国際融合科学論/先端融合科学論

LECTURE 04
Quantum Mechanics I: Introduction to Quantum Mechanics

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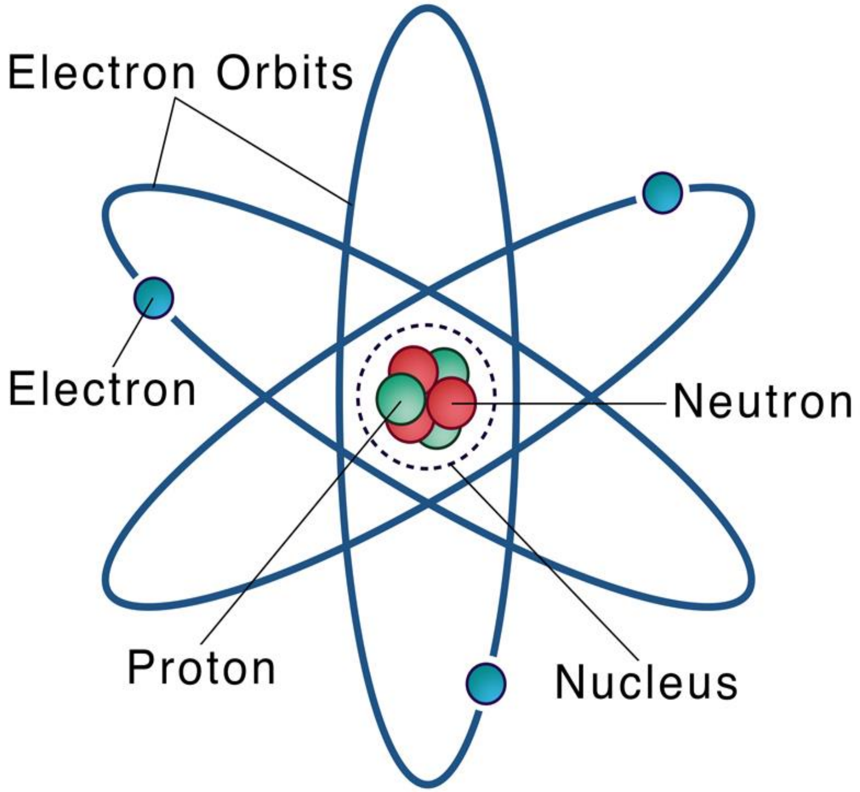
Lecture Outline

1) A brief introduction to Quantum Mechanics
2) Quantum Computing
   - Quantum Bit: QUBIT
   - Quantum Gates: Single and multiple qubit gates
   - Quantum Circuits
   - Quantum Algorithm: Deutsch Algorithm

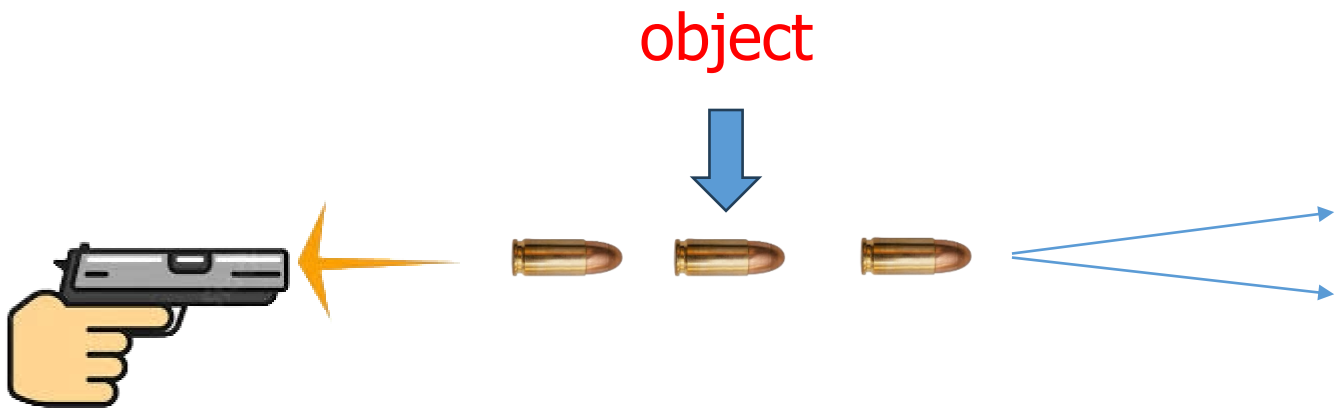
A brief introduction to Quantum Mechanics

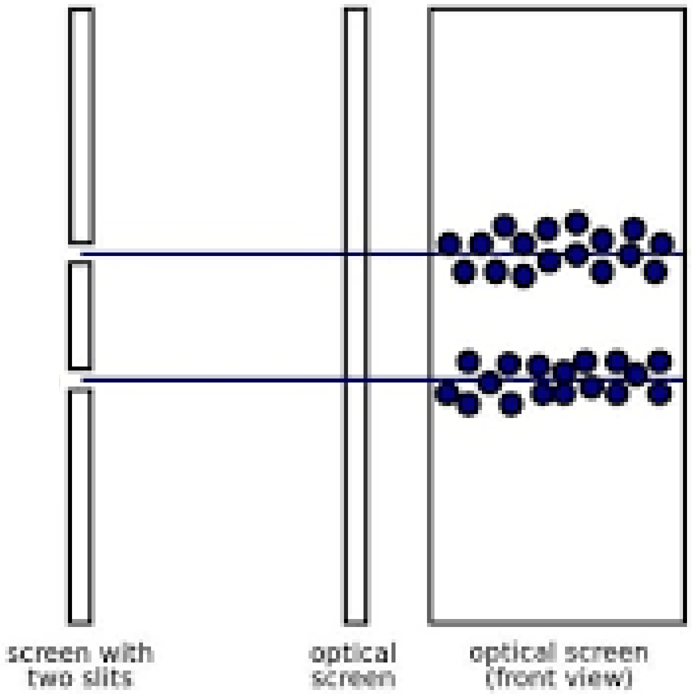
- Why Quantum mechanics?

  - It was developed to explain physical phenomena that Newtonian mechanics could not adequately describe, such as the behavior of particles at atomic and subatomic scales.



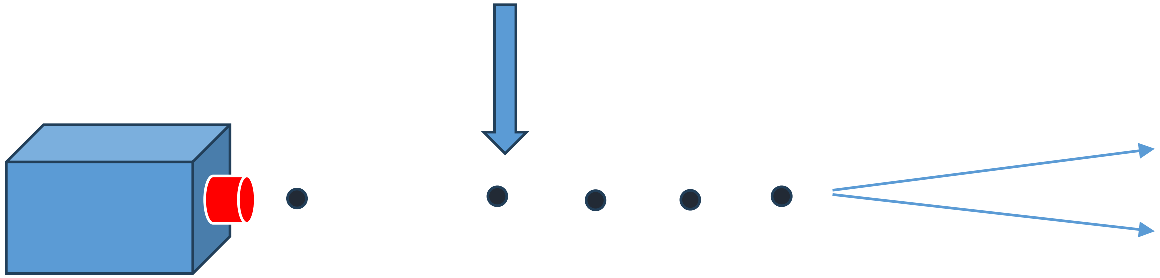
Double-slit experiment: Newton mechanics

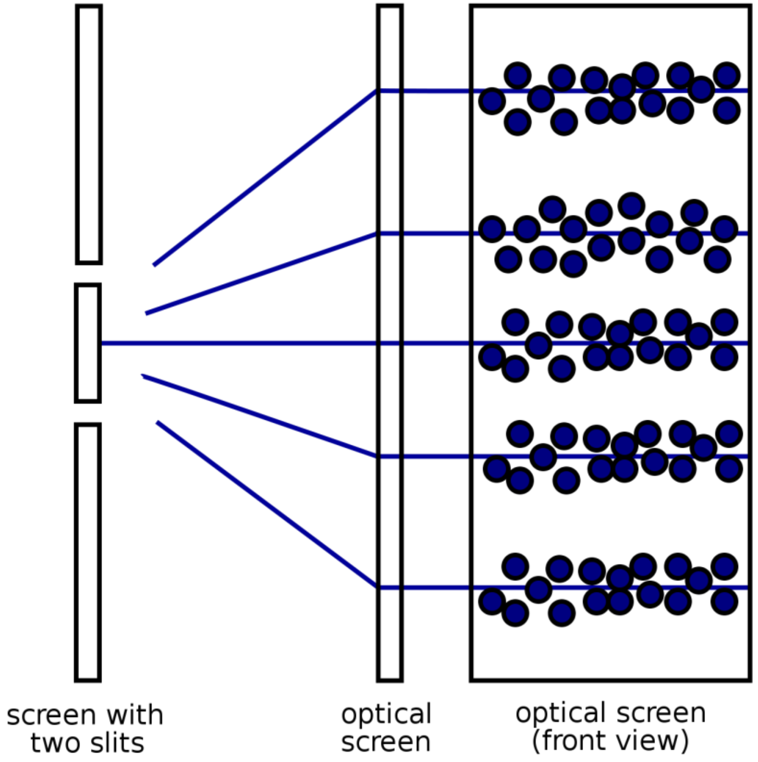




Double-slit experiment: Quantum mechanics

Electrons or any entities
of exceedingly small size.

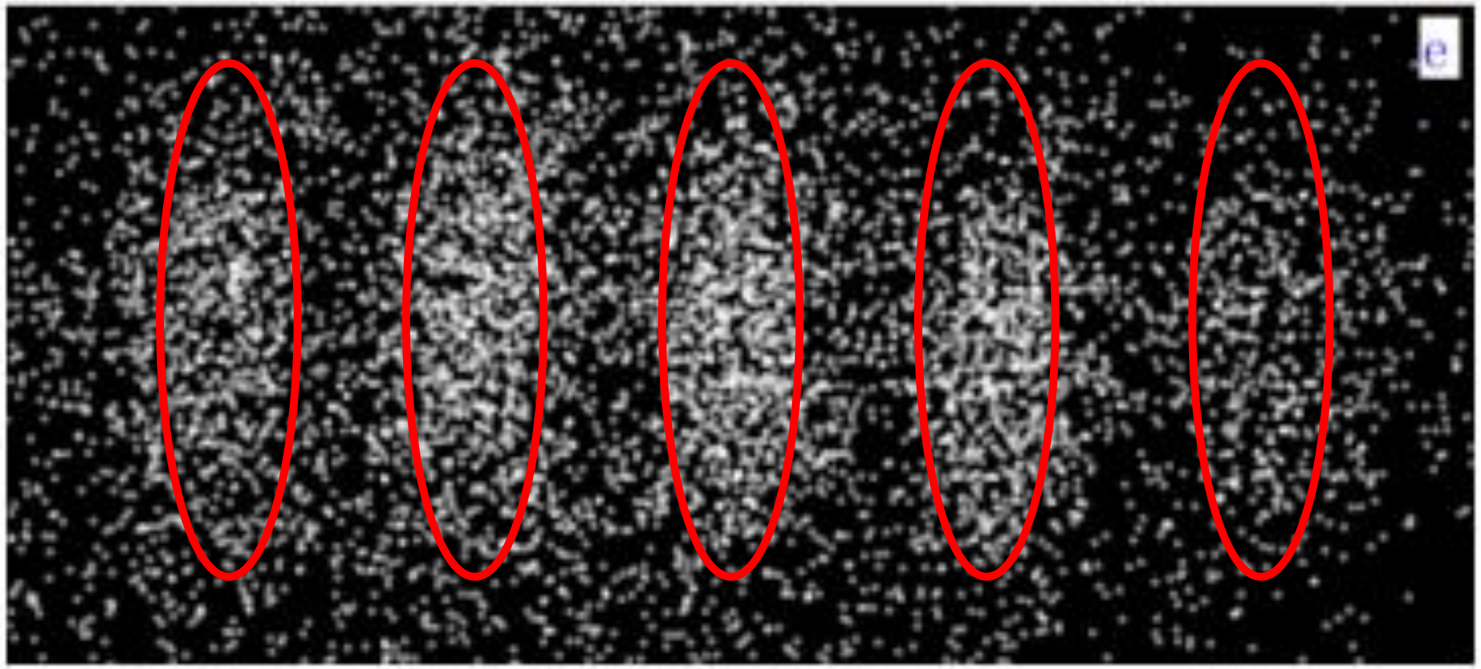




Interference pattern

Double-slit experiment: Quantum mechanics

Interference pattern



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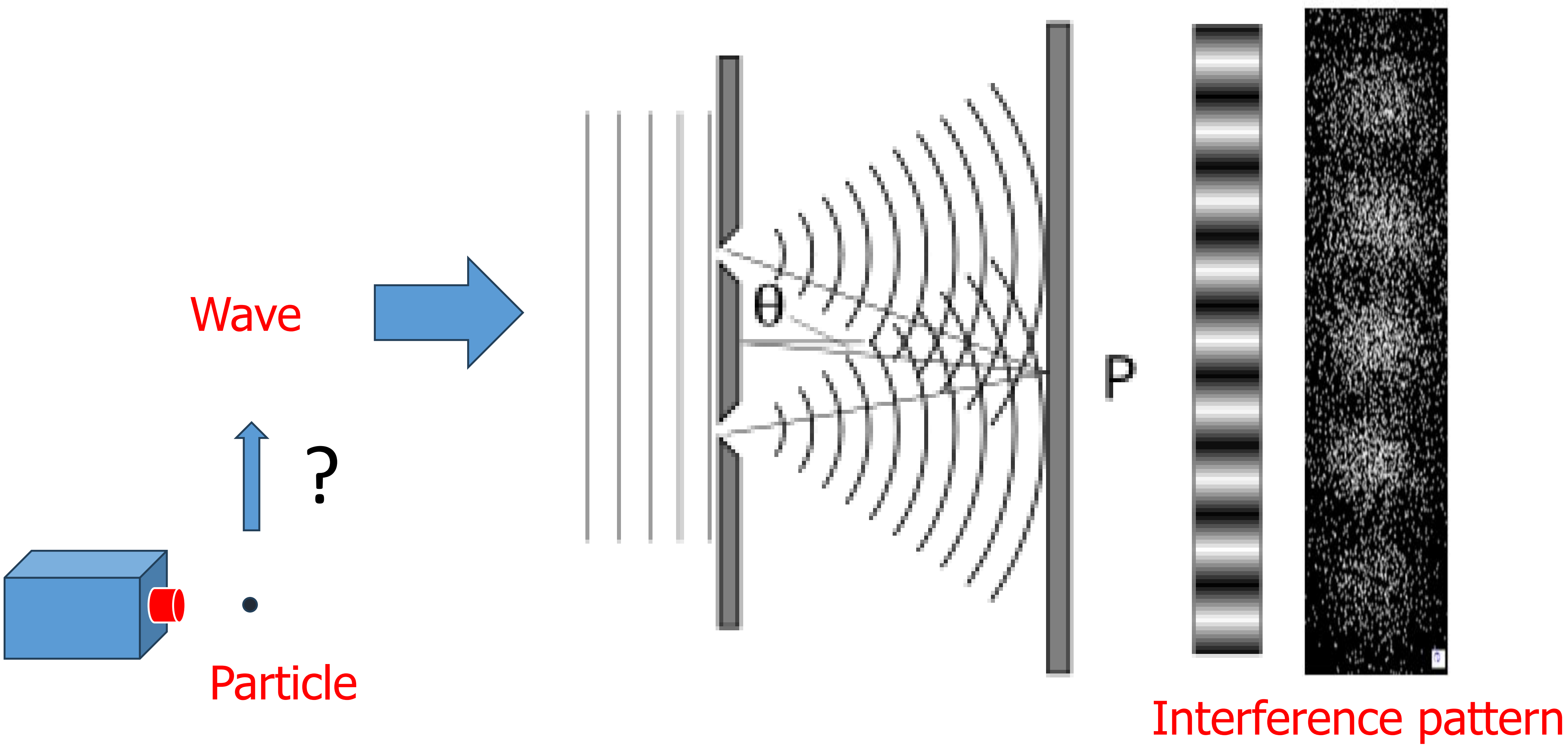
Double-slit experiment: Quantum mechanics: wave-particle duality



What is Quantum mechanics?

- a mathematical framework or set of rules for the construction of physical theories.
- a fundamental theory in physics that describes the physical phenomenon of nature at the scale of atoms and subatomic particles.
- Some are counter-intuitive even for experts

What is Quantum computing?

- A technology that uses the principles of quantum mechanics to perform computations far better than classical computers.

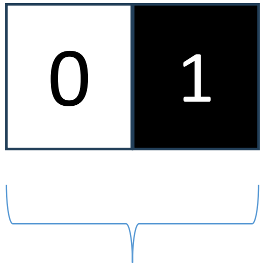
Quantum Computing

Quantum Bit: QUBIT

Quantum Bit: QUBIT

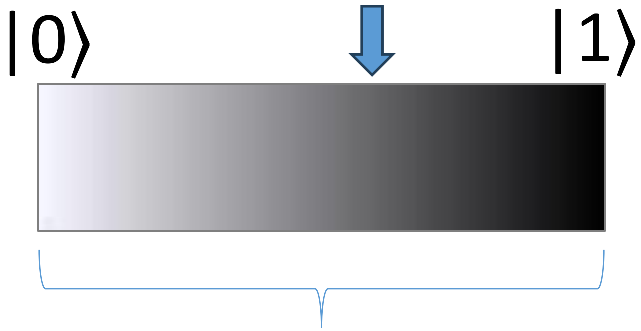
- The quantum bit or qubit for short is its analogous concept to the bit in classical computing or information.

Classical Bit



- One bit has two states.

Quantum Bit: Qubit



- One qubit has an infinite number of states.
- When **observed**, the state becomes either $|0\rangle$ or $|1\rangle$.
- Thus, before we observe, a qubit has both $|0\rangle$ and $|1\rangle$ states **simultaneously**, which is known as "**super position**".

Quantum Bit: QUBIT

- The quantum bit or qubit for short is its analogous concept to the bit in classical computing or information.
- A qubit state is represented as $|\psi\rangle = a|0\rangle + b|1\rangle$,
  - Notation like "⟨ | ⟩" is called, ***bra-ket*** or ***Dirac*** notation,
  - ⟨ |: we read it as "bra": row vector,
  - | ⟩: we read it as "ket": column vector,
  - $|0\rangle$ and $|1\rangle$: a two-dimensional vector $[1, 0]^T$ and $[0, 1]^T$,
  - a and b are complex numbers, $|a|^2 + |b|^2 = 1$
  - $|\psi\rangle = a|0\rangle + b|1\rangle = a\begin{bmatrix}1\\0\end{bmatrix} + b\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}a\\b\end{bmatrix} = \begin{bmatrix}p+qi\\v+wi\end{bmatrix}$

Quantum Bit: QUBIT

- **Inner product** between the vectors $|\varphi\rangle$ and $|\psi\rangle$
- Represented as

$$\langle \varphi | \psi \rangle$$

- Its outcome is **a scalar value**

$$\langle 0||1\rangle = \langle 0|1\rangle = [1,0]\begin{bmatrix}0\\1\end{bmatrix} = 0$$

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

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

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

$$\langle 1|1\rangle = 1$$

Quantum Bit: QUBIT

- **Inner product** between $|\varphi\rangle$ and $A|\psi\rangle$: A is a matrix operator
- Represented as

$$\langle \varphi | A | \psi \rangle$$

- Its outcome is **a scalar value**

$$\langle 0|A|1\rangle = [1,0]\begin{bmatrix} e_{11} e_{12} \\ e_{21} e_{22} \end{bmatrix}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = [1,0]\begin{bmatrix} e_{12} \\ e_{22} \end{bmatrix} = e_{12}$$

- **<u>Tensor product</u>** of the vectors $|\varphi\rangle$ and $|\psi\rangle$
- Represented as

$$|\varphi\rangle \otimes |\psi\rangle = |\varphi\rangle|\psi\rangle = |\varphi\psi\rangle$$

- Its outcome is **<u>a vector</u>**

$$|0\rangle|1\rangle = |01\rangle = \begin{bmatrix}1\\0\end{bmatrix}\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}1\begin{bmatrix}0\\1\end{bmatrix}\\0\begin{bmatrix}0\\1\end{bmatrix}\end{bmatrix} = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$$

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

$$|01\rangle = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$$

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

$$|11\rangle = \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

- **Tensor product** of the $|\varphi\rangle$, k times
- Represented as

$$|\varphi\rangle^{\otimes k} = |\varphi\rangle \otimes |\varphi\rangle \otimes \ldots \otimes |\varphi\rangle$$

- Its outcome is **a vector**

$$|\varphi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$$

$$|\varphi\rangle^{\otimes 2} = ?$$

$$|\varphi\rangle = \left(\begin{bmatrix}1\\0\end{bmatrix} + \begin{bmatrix}0\\1\end{bmatrix}\right)/\sqrt{2}$$

$$= \begin{bmatrix}1\\1\end{bmatrix}/\sqrt{2}$$

$$|\varphi\rangle^{\otimes 2} = \begin{bmatrix}1\\1\end{bmatrix}/\sqrt{2} \otimes \begin{bmatrix}1\\1\end{bmatrix}/\sqrt{2}$$

$$=(1/\sqrt{2})^2 \begin{bmatrix}1\\1\end{bmatrix} \otimes \begin{bmatrix}1\\1\end{bmatrix}$$

$$=(1/2)\begin{bmatrix}1\\1\\1\\1\end{bmatrix}$$

- **<u>Outer product</u>** of the vectors $|\varphi\rangle$ and $\langle\psi|$
- Represented as

$$|\varphi\rangle\langle\psi|$$

- Its outcome is **<u>an operator matrix</u>**

$$|1\rangle\langle 1| = \begin{bmatrix}0\\1\end{bmatrix}[0,1] = \begin{bmatrix}00\\01\end{bmatrix}$$

$$|0\rangle\langle 0| = \begin{bmatrix}10\\00\end{bmatrix}$$

$$|0\rangle\langle 1| = \begin{bmatrix}01\\00\end{bmatrix}$$

$$|1\rangle\langle 0| = \begin{bmatrix}00\\10\end{bmatrix}$$

$$|1\rangle\langle 1| = \begin{bmatrix}00\\01\end{bmatrix}$$

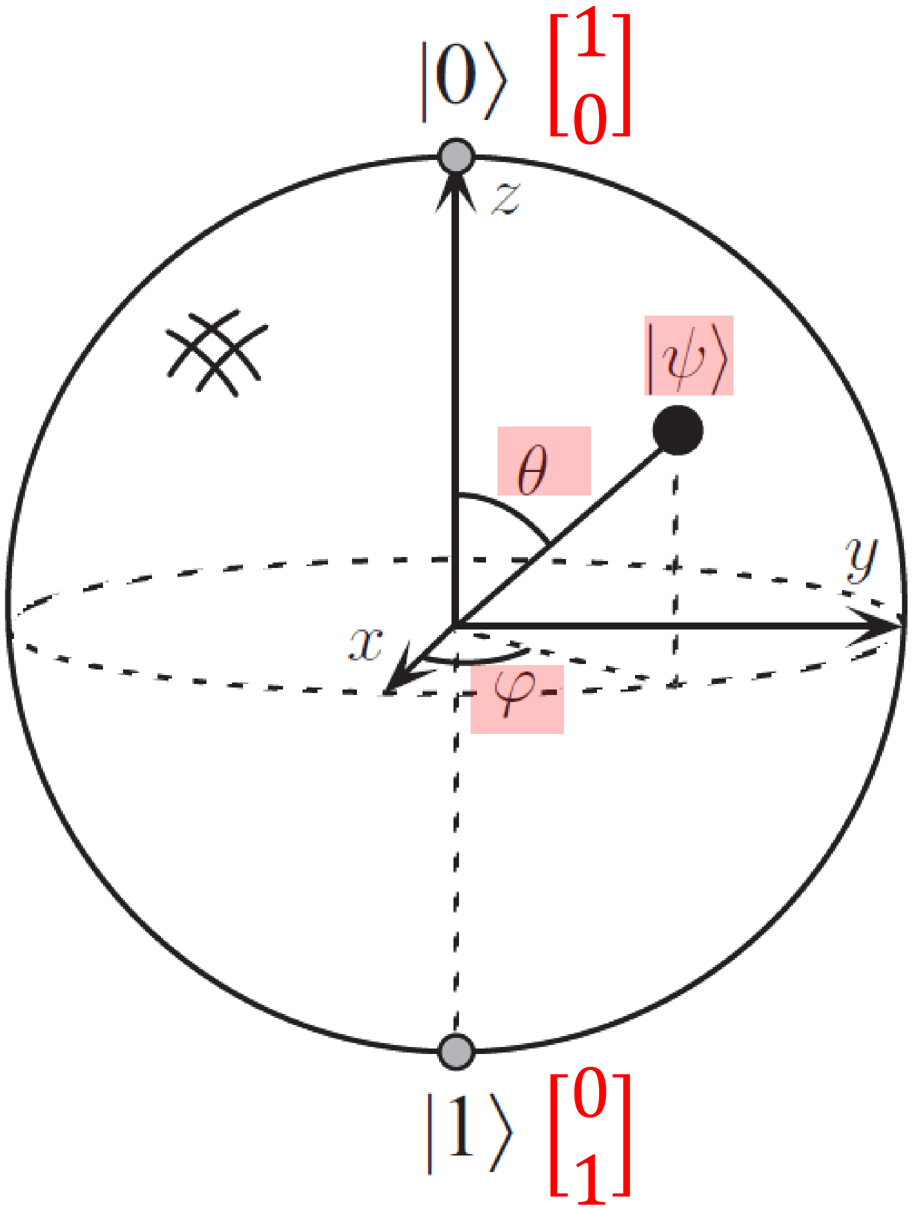
Quantum Bit: its geometric representation

$|\psi\rangle = a|0\rangle + b|1\rangle$

- A qubit state is initially described by four real parameters (p,q,v,w);

  a=p+qi, b=v+wi

- A qubit state can be mapped onto a single point on the sphere known as "**Bloch Sphere**."



4 parameters (p,q,v,w) → 2 parameters (φ , θ)

Quantum Bit control:

Single Qubit Gates

Quantum Bit control: single qubit gate

- A single qubit gate is a function (matrix operator) which takes a single qubit state as an input and returns its value as an output.
- Some important single qubit gates

Pauli Transformation Gates

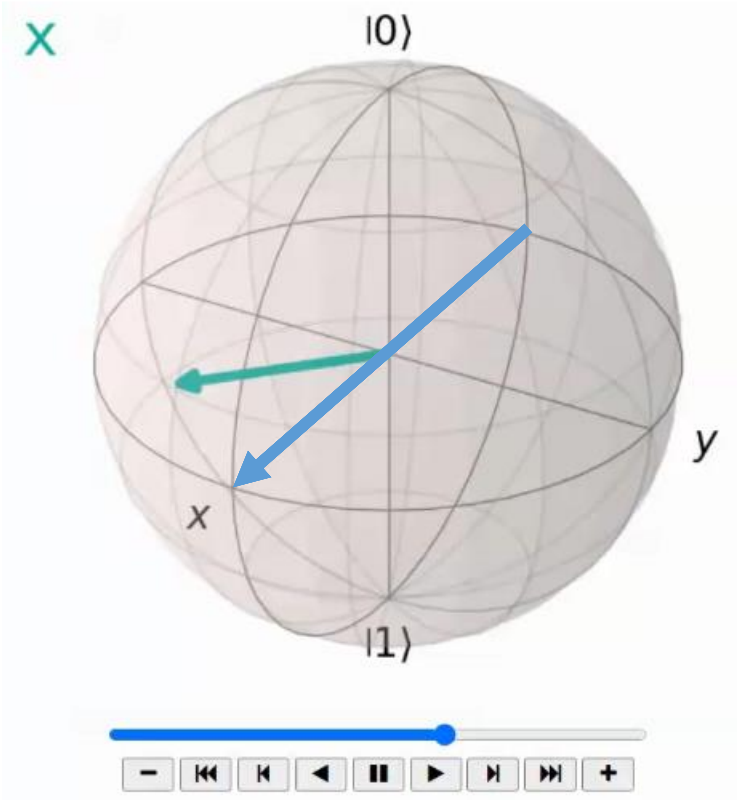
$$I \equiv \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad X \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$Y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad Z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

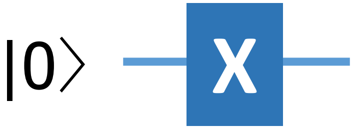
Hadamard Gate

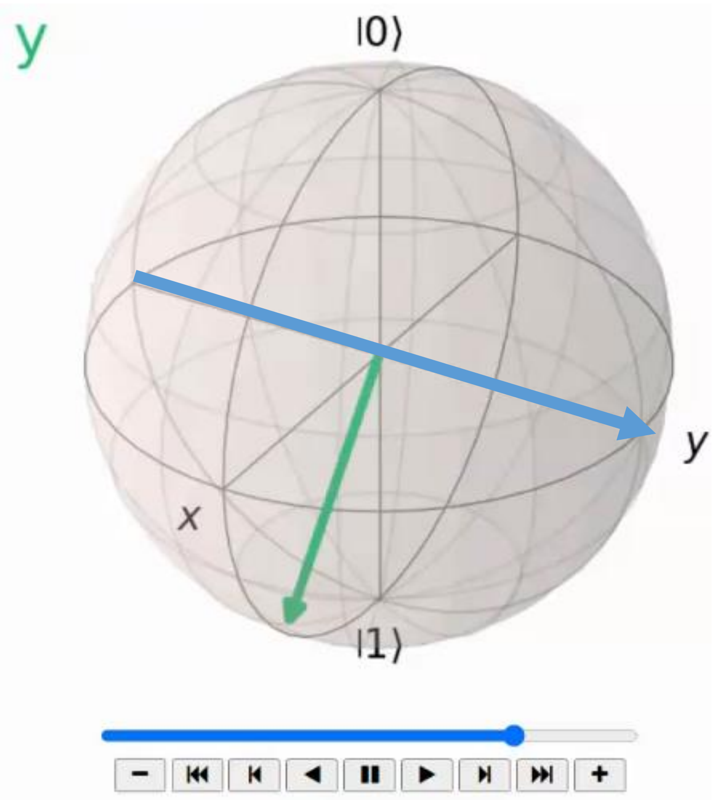
$$H \equiv \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Quantum Bit: its geometric representation

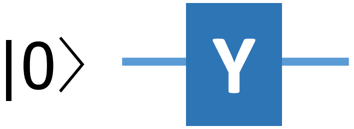


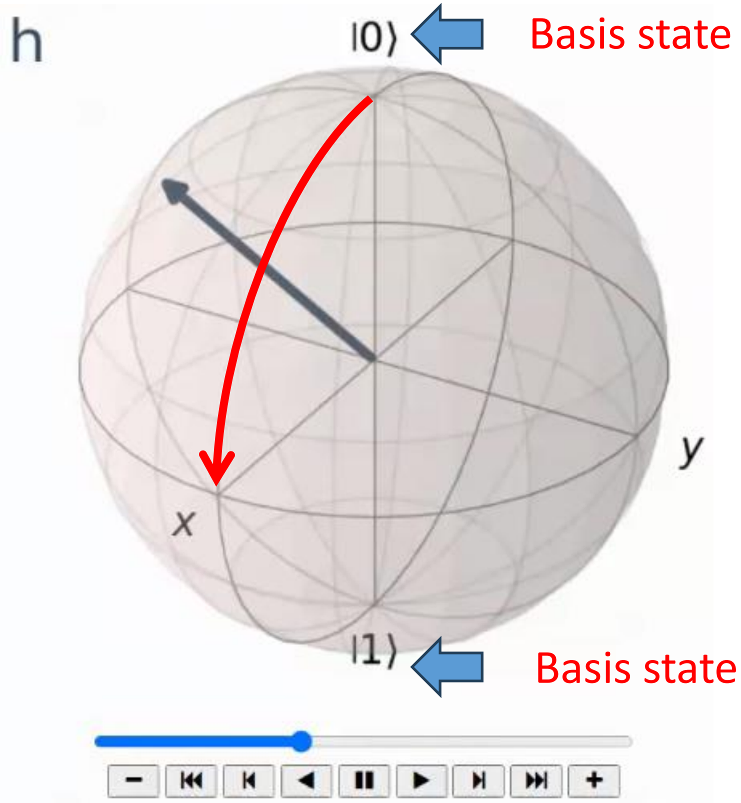
X gate
Rotating around the X-axis



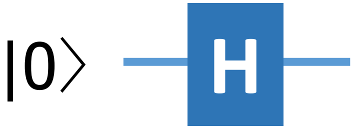


Y gate
Rotating around the Y-axis

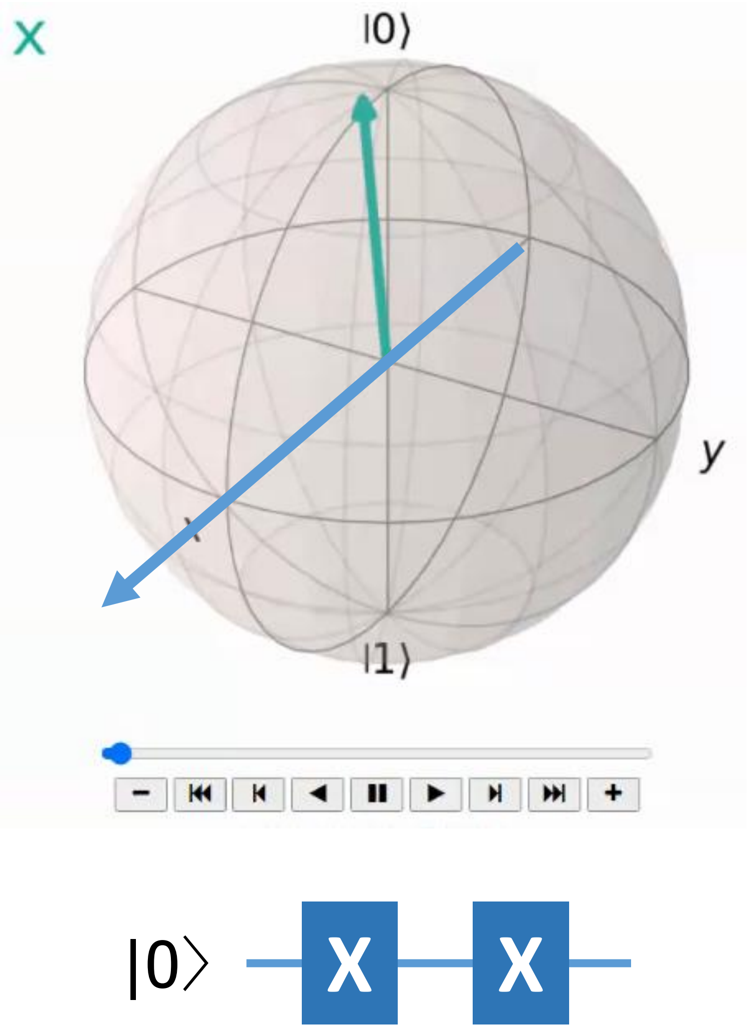


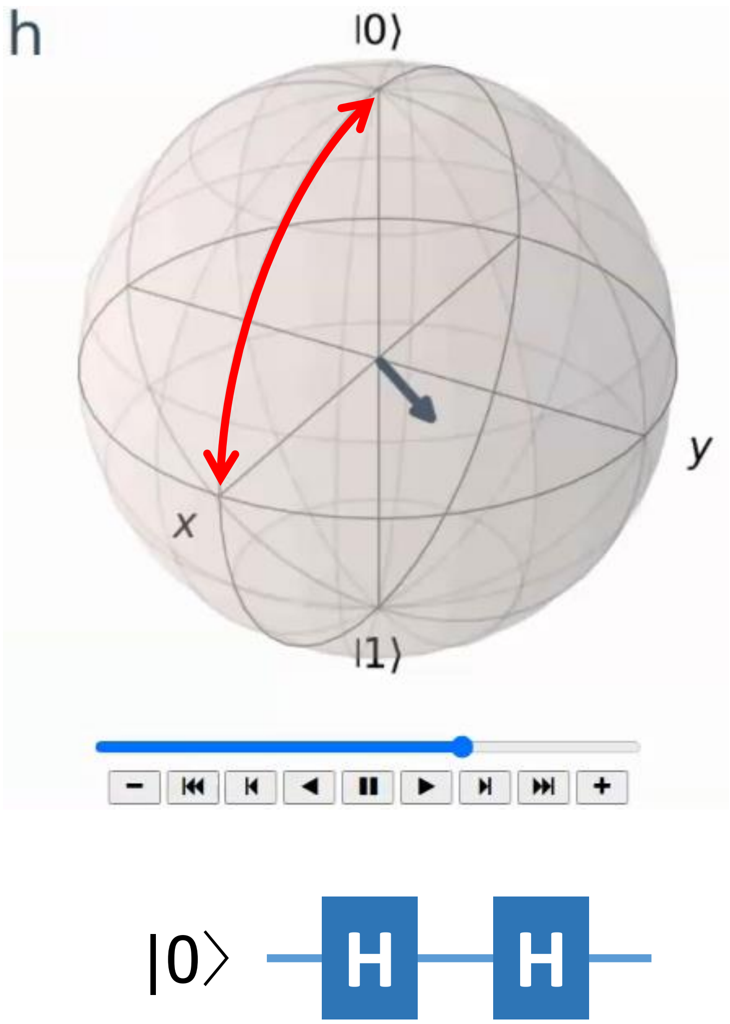


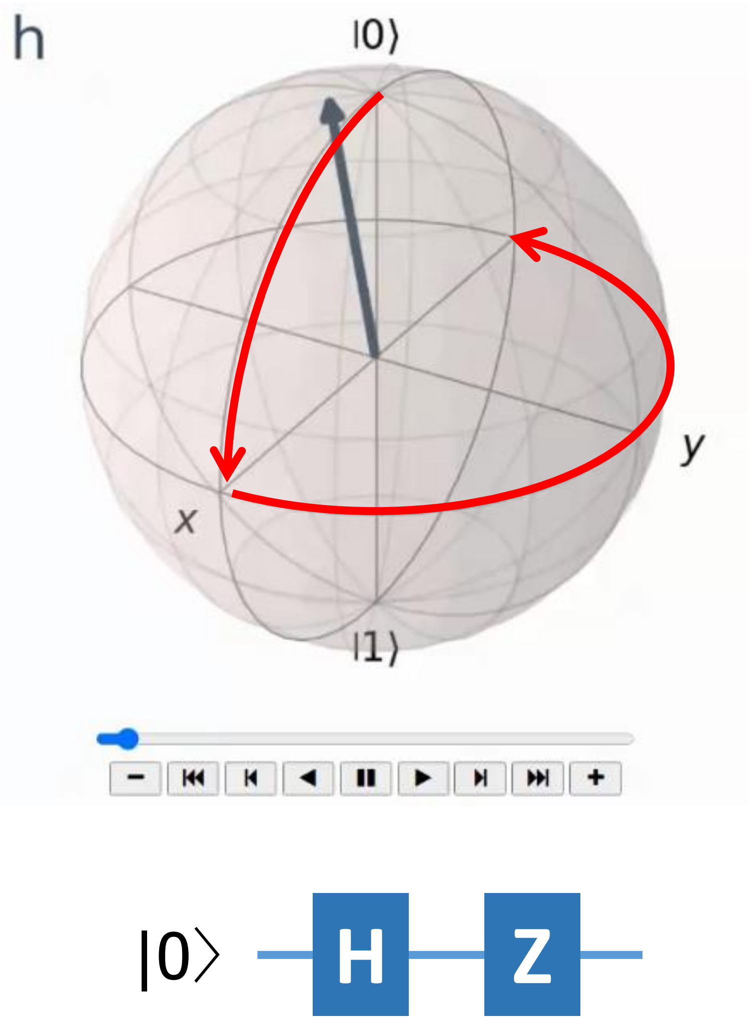
Hadamard gate



Quantum Bit: its geometric representation



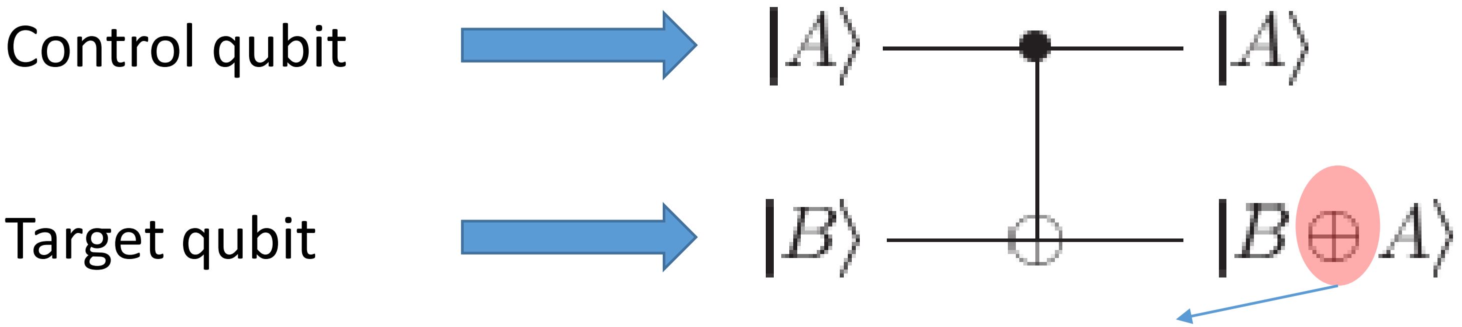




Quantum Bit control:

Gate for multiple Qubits

- Controlled-NOT gate
  - In short, **CNOT** Gate or **CX** Gate.
  - It has two input qubits; the control qubit and the target qubit.
  - If the control bit is 0, the target bit does not change.
  - If the control bit is 1, the target bit is flipped.



Addition modulo two: remainder after diving the summation of A and B by two

- <u>Addition modulo two: $\oplus$</u>
  - $0 \oplus 0$ => 0 so 0%2 = 0
  - $0 \oplus 1$ => 1 so 1%2 = 1
  - $1 \oplus 0$ => 1 so 1%2 = 1
  - $1 \oplus 1$ => 2 so 2%2 = 0

$|B\rangle$ $|A\rangle$

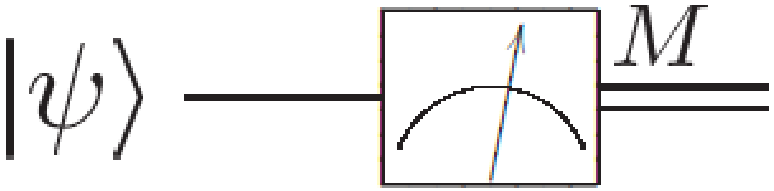
Quantum Bit control: multiple qubit gate

- One important thing you need to remember is
  - There are many interesting qubit gates however CNOT gate and single qubit gates are the prototypes for all other gates.
    - Any multiple qubit logic gate may be composed from CNOT gate and single qubit gates.

Quantum Circuits

Quantum Circuits

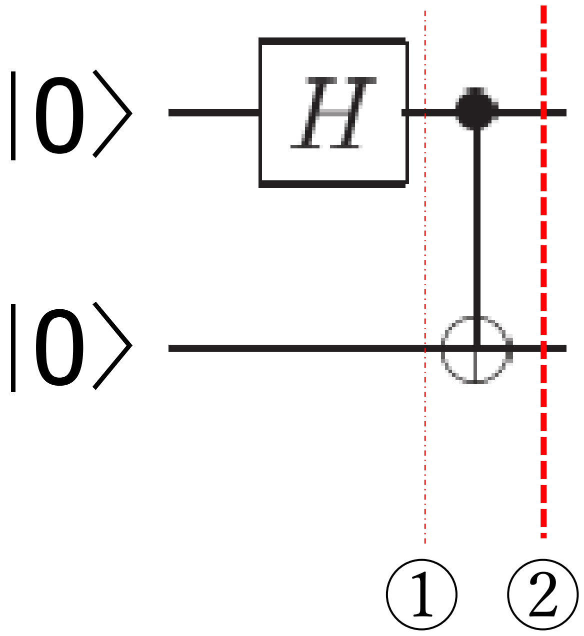
- A quantum circuit is a sequence of quantum gates and measurements designed to perform a specific quantum computation or algorithm on qubits.
- The circuit is read from left-to-right. The state input to the circuit is usually the state consisting of all $|0\rangle$s unless otherwise noted.



Quantum circuit symbol for measurement

Quantum Circuits: Bell state

- A quantum circuit for creating Bell state, also known as entanglement state.
- Entangled quantum state of two qubits says,
  - Knowing the state of one qubit automatically reveals the state of the other qubit regardless of the geographical locations of the two qubits.
- Bell state is created by Hadamard Gate followed by CNOT gate.



① **Hadamard Gate**:

creating an equal superposition of the two basis states.

Control bit

$$(H|0\rangle)\otimes|0\rangle = 1/\sqrt{2}\,(|0\rangle + |1\rangle)\otimes|0\rangle$$

$$= 1/\sqrt{2}\,(|00\rangle + |10\rangle)$$

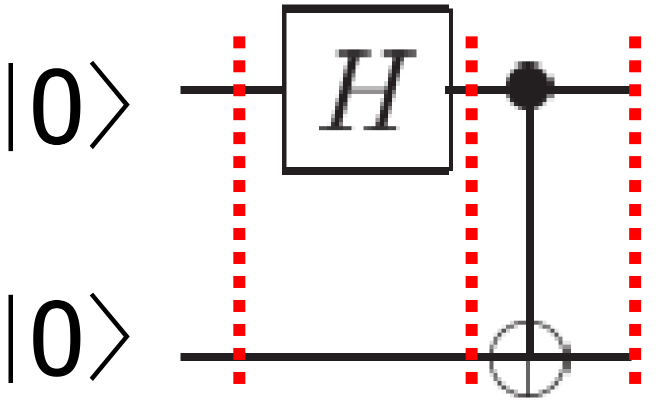
Control bit 0 : not changing

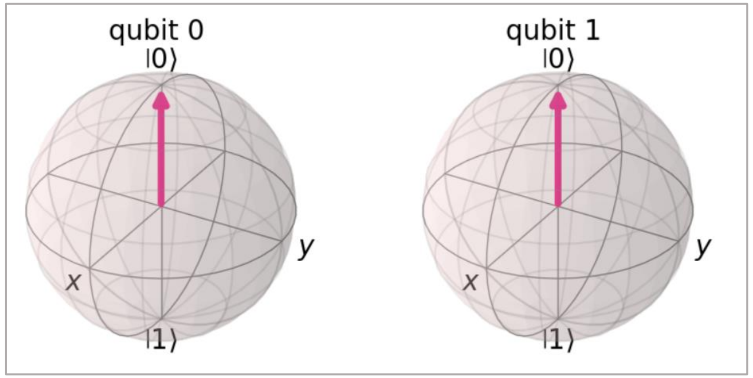
② **CNOT Gate**:

Control bit 1 : changing 0 to 1

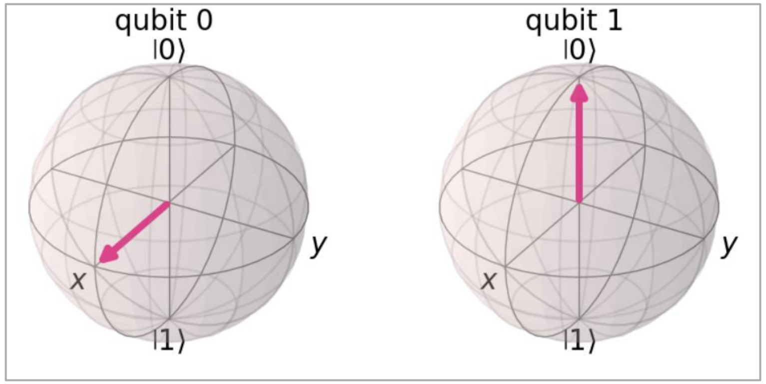
$$1/\sqrt{2}\,|00\rangle + 1/\sqrt{2}\,|11\rangle$$

Quantum Circuits: Bell state





(a)



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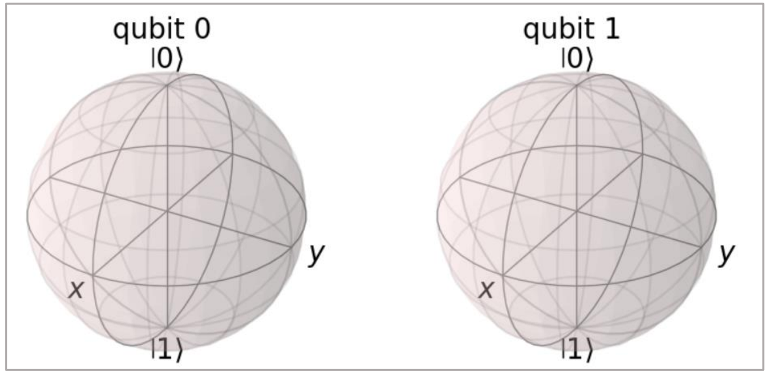
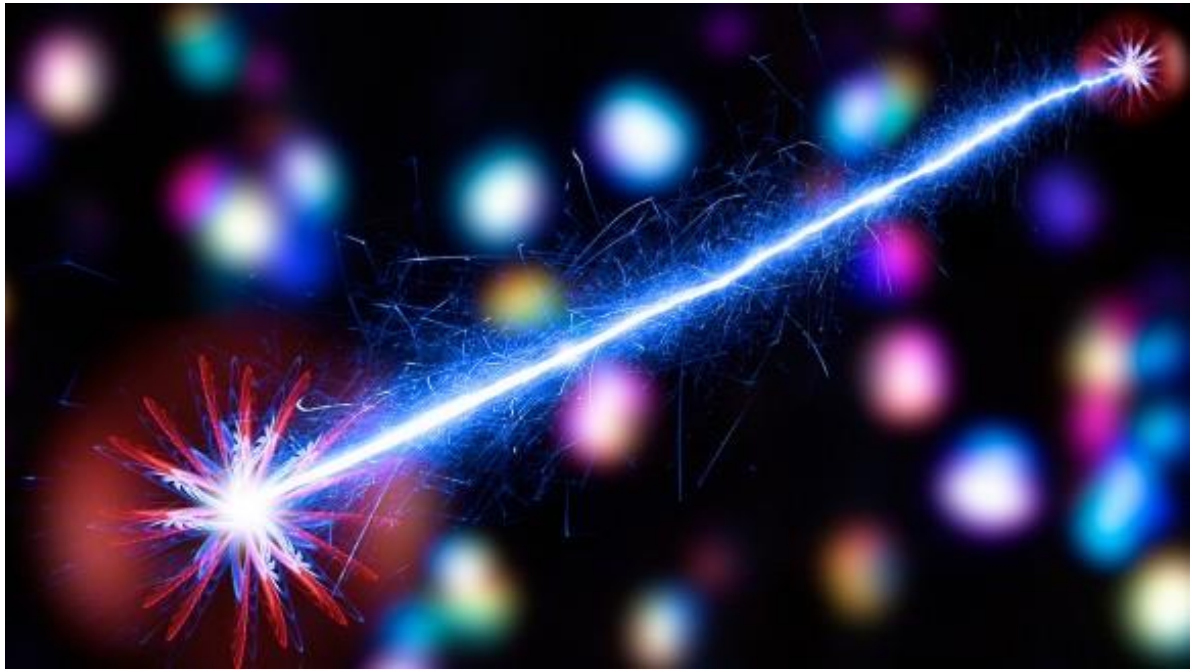


(c)

Quantum Circuits: Bell state: entanglement

- When the quantum states of two particles (e.g. photons) cannot be considered independently, we refer to quantum entanglement.
- In the case of two entangled particles, for example, this means that a measurement of one particle collapses not only its wave-function (and therefore determines its state), but also that of its twin.



https://www.nature.com/collections/aegdeibjfi

Quantum Algorithm

Deutsch algorithm

Quantum Algorithm: Deutsch's algorithm

- Given a binary function f(x), tell me whether it is either
  - Constant function: f(A) == f(B) or
  - Balanced function: f(A) != f(B)
- In a classic computing, it requires two evaluations to identify whether the function is constant or balanced function.
- In a quantum computing, it requires only one evaluation!
- One of the first examples which demonstrates a quantum algorithm is better than a classical algorithm.

Quantum Algorithm: Deutsch's algorithm

- Assuming that the binary function takes (n=3) bits as input and it gives you one bit as output.
- In a classic computing, how many queries need to identify whether it is constant or balanced function?

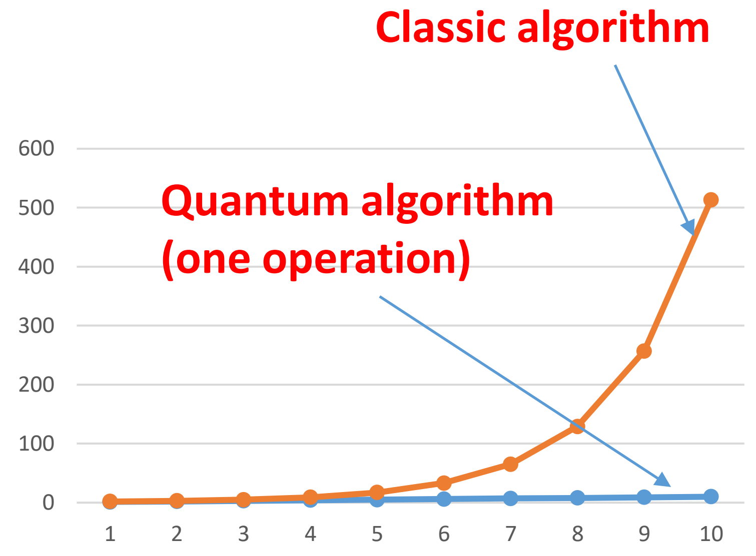
Constant function	Balanced function
f(000) = 0	f(000) = 0
f(001) = 0	f(001) = 0
f(010) = 0	f(010) = 0
f(011) = 0	f(011) = 0
f(100) = 0	f(100) = 1
f(101) = 0	f(101) = 1
f(110) = 0	f(110) = 1
f(111) = 0	f(111) = 1

2^{n-1}

$2^{n-1}+1$

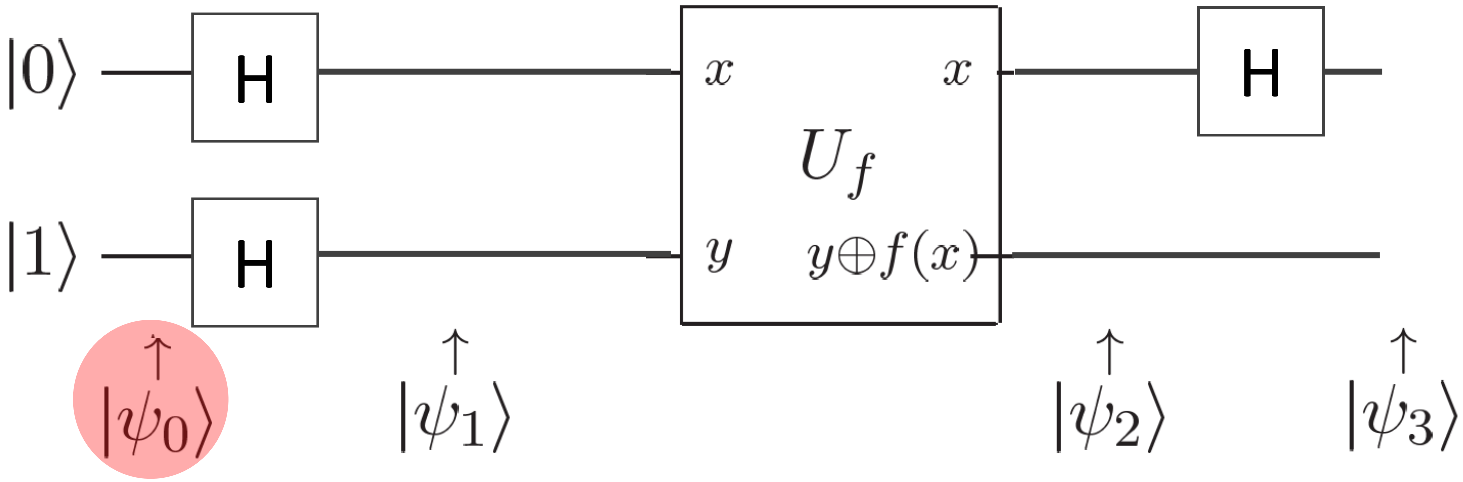
<u>In the worst case</u>, you need to make queries as many as this number

# of queries to verify if it is constant or balanced function.



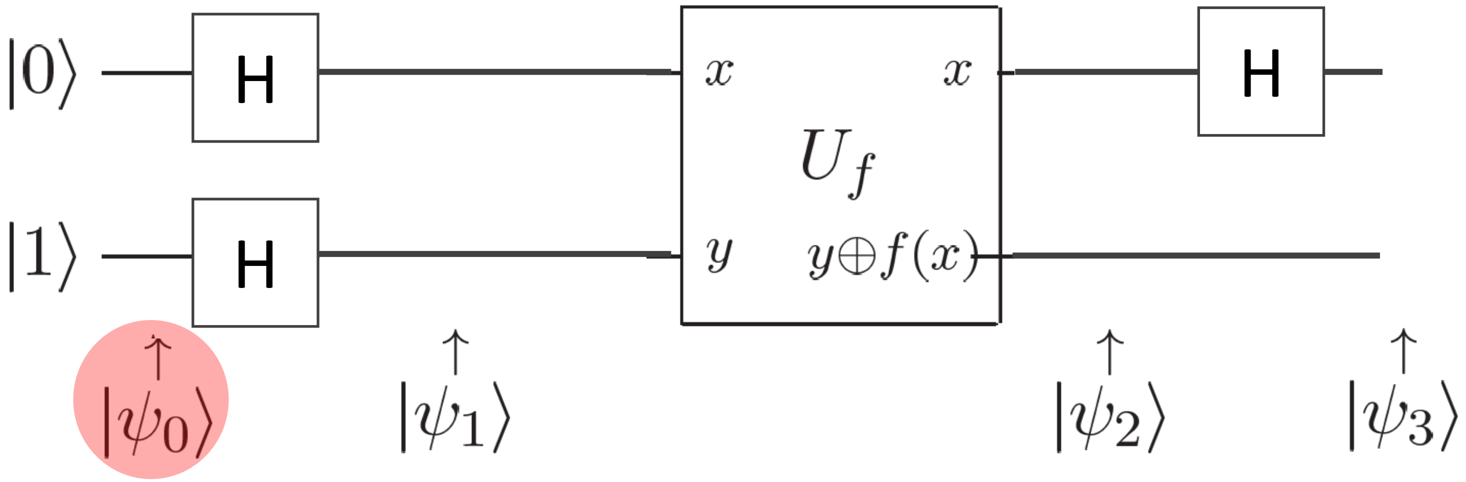
n: the number of input bits

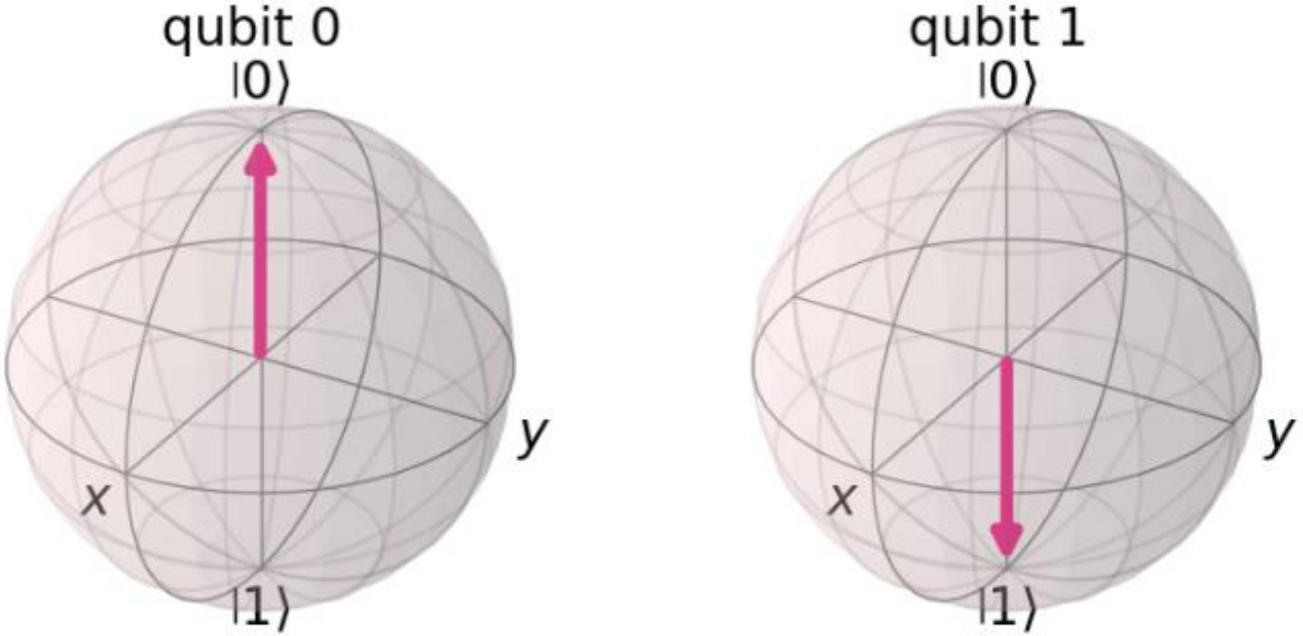
Quantum Algorithm: Deutsch's algorithm



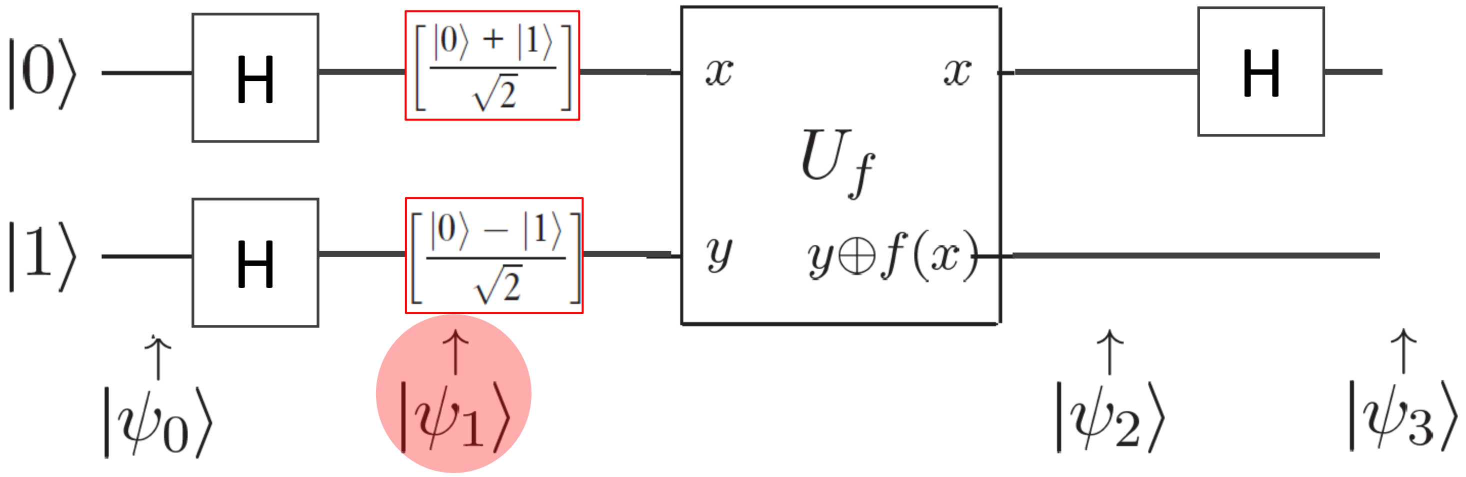
- Here we want to verify whether the function **f(x)** is constant or balanced function.
- First, the input state, $|\psi_0\rangle = |01\rangle$, is fed into the quantum circuit.

Quantum Algorithm: Deutsch's algorithm





Quantum Algorithm: Deutsch's algorithm

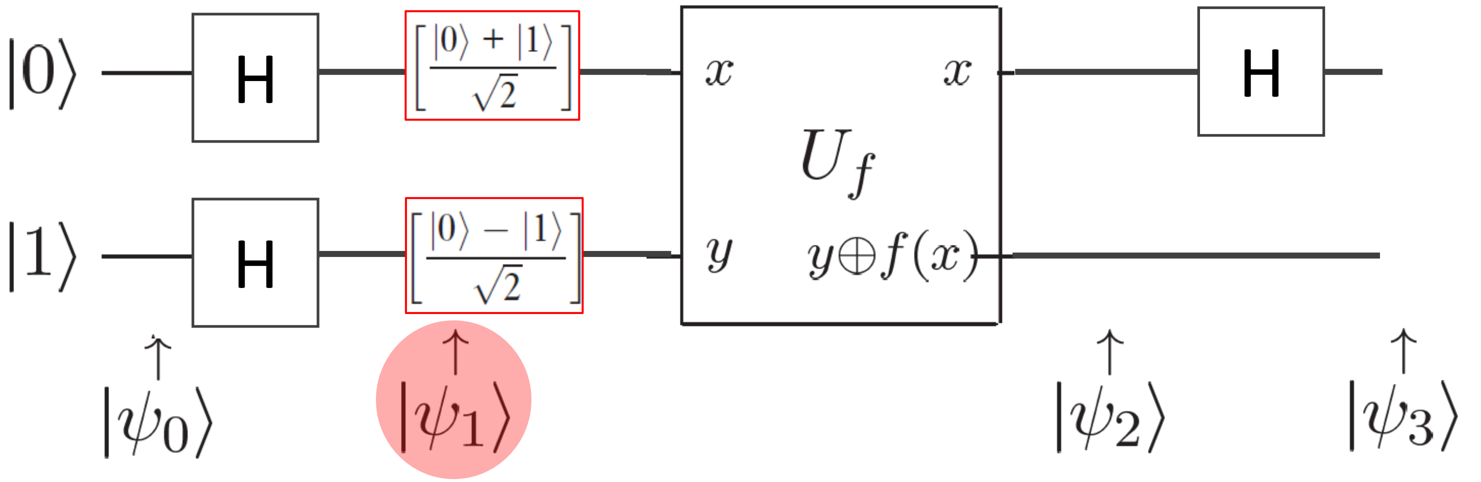


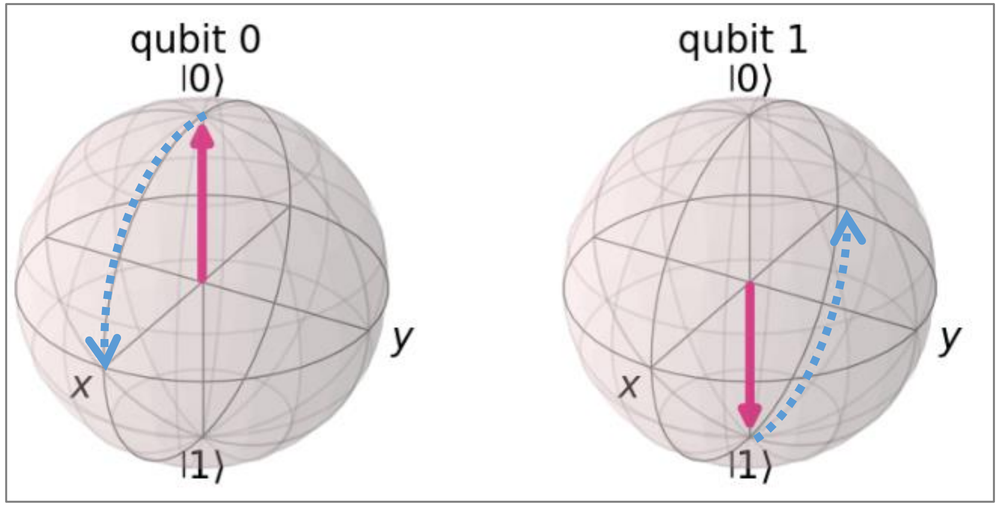
- Each of the qubit, $|0\rangle$ and $|1\rangle$, is sent through two Hadamard gates,
  - Hadamard gate: creating an equal superposition of the two basis states

Hadamard Gate

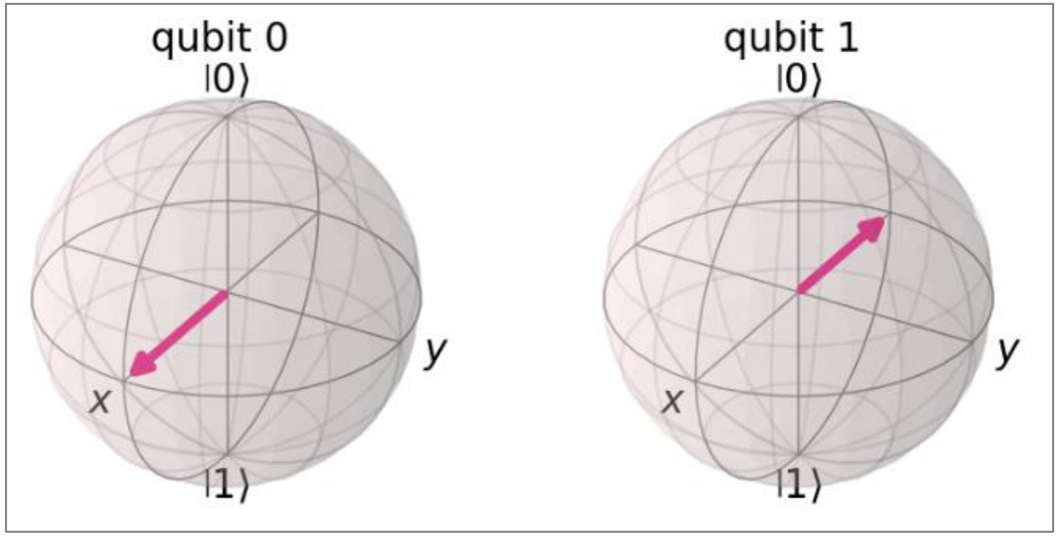
$$H \equiv \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Quantum Algorithm: Deutsch's algorithm



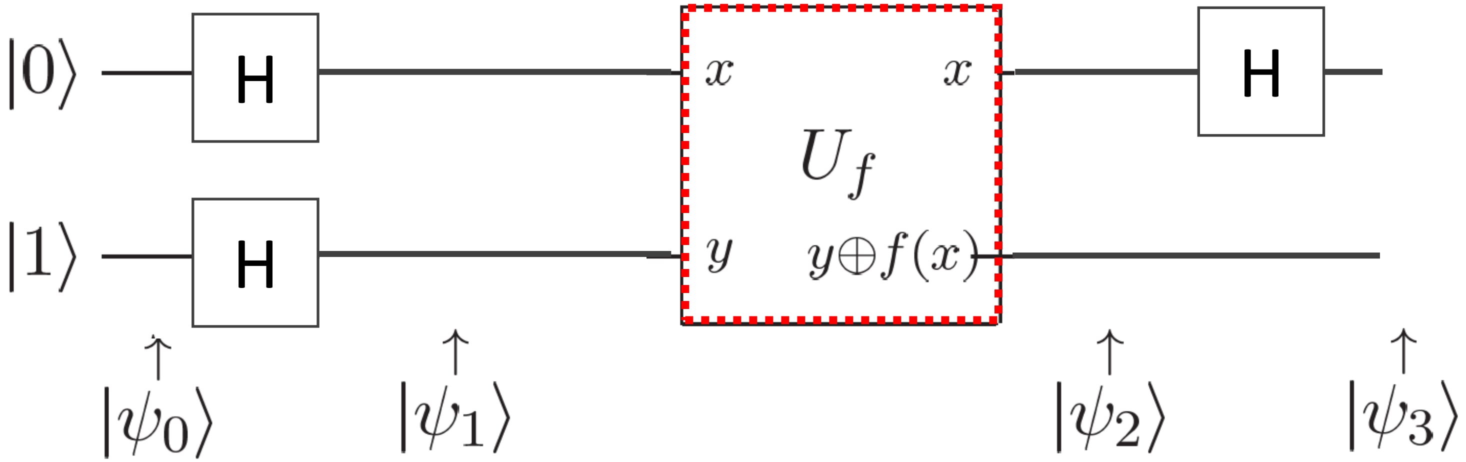


$|\psi_0\rangle$



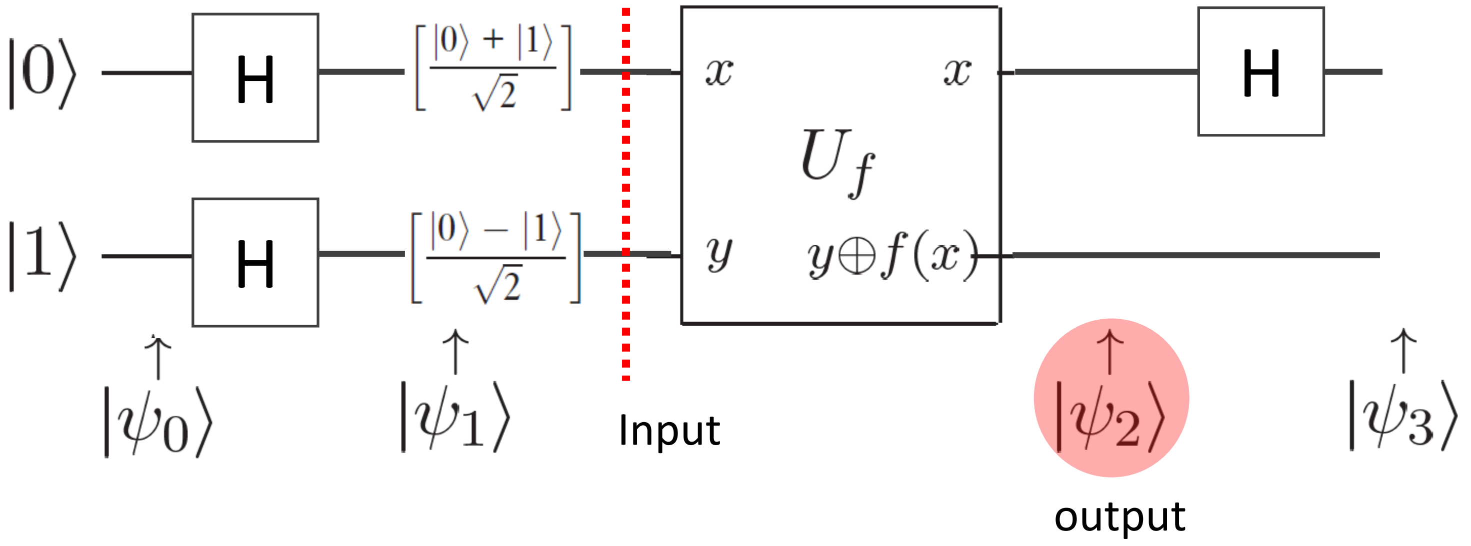
$|\psi_1\rangle$

Quantum Algorithm: Deutsch's algorithm



- **<u>Oracle function (U_f)</u>**
  - In ancient Greece, an oracle was a priest who made statements about future events or about the truth
  - Then, an oracle function is similar in a way that we don't know what the function produces given input value …

Quantum Algorithm: Deutsch's algorithm



- Input:

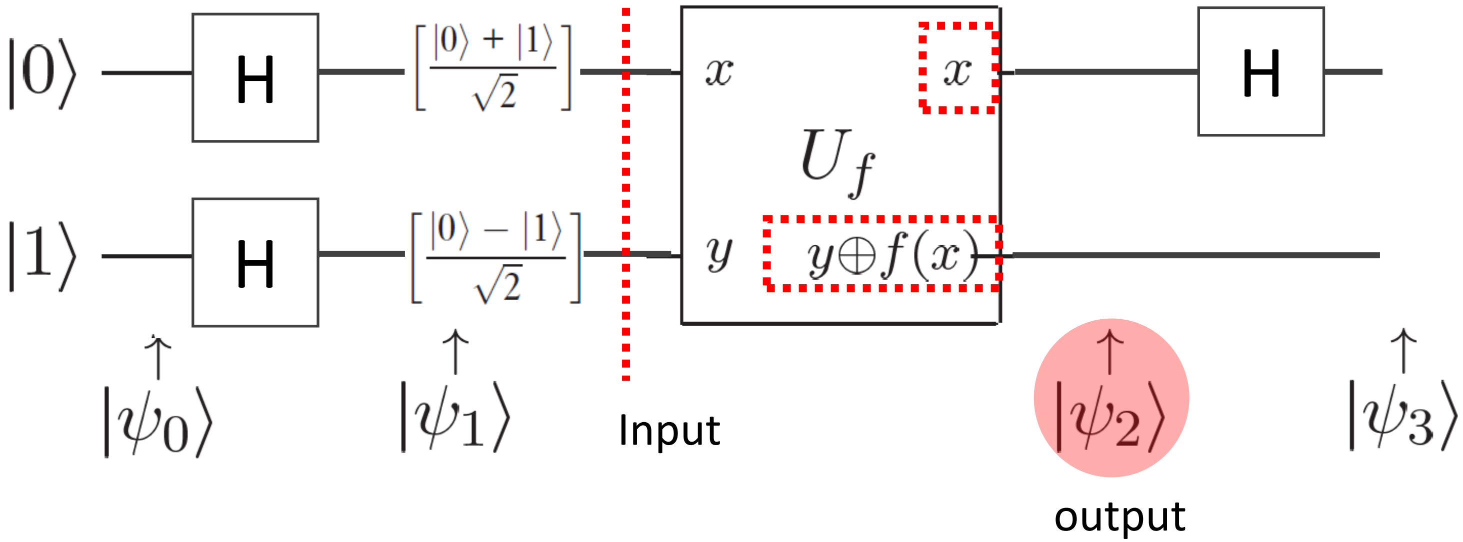
x y

$$|\psi_1\rangle = \left[\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right] = 1/2\,[|00\rangle + |10\rangle - |01\rangle - |11\rangle]$$

- Output:

$$|\psi_2\rangle = 1/2\,[|0, 0\oplus f(0)\rangle + |1, 0\oplus f(1)\rangle - |0, 1\oplus f(0)\rangle - |1, 1\oplus f(1)\rangle]$$

Quantum Algorithm: Deutsch's algorithm



- Input:

$$|\psi_1\rangle = \left[\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right] = 1/2\,[|00\rangle + |10\rangle - |01\rangle - |11\rangle]$$

x y

- Output:

$$|\psi_2\rangle = 1/2\,[|0, 0\oplus f(0)\rangle + |1, 0\oplus f(1)\rangle - |0, 1\oplus f(0)\rangle - |1, 1\oplus f(1)\rangle]$$

$x \quad y\oplus f(x)$

- ❑ **Output:**

$|\psi_2\rangle$ = 1/2 $[|0, 0\oplus f(0)\rangle + |1, 0\oplus f(1)\rangle - |0, 1\oplus f(0)\rangle - |1, 1\oplus f(1)\rangle]$

❖ Addition modulo two: $\oplus$

- $0\oplus 0$ => 0 so 0%2 = 0
- $0\oplus 1$ => 1 so 1%2 = 1
- $1\oplus 0$ => 1 so 1%2 = 1
- $1\oplus 1$ => 2 so 2%2 = 0

Constant function: f(0) == f(1)

$= 1/2\ [|0, f(0)\rangle + |1, f(1)\rangle - |0, \overline{f(0)}\rangle - |1, \overline{f(1)}\rangle]$

$= 1/2\ [|0, f(0)\rangle + |1, f(0)\rangle - |0, \overline{f(0)}\rangle - |1, \overline{f(0)}]$

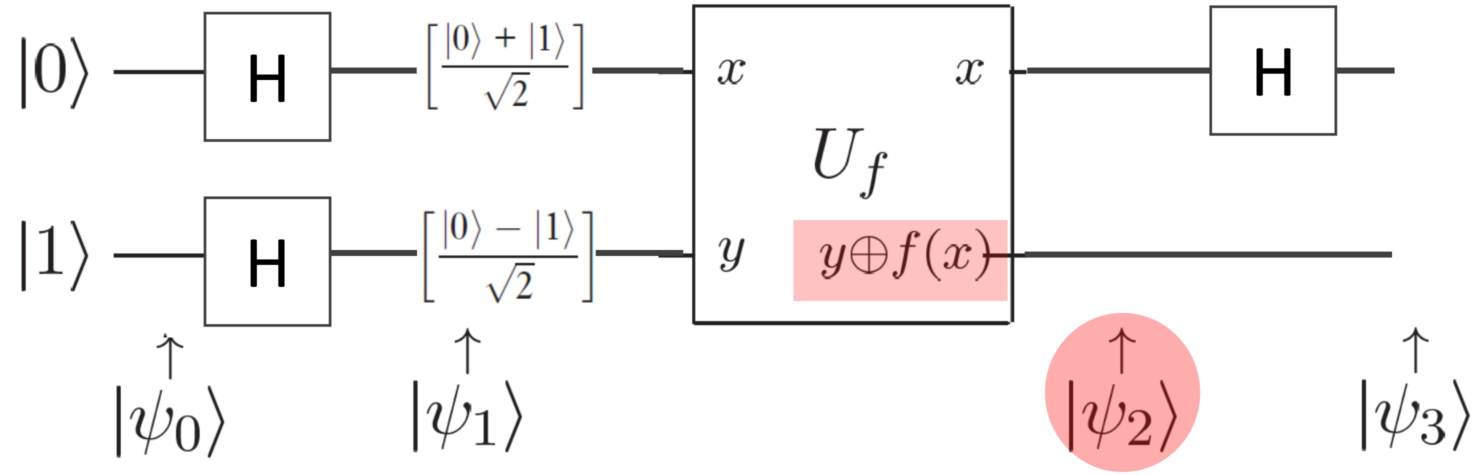
$= 1/2\ [(|0\rangle + |1\rangle)(f(0) - \overline{f(0)})\ ]$

$= \pm\ 1/2\ [(|0\rangle + |1\rangle)(|0\rangle - |1\rangle)]$

$= \pm \left[\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$

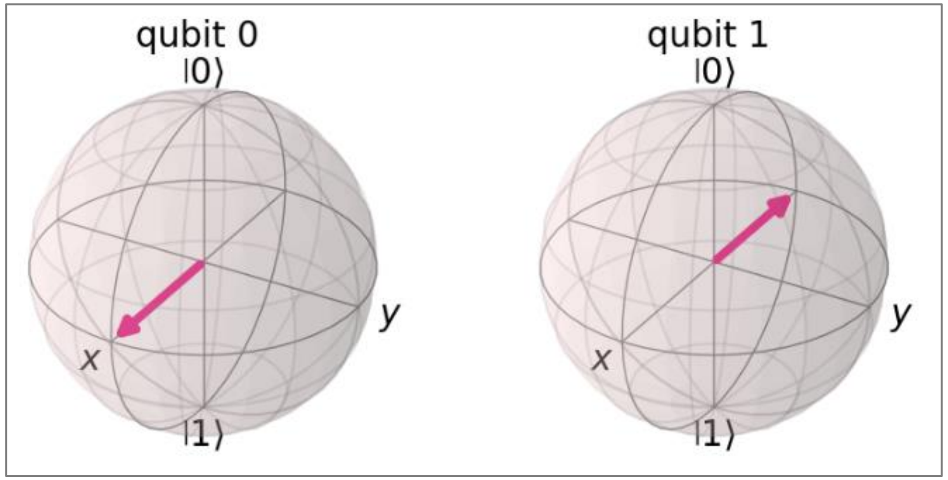
$$|\psi_2\rangle = \pm \left[\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$

Quantum Algorithm: Deutsch's algorithm

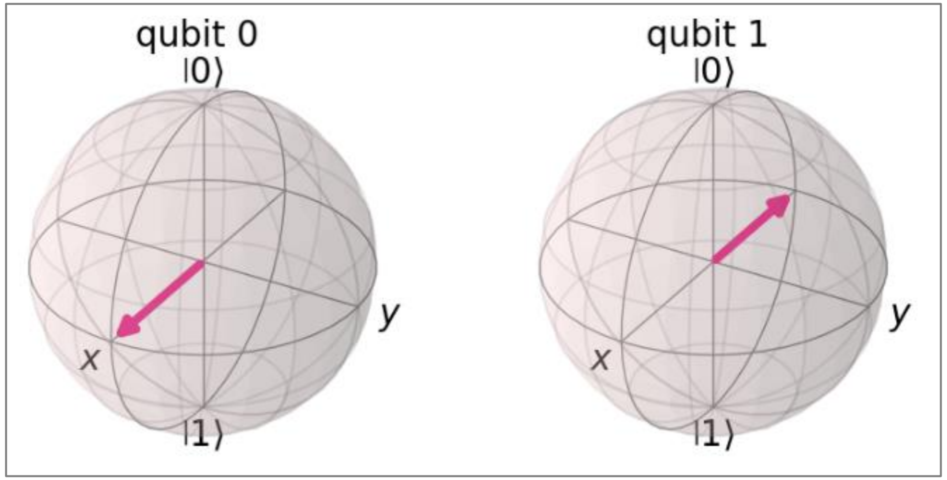


Constant function: f(0) == f(1)

$$|\psi_2\rangle = \pm\left[\frac{|0\rangle+|1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right]$$



$|\psi_1\rangle$



$|\psi_2\rangle$

- ❖ Addition modulo two: $\oplus$
  - $0 \oplus 0$ => 0 so 0%2 = 0
  - $0 \oplus 1$ => 1 so 1%2 = 1
  - $1 \oplus 0$ => 1 so 1%2 = 1
  - $1 \oplus 1$ => 2 so 2%2 = 0

❑ Output:

$|\psi_2\rangle = 1/2\, [|0, 0\oplus f(0)\rangle + |1, 0\oplus f(1)\rangle - |0, 1\oplus f(0)\rangle - |1, 1\oplus f(1)\rangle]$

Balanced function: f(0) != f(1)

$= 1/2\, [|0, f(0)\rangle + |1, f(1)\rangle - |0, \overline{f(0)}\rangle - |1, \overline{f(1)}\rangle]$

$= 1/2\, [|0, f(0)\rangle + |1, f(1)\rangle - |0, f(1)\rangle - |1, f(0)]$

$= 1/2\, [(|0\rangle - |1\rangle)(f(0) - f(1))]$

$= \pm\, 1/2\, [(|0\rangle - |1\rangle)(|0\rangle - |1\rangle)]$

$$= \pm \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$

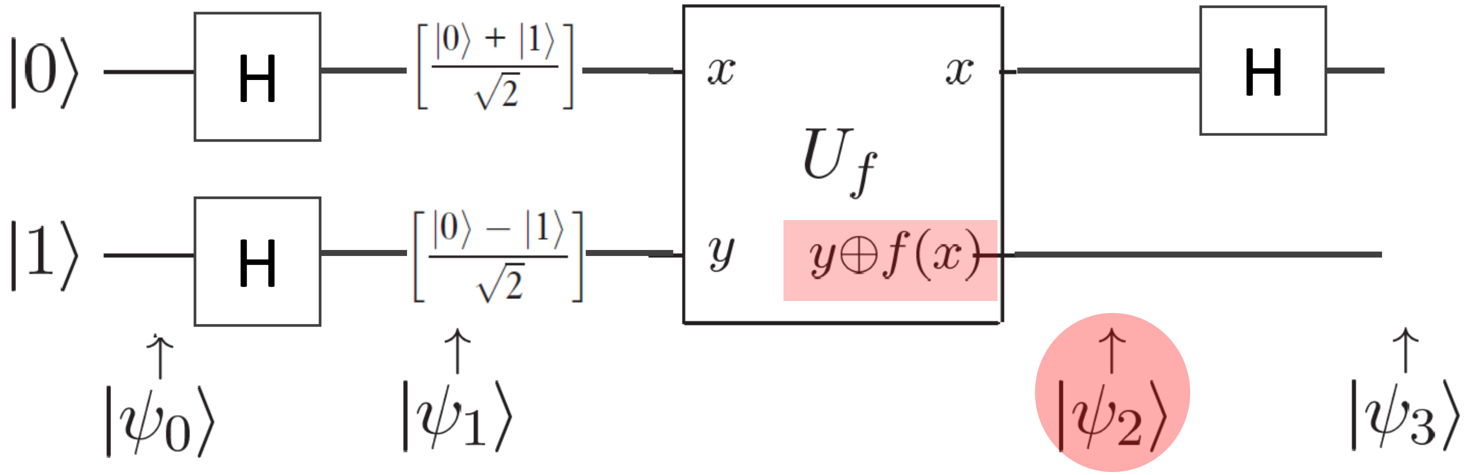
There are two cases;

1) f(0) = $|0\rangle$, f(1) = $|1\rangle$
2) f(0) = $|1\rangle$, f(1) = $|0\rangle$,

Thus, $(f(0)-f(1))$ becomes $\pm\,(|0\rangle - |1\rangle)$

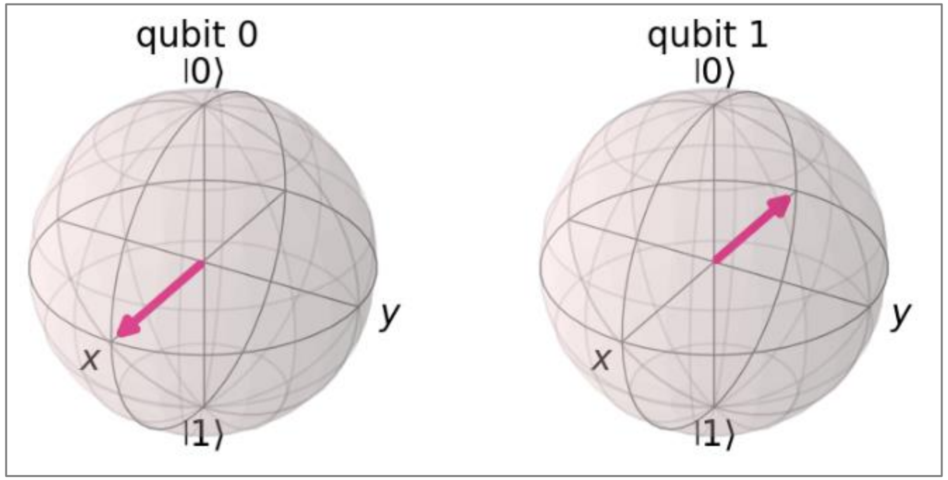
$$|\psi_2\rangle = \pm \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$

Quantum Algorithm: Deutsch's algorithm

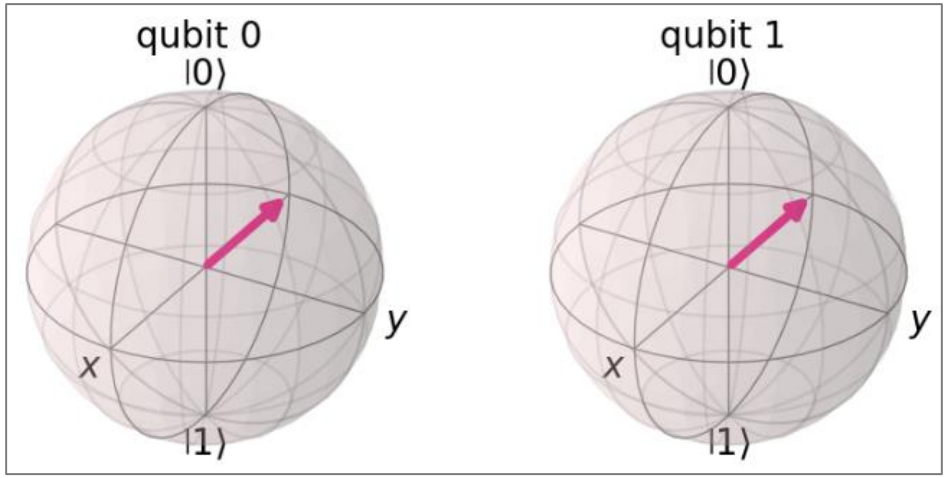


Balanced function: f(0) == f(1)

$$|\psi_2\rangle = \pm\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$

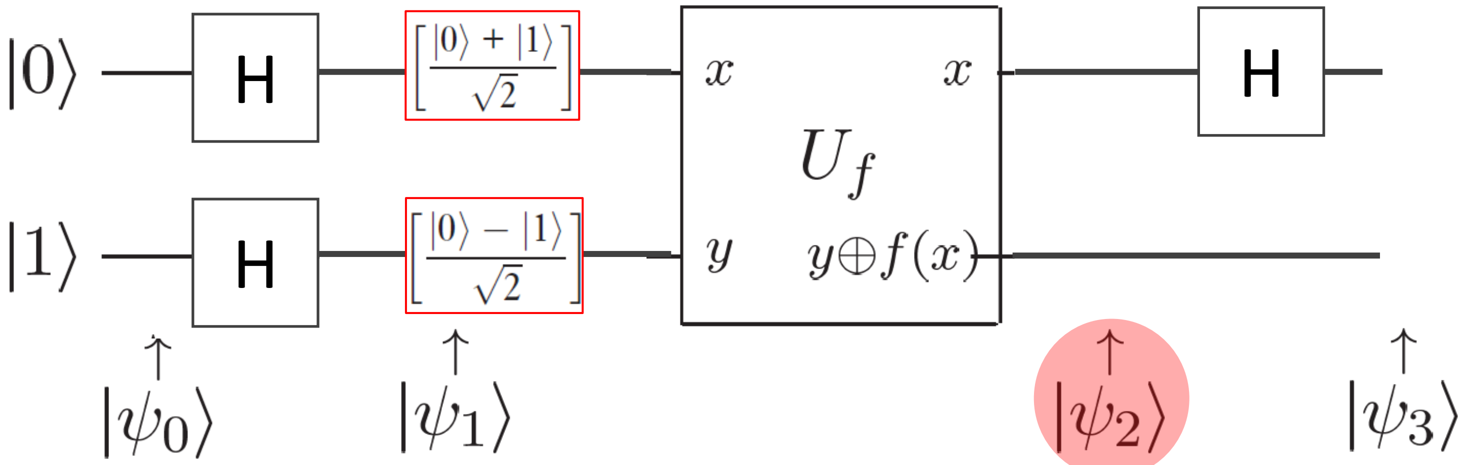


$|\psi_1\rangle$



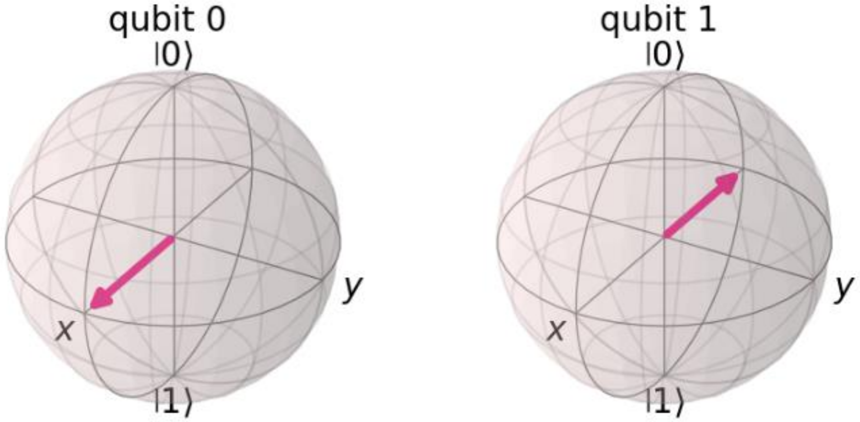
$|\psi_2\rangle$

Quantum Algorithm: Deutsch’s algorithm



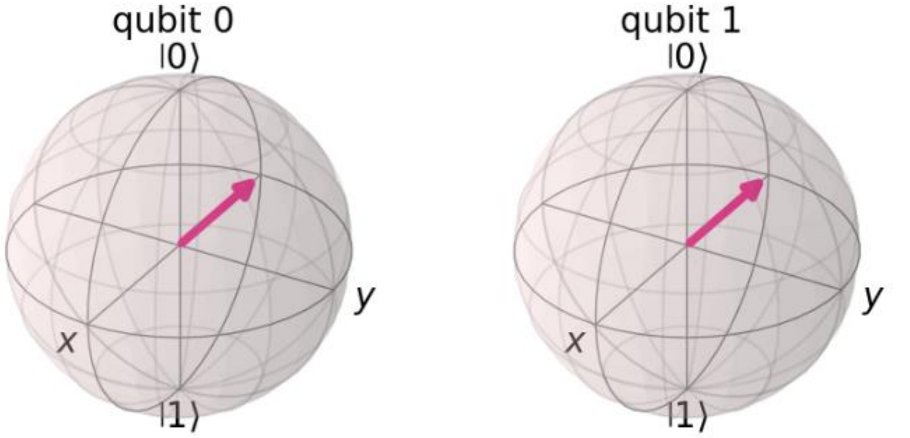
Constant function: f(0) == f(1)

$$|\psi_2\rangle = \pm\left[\frac{|0\rangle+|1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right]$$

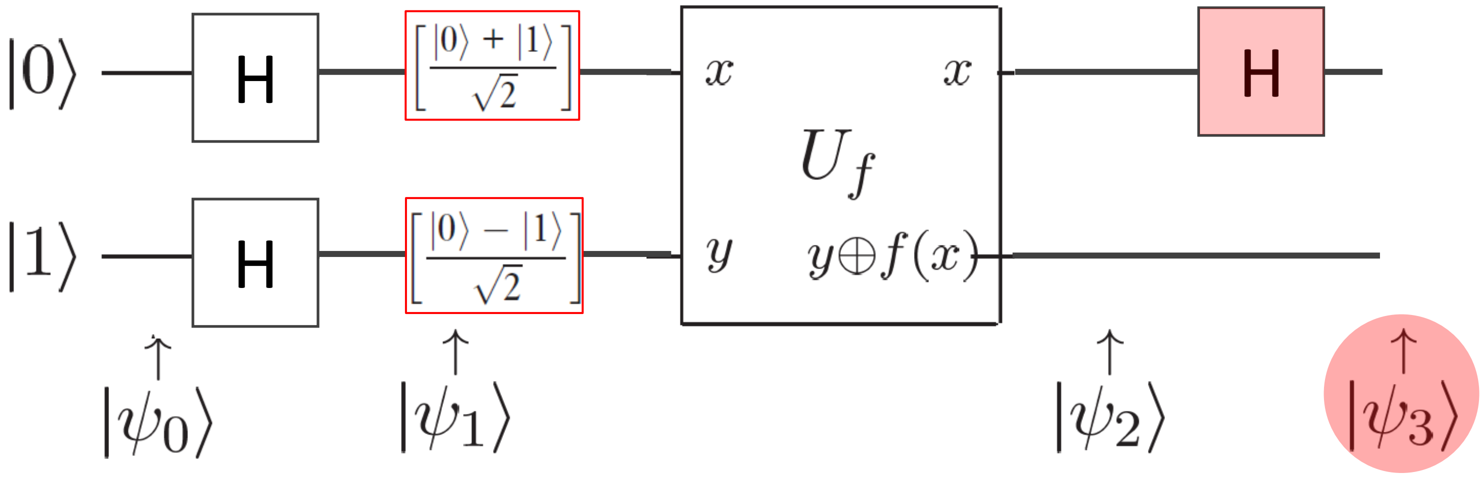


Balanced function: f(0) != f(1)

$$|\psi_2\rangle = \pm\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right]$$



Quantum Algorithm: Deutsch's algorithm



Constant function: f(0) == f(1)

$$|\psi_2\rangle = \pm\left[\frac{|0\rangle+|1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right]$$

$$|\psi_3\rangle = \pm\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}\left[\frac{|0\rangle+|1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right]$$

$$= \pm\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right]$$

$$= \pm\begin{bmatrix}1\\0\end{bmatrix}\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right] = \pm|0\rangle\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right]$$

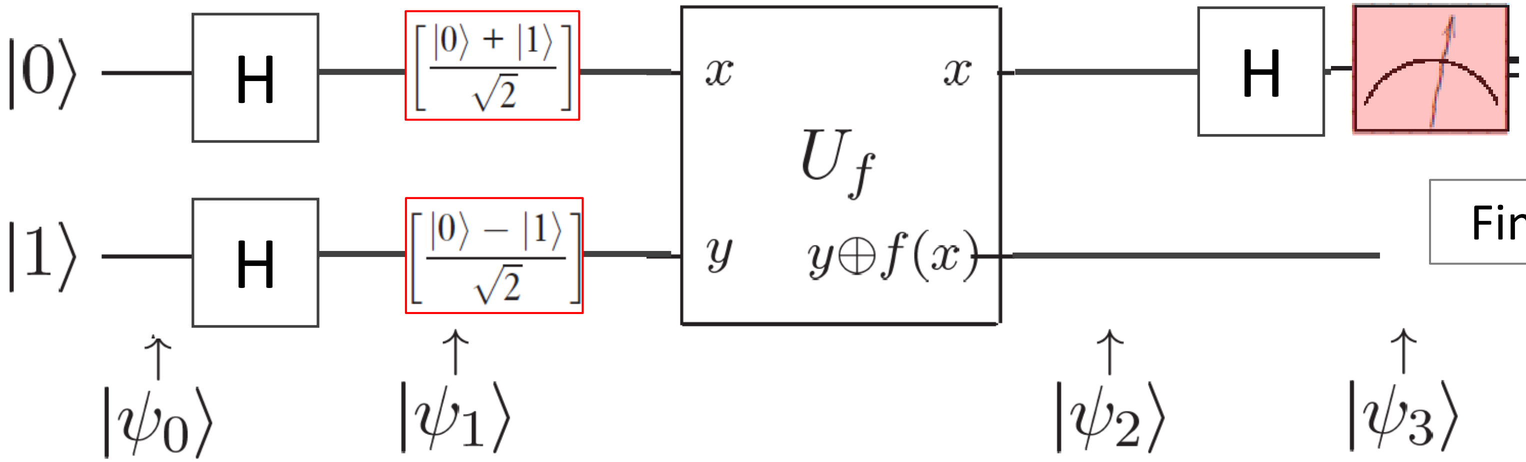
Balanced function: f(0) != f(1)

$$|\psi_2\rangle = \pm\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right]$$

$$|\psi_3\rangle = \pm\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right]$$

$$= \pm\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right]$$

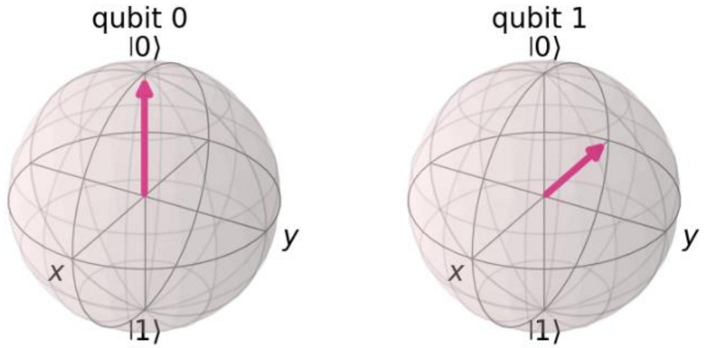
$$= \pm\begin{bmatrix}0\\1\end{bmatrix}\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right] = \pm|1\rangle\left[\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right]$$



Finally, we measure

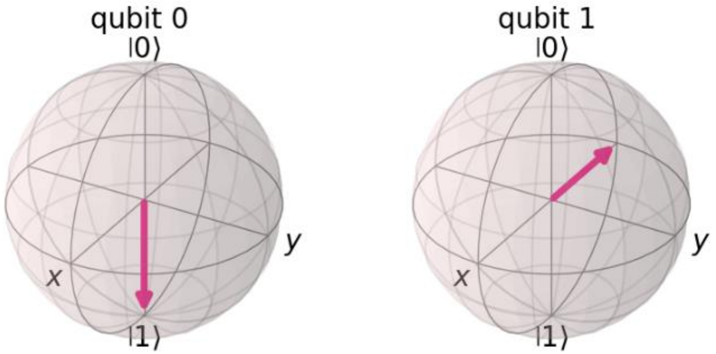
Constant function

$$\pm|0\rangle \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$



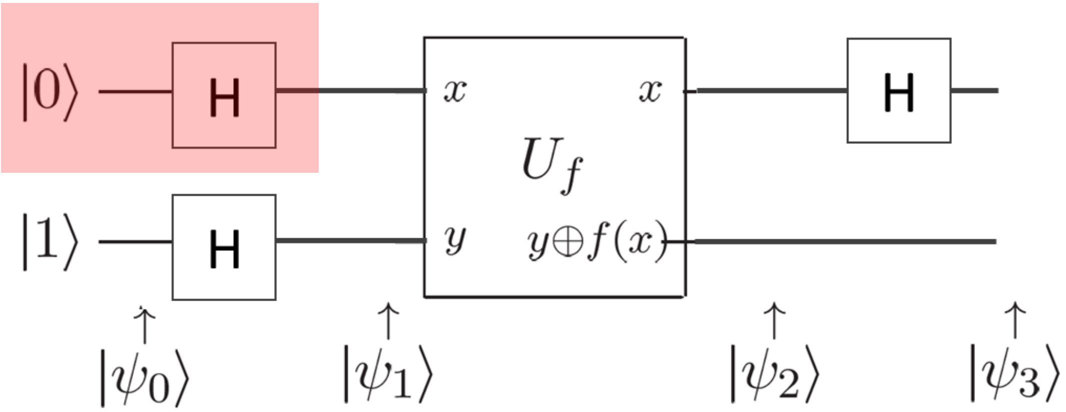
Balanced function

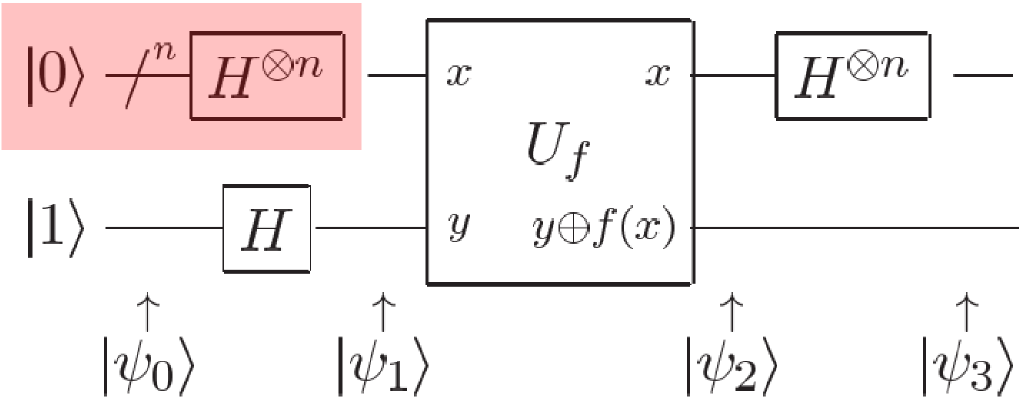
$$\pm|1\rangle \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$



- Measurement is done
  - If it's 0: f(x) is constant
  - If it's 1: f(x) is balanced

- The Deutsch-Jozsa algorithm is a generalized version of the Deutsch algorithm for multiple bits input.





- Deutsch algorithm
  - Single-bit input

- Deutsch Jozsa algorithm
  - Multiple-bits input

Summary

- Quantum mechanics is a mathematical framework or set of rules for the construction of physical theories.
- Quantum bit, its control through quantum gates and quantum circuits were explained as tools for the study of quantum mechanics.
- As an application scenario of quantum mechanics, Deutsch algorithm was introduced to demonstrate the superiority of quantum computing to classical computing.