

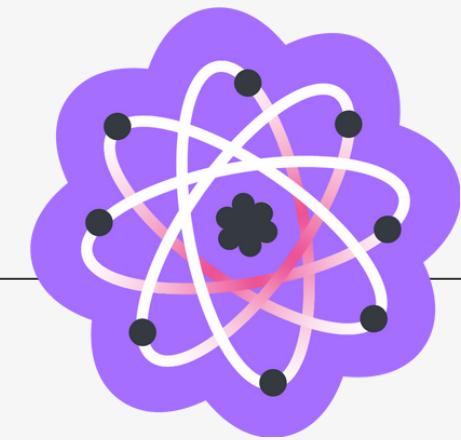


Quantum Fall Festival @ Yonsei University

Basics of Quantum Informatics

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Hamiltonian &
Unitary

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04

Superposition &
Entanglement



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01. Hamiltonian & Unitary

What is hamiltonian?

Hamiltonian

What is Unitary?

Observable

Unitary

Hermitian

01. Hamiltonian & Unitary

1) Hamiltonian

- Def

해밀토니언(Hamiltonian, \hat{H} 또는 H 로 표기)은 양자 상태의 시간 변화를 생성하는 [에르미트](#) 연산자이다.

이는 고전 [해밀턴 역학](#)에서 [해밀토니언을 양자화](#)하여 얻을 수 있고, 고전적인 [에너지](#)를 나타낸다.

- Hermitian
(self-adjoint)

$$\hat{H} = \hat{H}^\dagger$$

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

01. Hamiltonian & Unitary

2) Observable

- Def

$$\hat{H} = \hat{H}^\dagger \quad \hat{H}|\Psi\rangle = E|\Psi\rangle$$

In physics, an **observable** is a **physical property** or **physical quantity** that can be **measured**. In **classical mechanics**, an observable is a **real-valued** "function" on the set of all possible system states, e.g., **position** and **momentum**. In **quantum mechanics**, an observable is an **operator**, or **gauge**, where the property of the **quantum state** can be determined by some sequence of **operations**. For example, these operations might involve submitting the system to various **electromagnetic fields** and eventually reading a value.

01. Hamiltonian & Unitary

2) Observable

- cf)

$$\hat{H} = \hat{H}^\dagger \quad \hat{H}|\Psi\rangle = E|\Psi\rangle$$

Problem 2.1 Prove the following three theorems:

- (a) For normalizable solutions, the separation constant E must be *real*. Hint: Write E (in Equation 2.7) as $E_0 + i\Gamma$ (with E_0 and Γ real), and show that if Equation 1.20 is to hold for all t , Γ must be zero.

$$\Psi(x, t) = \psi(x)e^{-iEt/\hbar},$$

$$\int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx = 1.$$



01. Hamiltonian & Unitary

3) Hermitian

- Def

$$\hat{H} = \hat{H}^\dagger$$

- Real eigenvalue

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

$$\begin{aligned} E &= \langle \Phi | \hat{H} | \Phi \rangle = (\langle \Phi | \hat{H}) | \Phi \rangle \\ &= (\hat{H} | \Phi \rangle)^\dagger | \Phi \rangle \\ &= \langle \Phi | \bar{E} | \Phi \rangle = \bar{E} \end{aligned}$$

01. Hamiltonian & Unitary

4) Unitary

- Def

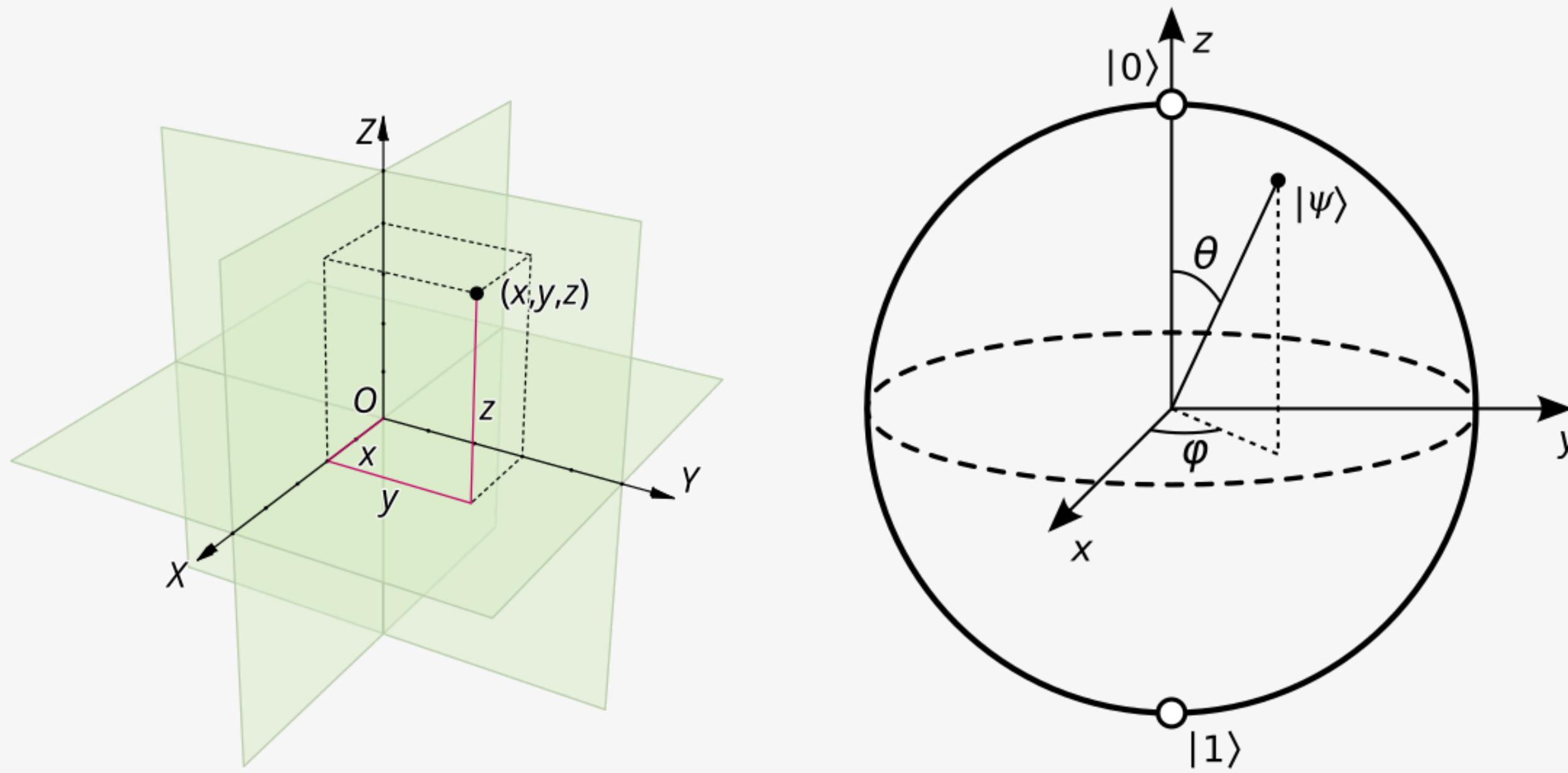
$$\hat{U}\hat{U}^\dagger = I \quad \hat{U}^\dagger = \hat{U}^{-1}$$

Problem 6.2 Show that, for a Hermitian operator \hat{Q} , the operator $\hat{U} = \exp[i\hat{Q}]$ is unitary.

Hint: First you need to prove that the adjoint is given by $\hat{U}^\dagger = \exp[-i\hat{Q}]$; then prove that $\hat{U}^\dagger \hat{U} = 1$. Problem 3.5 may help.

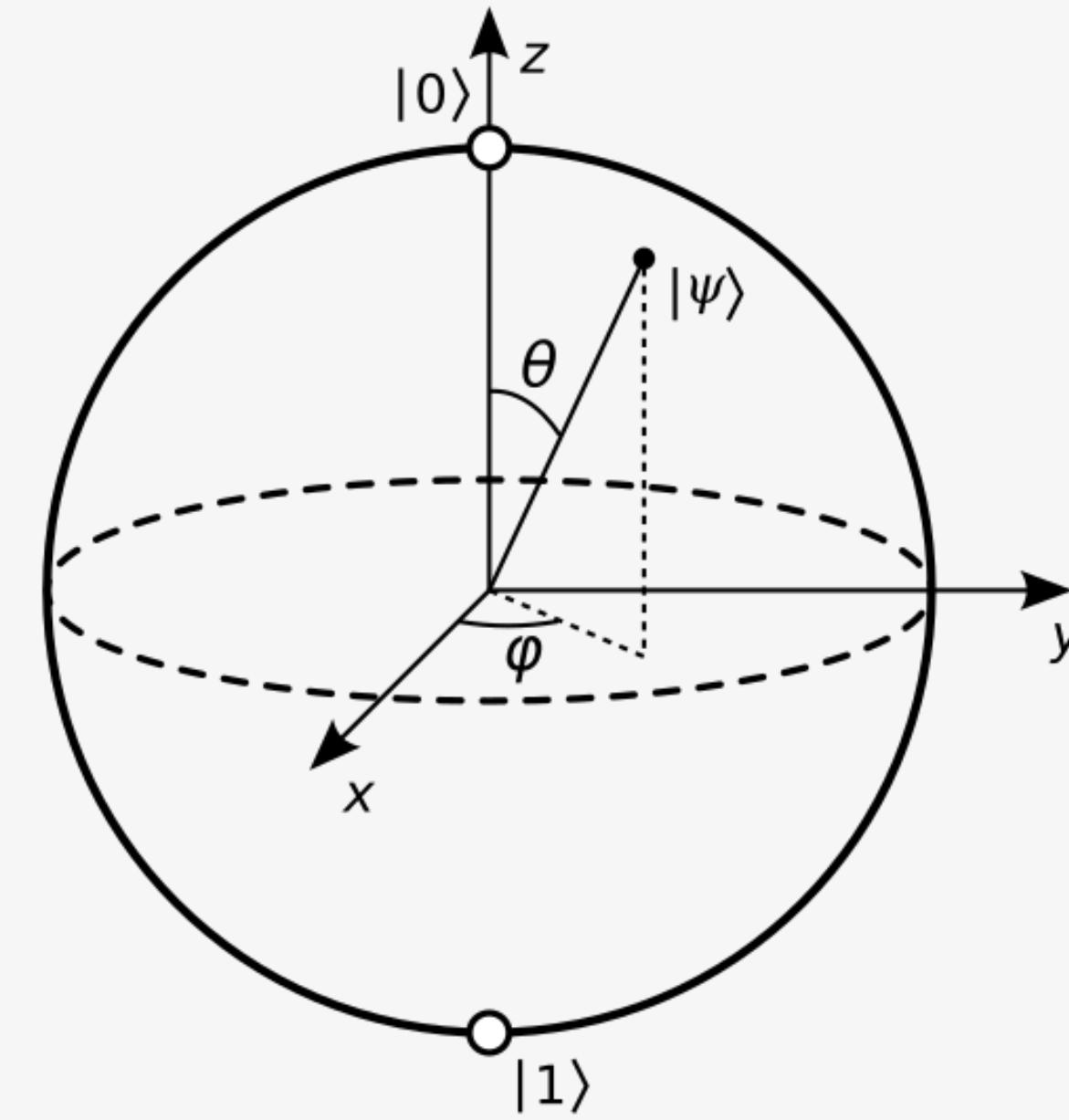
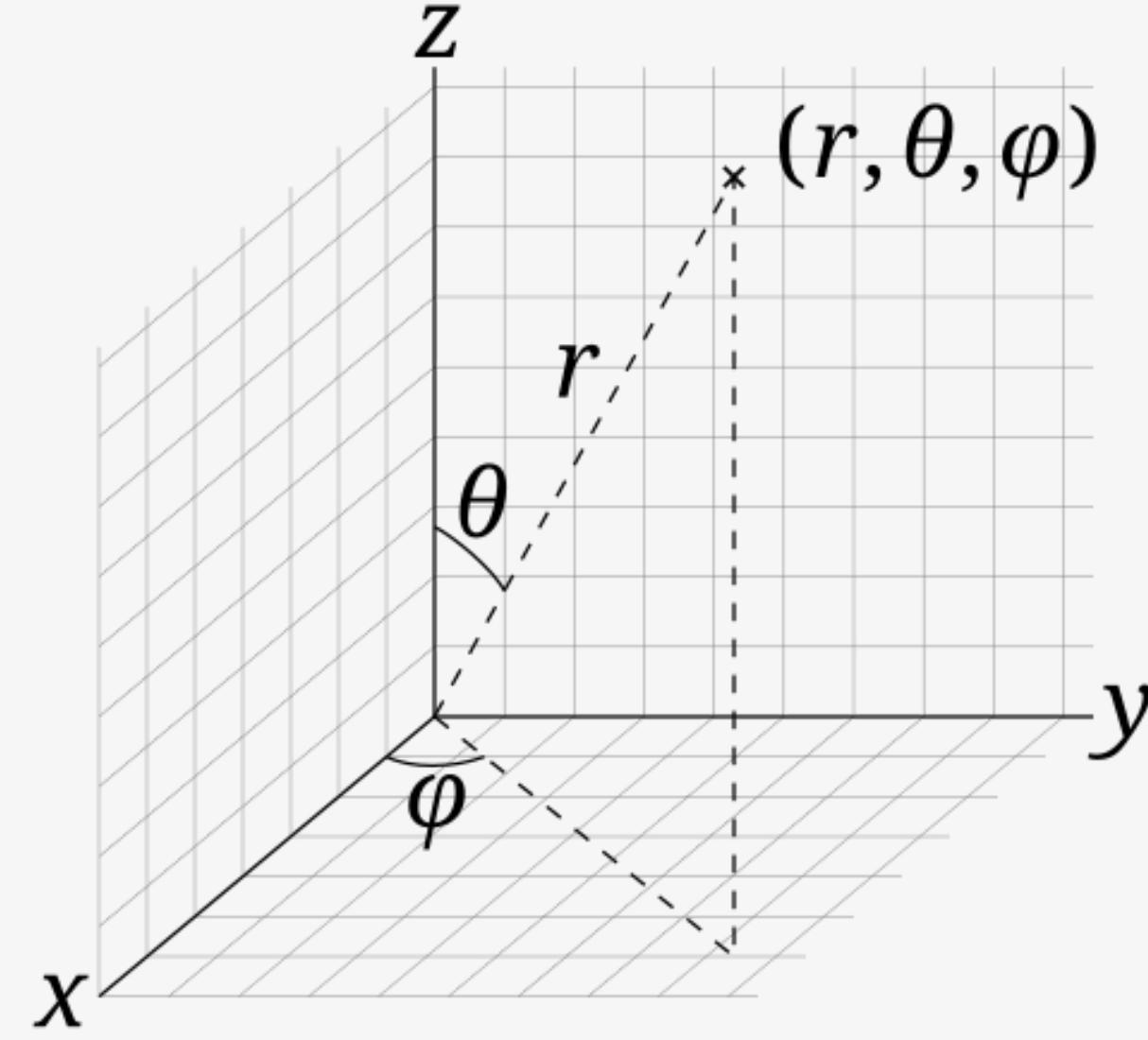
02. Bloch sphere

1) Cartesian Coord. vs. Bloch sphere



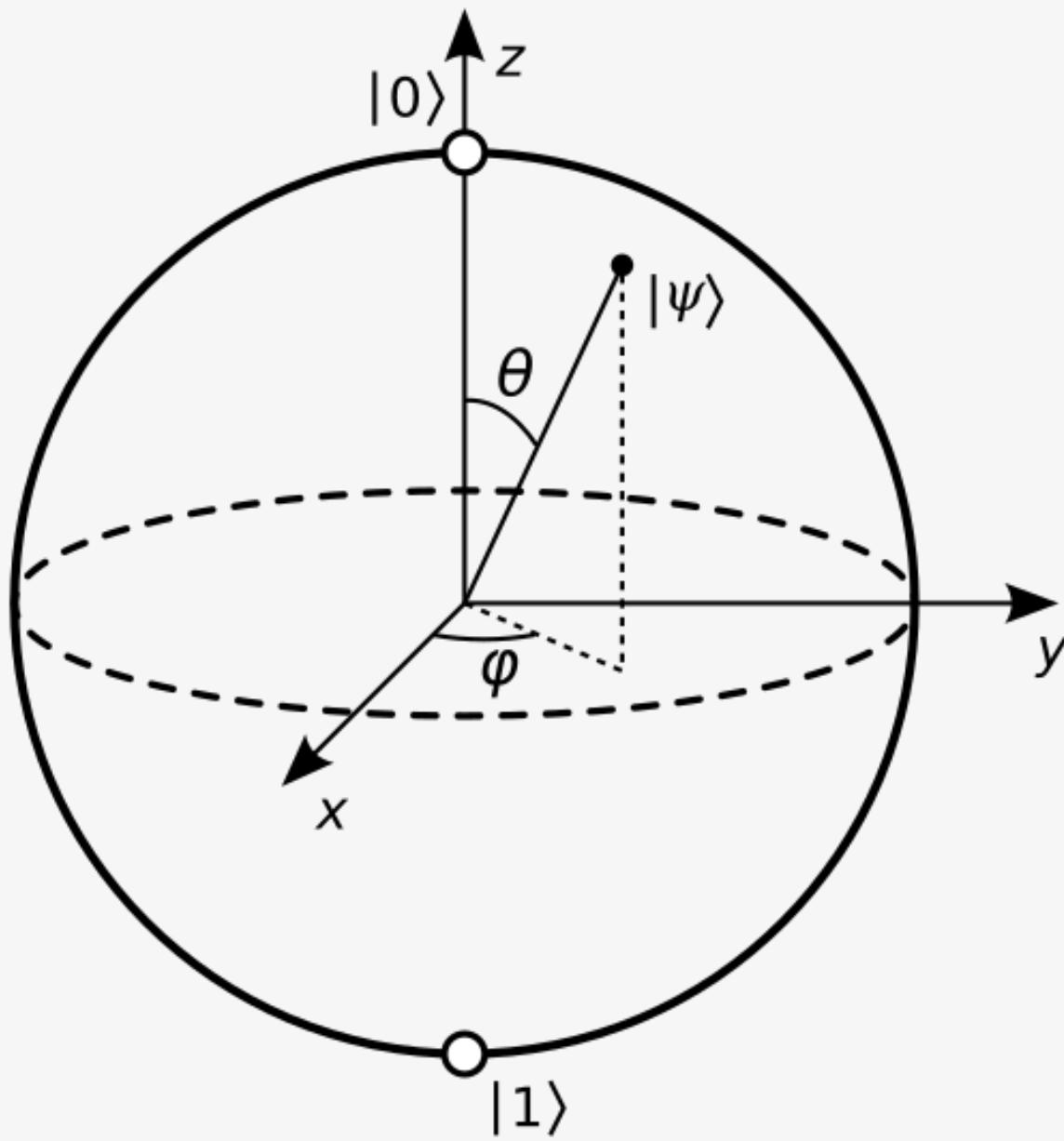
02. Bloch sphere

2) Spherical Coord. vs. Bloch sphere



02. Bloch sphere

3) Bloch sphere



z-axis

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

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

y-axis

$$|+i\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} = \frac{|0\rangle + i|1\rangle}{\sqrt{2}}$$

$$|-i\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix} = \frac{|0\rangle - i|1\rangle}{\sqrt{2}}$$

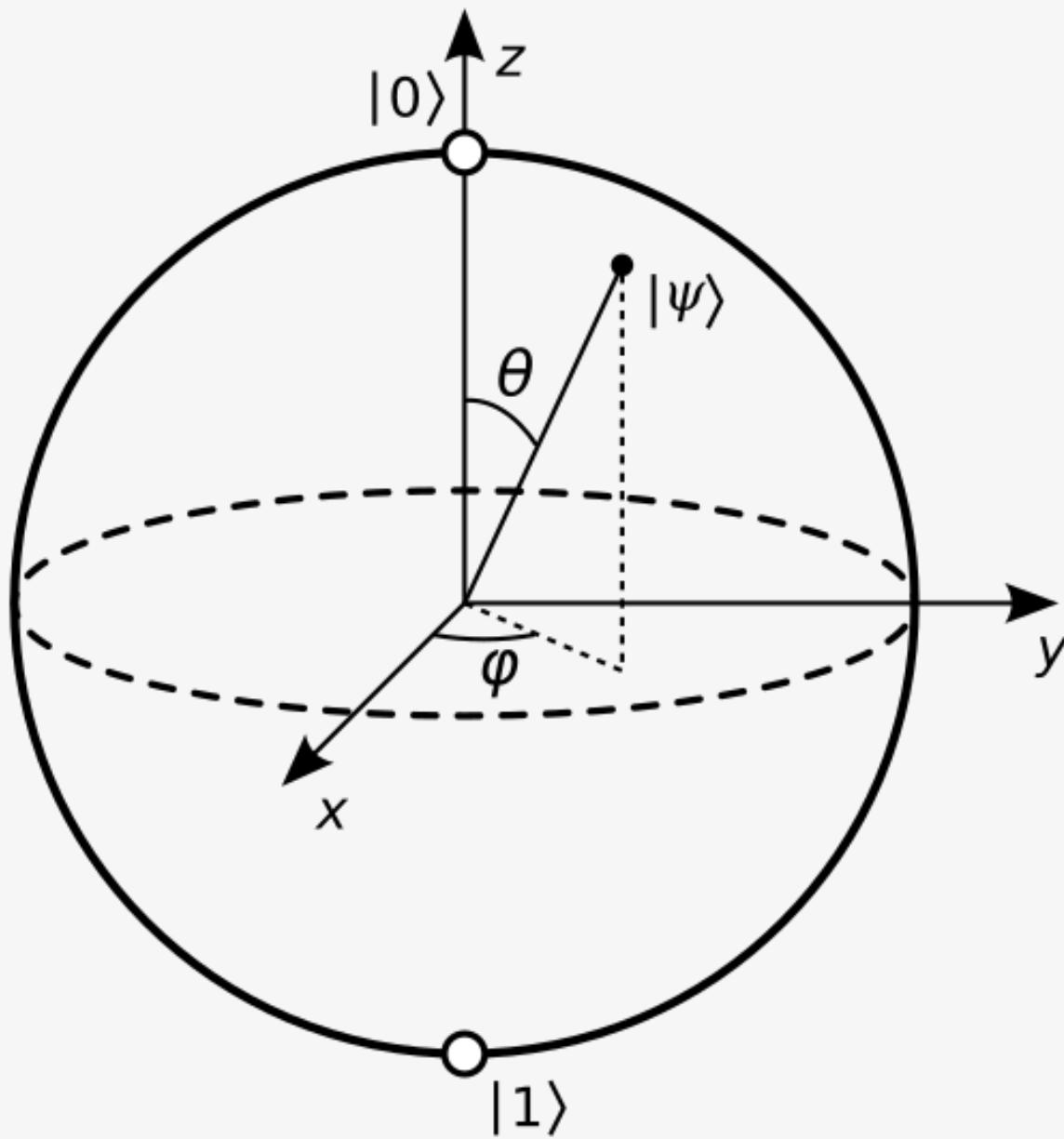
x-axis

$$|+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

$$|-\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

02. Bloch sphere

3) Bloch sphere (cont.)



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

$$|\psi\rangle = \cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle \text{ (surface-pure)}$$

$$\rho = \frac{1}{2}(I + \vec{a} \cdot \vec{\sigma}) = \begin{bmatrix} 1 + a_z & a_x - ia_y \\ a_x + ia_y & 1 - a_z \end{bmatrix} \text{ (inside-mixed)}$$

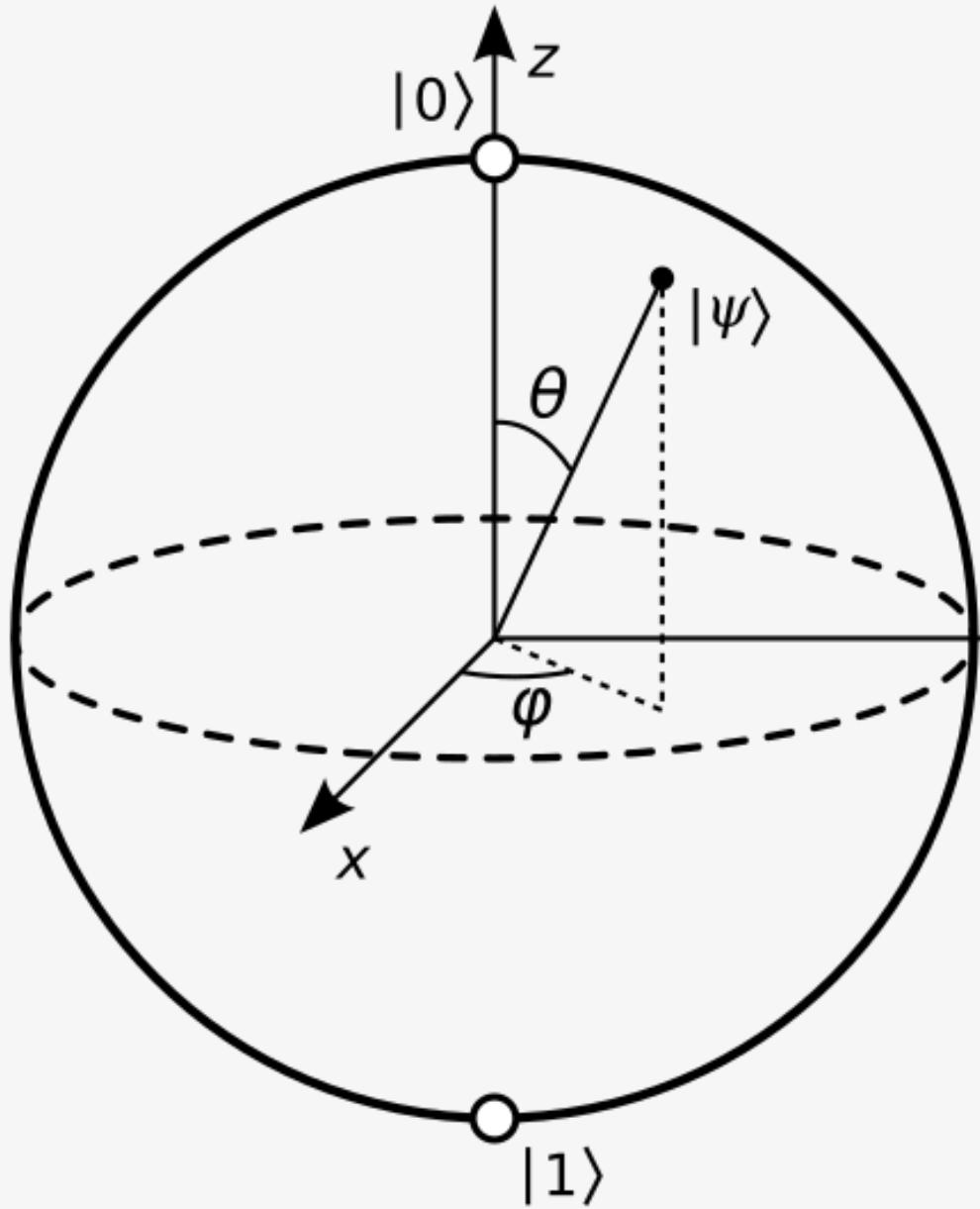
cf) Pauli matrix

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$



02. Bloch sphere

3) Bloch sphere (cont.)



rotation

$$R_x(\theta) = e^{-i\frac{\theta}{2}\sigma_x} = \begin{bmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{bmatrix}$$

$$R_y(\theta) = e^{-i\frac{\theta}{2}\sigma_y} = \begin{bmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{bmatrix}$$

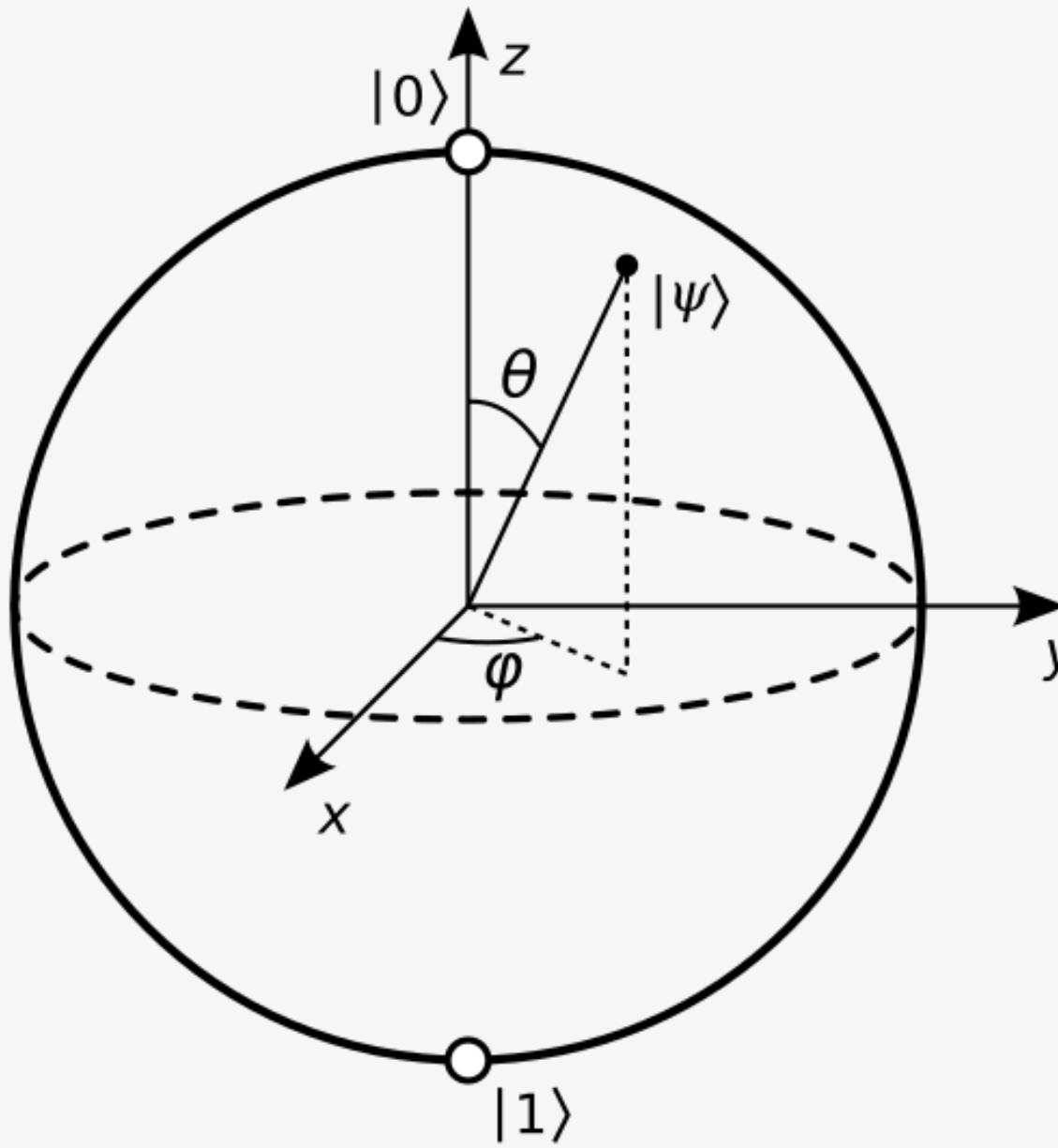
$$R_z(\theta) = e^{-i\frac{\theta}{2}\sigma_z} = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}$$

$$R_{\hat{n}}(\theta) = e^{-i\frac{\theta}{2}\hat{n}\cdot\vec{\sigma}} = \cos(\theta/2) - i\sin(\theta/2)\hat{n}\cdot\vec{\sigma}$$



02. Bloch sphere

cf) Taylor expansion



$$\text{ex)} \quad R_x(\theta) = e^{-i\frac{\theta}{2}\sigma_x} = \begin{bmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{bmatrix}$$

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_x^2 = I \quad e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

$$e^{-i\frac{\theta}{2}\sigma_x} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-i \frac{1}{2} \theta \right)^n \sigma_x^n$$

$$e^{-i\frac{\theta}{2}\sigma_x} = \begin{bmatrix} 1 - \frac{1}{2!} \left(\frac{\theta}{2} \right)^2 + \frac{1}{4!} \left(\frac{\theta}{2} \right)^4 + \dots & -i \left(\frac{\theta}{2} \right) + i \frac{1}{3!} \left(\frac{\theta}{2} \right)^3 + \dots \\ -i \left(\frac{\theta}{2} \right) + i \frac{1}{3!} \left(\frac{\theta}{2} \right)^3 + \dots & 1 - \frac{1}{2!} \left(\frac{\theta}{2} \right)^2 + \frac{1}{4!} \left(\frac{\theta}{2} \right)^4 + \dots \end{bmatrix}$$



03. Qubits & Gates

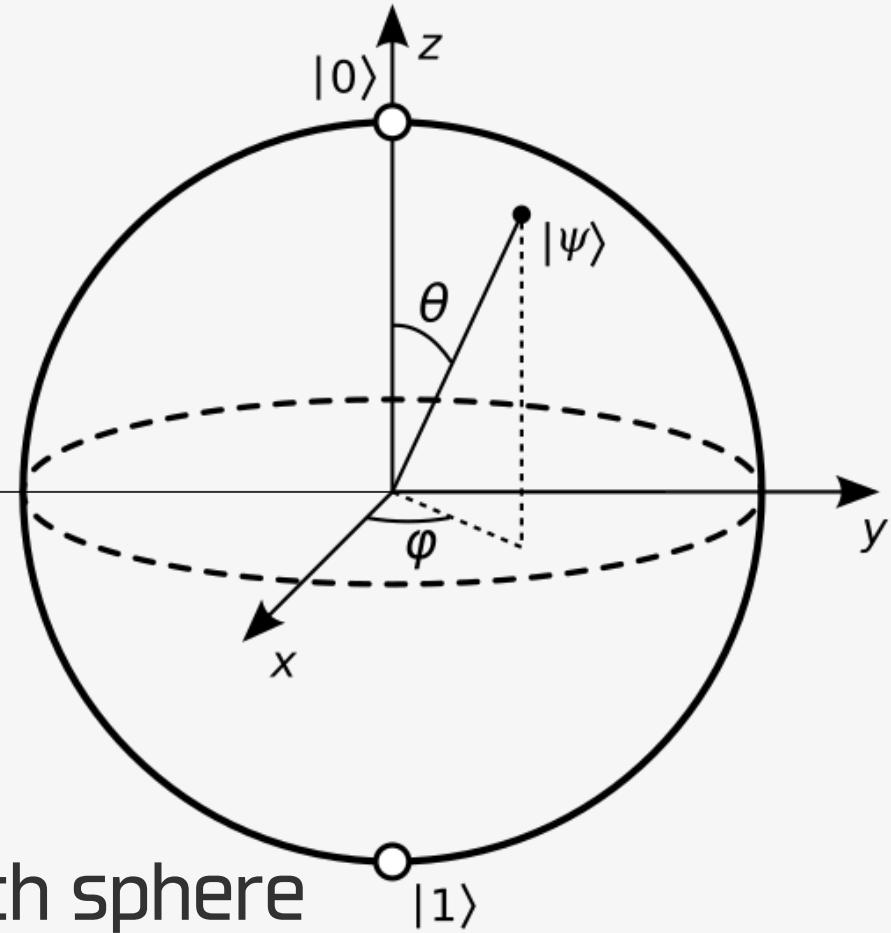
1) Clbits vs. Qubits

- Binary Digits
- Represent true/false, on/off, normal/abnormal, etc.
- (exclusive state).

$$\Sigma = \{0, 1\}^n$$

- Quantum state on Bloch sphere
- Complex

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



03. Qubits & Gates

2) Logic gate vs. Quantum Logic gate

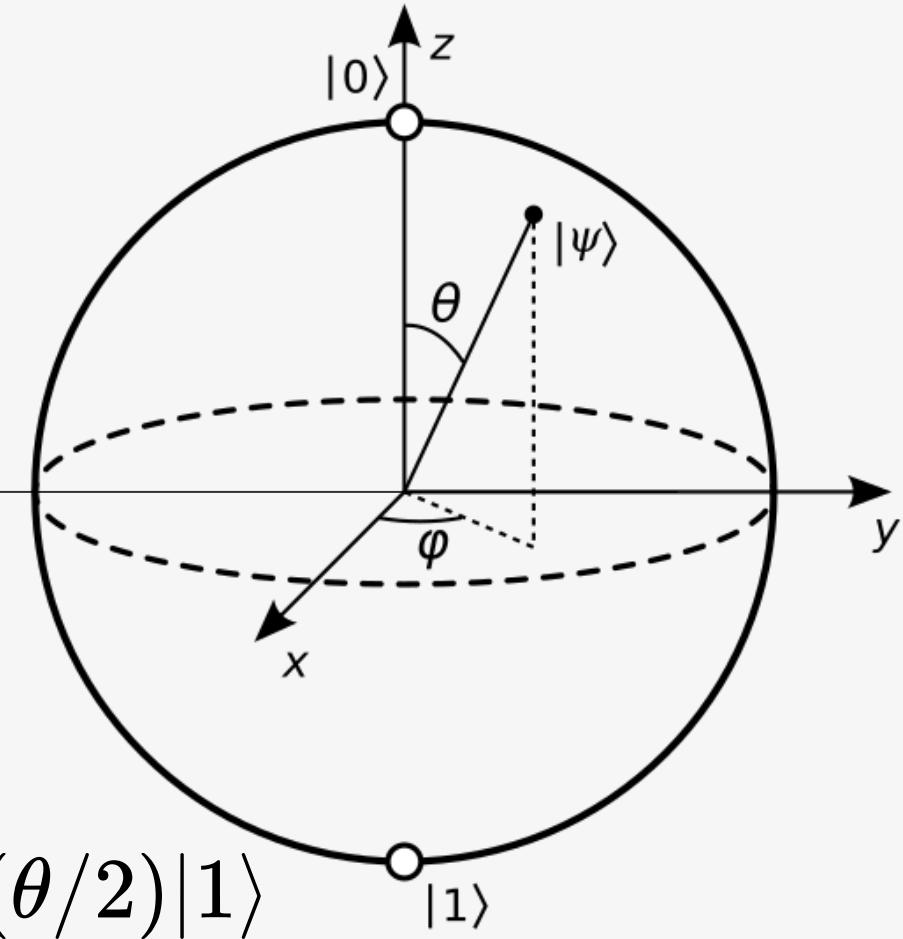
$$\Sigma = \{0, 1\}^n$$

- Logic gates(and, or, nand, nor, ...)



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

- Universal gate set
- Clifford set({CNOT, H, S}) + T-gate
- Rotation + CNOT
- Toffoli + H



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03. Qubits & Gates

3) Quantum Logic gate (1-qubit)

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

- Hadamard

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

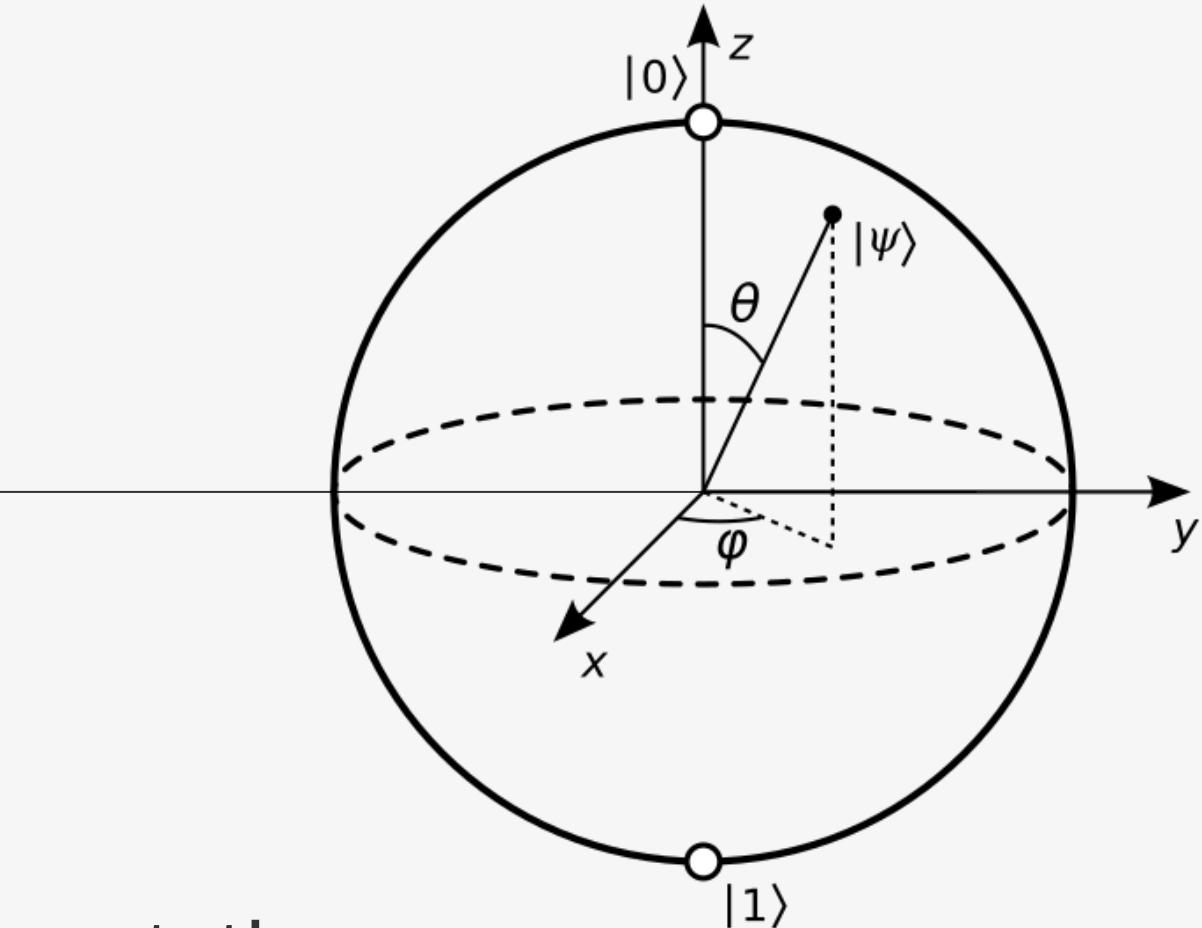
- Phase

$$P(\phi) = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix} = e^{-i\frac{\phi}{2}} \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix} = -iR_z(\phi)$$

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = P(\pi)$$

$$S = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{2}} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix} = P\left(\frac{\pi}{2}\right)$$

$$T = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{bmatrix} = P\left(\frac{\pi}{4}\right)$$



- rotation

$$R_{\hat{n}}(\theta) = e^{-i\frac{\theta}{2}\hat{n}\cdot\vec{\sigma}} = \cos(\theta/2) - i \sin(\theta/2)\hat{n}\cdot\vec{\sigma}$$

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = iR_x(\pi)$$

$$Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = iR_y(\pi)$$



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03. Qubits & Gates

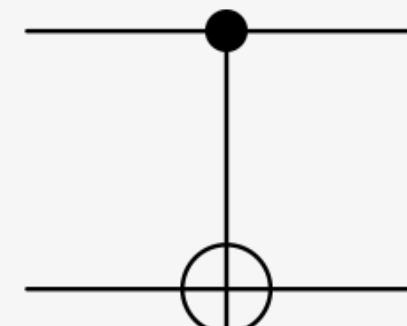
3) Quantum Logic gate (2-qubit)

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

- CNOT(CX)

$$\begin{aligned} CNOT|a\rangle|b\rangle &= |a\rangle|a \oplus b\rangle \\ CNOT &= |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes X \end{aligned}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

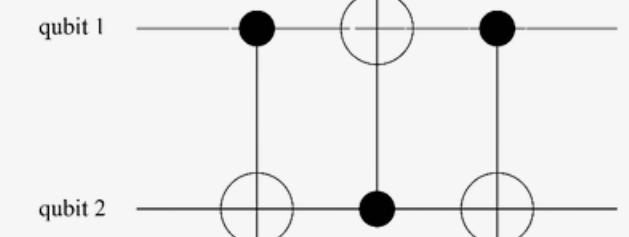
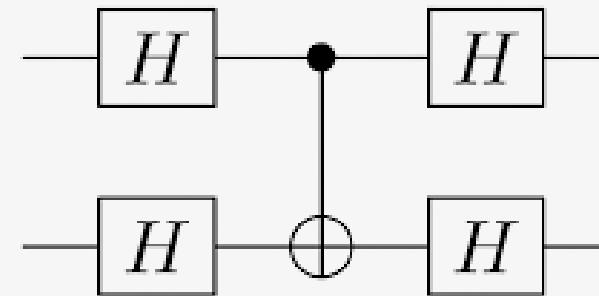
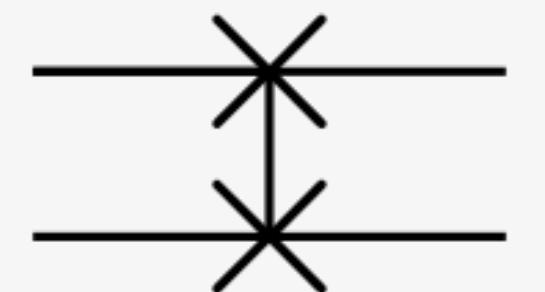


- SWAP

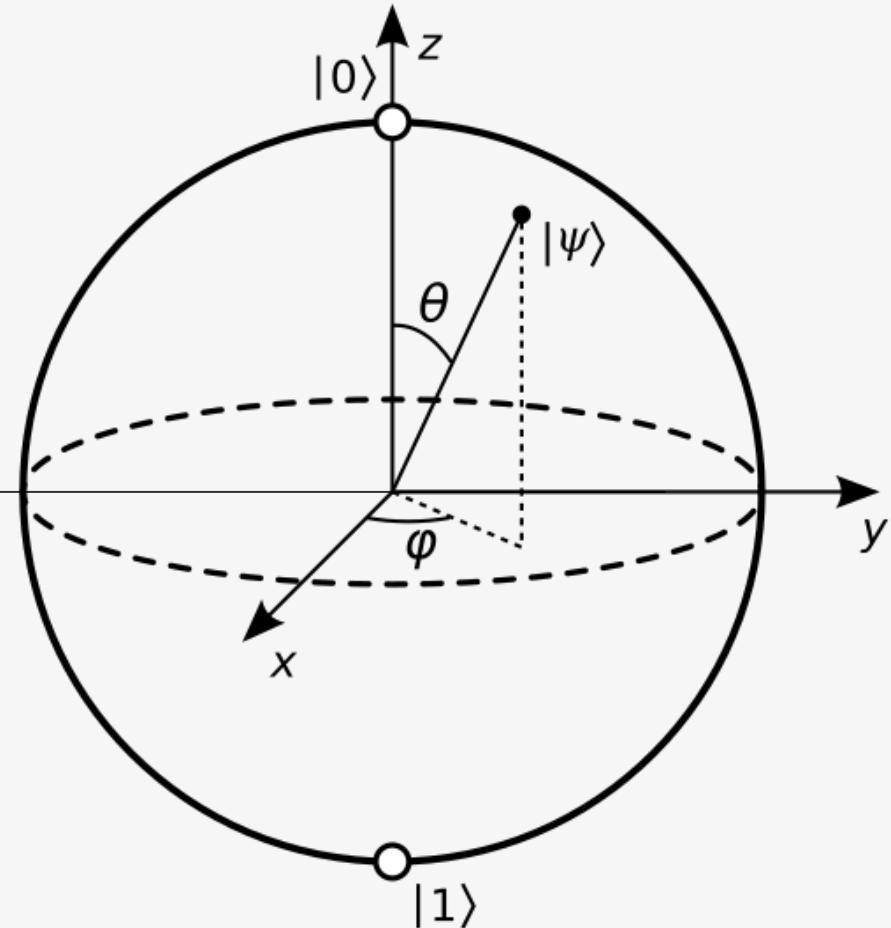
$$\begin{aligned} SWAP|a\rangle|b\rangle &= |b\rangle|a\rangle \\ SWAP &= |0\rangle\langle 0| \otimes |0\rangle\langle 0| + \end{aligned}$$

$$\begin{aligned} &|0\rangle\langle 1| \otimes |1\rangle\langle 0| + \\ &|1\rangle\langle 0| \otimes |0\rangle\langle 1| + \\ &|1\rangle\langle 1| \otimes |1\rangle\langle 1| \end{aligned}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$



$$= \begin{array}{c} \text{circle with cross inside} \\ \text{---} \\ \text{black dot} \end{array}$$



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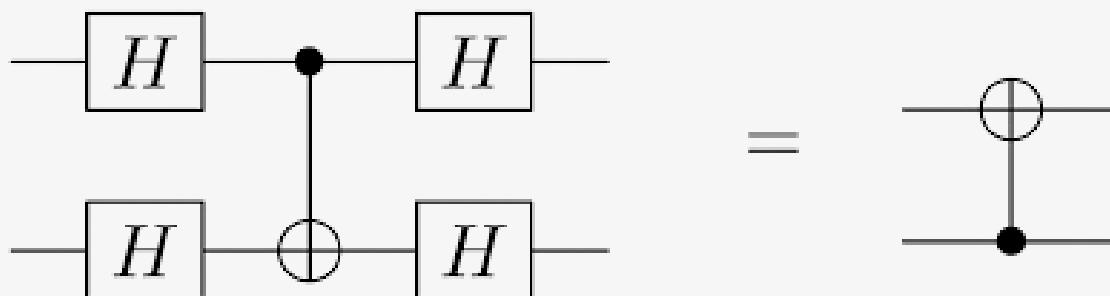
03. Qubits & Gates

cf) Sylvester's construction

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

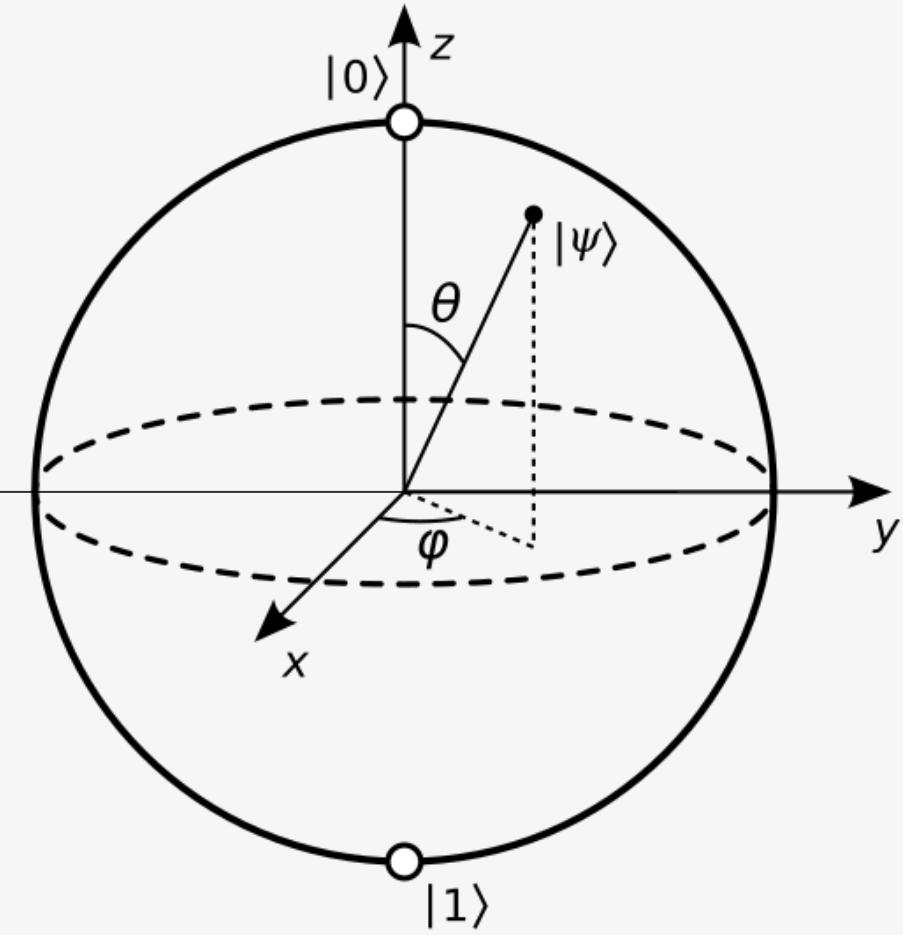
$$CNOT = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes X$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$



$$H_{2^k} = H_2 \otimes H_{2^{k-1}}$$

$$H_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \rightarrow H_4 = \frac{1}{\sqrt{2}} \begin{bmatrix} H_2 & H_2 \\ H_2 & -H_2 \end{bmatrix} = H_2 \otimes H_2$$

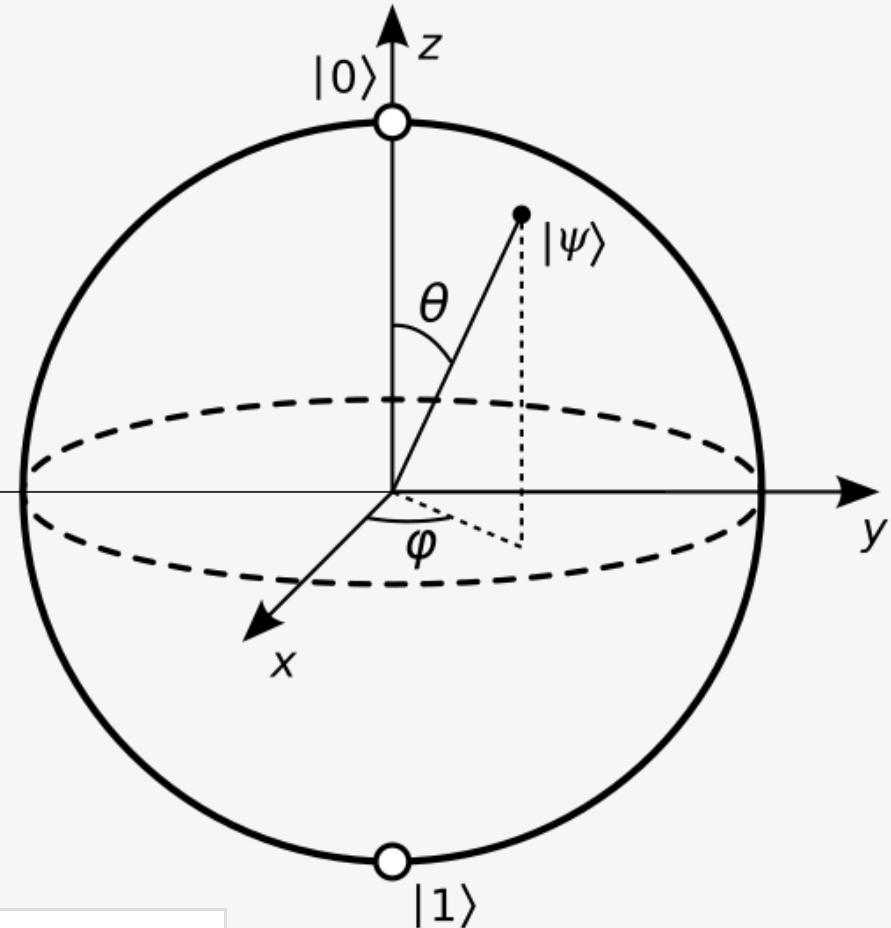


03. Qubits & Gates

4) Summary

| Operator | Gate(s) | Matrix |
|----------------------------------|---|--|
| Pauli-X (X) |  | $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ |
| Pauli-Y (Y) |  | $\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ |
| Pauli-Z (Z) |  | $\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ |
| Hadamard (H) |  | $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ |
| Phase (S, P) |  | $\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$ |
| $\pi/8$ (T) |  | $\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$ |
| Controlled Not (CNOT, CX) |  | $\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$ |
| Controlled Z (CZ) |  | $\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$ |
| SWAP |  | $\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$ |
| Toffoli (CCNOT, CCX, TOFF) |  | $\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$ |

| Operator | Gate(s) | Matrix |
|----------------------------------|---|--|
| Pauli-X (X) |  | $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ |
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| Hadamard (H) |  | $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ |
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Quantum logic gate

In quantum computing and specifically the quantum circuit model of computation, a quantum logic gate is a basic quantum...

[Wikipedia](#)



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03. Qubits & Gates

cf) ???



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03. Qubits & Gates

c) TOMORROW X TOGETHER (TXT)



투모로우바이투게더

투모로우바이투게더(영어: TOMORROW X TOGETHER · TXT)는 2019년 3월 4일에 데뷔한 대한민국 빅히트 뮤직 소속의 5인조 다국적 보이 그룹이다.

w Wikipedia

$$\sim \begin{bmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{bmatrix}$$

04. Superposition & Entanglement

1) Superposition

- linear, homogeneous PDE / eigenvalues & eigenvectors

$$\Psi = \sum_i c_i \psi_i \quad \hat{A} \psi_i = \lambda_i \psi_i$$

- Quantum information processing

$$|\Psi\rangle = c_0|0\rangle + c_1|1\rangle \quad (\text{where } |c_0|^2 + |c_1|^2 = 1)$$

04. Superposition & Entanglement

1) Superposition

- Quantum information processing

$$|\Psi\rangle = c_0|0\rangle + c_1|1\rangle \quad (\text{where } |c_0|^2 + |c_1|^2 = 1)$$

ex) Hadamard for superposition

$$H|0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

$$H|1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

04. Superposition & Entanglement

2) Entanglement

- Pure state - separable tensor product

$$|\psi\rangle_a \otimes |\psi\rangle_b$$

- Mixed state - no separable(entangled)

ex) Bell state

$$|\Phi\rangle_+ = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \quad GHZ = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$$

$$|\Phi\rangle_- = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \quad ex) W \text{ state}$$

$$|\Psi\rangle_+ = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \quad W = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle)$$

$$|\Psi\rangle_- = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$



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04. Superposition & Entanglement

2) Entanglement

- Mixed state – no separable(entangled)

ex) Bell state

$$|\Phi\rangle_+ = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

$$|\Phi\rangle_- = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$$

$$|\Psi\rangle_+ = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$$

$$|\Psi\rangle_- = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$

$$|\psi\rangle_1 = a|0\rangle + b|1\rangle$$

$$|\psi\rangle_2 = c|0\rangle + d|1\rangle$$

where ($|a|^2 + |b|^2 = 1, |c|^2 + |d|^2 = 1$)

$$|\psi\rangle_1 |\psi\rangle_2 = (a|0\rangle + b|1\rangle)(c|0\rangle + d|1\rangle)$$

$$= ac|00\rangle + ad|01\rangle + bc|10\rangle + bd|11\rangle$$

- impossible to make Bell states

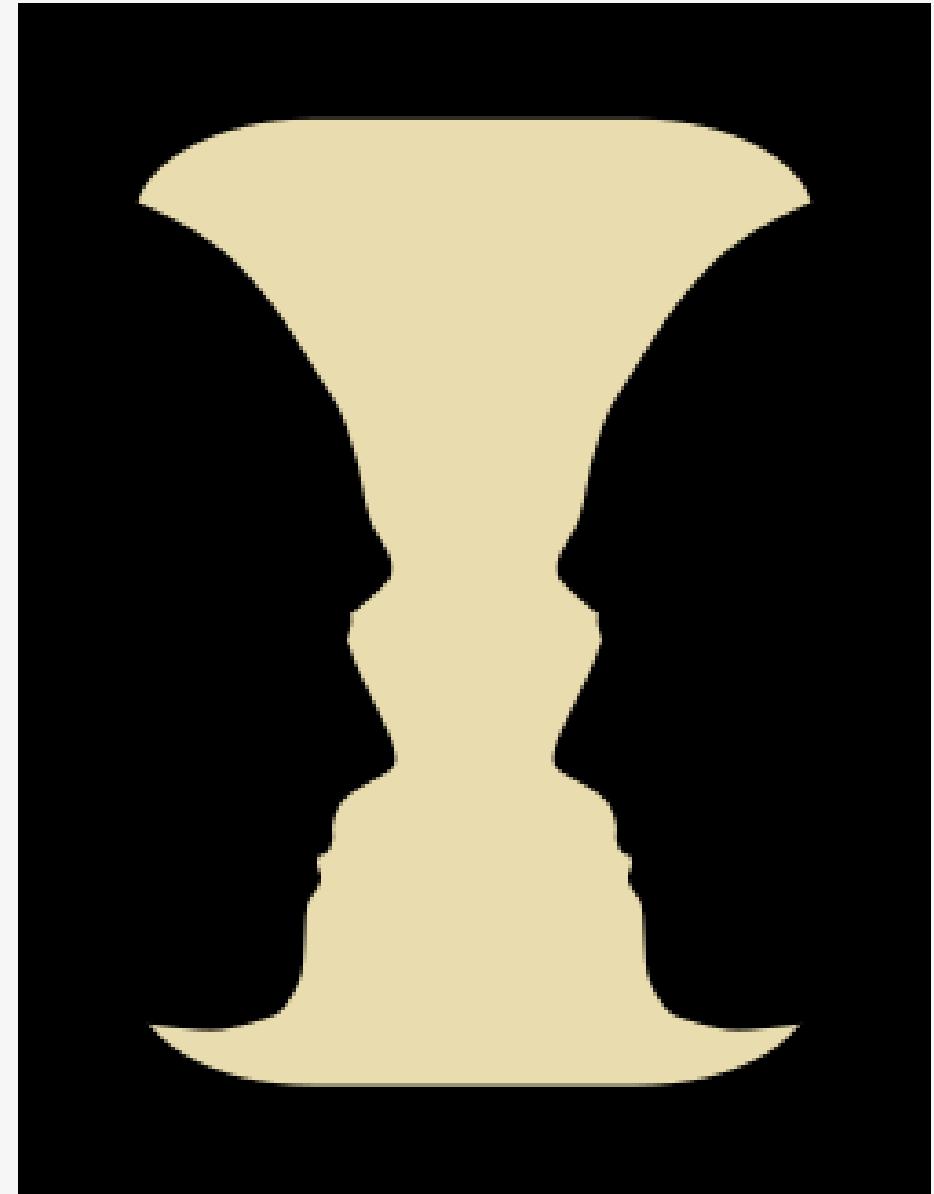
04. Superposition & Entanglement

2) Entanglement

It is possible to be pure state and mixed state concurrently, depending on which system you focus on.

ex)

$$|\Psi\rangle_{total} = |\Phi\rangle_+ |+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$



04. Superposition & Entanglement

2) Entanglement

- Density matrix

By spectral theorem,

$$\rho = \sum_i w_i |\psi_i\rangle\langle\psi_i|$$

- pure state

$$\text{Tr}(\rho^2) = 1$$

- mixed state

$$\text{Tr}(\rho^2) < 1$$

ex) Bell state

$$\rho_{total} = |\Phi_+\rangle\langle\Phi_+| = \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

$$\text{Tr}(\rho_{total}^2) = 1$$

- partial trace

$$\rho_{partial} = \frac{1}{2} I$$

$$\text{Tr}(\rho_{partial}^2) = 1/2 < 1$$

$$\begin{bmatrix} a & b & c & d \\ e & f & g & h \\ i & j & k & l \\ m & n & o & p \end{bmatrix} \rightarrow \begin{bmatrix} a+f & c+h \\ i+n & k+p \end{bmatrix}$$





Reference

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- https://en.wikipedia.org/wiki/Unitary_matrix
 - https://en.wikipedia.org/wiki/Hermitian_matrix
 - https://en.wikipedia.org/wiki/Bloch_sphere
 - https://en.wikipedia.org/wiki/Logic_gate
 - <https://en.wikipedia.org/wiki/Bit>
 - https://en.wikipedia.org/wiki/Quantum_logic_gate
 - https://en.wikipedia.org/wiki/Hadamard_matrix
 - https://en.wikipedia.org/wiki/Quantum_superposition
 - https://en.wikipedia.org/wiki/Quantum_entanglement
 - https://en.wikipedia.org/wiki/Partial_trace
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THANK YOU