



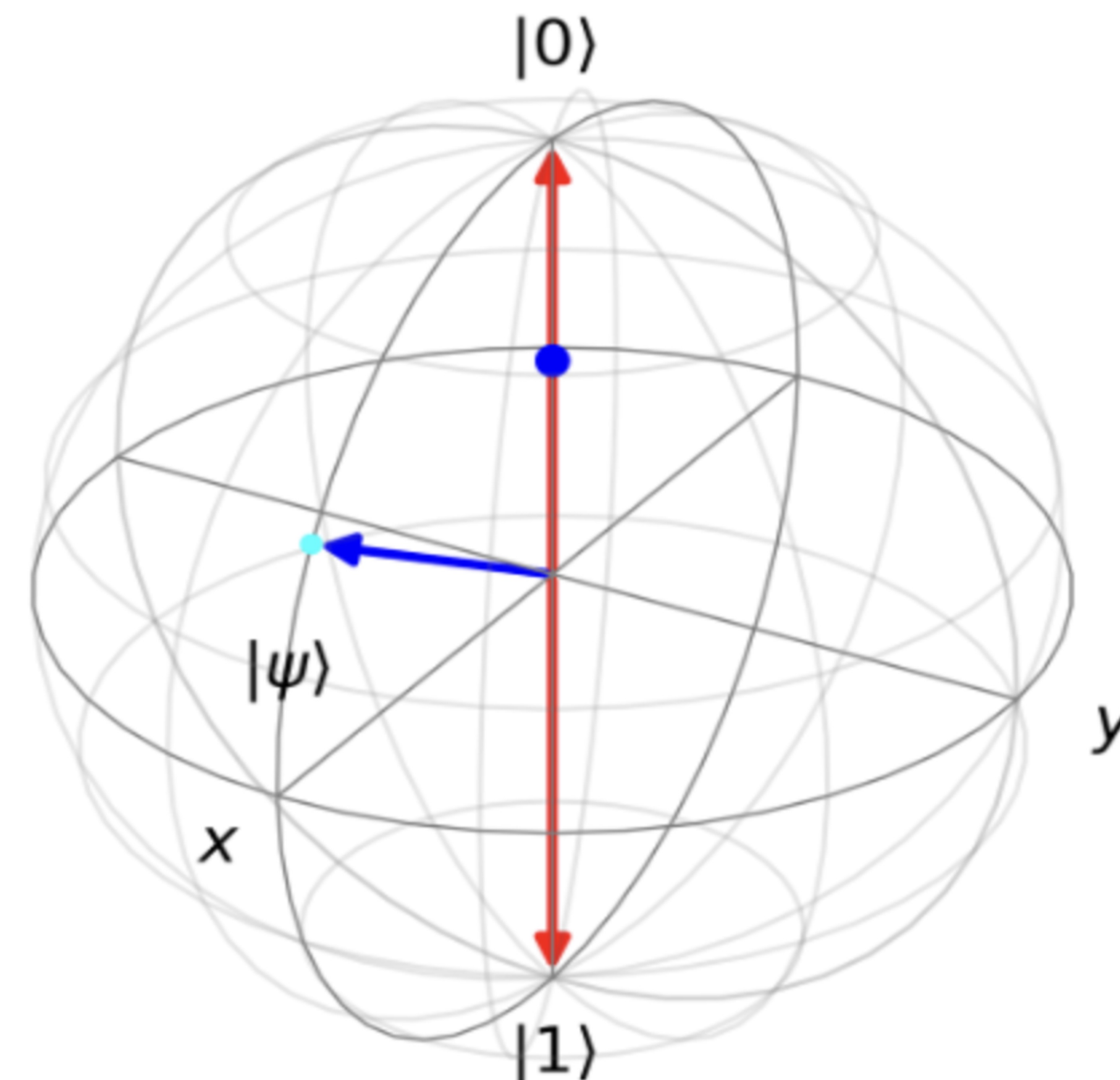
# A Hand-on Introduction to Quantum Computing with NVIDIA's CUDA-Q

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# Classical bit vs. quantum bit



Quantum states  $|0\rangle$  and  $|1\rangle$  form orthonormal basis also called computational basis or canonical basis.

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

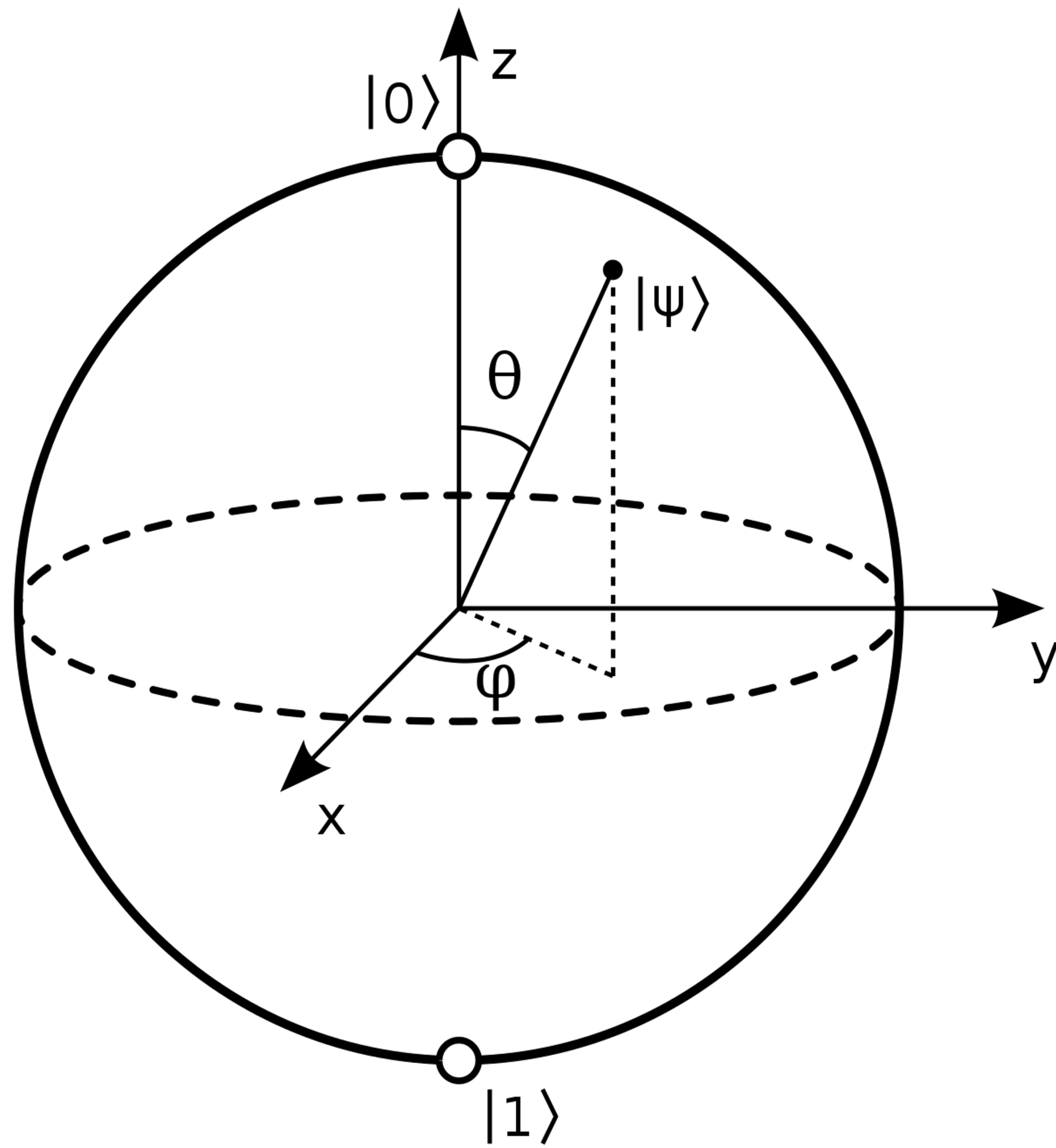
Qubit is a two-dimensional complex vector:

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

- Classical bit can be either  $|0\rangle$  or  $|1\rangle$
- Quantum bit (qubit): can exist in  $|0\rangle$  state,  $|1\rangle$  state, or any state that is a linear combination of  $|0\rangle$  and  $|1\rangle$ . The state of a qubit can be expressed as:

$$|\phi\rangle = \alpha |0\rangle + \beta |1\rangle \quad \text{where } \alpha, \beta \text{ are complex numbers.} \quad \longrightarrow \quad |\alpha|^2 + |\beta|^2 = 1$$

# System of qubits



- Mathematical structure of a qubit generalized to higher dimensional quantum systems.
- The state of any quantum system is a normalized vector (a vector of norm 1) in a complex vector space.
- The joint state of a system of qubits is described using an operation known as the tensor product.

$$|\phi\rangle \otimes |\phi'\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \otimes \begin{pmatrix} \alpha' \\ \beta' \end{pmatrix} = \begin{pmatrix} \alpha\alpha' \\ \alpha\beta' \\ \beta\alpha' \\ \beta\beta' \end{pmatrix}$$

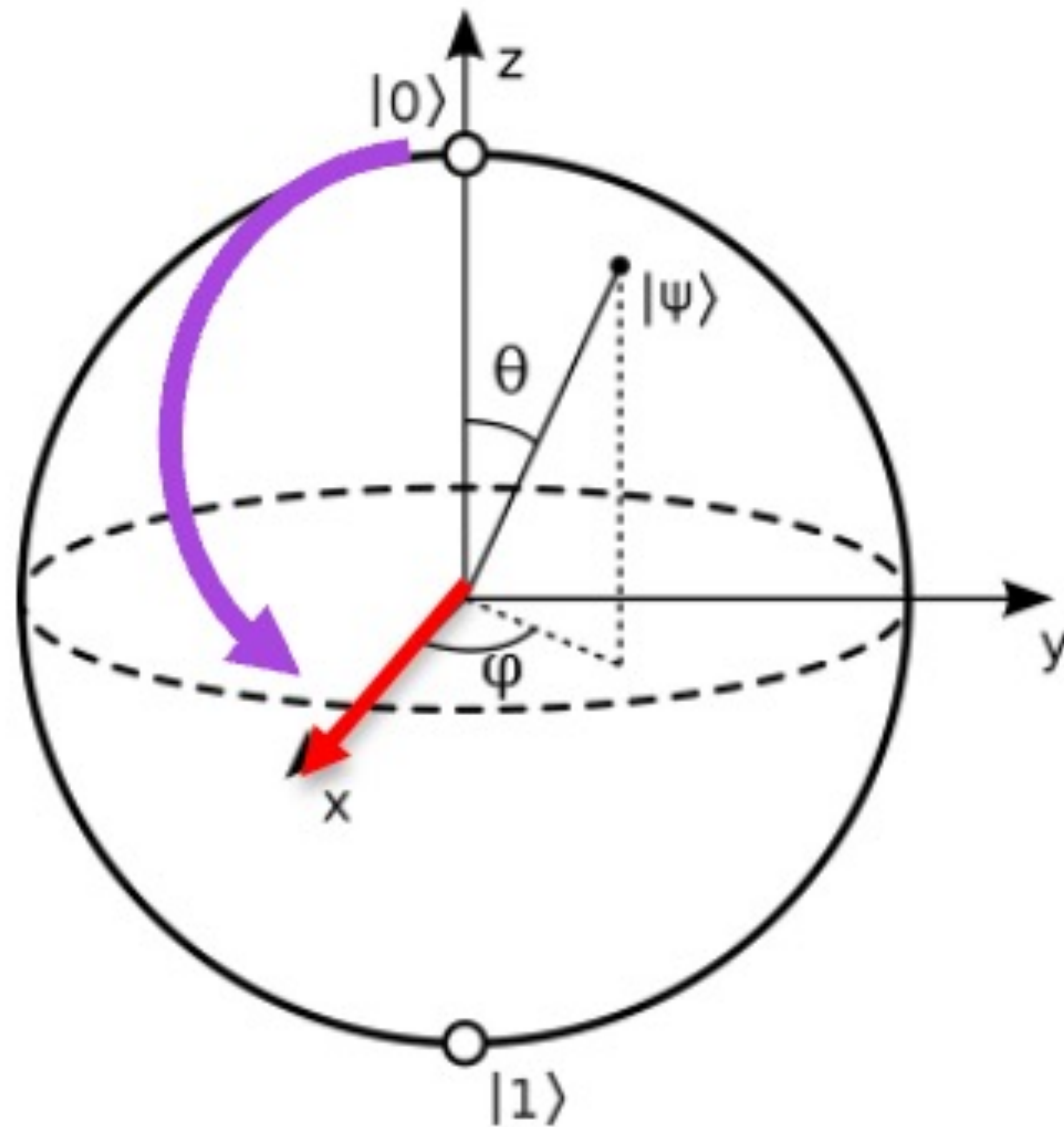
$$|\gamma_1\gamma_2\gamma_3\rangle = |\gamma_1\rangle \otimes |\gamma_2\rangle \otimes |\gamma_3\rangle$$

$$= \alpha_1\alpha_2\alpha_3 |000\rangle + \alpha_1\alpha_2\beta_3 |001\rangle + \alpha_1\beta_2\alpha_3 |010\rangle + \alpha_1\beta_2\beta_3 |011\rangle \\ + \beta_1\alpha_2\alpha_3 |100\rangle + \beta_1\alpha_2\beta_3 |101\rangle + \beta_1\beta_2\alpha_3 |110\rangle + \beta_1\beta_2\beta_3 |111\rangle$$

$$|\gamma_j\rangle = \alpha_j |0\rangle + \beta_j |1\rangle$$



# Superposition and entanglement



- **Superposition:** Any quantum state can be expressed as a linear combination of a few basis state.
- Qubit can be expressed as a linear combination of  $|0\rangle$ ,  $|1\rangle$ . Similarly, the state of any  $n$  qubit system.
- Three qubits: complete state was the tensor product of three different single qubit state.
- **Entanglement:** state cannot be written as a tensor product of states of its individual subsystems.

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

# Inner product and outer product

- **Inner product:** overlap between two quantum state.
- Quantum states are vectors in complex vectors spaces.

$$|\phi\rangle = \alpha |0\rangle + \beta |1\rangle \text{ and } |\psi\rangle = \gamma |0\rangle + \delta |1\rangle$$

$$\langle\psi|\phi\rangle = \gamma^* \alpha + \delta^* \beta, \quad |\phi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad \langle\phi| = (\alpha^* \quad \beta^*)$$

- Overlap of a state with a bit string state will produce the corresponding coefficient.  $\langle 0|\phi\rangle = \alpha$  and  $\langle 1|\phi\rangle = \beta$ .  $\langle 001|\gamma_1\gamma_2\gamma_3\rangle = \alpha_1\alpha_2\beta_3$

- **Outer product** of two states produces a matrix.

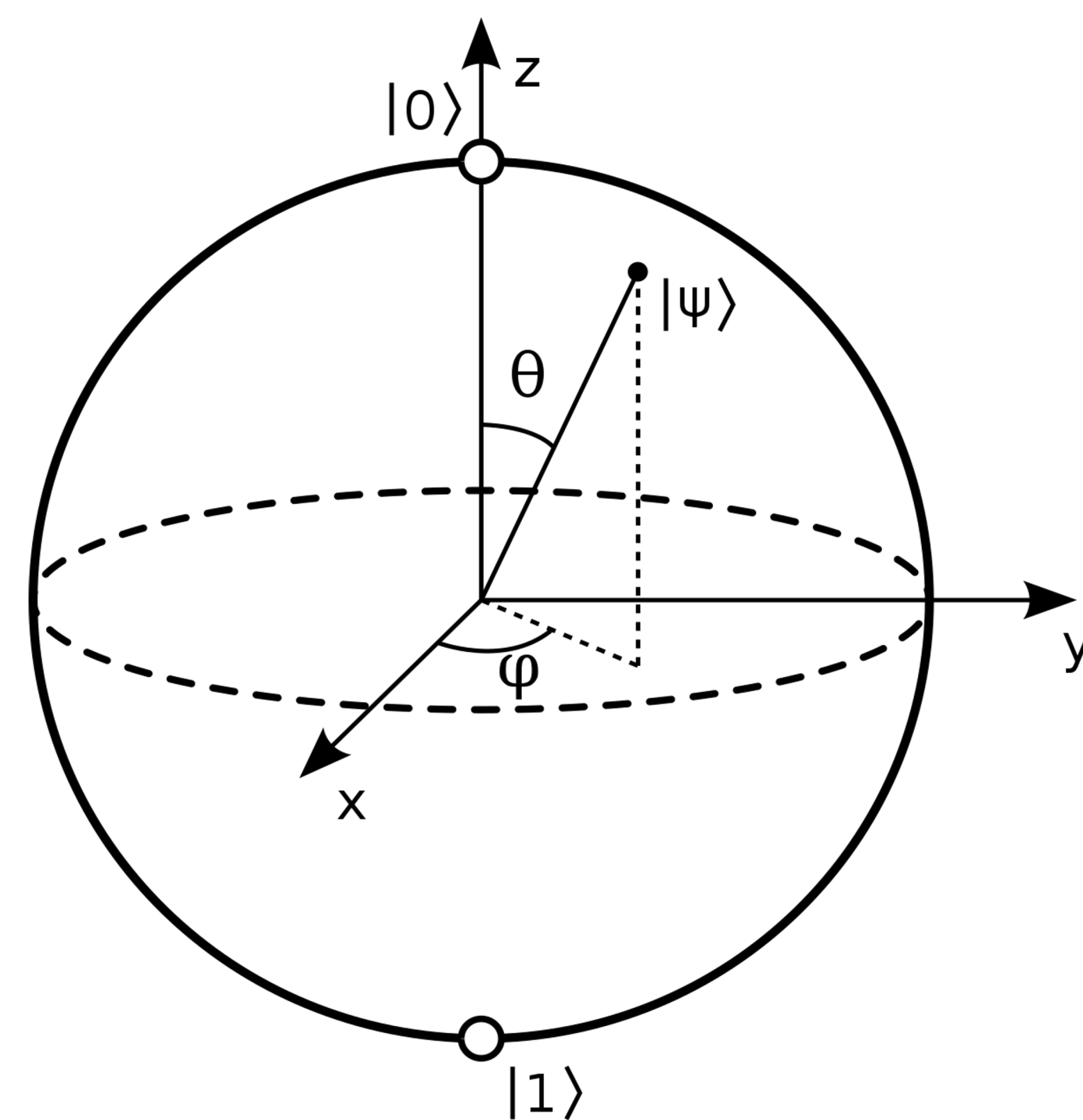
$$|\psi\rangle \langle\phi| = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} (\gamma^* \quad \delta^*) = \begin{pmatrix} \alpha\gamma^* & \alpha\delta^* \\ \beta\gamma^* & \beta\delta^* \end{pmatrix}$$

- Any matrix can be written as a linear combination of outer product between bit-string.

$$A = \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix} = A_{00} |0\rangle \langle 0| + A_{01} |0\rangle \langle 1| + A_{10} |1\rangle \langle 0| + A_{11} |1\rangle \langle 1|$$

- Acting on a state with a matrix: overlap between states

$$\begin{aligned} A|\phi\rangle &= A_{00} |0\rangle \langle 0|\phi\rangle + A_{01} |0\rangle \langle 1|\phi\rangle + A_{10} |1\rangle \langle 0|\phi\rangle + A_{11} |1\rangle \langle 1|\phi\rangle, \\ &= (A_{00}\alpha + A_{01}\beta) |0\rangle + (A_{10}\alpha + A_{11}\beta) |1\rangle = \begin{pmatrix} A_{00}\alpha + A_{01}\beta \\ A_{10}\alpha + A_{11}\beta \end{pmatrix}. \end{aligned}$$

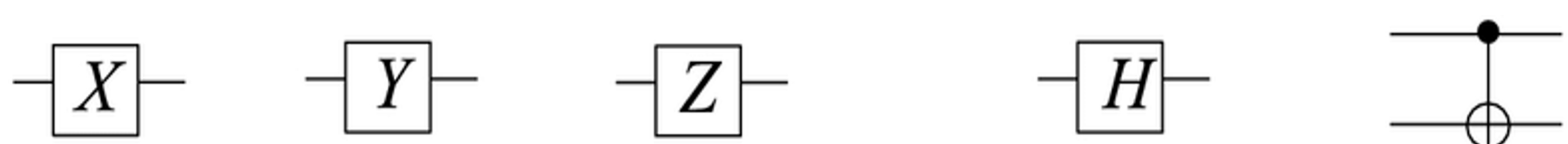


$$|\phi\rangle = \alpha |0\rangle + \beta |1\rangle$$

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$



# Unitary transformation and quantum gates



Quantum circuit diagram showing the following gates in sequence: X, Y, Z, H, and a CNOT gate (control on the top line, target on the bottom line).

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

- Gates are unitary transformation
- Quantum gates are reversible
- Reversible means that the gate's input can always be reconstructed from the gate's output.

- A qubit or a system of qubits changes its state by going through a series of unitary transformation.
- A matrix  $U$  is called unitary if:

$$UU^\dagger = U^\dagger U = I$$

$U^\dagger$   The transposed, complex conjugate of  $U$  (Hermitian operator)

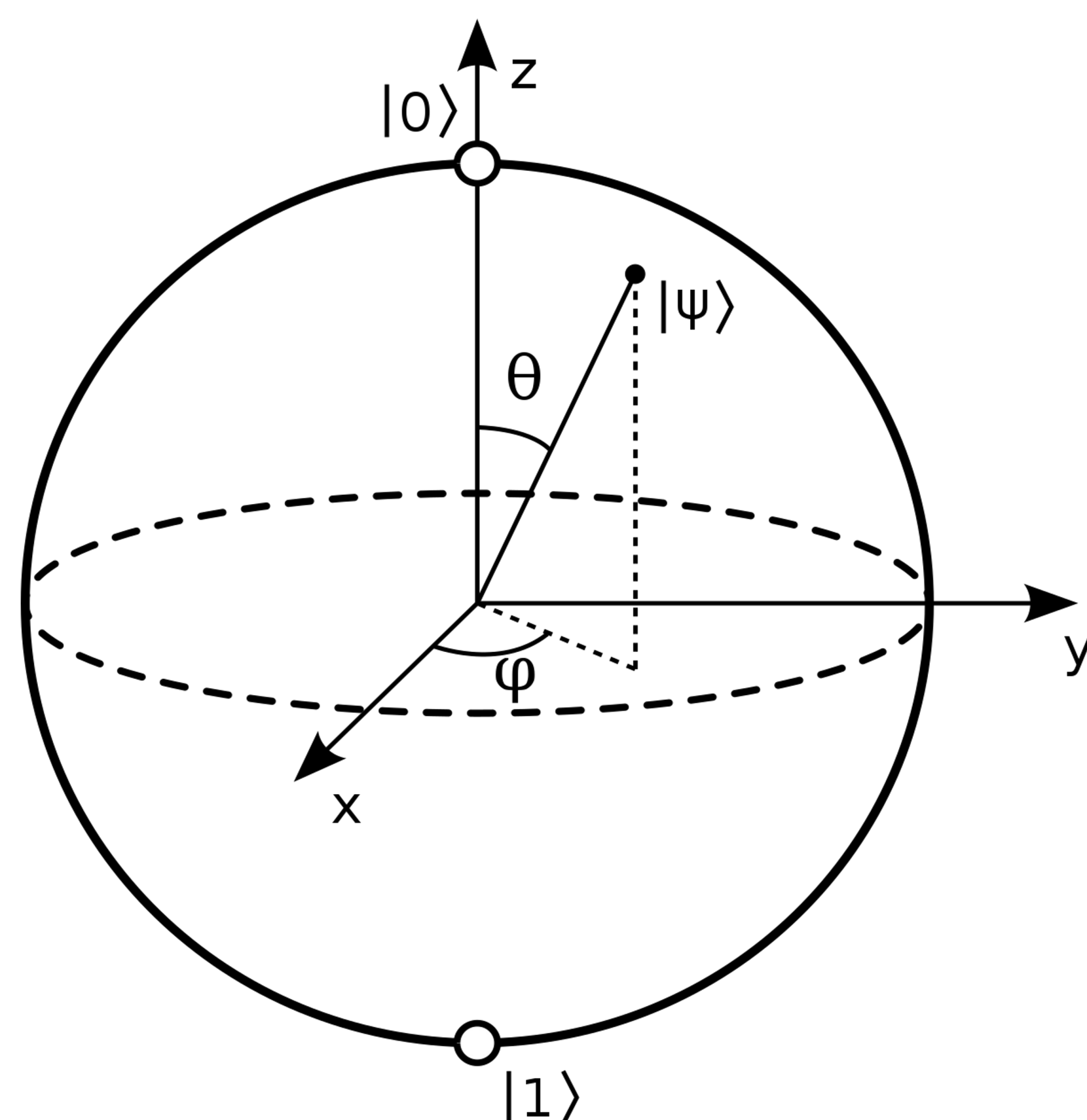
- A qubit state  $|\phi\rangle = \alpha|0\rangle + \beta|1\rangle$  evolves under the action of  $2 \times 2$  matrix  $U$  as

$$|\phi\rangle \rightarrow U|\phi\rangle = \begin{pmatrix} U_{00} & U_{01} \\ U_{10} & U_{11} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} U_{00}\alpha + U_{01}\beta \\ U_{10}\alpha + U_{11}\beta \end{pmatrix}$$

- Operators acting on different qubits can be combined using tensor product.  $U_1 \otimes U_2$

# Measurement in computational basis

- Measurement corresponds to transforming the quantum information into classical information.
- Measuring a qubit typically corresponds to reading out a classical bit.



$$|\phi\rangle = \alpha |0\rangle + \beta |1\rangle$$

- The probability of obtaining  $|0\rangle$  after measurement is  $|\langle 0|\phi\rangle|^2$
- The probability of obtaining  $|1\rangle$  after measurement is  $|\langle 1|\phi\rangle|^2$
- Measurement can be represented as the squared absolute values of overlaps.
- A central principle of quantum mechanics is that measurement outcomes are probabilistic.
- Generalizing: the probability of getting the bit string  $|x_1 \dots x_n\rangle$

after measuring an n qubit state  $|\phi\rangle$  is then  $|\langle x_1 \dots x_n|\phi\rangle|^2$

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle) \longrightarrow \text{Probability is 0.5}$$

# Sampling

- . Quantum mechanics is inherently probabilistic in nature.
- . Running the quantum circuit repeatedly and measuring the qubits at the end of the computation.
- . The result is a classical bitstring, where each bit represents the outcome of measuring a qubit.
- . Provides the distribution of possible measurement outcomes.



## Observable and expectation values

$$\langle \phi | Z | \phi \rangle = \langle \phi | 0 \rangle \langle 0 | \phi \rangle - \langle \phi | 1 \rangle \langle 1 | \phi \rangle = |\alpha|^2 - |\beta|^2$$

$$|\phi\rangle = \alpha |0\rangle + \beta |1\rangle \quad Z = |0\rangle \langle 0| - |1\rangle \langle 1| = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$Z$  operator is called the observable. And the quantity  $\langle \phi | Z | \phi \rangle$  is called its expectation value.

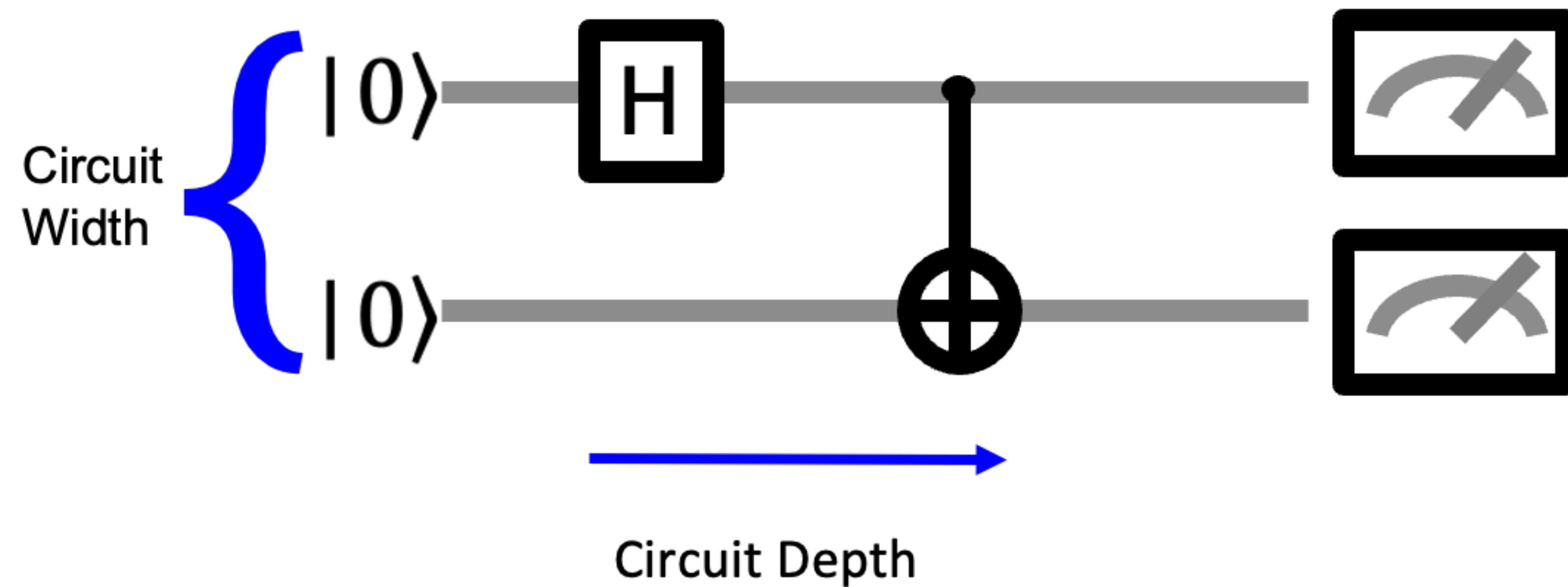
$$O \equiv \sum_i a_i |\Phi_i\rangle \langle \Phi_i|, \quad \langle \psi | O | \psi \rangle = \sum_i a_i \langle \psi | \Phi_i \rangle \langle \Phi_i | \psi \rangle = \sum_i a_i |\langle \Phi_i | \psi \rangle|^2$$

$O$  is called Hermitian operator. These operators are equal to their Hermitian conjugates ( $O = O^\dagger$ ).

In quantum mechanics, any Hermitian operator is a valid observable.

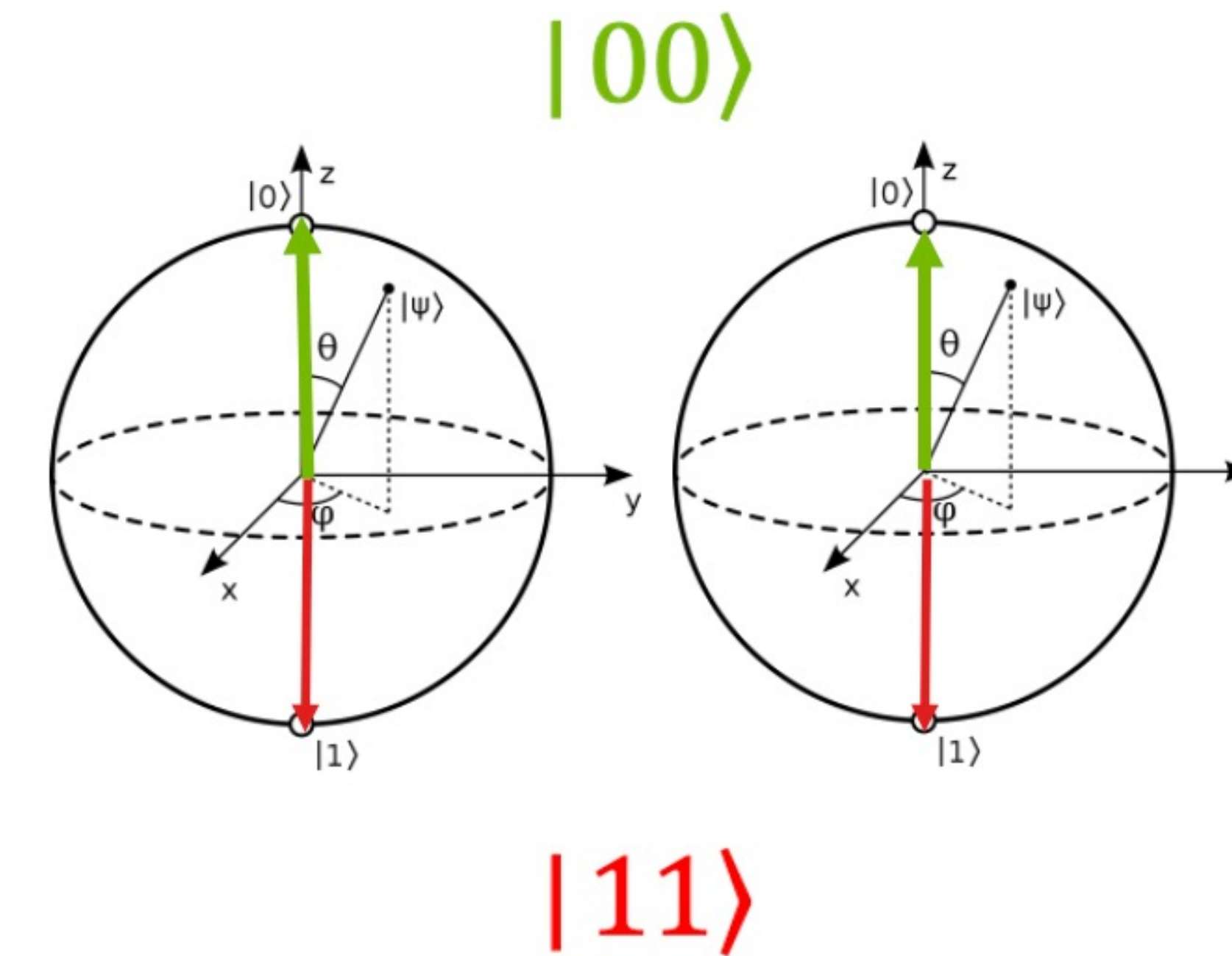


# Quantum circuit



Hadamard Gate:  
 $\text{Had}|0\rangle = |0\rangle + |1\rangle$   
 $\text{Had}|1\rangle = |0\rangle - |1\rangle$

CNOT Gate:  
 $\text{CNOT}|10\rangle = |11\rangle$   
 $\text{CNOT}|11\rangle = |10\rangle$



$$\text{CNOT}_{12} (H \otimes I) |00\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle).$$

$$H \otimes I |00\rangle = (H |0\rangle) \otimes (I |0\rangle) = \left( \frac{|0\rangle + |1\rangle}{\sqrt{2}} \right) \otimes |0\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |10\rangle)$$

$$\text{CNOT}_{12} \left( \frac{1}{\sqrt{2}} (|00\rangle + |10\rangle) \right) = \frac{1}{\sqrt{2}} (\text{CNOT}_{12} |00\rangle + \text{CNOT}_{12} |10\rangle) = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$$



# No-cloning theorem

No-cloning theorem: copying of state is prohibited.

$$U |\varphi\rangle |0\rangle = |\varphi\rangle |\varphi\rangle, \quad U |\phi\rangle |0\rangle = |\phi\rangle |\phi\rangle$$

It follows from linearity that

$$U (a |\varphi\rangle + b |\phi\rangle) |0\rangle = a U |\varphi\rangle |0\rangle + b U |\phi\rangle |0\rangle = a |\varphi\rangle |\varphi\rangle + b |\phi\rangle |\phi\rangle$$

But if U cloned arbitrary inputs, we would have

$$\begin{aligned} U(a |\varphi\rangle + b |\phi\rangle) |0\rangle &= (a |\varphi\rangle + b |\phi\rangle)(a |\varphi\rangle + b |\phi\rangle) \\ &= a^2 |\varphi\rangle |\varphi\rangle + b^2 |\phi\rangle |\phi\rangle + ab |\varphi\rangle |\phi\rangle + ba |\phi\rangle |\varphi\rangle \end{aligned}$$





To jupyter notebook