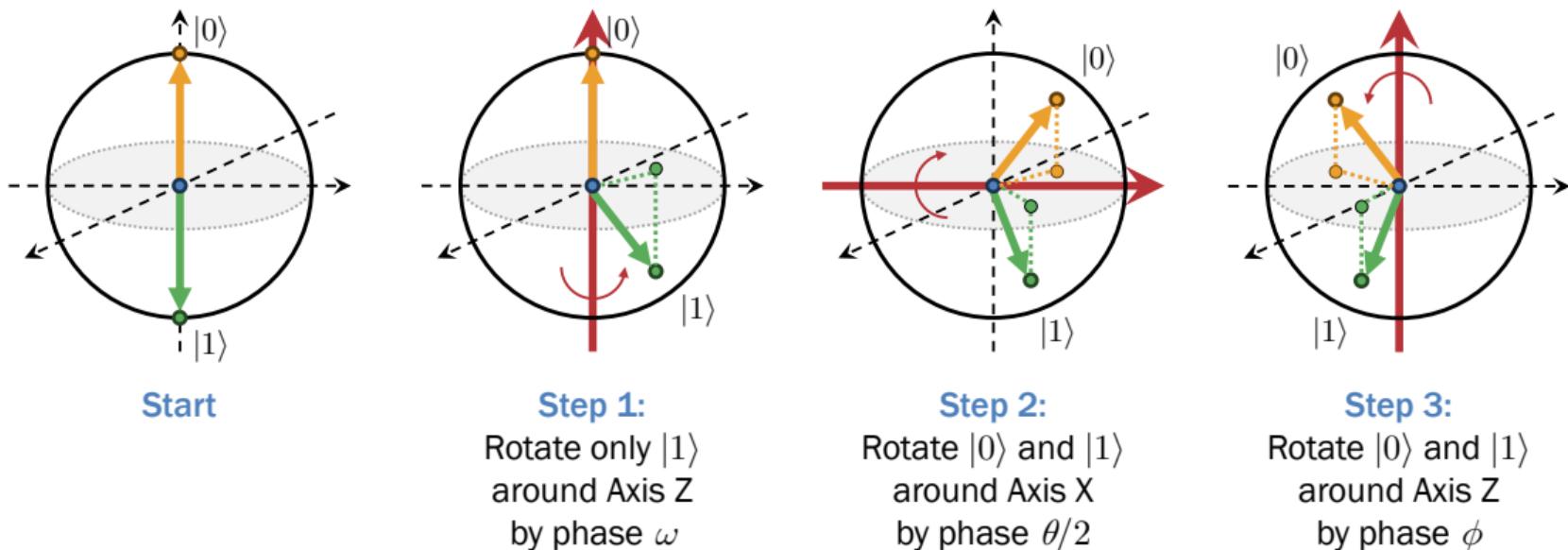


Figure 3: Universal rotation

## Universal Rotation Operator: $U_3$

- All quantum operators are essentially a rotation operator for spinors

$$U_3(\phi, \theta, \omega) = \begin{bmatrix} \cos \frac{\theta}{2} & -\text{cis} \omega \sin \frac{\theta}{2} \\ \text{cis} \phi \sin \frac{\theta}{2} & \text{cis}(\phi + \omega) \cos \frac{\theta}{2} \end{bmatrix}$$

This matrix representation was first proposed by IBM Quantum Platform

- The rotation matrix  $U_3(\phi, \theta, \omega)$  can also be seen as a state mapping

$$|0\rangle \mapsto \cos \frac{\theta}{2} |0\rangle + \text{cis} \phi \sin \frac{\theta}{2} |1\rangle$$

$$|1\rangle \mapsto -\text{cis} \omega \sin \frac{\theta}{2} |0\rangle + \text{cis}(\phi + \omega) \cos \frac{\theta}{2} |1\rangle$$

- Inventing the rotation matrix:

- Previously, we found that any quantum operator can be rewritten as

$$U = \begin{bmatrix} a & c \\ b & d \end{bmatrix} = \begin{bmatrix} a & -\bar{b} \text{cis} \lambda \\ b & \bar{a} \text{cis} \lambda \end{bmatrix}$$

- Since  $U$  is unitary, each column should be a unit vector; i.e.  $a\bar{a} + b\bar{b} = 1$
- Motivated by  $\cos^2 x + \sin^2 x = 1$ , we choose  $a = \cos \frac{\theta}{2}$  due to the spinors
- To make  $b$  a complex number, we choose  $b = \text{cis} \phi \sin \frac{\theta}{2}$
- Letting  $\lambda = \omega + \phi$ , we choose  $c = -\bar{b} \text{cis}(\omega + \phi) = -\text{cis} \omega \sin \frac{\theta}{2}$
- Therefore,  $d = \cos \frac{\theta}{2} \text{cis}(\omega + \phi)$

## Conversion to $U_3$

- Any quantum operator  $Q$  can be converted to  $U_3(\phi, \theta, \omega)$
- Example: Let's convert  $Q$  to  $U_3$

$$Q = \begin{bmatrix} a_1 \text{cis} \lambda_1 & -a_2 \text{cis} \lambda_3 \\ a_2 \text{cis} \lambda_2 & a_1 \text{cis} \lambda_4 \end{bmatrix}$$

where all  $a_k, \lambda_k$  are real numbers

### Steps:

- Rewrite  $Q$  with the global phase  $\lambda_1$

$$Q' = \begin{bmatrix} a_1 & -a_2 \text{cis}(\lambda_3 - \lambda_1) \\ a_2 \text{cis}(\lambda_2 - \lambda_1) & a_1 \text{cis}(\lambda_4 - \lambda_1) \end{bmatrix}$$

- We obtain  $\theta, \phi, \omega$  via

$$\theta = 2 \arccos \frac{a_1}{\sqrt{a_1^2 + a_2^2}}, \quad \phi = \lambda_2 - \lambda_1, \quad \omega = \lambda_3 - \lambda_1$$

- We rewrite  $Q$  with the global phase 0

$$Q = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$Q' = \begin{bmatrix} 1 & -1 \text{cis} \pi \\ 1 \text{cis} 0 & 1 \text{cis} \pi \end{bmatrix}$$

- We extract  $\theta, \phi, \omega$  via:

$$\theta = 2 \arccos \frac{1}{\sqrt{1^2 + 1^2}} = \frac{\pi}{2}$$

$$\phi = 0$$

$$\omega = \pi$$

## Exercise 2.3: Rotation Matrix $\mathbf{U}_3$

Convert the following quantum operators into the equivalent rotation matrices.

$$1. \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$2. \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$3. \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

$$4. \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$5. \frac{1}{\sqrt{2}} \begin{bmatrix} \text{cis } \frac{\pi}{4} & \text{cis } \frac{\pi}{4} \\ \text{cis } (-\frac{\pi}{4}) & -\text{cis } (-\frac{\pi}{4}) \end{bmatrix}$$

Answer the following questions.

6. Show that for any quantum operator

$$\mathbf{Q} = \begin{bmatrix} a_1 \text{cis } \lambda_1 & -a_2 \text{cis } \lambda_3 \\ a_2 \text{cis } \lambda_2 & a_1 \text{cis } \lambda_4 \end{bmatrix}$$

we can extract  $\theta, \phi, \omega$  for  $\mathbf{U}_3$  via:

$$\theta = 2 \arccos \frac{a_1}{\sqrt{a_1^2 + a_2^2}}$$

$$\phi = \lambda_2 - \lambda_1$$

$$\omega = \lambda_3 - \lambda_1$$

## Exercise 2.3 (cont'd): Rotation Matrix $U_3$

Convert the following state mappings into the equivalent rotation matrices.

7.  $|0\rangle \mapsto |1\rangle$  and  $|1\rangle \mapsto |0\rangle$
8.  $|0\rangle \mapsto i|1\rangle$  and  $|1\rangle \mapsto -i|0\rangle$
9.  $|0\rangle \mapsto |0\rangle$  and  $|1\rangle \mapsto -|1\rangle$
10.  $|0\rangle \mapsto |0\rangle$  and  $|1\rangle \mapsto i|1\rangle$
11.  $|0\rangle \mapsto |0\rangle$  and  $|1\rangle \mapsto \text{cis}(-\frac{\pi}{4})|1\rangle$
12.  $|0\rangle \mapsto \frac{|0\rangle+|1\rangle}{\sqrt{2}}$  and  $|1\rangle \mapsto \frac{|0\rangle-|1\rangle}{\sqrt{2}}$
13.  $\frac{|0\rangle+|1\rangle}{\sqrt{2}} \mapsto |0\rangle$  and  $\frac{|0\rangle-|1\rangle}{\sqrt{2}} \mapsto |1\rangle$
14.  $\text{cis}\frac{\pi}{4}|0\rangle \mapsto \text{cis}\frac{\pi}{4}|1\rangle$  and  $\text{cis}\frac{\pi}{4}|1\rangle \mapsto \text{cis}\frac{\pi}{4}|0\rangle$
15.  $\frac{\text{cis}(-\pi/4)|0\rangle+\text{cis}(-\pi/4)|1\rangle}{\sqrt{2}} \mapsto |0\rangle$  and  $\frac{\text{cis}(\pi/4)|0\rangle-\text{cis}(\pi/4)|1\rangle}{\sqrt{2}} \mapsto |1\rangle$

Answer the following questions.

16. Explain briefly why it takes a  $720^\circ$  full rotation to return to the origin on a one-twist Möbius strip.
17. Show that

$$\begin{aligned} & U_3(\phi_1, \theta_1, \omega_1)U_3(\theta_2, \phi_2, \omega_2) \\ &= U_3(\phi_1 + \phi_2, \theta_1 + \theta_2, \omega_1 + \omega_2) \end{aligned}$$

18. Show that

$$U_3^*(\phi, \theta, \omega) = U_3(-\omega, -\theta, -\phi)$$

## Mixed States

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# Multi-Qubit and Mixed State

- Multi-qubit is equivalent to bitstring in classical computers, e.g.  $|10011\rangle$  is equivalent to binary **10011** (decimal 19)
- Multi-qubit of length  $N$  is a one-hot vector of  $2^N$  dimensions, where  $|s\rangle$  has the one-hot position at  $s$  starting from 0
- Example:

$$|00\rangle = \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}^\top$$

$$|10\rangle = \begin{bmatrix} 0 & 0 & 1 & 0 \end{bmatrix}^\top$$

$$|000\rangle = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^\top$$

$$|101\rangle = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}^\top$$

- Mixed state is a mixture of multi-qubits  $|\phi_k\rangle$  and their complex coefficients  $\alpha_k$ :

$$|\phi\rangle = \alpha_1 |\phi_1\rangle + \dots + \alpha_K |\phi_K\rangle$$

where the probability distribution for each multi-qubit is  $P(\phi_k|\phi) = |\alpha_k|^2$

- Example: Consider the mixed state  $|\phi\rangle$

$$|\phi\rangle = \frac{1}{\sqrt{2}} |00\rangle + \frac{1}{\sqrt{2}} |11\rangle$$

The distribution for each outcome is

$$P(00|\phi) = (1/\sqrt{2})^2 = 0.5$$

$$P(11|\phi) = (1/\sqrt{2})^2 = 0.5$$

## Exercise 2.4: Mixed State

Convert the following mixed states to the equivalent vectors.

1.  $|1\rangle$
2.  $\frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle$
3.  $\frac{\sqrt{3}}{2}|10\rangle + \frac{1}{2}|11\rangle$
4.  $\frac{1}{\sqrt{2}}(-i|0\rangle + i|1\rangle)$
5.  $\frac{1}{2}(|00\rangle - |01\rangle + |10\rangle - |11\rangle)$
6.  $\frac{1}{\sqrt{2}}(|010\rangle + |101\rangle)$
7.  $\frac{1}{\sqrt{2}}(\text{cis}\frac{\pi}{4}|0110\rangle - \text{cis}(-\frac{\pi}{4})|1110\rangle)$
8.  $\frac{1}{\sqrt{8}}\sum_{k=000}^{111} \text{cis}\frac{k\pi}{4}|k\rangle$

Convert the following vectors to the equivalent mixed states.

9.  $\begin{bmatrix} 1 & 0 \end{bmatrix}^\top$
10.  $\frac{1}{\sqrt{2}}\begin{bmatrix} i & -i \end{bmatrix}^\top$
11.  $\frac{1}{\sqrt{2}}\begin{bmatrix} \text{cis}\frac{\pi}{4} & \text{cis}(-\frac{\pi}{4}) \end{bmatrix}^\top$
12.  $\frac{1}{\sqrt{3}}\begin{bmatrix} 1 & 0 & -1 & 1 \end{bmatrix}^\top$
13.  $\frac{1}{2}\begin{bmatrix} 1 & 0 & 0 & i & 0 & -1 & -i & 0 \end{bmatrix}^\top$
14.  $\begin{bmatrix} \frac{1}{2}\text{cis}\frac{\pi}{3} & 0 & 0 & \frac{\sqrt{3}}{2}\text{cis}\frac{2\pi}{3} \end{bmatrix}^\top$

# Tensor Product

- Tensor product: We can construct a longer multi-qubit by enumeratively concatenating shorter multi-qubits
- Suppose we have

$$|\psi\rangle = \alpha_1 |\psi_1\rangle + \dots + \alpha_K |\psi_K\rangle$$

$$|\phi\rangle = \beta_1 |\phi_1\rangle + \dots + \beta_M |\phi_M\rangle$$

- Their tensor product is

$$|\psi\rangle \otimes |\phi\rangle = \sum_{k=1}^K \sum_{m=1}^M \alpha_k \beta_m |\psi_k \phi_m\rangle$$

where the distribution for outcome  $\psi_k \phi_m$  becomes  $P(\psi_k \phi_m) = |\alpha_k \beta_m|^2$

- Example: Let

$$|\psi\rangle = \frac{1}{\sqrt{2}} |01\rangle + \frac{1}{\sqrt{2}} |10\rangle$$

$$|\phi\rangle = \frac{1}{\sqrt{2}} |00\rangle + \frac{1}{\sqrt{2}} |11\rangle$$

We then have

$$\begin{aligned} |\psi\rangle \otimes |\phi\rangle &= \frac{1}{2} |0100\rangle + \frac{1}{2} |0111\rangle \\ &\quad + \frac{1}{2} |1000\rangle + \frac{1}{2} |1011\rangle \end{aligned}$$

Note that each outcome has equal probabilities  $(1/2)^2 = 0.25$

# Factorization of Mixed States

Example: Factorize  $\frac{1}{\sqrt{2}}(|00\rangle + |01\rangle)$ .

1. Factorization of two qubits means

$$(a|0\rangle + b|1\rangle) \otimes (c|0\rangle + d|1\rangle) \\ = ac|00\rangle + ad|01\rangle + bc|10\rangle + bd|11\rangle$$

2. We obtain the following equations

$$ac = ad = 1/\sqrt{2} \quad bc = bd = 0$$

3. Since  $c, d \neq 0$ , therefore  $b = 0$ .

4. Since  $c = d$ , we therefore obtain

Case 1:  $a = 1/\sqrt{2}, b = 0, c = d = 1$

Case 2:  $a = 1, b = 0, c = d = 1/\sqrt{2}$

Example: Factorize  $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ .

1. Factorization of two qubits means

$$(a|0\rangle + b|1\rangle) \otimes (c|0\rangle + d|1\rangle) \\ = ac|00\rangle + ad|01\rangle + bc|10\rangle + bd|11\rangle$$

2. We obtain the following equations

$$ac = bd = 1/\sqrt{2} \quad ad = bc = 0$$

3. Since  $a, b, c, d \neq 0$ , there are no ways to allow  $ad = bc = 0$ .

4. Therefore, there are no solutions for these equations. This mixed state cannot be factorized any further.

## Factorization Formulae

- Common prefix  $|w\rangle$

$$\sum_{k=1}^N a_k |ws_k\rangle = |w\rangle \otimes \left( \sum_{k=1}^N a_k |s_k\rangle \right)$$

- Common suffix  $|w\rangle$

$$\sum_{k=1}^N a_k |s_k w\rangle = \left( \sum_{k=1}^N a_k |s_k\rangle \right) \otimes |w\rangle$$

- Bit-flipped prefixes  $|w\rangle$  and  $|\overline{w}\rangle$

$$\sum_{k=1}^N a_k (b|ws_k\rangle + c|\overline{w}s_k\rangle) = (b|w\rangle + c|\overline{w}\rangle) \otimes \left( \sum_{k=1}^N a_k |s_k\rangle \right)$$

$$\sum_{k=1}^N a_k (b|s_k w\rangle + c|s_k \overline{w}\rangle) = \left( \sum_{k=1}^N a_k |s_k\rangle \right) \otimes (b|w\rangle + c|\overline{w}\rangle)$$

## Exercise 2.5: Tensor Product and Factorization

Compute the following tensor products.

Compare each of them against a lattice.

$$1. |0\rangle \otimes |1\rangle$$

$$2. \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

$$3. \frac{|00\rangle + |11\rangle}{\sqrt{2}} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

$$4. \frac{|00\rangle + |11\rangle}{\sqrt{2}} \otimes \frac{|01\rangle + |10\rangle}{\sqrt{2}}$$

$$5. |0\rangle \otimes \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |1\rangle$$

$$6. \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

$$7. \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes \frac{|01\rangle + |10\rangle}{\sqrt{2}} \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

$$8. \frac{|00\rangle + |01\rangle + |10\rangle}{\sqrt{3}} \otimes \frac{|01\rangle + |10\rangle + |11\rangle}{\sqrt{3}}$$

Factorize the following mixed states into as many tensor products as possible.

$$9. \frac{1}{\sqrt{2}} (|100\rangle + |101\rangle)$$

$$10. \frac{1}{\sqrt{2}} (|001\rangle + |101\rangle)$$

$$11. \frac{1}{2} (|000\rangle + |001\rangle + |110\rangle + |111\rangle)$$

$$12. \frac{1}{\sqrt{2}} (|001011\rangle + |000111\rangle)$$

$$13. \frac{1}{2} (|1100\rangle + |1101\rangle + |1110\rangle + |1111\rangle)$$

$$14. \frac{2}{\sqrt{10}} |100000\rangle - \frac{1}{\sqrt{10}} |100100\rangle + \frac{1}{\sqrt{10}} |101000\rangle - \frac{2}{\sqrt{10}} |101100\rangle$$

$$15. \frac{1}{\sqrt{2}} (|001100\rangle - |111111\rangle)$$

$$16. \frac{1}{\sqrt{3}} (|1000\rangle + |0100\rangle + |0010\rangle) \text{ [hard]}$$

## Exercise 2.5 (cont'd): Tensor Product and Factorization

Answer the following questions.

17. Show that we cannot factorize  $\frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$  any further.
18. Show that if  $|w\rangle$  is a multi-qubit of length  $N > 1$ , then we cannot factorize  $\frac{1}{\sqrt{2}}(|w\rangle + |\overline{w}\rangle)$  any further
19. Show that if  $|w\rangle$  and each  $|s_k\rangle$  are multi-qubits, then

$$\sum_{k=1}^N a_k |ws_k\rangle = |w\rangle \otimes \sum_{k=1}^N a_k |s_k\rangle$$

20. Show that if  $|w\rangle$  and each  $|s_k\rangle$  are multi-qubits, then

$$\sum_{k=1}^N a_k |s_k w\rangle = \left( \sum_{k=1}^N a_k |s_k\rangle \right) \otimes |w\rangle$$

## Quantum Entanglement

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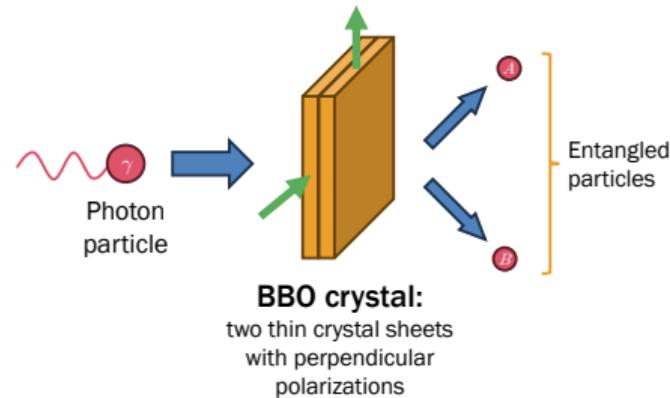
# Quantum Entanglement

- Entanglement: is the phenomenon, where quantum state of each particle in a group cannot be described independently of the others

- If a mixed state is factorizable, it can be decomposed into separate qubits
- However, if it is unfactorizable, we say it is an entangled state

- Properties

- Measuring one particle in a group will destroy the superposition, causing all of them to reveal their pure states
- Entangled state can be used for secure data sharing, where each particle carries shared secret information



**Figure 4:** Entangled states are created with the SPDC process (spontaneous parametric down-conversion) using Beta-Barium Borate (BBO) crystals. In 2024, it takes  $10^6$  photon pumps to create 1 pair of entangled particles. Quantum entanglement is such an expensive resource!

# Categories of Quantum Entanglement

- Category 1: Bell state

$$|\Psi^+\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

$$|\Psi^-\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}}$$

$$|\Phi^+\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}$$

$$|\Phi^-\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}$$

- We refer to each qubit of the entangled state with letters A, B, C, ...
- For example,  $|\Psi_A^+\rangle$  and  $|\Psi_B^+\rangle$  are either (0,0) or (1,1)

- Category 2: GHZ state (Greenberger, Horne, and Zellinger)

$$|GHZ_N\rangle = \frac{|0\rangle^{\otimes N} + |1\rangle^{\otimes N}}{\sqrt{2}}$$

where  $|\psi\rangle^{\otimes N}$  is the  $N$  repetitions of  $|\psi\rangle$

- Category 3: W-state

$$|W_N\rangle = \frac{1}{\sqrt{N}} \sum_{k=1}^N |\text{onehot}(k)\rangle$$

where  $\text{onehot}(k)$  is the one-hot vector at position  $k$

# Quantum Robustness

- Repetition  $|b\rangle^{\otimes N}$  is more prone to **quantum decoherence** than  $|\text{onehot}(k)\rangle$
- One corrupted qubit (projected to either  $|0\rangle$  or  $|1\rangle$ ) makes the remaining qubits disentangled
- Example: Corruption on the third bit to  $|0\rangle$  of the 3-qubit states is the projector:

$$\begin{aligned} P = & |00\rangle\langle 00\underline{0}| + |01\rangle\langle 01\underline{0}| \\ & + |10\rangle\langle 10\underline{0}| + |11\rangle\langle 11\underline{0}| \end{aligned}$$

Note that all multi-qubits ending with  $|1\rangle$  are eliminated

- Case 1: We have a 3-qubit GHZ state

$$|GHZ_3\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$$

- The superposition collapses to the subspace whose third qubit is  $|0\rangle$

$$\begin{aligned} P|GHZ_3\rangle &= P\left(\frac{1}{\sqrt{2}}|00\underline{0}\rangle + |11\underline{1}\rangle\right) \\ &= |00\rangle \\ &= |0\rangle \otimes |0\rangle \end{aligned}$$

The result is not an entangled state

- GHZ state is fragile and intolerant to corrupted qubits

- Repetition  $|b\rangle^{\otimes N}$  is more prone to **quantum decoherence** than  $|\text{onehot}(k)\rangle$
- One corrupted qubit (projected to either  $|0\rangle$  or  $|1\rangle$ ) makes the remaining qubits disentangled
- Example: Corruption on the third bit to  $|0\rangle$  of the 3-qubit states is the projector:

$$\begin{aligned} P = & |00\rangle\langle 00\underline{0}| + |01\rangle\langle 01\underline{0}| \\ & + |10\rangle\langle 10\underline{0}| + |11\rangle\langle 11\underline{0}| \end{aligned}$$

Note that all multi-qubits ending with  $|1\rangle$  are eliminated

- Case 2: We have a 3-qubit W-state

$$|W_3\rangle = \frac{1}{\sqrt{3}} (|10\underline{0}\rangle + |01\underline{0}\rangle + |00\underline{1}\rangle)$$

- The superposition collapses to the subspace whose third qubit is  $|0\rangle$

$$\begin{aligned} P|W_3\rangle &= P \left( \frac{1}{\sqrt{3}} |10\underline{0}\rangle + |01\underline{0}\rangle + |00\underline{1}\rangle \right) \\ &= \frac{1}{\sqrt{2}} (|10\rangle + |01\rangle) \end{aligned}$$

The result is still an entangled state

- W-state is more robust and tolerant to corrupted qubits

# Quantum Robustness

	Bell State	GHZ State	W-State
Qubit counts	2	3 or more	3 or more
Robustness	Not applicable	Fragile	Robust
Creation complexity	Simple	Moderate	Hard
Error tolerance	Moderate	Low	High
Applications	Fundamental experiments	Distributed quantum computing	Distributed quantum computing

Table 1: Comparison of quantum entanglement

## Exercise 2.6: Entanglement

Answer the following questions.

1. Compute the projector matrix  $\mathbf{P}_{4@2}$  for corruption on the second bit to  $|1\rangle$  of the 4-qubit states.
2. Compute a 4-qubit GHZ state  $|\text{GHZ}_4\rangle$ , and show that  $\mathbf{P}_{4@2}|\text{GHZ}_4\rangle$  is not an entangled state anymore.
3. Compute a 4-qubit W-state  $|W_4\rangle$ , and show that  $\mathbf{P}_{4@2}|W_4\rangle$  is still entangled.
4. Compute the projector matrix  $\mathbf{P}_{N@1}$  for corruption on the first bit to  $|1\rangle$  of the  $N$ -qubit states.

5. Show that  $|\text{GHZ}_N\rangle$  is more fragile than  $|W_N\rangle$  using the projector matrix  $\mathbf{P}_{N@1}$ .
6. Suppose we have invented a new entangled state

$$|Q_N\rangle = \frac{|0\rangle^{\otimes N} \otimes |1\rangle^{\otimes N} + |1\rangle^{\otimes N} \otimes |0\rangle^{\otimes N}}{\sqrt{2}}$$

Show that  $|Q_N\rangle$  is still as fragile as  $|\text{GHZ}_{2N}\rangle$  using the projector matrix.

7. Explain why it is hard to create an entangled state with the SPDC process.

## Multi-Qubit Quantum Operators

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# Multi-Qubit Operators

- Quantum operator: is a unitary matrix

$$\mathbf{U} = \sum_{k=1}^K |\phi_k\rangle\langle\psi_k|$$

where each  $(\psi_k, \phi_k)$  is a pair of input and output states, single- or multi-qubit

- That means  $\mathbf{U}$  is always a square matrix (unlike projectors which can also be non-square)
- Due to frugality reasons, multi-qubit quantum operators partially manipulate the input state to return the output

- Example: Let's construct a quantum operator that flips the second qubit if the first qubit is  $|1\rangle$ ; i.e.

$$\begin{array}{ll} |00\rangle \mapsto |00\rangle & |01\rangle \mapsto |01\rangle \\ |10\rangle \mapsto |11\rangle & |11\rangle \mapsto |10\rangle \end{array}$$

- Our quantum operator becomes

$$\begin{aligned} \text{CNOT} &= |00\rangle\langle 00| + |01\rangle\langle 01| \\ &\quad + |11\rangle\langle 10| + |10\rangle\langle 11| \\ &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \end{aligned}$$

# Multi-Qubit Operators

- Quantum operator: is a unitary matrix

$$\mathbf{U} = \sum_{k=1}^K |\phi_k\rangle\langle\psi_k|$$

where each  $(\psi_k, \phi_k)$  is a pair of input and output states, single- or multi-qubit

- That means  $\mathbf{U}$  is always a square matrix (unlike projectors which can also be non-square)
- Due to frugality reasons, multi-qubit quantum operators partially manipulate the input state to return the output

- Example: Let's construct a quantum operator that swaps both input qubits

$$\begin{array}{ll} |00\rangle \mapsto |00\rangle & |01\rangle \mapsto |10\rangle \\ |10\rangle \mapsto |01\rangle & |11\rangle \mapsto |11\rangle \end{array}$$

- Our quantum operator becomes

$$\begin{aligned} \text{SWAP} &= |00\rangle\langle 00| + |10\rangle\langle 01| \\ &\quad + |01\rangle\langle 10| + |11\rangle\langle 11| \\ &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{aligned}$$

## Exercise 2.7: Multi-Qubit Operators

Compute multi-qubit operators from the following state mappings.

1.  $|00\rangle \mapsto |01\rangle$ ,  $|01\rangle \mapsto |00\rangle$ ,  $|10\rangle \mapsto |10\rangle$ , and  $|11\rangle \mapsto |11\rangle$
2.  $|00\rangle \mapsto |01\rangle$ ,  $|01\rangle \mapsto |00\rangle$ ,  $|10\rangle \mapsto i|11\rangle$ , and  $|11\rangle \mapsto i|10\rangle$
3.  $|00\rangle \mapsto |00\rangle$ ,  $|01\rangle \mapsto |01\rangle$ ,  $|10\rangle \mapsto \frac{|10\rangle + |11\rangle}{\sqrt{2}}$ , and  $|11\rangle \mapsto \frac{|10\rangle - |11\rangle}{\sqrt{2}}$
4.  $\frac{|00\rangle + |01\rangle}{\sqrt{2}} \mapsto |00\rangle$ ,  $\frac{|00\rangle - |01\rangle}{\sqrt{2}} \mapsto |01\rangle$ ,  $|10\rangle \mapsto |10\rangle$ , and  $|11\rangle \mapsto |11\rangle$
5.  $\text{cis} \frac{\pi}{4} |00\rangle \mapsto |01\rangle$ ,  $\text{cis}(-\frac{\pi}{4}) |01\rangle \mapsto |00\rangle$ ,  $|10\rangle \mapsto |10\rangle$ , and  $|11\rangle \mapsto |11\rangle$

Answer the following questions.

6. Design a quantum operator whose state mapping is  $|0x\rangle \mapsto |0x\rangle$  and  $|1x\rangle \mapsto |1\bar{x}\rangle$ , where  $\bar{x}$  denotes the bit flipping of  $x$ .
7. Design a quantum operator that imitates the NAND gate, whose state mapping is  $|xy\rangle \mapsto |\overline{x \wedge y}\rangle \otimes |y\rangle$ .
8. Design a quantum operator that bit-flips the third qubit only if the first and second qubits are  $|1\rangle$ , or preserves the third qubit otherwise.
9. Design a quantum operator whose state mapping is  $|xy\rangle \mapsto |x \wedge y\rangle \otimes |x \vee y\rangle$ .

## Conclusion

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# Conclusion

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- Quantum bits
- Quantum operators
- Universal rotation
- Mixed states
- Quantum entanglement
- Multi-qubit quantum operators

Questions?

# Target Learning Outcomes/1

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- Master Dirac Notation and Quantum State Representation
  1. Translate between bitstring distributions, column vectors (kets), and row vectors (bras).
  2. Calculate the adjoint of both pure and mixed quantum states.
  3. Normalize complex vectors to represent valid mixed states (superpositions) where the sum of squared magnitudes equals 1.
  4. Evaluate state similarity using the inner product and understand the concept of phase synchronicity.
- Construct and Interpret Quantum Operators
  1. Define a quantum operator as a unitary matrix and explain its function as a state mapping mechanism.
  2. Synthesize quantum operators from specified state mappings using the outer product or "positional tricks" for matrix construction.
  3. Analyze existing unitary matrices to extract their underlying state mappings.

## Target Learning Outcomes/2

- Apply Universal Rotation Theory
  1. Visualize quantum states using the Bloch Sphere and understand spin coordinates in terms of polar and azimuthal angles.
  2. Decompose any quantum operator into a 3-step rotation using the  $\mathbf{U}_3$  matrix representation.
  3. Convert standard quantum operators into their equivalent  $\mathbf{U}_3$  parameters by accounting for global phase.
- Manipulate Multi-Qubit Systems and Mixed States
  1. Represent multi-qubit bitstrings as high-dimensional one-hot vectors (e.g.,  $2^N$  dimensions for  $N$  qubits).
  2. Perform tensor products to construct longer multi-qubits from shorter ones.
  3. Execute factorization of mixed states to determine if a multi-qubit system can be decomposed into independent qubits.

## Target Learning Outcomes/3

- Evaluate Quantum Entanglement and Robustness
  1. Identify entangled states as mixed states that are unfactorizable.
  2. Distinguish between major entanglement categories, including Bell states, GHZ states, and W-states.
  3. Assess quantum robustness by calculating how projectors (representing bit corruption) affect the entanglement of different states.
  4. Compare the creation complexity and error tolerance of various entangled states in distributed quantum computing contexts.
- Design Multi-Qubit Logic Gates
  1. Construct complex multi-qubit operators like CNOT and SWAP from conditional state mappings.
  2. Design functional quantum gates that imitate classical logic, such as the NAND gate or conditional bit-flippers (Toffoli-style gates).