

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**

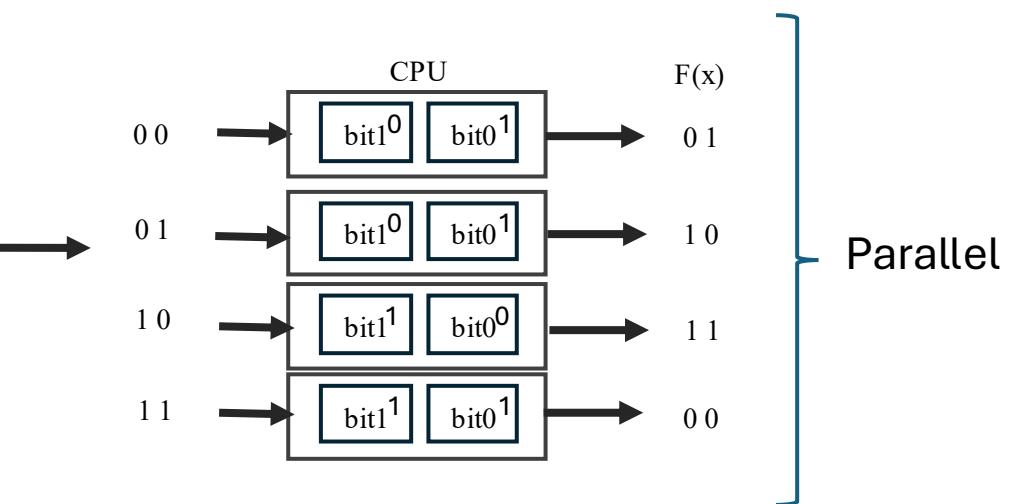
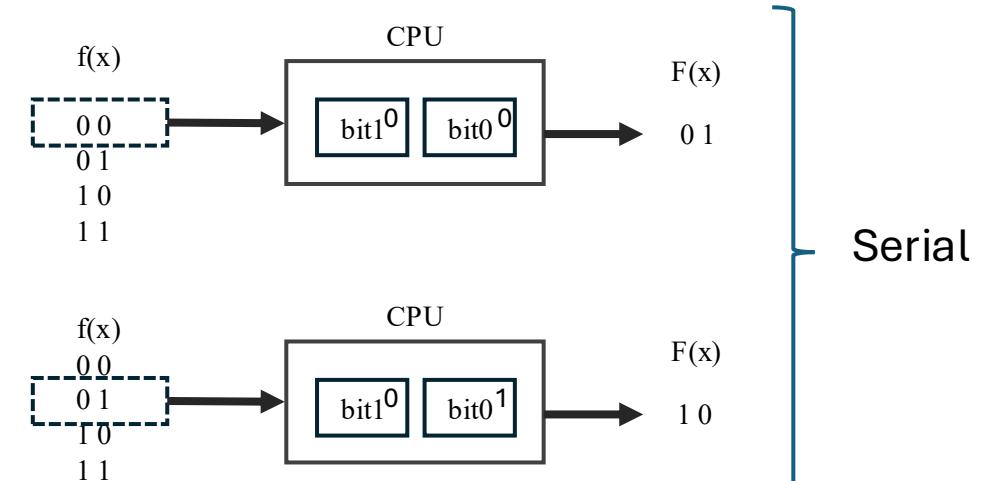
- Data in **binary** form (bits)
- Processed by **logical operations** (AND, OR, NOT, etc.) on registers

- **Output**

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

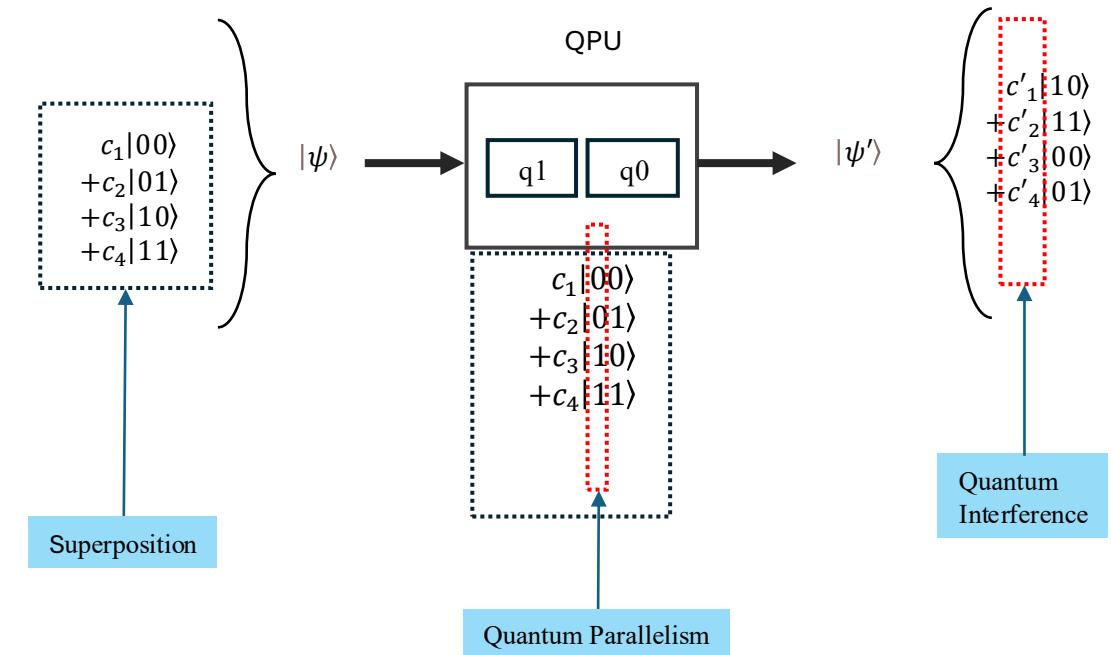
- **Key Point**

- 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*.



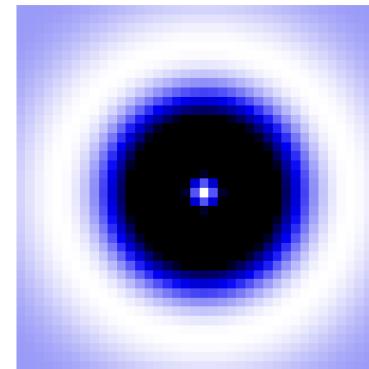
Visualizing Time Evolution of the Quantum Wavefunction

Hydrogen Atom Wave Function Evolution

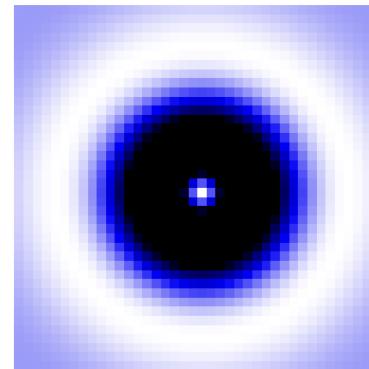
n (1-3): l (0-2):

3

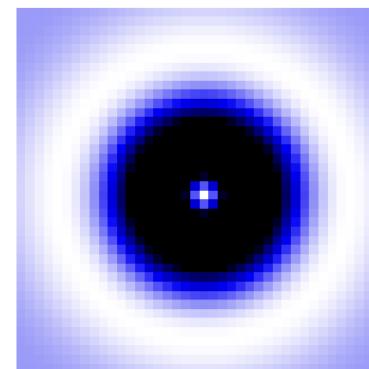
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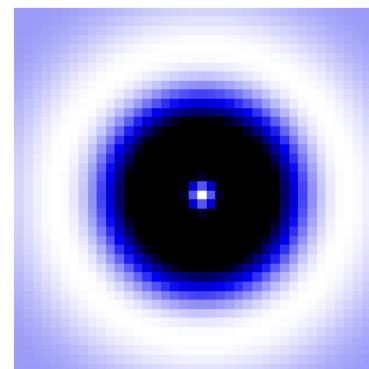
$t = 0.00$ fs



$t = 0.68$ 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**

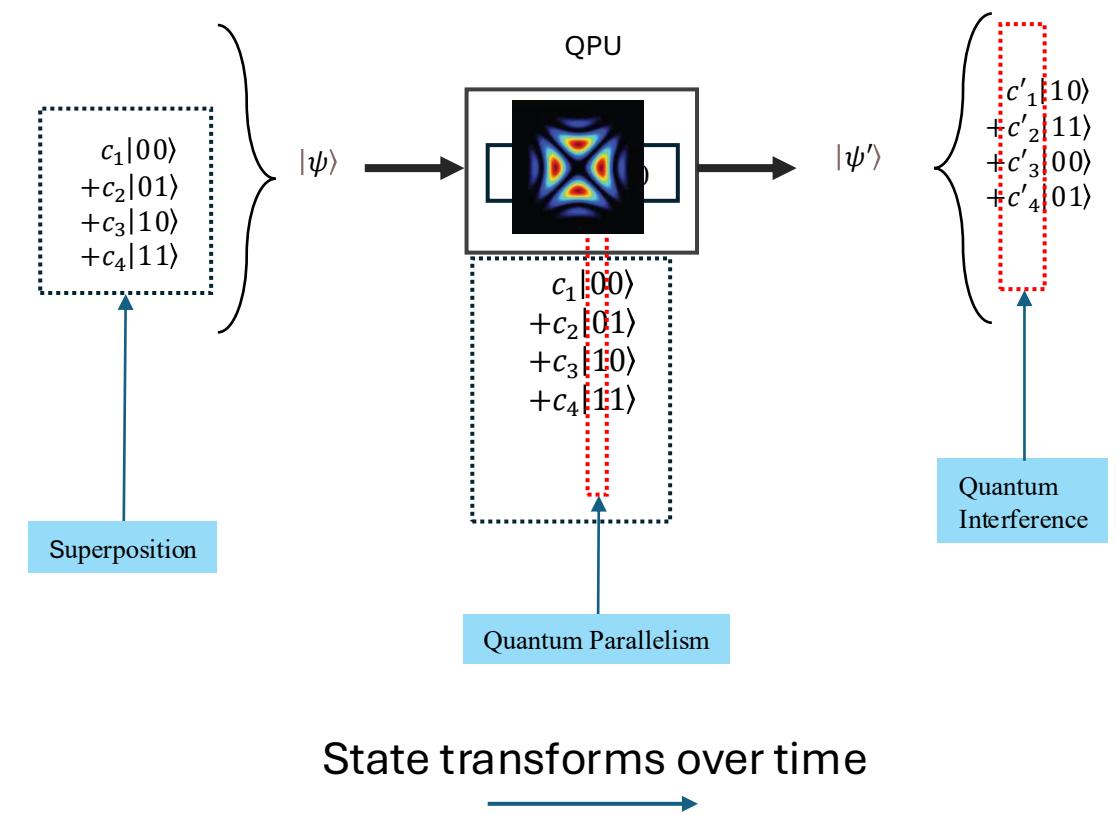
- We **encode** classical information into a **quantum wavefunction** $|\psi\rangle$
- For two qubits, we might have
 - Sss

- Processing via Quantum Circuit

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

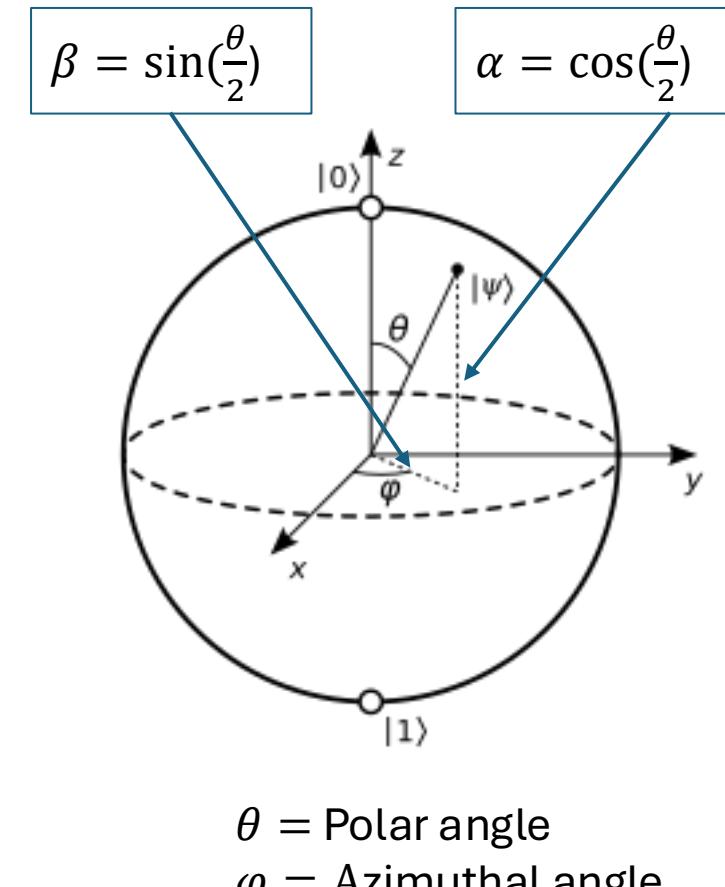
- **Mathematical Tools**

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



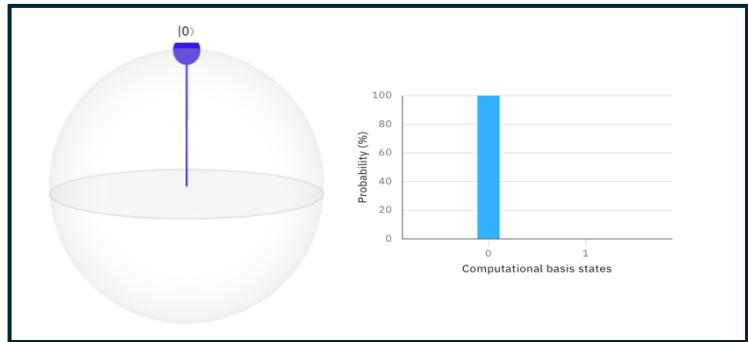
θ = Polar angle

φ = Azimuthal angle

Bloch Sphere: 1 qubit

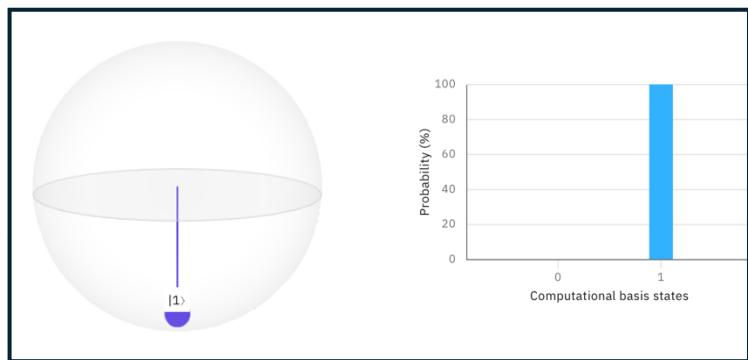
$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

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



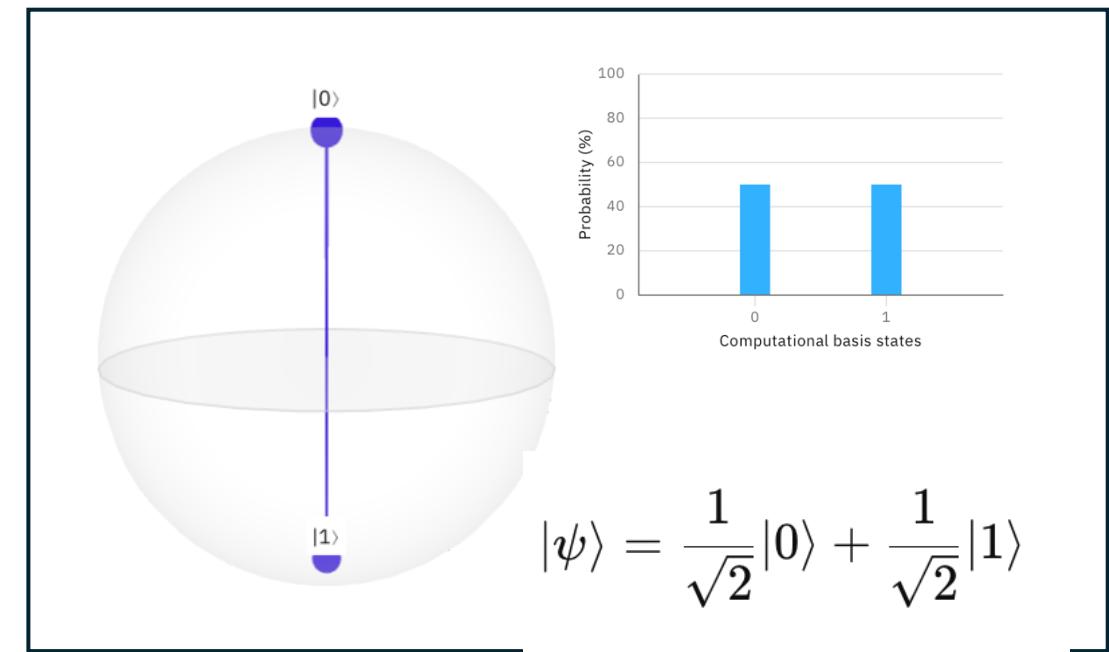
$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\cos(180^\circ/2) = 0$$
$$\sin(180^\circ/2) = 1$$



Single Qubit, Basis State

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



Single Qubit, Superposition State

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

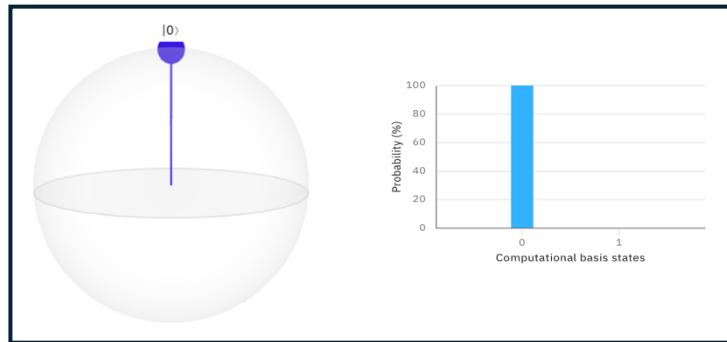
$$\beta = \frac{1}{\sqrt{2}}, \text{ so } |\beta|^2 = 0.5.$$

Bloch Sphere: single qubit

Basis State

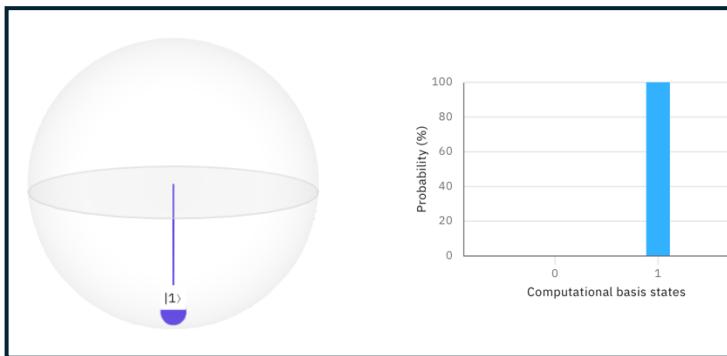
$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

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



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

$$\cos(180^\circ/2) = 0$$
$$\sin(180^\circ/2) = 1$$

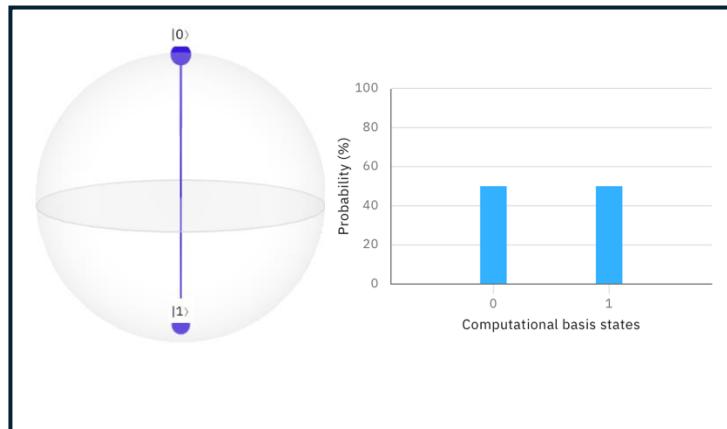


Superposition State

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

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

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



As column vector: $[1 + 0i]$
In basis notation: $1|0\rangle + 0|1\rangle$

As column vector: $[0 + 0i]$
In basis notation: $0|0\rangle + 1|1\rangle$

As column vector: $[1/\sqrt{2} + 0i]$
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:
$[1 + 0i]$	$ 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:
$[0 + 0i]$	$ 01\rangle = 0 00\rangle + 1 01\rangle + 0 10\rangle + 0 11\rangle$
$[1 + 0i]$	
$[0 + 0i]$	
$[0 + 0i]$	

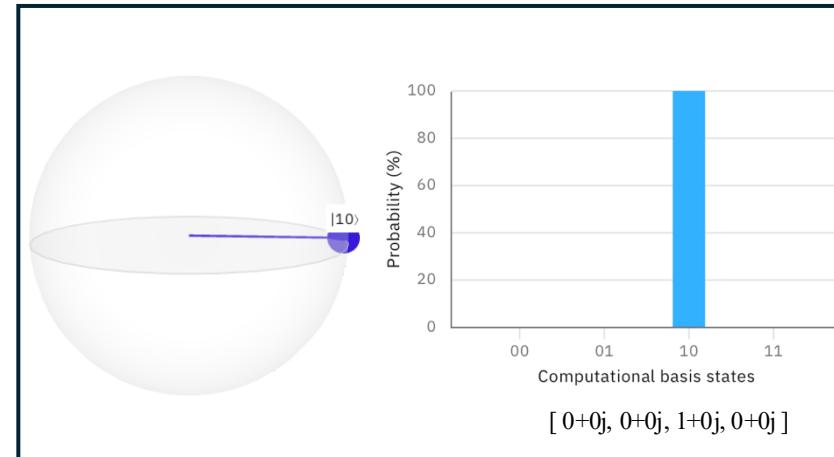
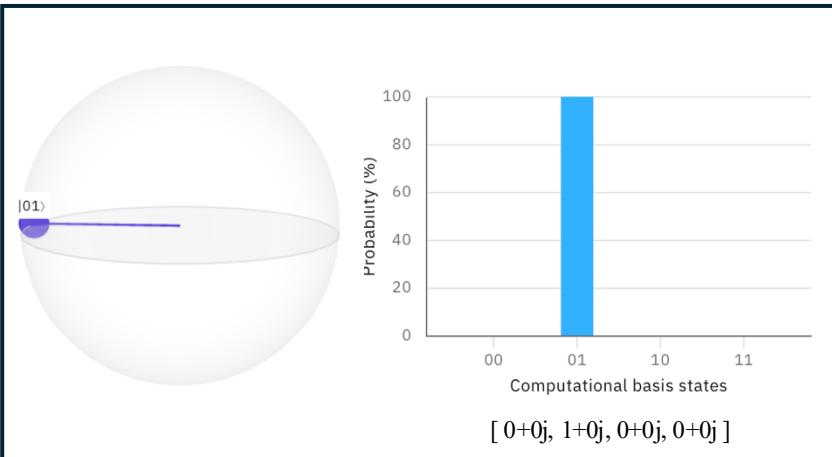
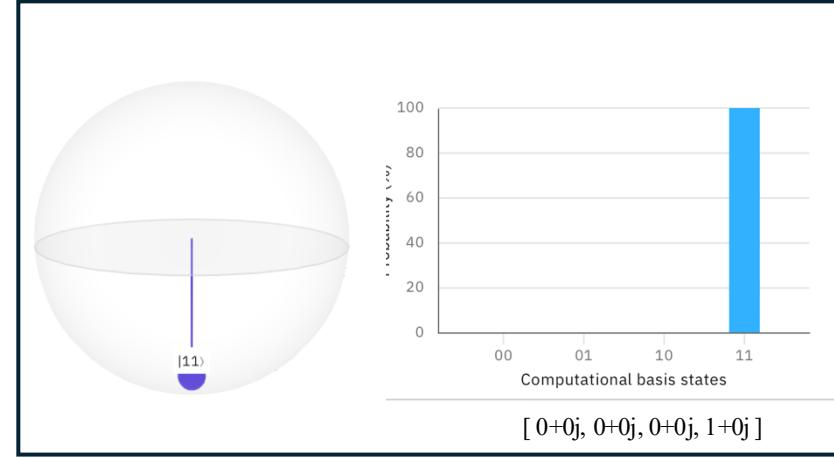
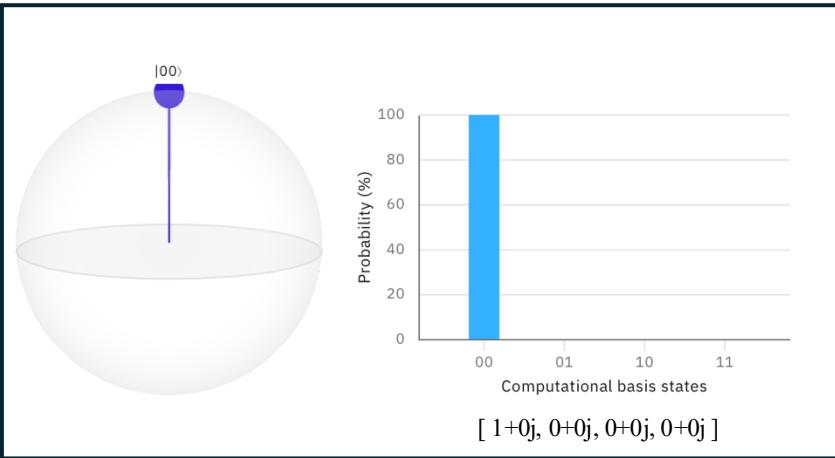
$|10\rangle$ State

Vector form:	Bra-ket form:
$[0 + 0i]$	$ 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:
$[0 + 0i]$	$ 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**

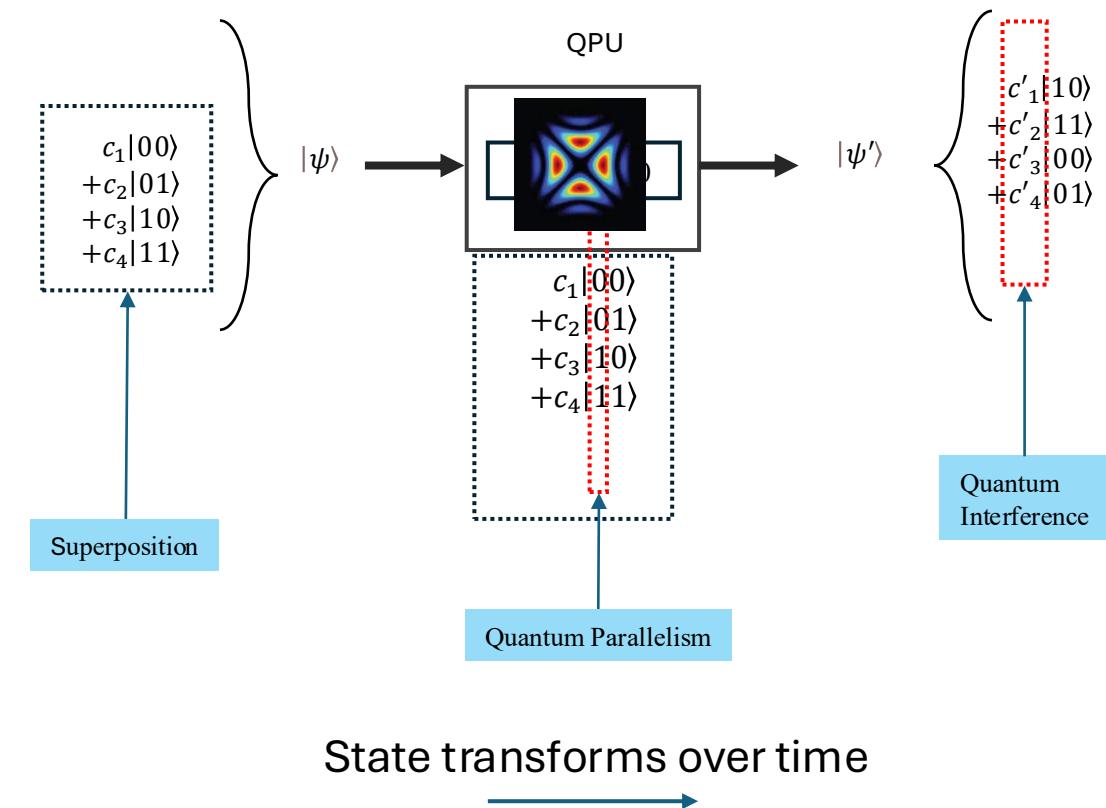
- A quantum computer's computing unit defines how it manipulates the quantum wavefunction to process algorithms.
- These units determine the type of quantum computer, shaping both the hardware and the way we implement quantum algorithms.

- **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:**

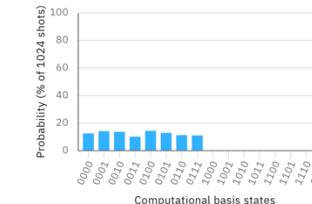
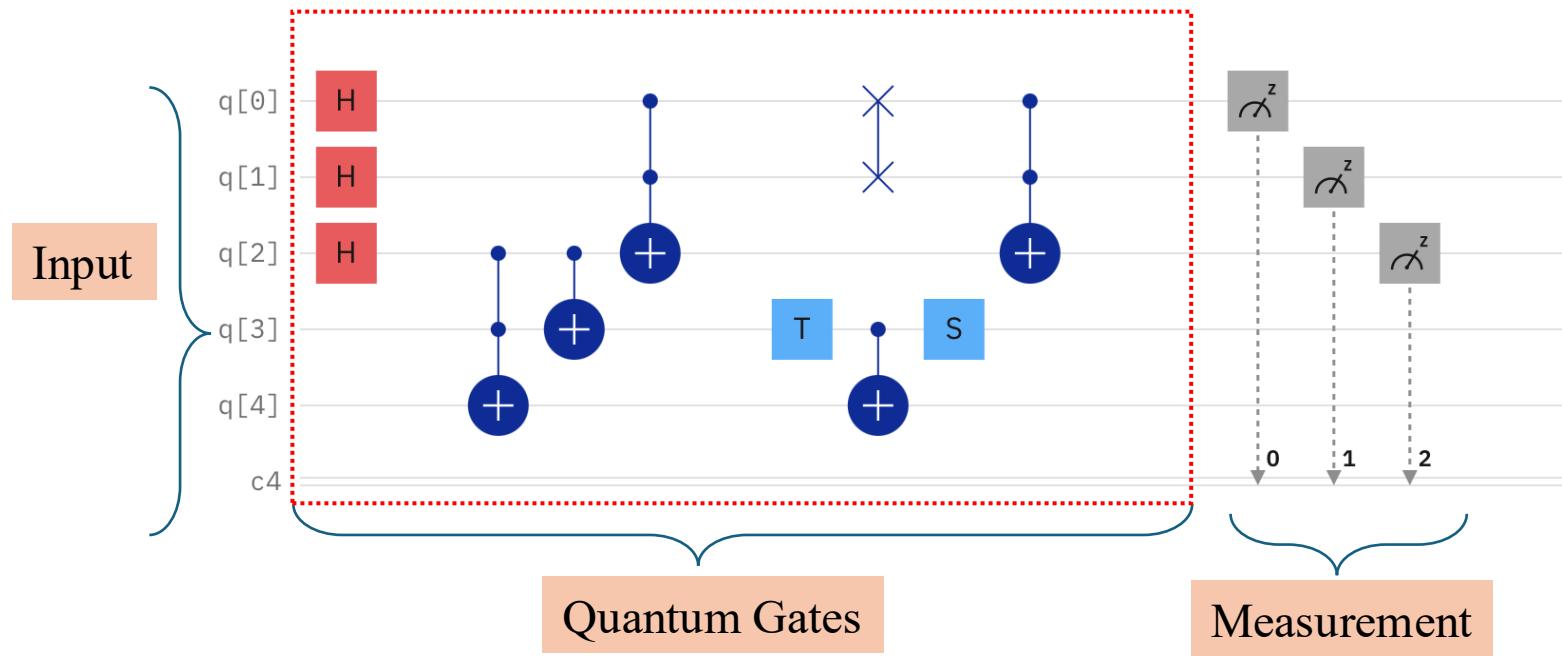
- How we design algorithms (gate-based, annealing, etc.)
- Hardware capabilities and limitations
- Efficiency for specific tasks



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} (*a unitary matrix*) $\Rightarrow \mathbb{U}^\top \mathbb{U} = \mathbb{I}$
 - 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 π radians about the x-axis	$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Y	Rotate by π radians about the y-axis	$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
Z	Rotate by π 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 π 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.

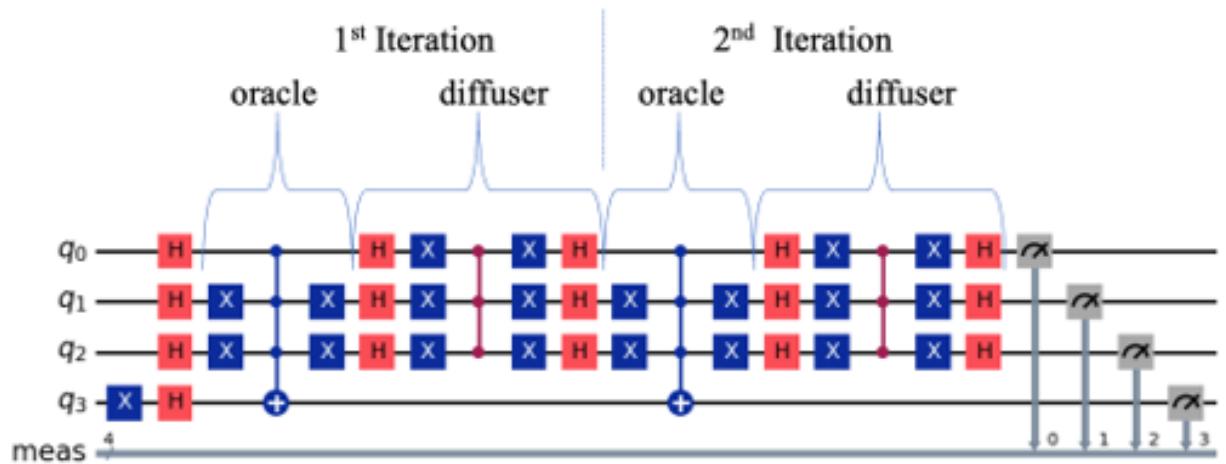


FIGURE 2-15 Quantum Circuit for Grover's Algorithm Implementation

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](#))

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

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

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

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

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

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 θ goes from 0 to π .