

# Understanding Quantum Computing: Qubits, Gates, and Circuits

Quantum Computing  
Parallelizing Data Processing Algorithm

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# Classical Computers — A Binary Input/Output Model

- **Input to CPU**

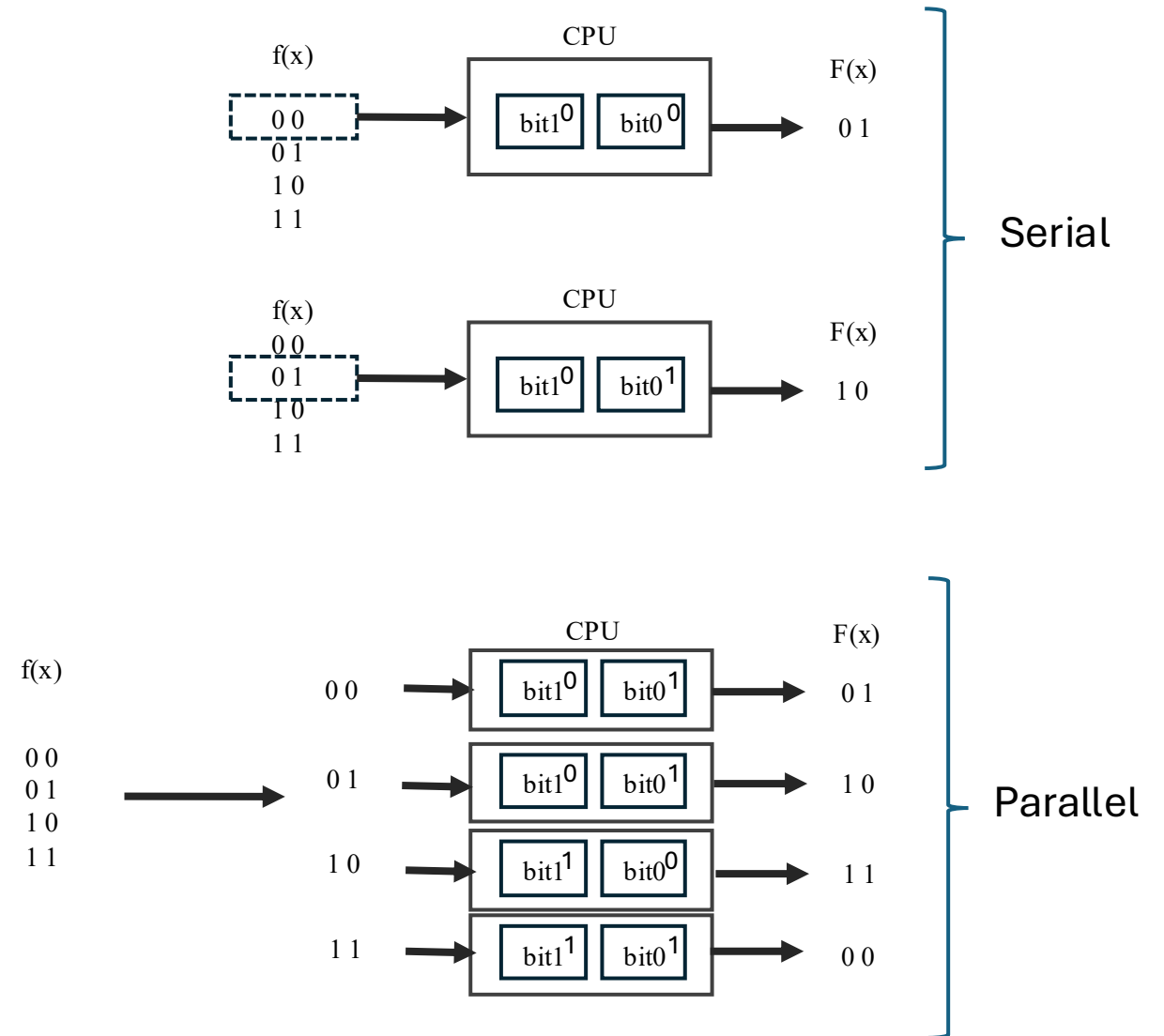
- Data in **binary** form (bits)
- Processed by **logical operations** (AND, OR, NOT, etc.) on registers

- **Output**

- Also, in **binary** (e.g., 0 or 1, or sets of bits)

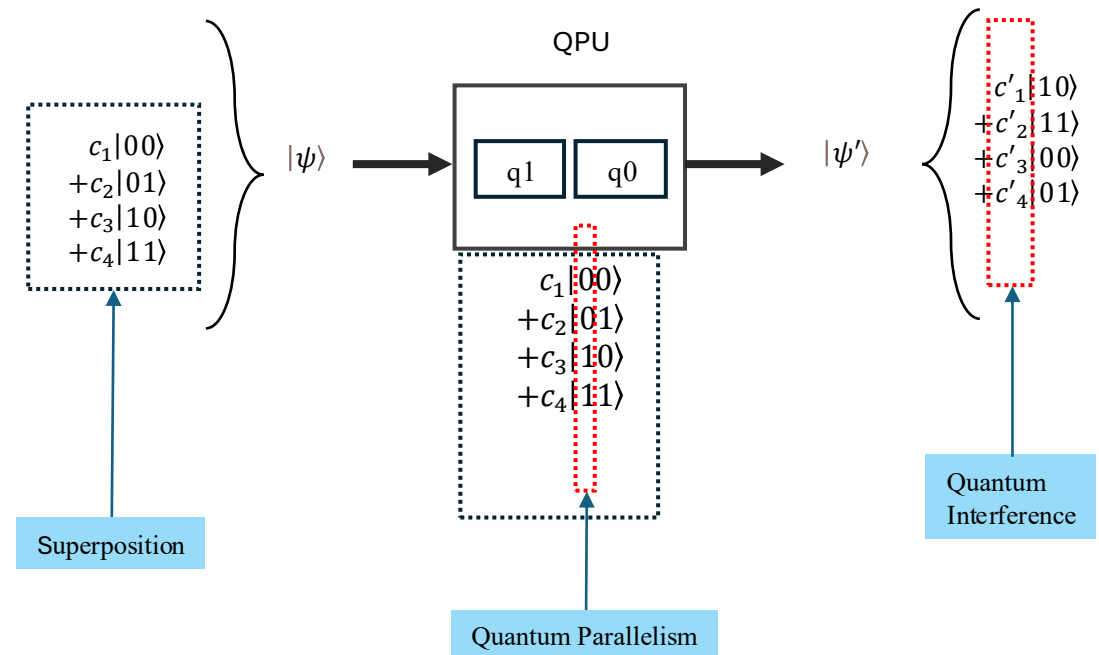
- **Key Point**

- All processing is effectively in a binary, **deterministic** framework
- Even parallel or multi-core approaches remain bound by binary logic



# Quantum Computing — Superposition & Wavefunction

- **Example:** 2 Qubits in Superposition
- **Actions Affect the Whole Wavefunction**
  - Applying a gate to one qubit transforms the **entire** wavefunction
  - This is fundamentally different from classical bitwise operations
- **Measurement**
  - **Single Shot:** Each measurement collapses the superposition to one outcome
  - **Probability Distribution:** Repeating the measurement many times (multiple “shots”) builds a statistical distribution reflecting



# Key Quantum Concepts: Wavefunction & Phenomena

- **Quantum Wavefunction**

- Represents **information** in quantum systems
- Complex amplitudes (phase + magnitude)
- Foundation for computing with qubits

- **Quantum Phenomena**

- **Superposition:** Qubits can exist in multiple basis states simultaneously
- **Entanglement:** Strong correlation between qubits that has no classical analogue
- **Interference:** Amplitudes can reinforce or cancel out, affecting measurement outcomes

- **Quantum Parallelism**

- Arises from these phenomena
- Allows certain computations to evaluate many possibilities “at once”

# Designing for Quantum Advantage

- **Key Takeaway**

- The goal of quantum computing design is to **define and encode information** into a **quantum wavefunction**, then **exploit** superposition, entanglement, and interference to achieve **quantum parallelism** and potential speedups.

- **Focus**

- *Harness* quantum phenomena as much as possible
- *Architect* circuits or annealing processes to maximize quantum advantage

# Quantum Wave Equation & Quantum Wavefunction

- **What is the Quantum Wave Equation?**

- **Schrödinger's Equation:** Governs how the quantum wavefunction  $|\psi\rangle$  evolves over time.
- Replaced classical deterministic trajectories with **probabilistic** descriptions.

- **Significance**

- *Foundation of Quantum Mechanics:* By solving Schrödinger's equation, physicists uncovered quantum phenomena (superposition, entanglement, interference).
- *Describes Dynamics:* Provides the rule for how  $\psi(x, t)$  changes under various potentials or interactions.

- **Key Insight**

- **Wavefunction:** Encodes **all possible outcomes** a system can exhibit.
- **Schrödinger's Equation:** Dictates **when and how** those possibilities evolve or interact.
- **Quantum Computing:** Utilizes the wavefunction as a **mathematical tool** to describe qubit states and engineer quantum operations.

- **Reference**

- E. Schrödinger (1926), *Quantisierung als Eigenwertproblem*, *Annalen der Physik*.
- R. P. Feynman, *The Feynman Lectures on Physics*, Vol. III.

# Visualizing Time Evolution of the Quantum Wavefunction

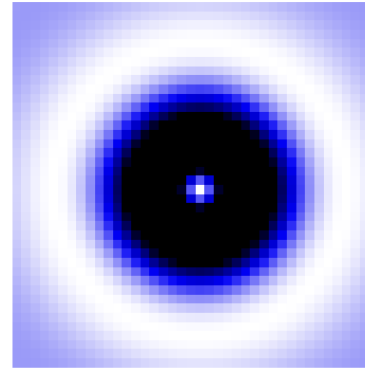
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## Hydrogen Atom Wave Function Evolution

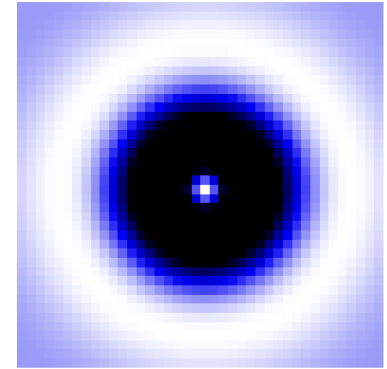
n (1-3): | (0-2):

3

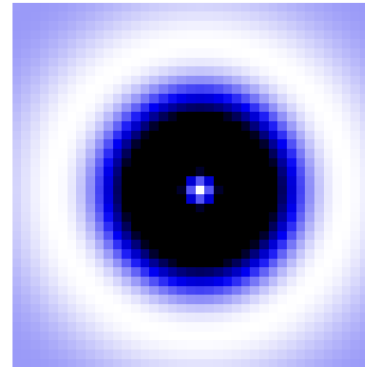
1



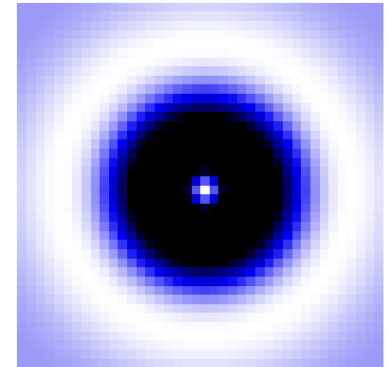
t = 0.00 fs



t = 0.68 fs



t = 1.37 fs



t = 2.05 fs

Showing probability density evolution for quantum numbers:  $n = 3$ ,  $l = 1$ ,  $m = 0$

# Encoding Data into the Wave function

- **Wave function as Data**

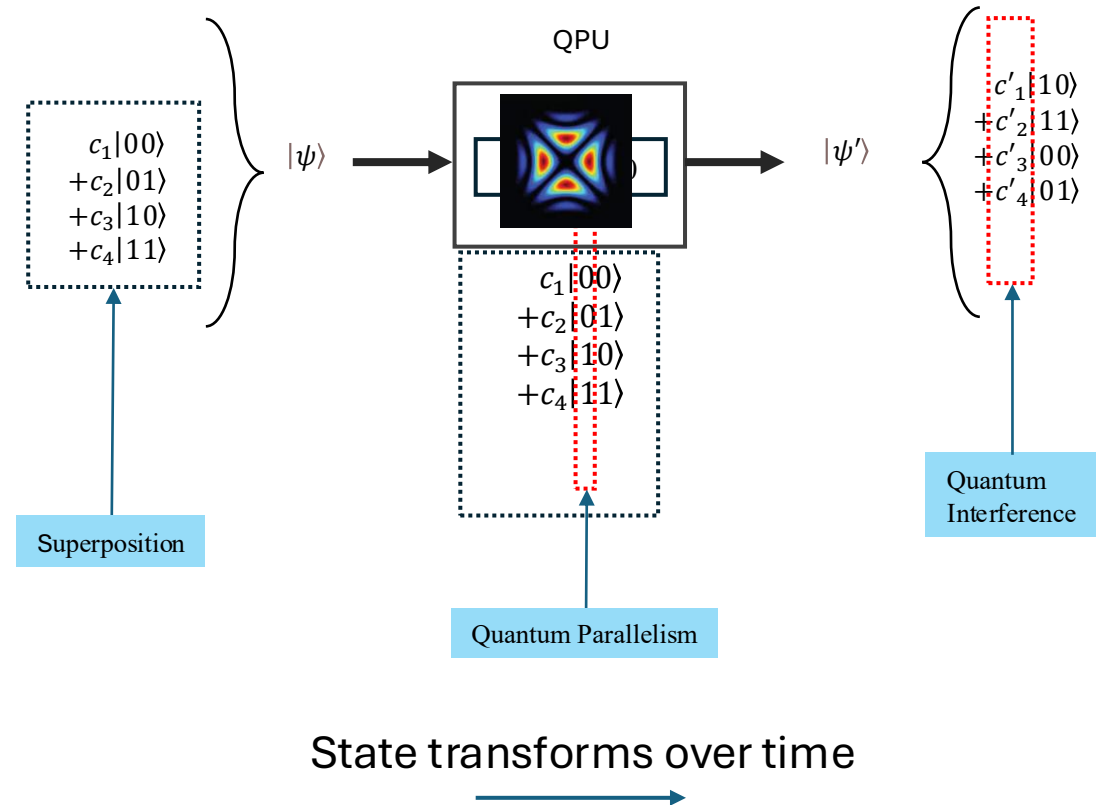
- We **encode** classical information into a **quantum wavefunction**  $|\psi\rangle$
- For two qubits, we might have
  - Sss

- **Processing via Quantum Circuit**

- A **quantum circuit** transforms  $|\psi\rangle$  over time
- Different circuit types or models  $\Rightarrow$  different quantum computing paradigms

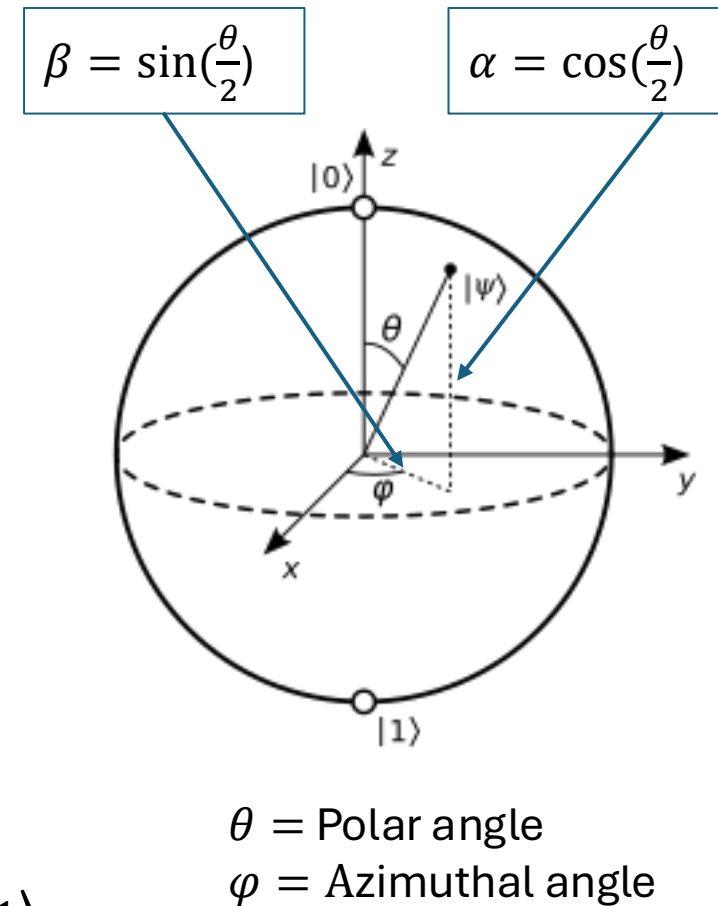
- **Mathematical Tools**

- **Linear algebra** (vectors, matrices)
- **Complex numbers** for phases and amplitudes
- Bra-ket notation



# Qubits, Bloch Sphere & Bra-Ket Notation

- **From Wavefunction to Qubit**
  - Abstracting quantum state into a **qubit**
- **Bra-Ket Notation**
  - **Dirac Notation:**  $|\psi\rangle$  (ket) and  $\langle\psi|$  (bra)
  - Represents **vectors** and **dual vectors** in Hilbert space
  - **Superposition** :  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$  , with  $|\alpha|^2 + |\beta|^2 = 1$
  - $|0\rangle$  and  $|1\rangle$  form the standard basis
- **Equivalent Mathematical Forms**
  - **Vector Form:**  $|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$
  - **Bra-Ket Form:**  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$
  - **State Vector :**  $|\psi\rangle = (a + bi)|0\rangle + (c + di)|1\rangle$
  - **Bloch Sphere Representation :**  $|\psi\rangle = \cos(\frac{\theta}{2})|0\rangle + e^{-i\varphi}\sin(\frac{\theta}{2})|1\rangle$

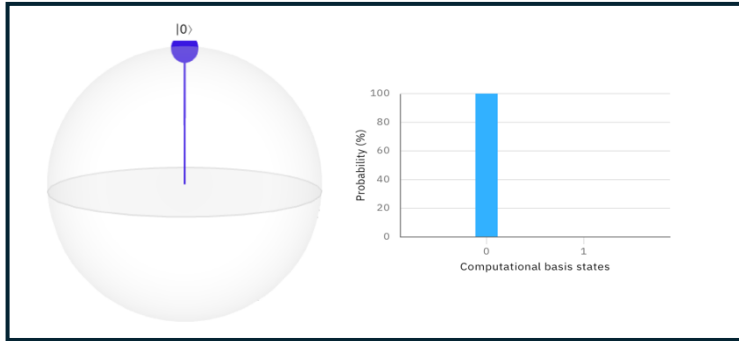


# Bloch Sphere: 1 qubit

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\cos(0/2) = 1$$

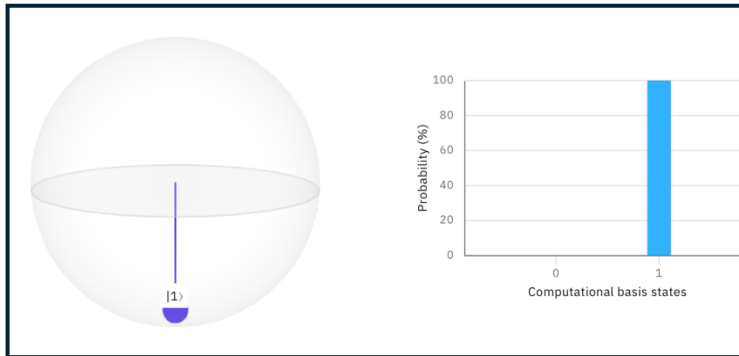
$$\sin(0/2) = 0$$



$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

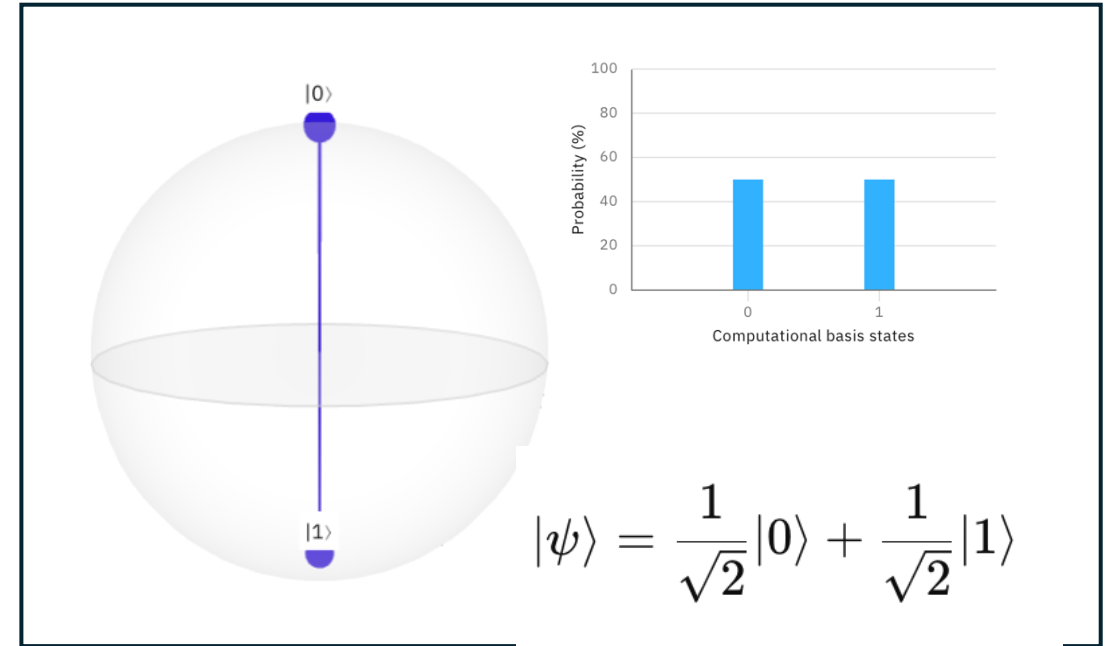
$$\cos(180^\circ/2) = 0$$

$$\sin(180^\circ/2) = 1$$



Single Qubit, Basis State

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



$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$$

Single Qubit, Superposition State

$$\alpha = \frac{1}{\sqrt{2}}, \text{ so } |\alpha|^2 = 0.5.$$

$$\beta = \frac{1}{\sqrt{2}}, \text{ so } |\beta|^2 = 0.5.$$

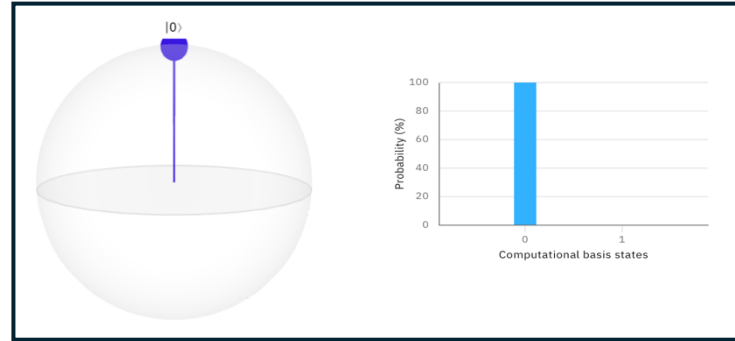
# Bloch Sphere: single qubit

Basis State

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\cos(0/2) = 1$$

$$\sin(0/2) = 0$$

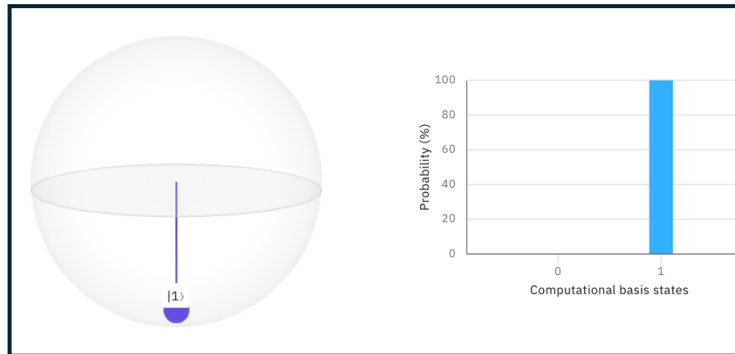


As column vector:  $\begin{bmatrix} 1 + 0i \\ 0 + 0i \end{bmatrix}$  In basis notation:  $1|0\rangle + 0|1\rangle$

$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\cos(180^\circ/2) = 0$$

$$\sin(180^\circ/2) = 1$$



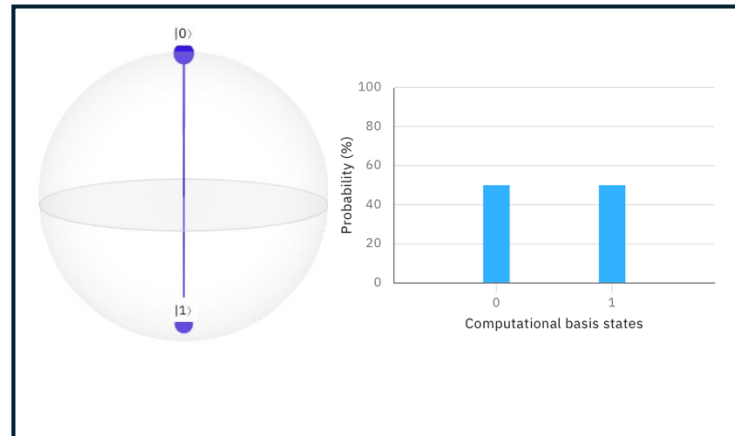
As column vector:  $\begin{bmatrix} 0 + 0i \\ 1 + 0i \end{bmatrix}$  In basis notation:  $0|0\rangle + 1|1\rangle$

Superposition State

$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$$

$$\alpha = \frac{1}{\sqrt{2}}, \text{ so } |\alpha|^2 = 0.5.$$

$$\beta = \frac{1}{\sqrt{2}}, \text{ so } |\beta|^2 = 0.5.$$



As column vector:  $\begin{bmatrix} 1/\sqrt{2} + 0i \\ 1/\sqrt{2} + 0i \end{bmatrix}$  In basis notation:  $(1/\sqrt{2})|0\rangle + (1/\sqrt{2})|1\rangle$

# 2 Qubits

## General Two-Qubit State

$$|\psi\rangle = [a + bi] = (a + bi)|00\rangle + (c + di)|01\rangle + (e + fi)|10\rangle + (g + hi)|11\rangle$$

Where:

- $a^2 + b^2 + c^2 + d^2 + e^2 + f^2 + g^2 + h^2 = 1$  (normalization)
- Each component represents amplitude for respective basis state:
  - First:  $(a + bi)$  for  $|00\rangle$
  - Second:  $(c + di)$  for  $|01\rangle$
  - Third:  $(e + fi)$  for  $|10\rangle$
  - Fourth:  $(g + hi)$  for  $|11\rangle$

### $|00\rangle$ State

Vector form:      Bra-ket form:

$$[1 + 0i] \quad |00\rangle = 1|00\rangle + 0|01\rangle + 0|10\rangle + 0|11\rangle$$

$$[0 + 0i]$$

$$[0 + 0i]$$

$$[0 + 0i]$$

### $|01\rangle$ State

Vector form:      Bra-ket form:

$$[0 + 0i] \quad |01\rangle = 0|00\rangle + 1|01\rangle + 0|10\rangle + 0|11\rangle$$

$$[1 + 0i]$$

$$[0 + 0i]$$

$$[0 + 0i]$$

### $|10\rangle$ State

Vector form:      Bra-ket form:

$$[0 + 0i] \quad |10\rangle = 0|00\rangle + 0|01\rangle + 1|10\rangle + 0|11\rangle$$

$$[0 + 0i]$$

$$[1 + 0i]$$

$$[0 + 0i]$$

### $|11\rangle$ State

Vector form:      Bra-ket form:

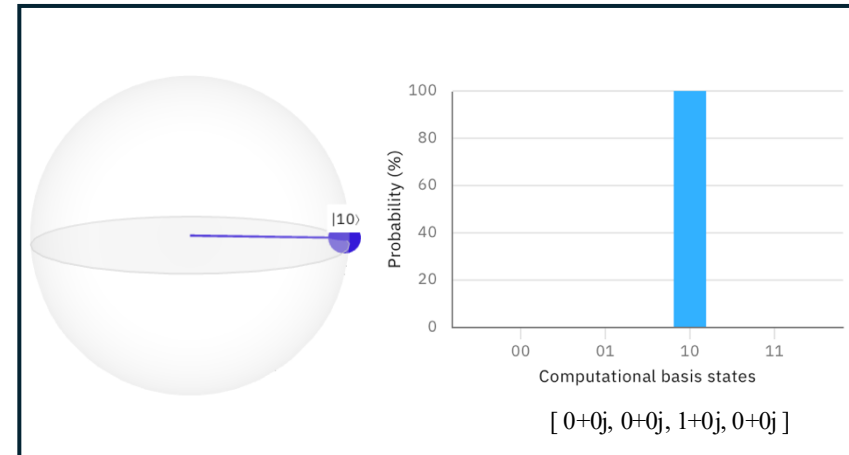
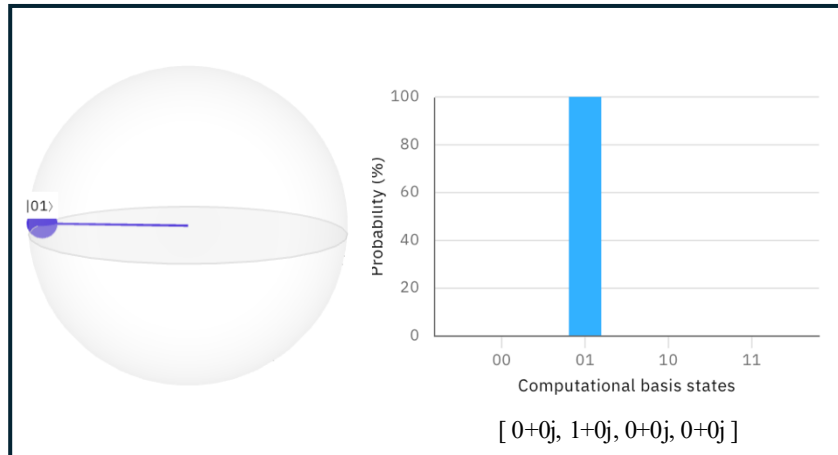
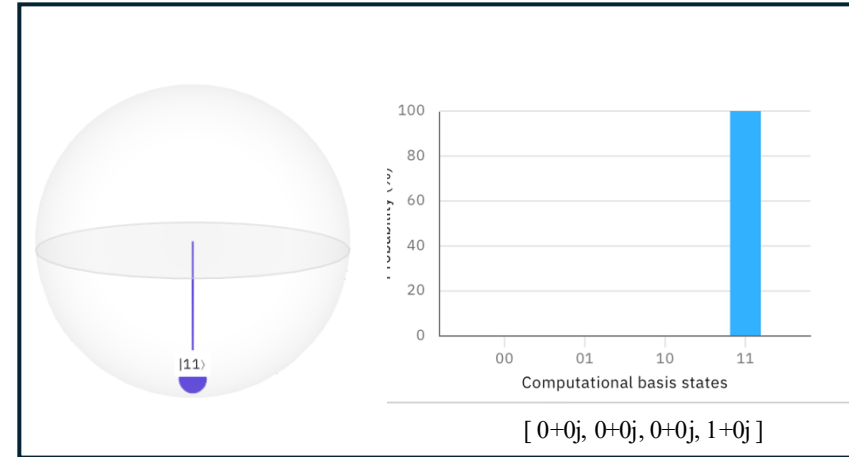
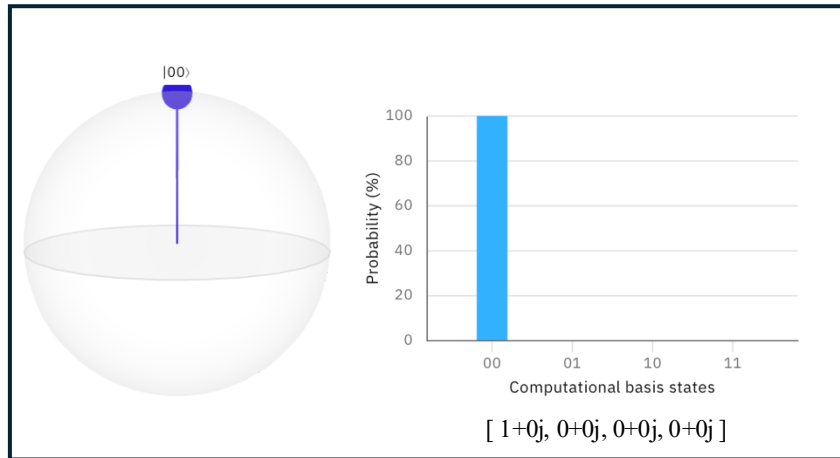
$$[0 + 0i] \quad |11\rangle = 0|00\rangle + 0|01\rangle + 0|10\rangle + 1|11\rangle$$

$$[0 + 0i]$$

$$[0 + 0i]$$

$$[1 + 0i]$$

# 2 Qubits, Basis State



2 Qubits, Basis State

# Lab 2-1 Introduction — Exploring the IBM Quantum Composer

- **Getting Started**
  - **Create an Account:** Visit <https://quantum.ibm.com> and sign up for a free account.
- **Access the Quantum Composer:**
  - Log in and open the **Quantum Composer** tool.
- **Key Features to Explore**
  - **Circuit Composer:** Drag and drop quantum gates to build quantum circuits.
  - **State Visualization:** View the qubit's state on the **Bloch sphere** after each gate operation.
- **Objectives for This Lab**
  - **Read and Interpret Output States:** Observe how quantum states (state vectors) change after applying gates.
  - **Explore the Bloch Sphere:**

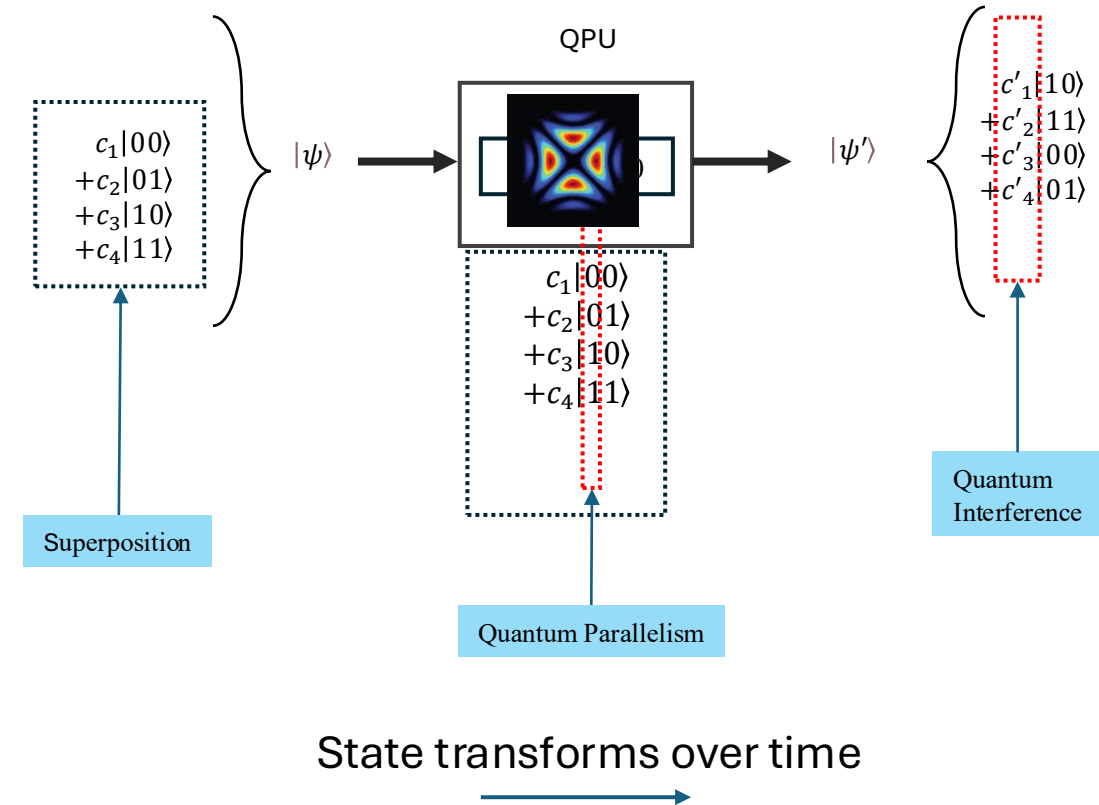
# Computing Units of a Quantum Computer

- **Quantum Computing Units**

- A quantum computer's computing unit defines how it manipulates the quantum wavefunction to process algorithms.
- These units determine the type of quantum computer, shaping both the hardware and the way we implement quantum algorithms.

- **Types of Quantum Computing Units**

- **Gate-Based Quantum Computers:** Use quantum gates and circuits (e.g., IBM, Google, Rigetti).
  - **Quantum Annealers:** Solve optimization problems by finding energy minima (e.g., D-Wave).
  - **Measurement-Based Quantum Computers:** Use entangled states and measurements to compute.
  - **Topological Quantum Computers:** Encode information into topological states for fault tolerance (e.g., Microsoft's approach).
- **The type of computing unit dictates:**
    - How we design algorithms (gate-based, annealing, etc.)
    - Hardware capabilities and limitations
    - Efficiency for specific tasks



# Gate-Based Quantum Computers

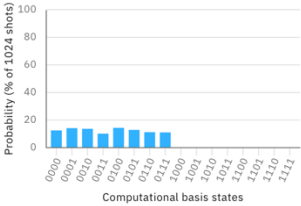
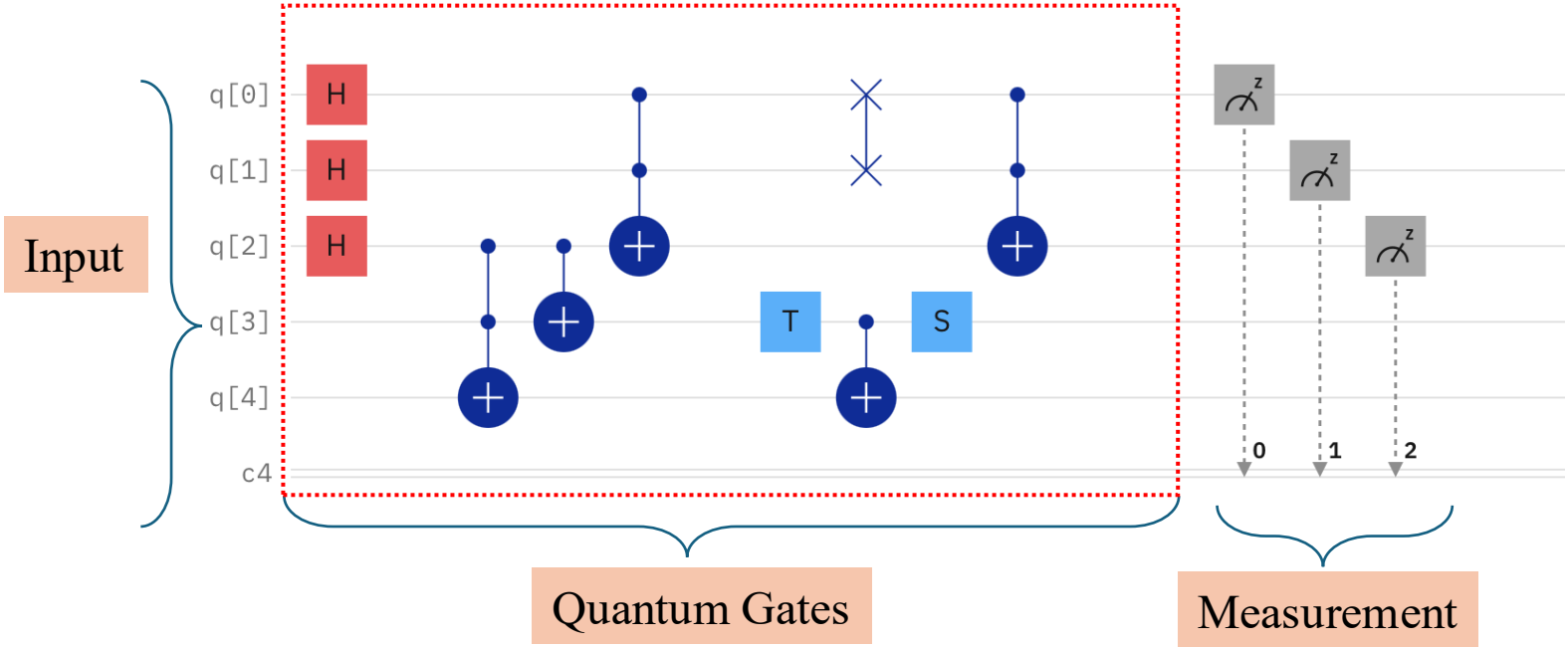
- **What is a Gate-Based Quantum Computer?**

- Processes quantum information using **quantum gates**.
- Quantum gates operate on qubits to manipulate their states (superposition, entanglement, interference).
- Like classical circuits but uses **unitary transformations** to modify the quantum wavefunction.

- **Mathematical Model**

- Quantum gates are represented as **unitary matrices**
  - $\mathbb{U}(\text{a unitary matrix}) \Rightarrow \mathbb{U}^\dagger \mathbb{U} = \mathbf{I}$
- A quantum state evolves as:  $|\psi'\rangle = \mathbb{U}|\psi\rangle$

# Gates-Based Quantum Computer



# The X Gate

- Mathematical Representation of the X Gate  $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
- The X gate is the **quantum equivalent of a classical NOT gate**, flipping the qubit state  $|0\rangle \rightarrow |1\rangle$   
 $|1\rangle \rightarrow |0\rangle$
- Applying X Gate to  $|0\rangle$

Start with the qubit state:

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Apply the X gate:

$$|\psi'\rangle = X|0\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Result:

$$|\psi'\rangle = |1\rangle$$

**TABLE 2-2** Example of Quantum Gates

Gate	Function	Matrix
I	No rotation	$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
X	Rotate by $\pi$ radians about the x-axis	$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Y	Rotate by $\pi$ radians about the y-axis	$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
Z	Rotate by $\pi$ radians about the z-axis	$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
S	Rotate by $\pi/2$ radians about z-axis	$S = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2} \end{pmatrix}$
H	Rotate by $\pi$ radians about a diagonal in x-z plane	$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

**Quantum algorithms** are designed by arranging gates in specific sequences to manipulate the wavefunction and produce desired measurement outcomes.

# Grover's Circuit — Designing Quantum Algorithms

- **Grover's Circuit Example**
  - Demonstrates a **quantum algorithm** designed to solve a search problem.
- **Structure:**
  - **Input:** Encodes the initial state of the qubits.
  - **Gates:** A series of operations applied step by step to transform the wavefunction.
  - **Output:** Measurement collapses the state to reveal the result.

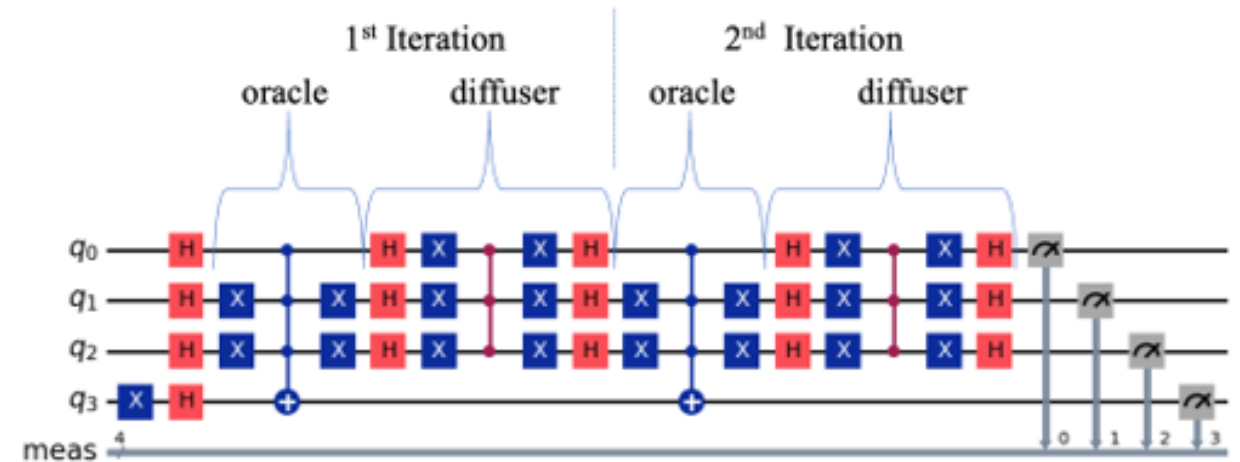


FIGURE 2-15 Quantum Circuit for Grover's Algorithm Implementation

# Lab 2-2 — Exploring Quantum Gates and Their Outputs

## •Lab Overview

- Explore how individual quantum gates manipulate qubit states.
- Use the **IBM Quantum Composer** to visualize the effect of gates on qubits, both mathematically (state vectors) and geometrically (Bloch sphere).

## •What You'll Do

- Start with a single qubit in the  $|0\rangle$  state
- Apply various quantum gates (e.g., X, H, Z, S, etc.) and observe:
  - **State Vector Updates:** How the qubit's mathematical representation changes.
  - **Bloch Sphere Visualization:** How the qubit's position on the Bloch sphere evolves.
  - Experiment with combinations of gates to understand their cumulative effects.

## •Goals of the Lab

- Develop intuition about how quantum gates manipulate qubit states.
- Understand the relationship between gates, state vectors, and the Bloch sphere.
- Build familiarity with the IBM Quantum Composer interface.

# Recommended Reading

- **Topics to Review**

- **Linear Algebra**

- Basics of vectors and matrices
    - Operations: addition, multiplication, dot product
    - Special matrices: unitary, Hermitian, and eigenvalues

- **Quantum Phenomena**

- Superposition
    - Entanglement
    - Quantum interference

- **Suggested Resources**

- **Linear Algebra**

- "*Linear Algebra and Its Applications*" by Gilbert Strang
    - Khan Academy: Linear Algebra Tutorials ([online free resource](#))
    - 3Blue1Brown's YouTube series: *The Essence of Linear Algebra*

- **Quantum Mechanics**

- "*Quantum Mechanics: The Theoretical Minimum*" by Leonard Susskind
    - MIT OpenCourseWare: *Introduction to Quantum Mechanics* ([online free resource](#))
    - IBM Quantum Documentation ([link](#))

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad (1)$$

$$\alpha = ae^{i\phi_a}, \quad (2)$$

$$\beta = be^{i\phi_b}, \quad (3)$$

$$|\psi\rangle = a|0\rangle + be^{i\phi}|1\rangle, \quad (4)$$

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

The normalization constraint of quantum states,  $|\alpha|^2 + |\beta|^2 = 1$ , allows you to parametrize  $a$  and  $b$  as

$$a = \cos(\theta/2), \quad (5)$$

$$b = \sin(\theta/2), \quad (6)$$

where  $\theta$  goes from 0 to  $\pi$ .