

Advanced Parallel School 2022

Quantum Computing – Day 1

Quantum Algorithms

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Quantum Computing @ CINECA

CINECA: Italian HPC center

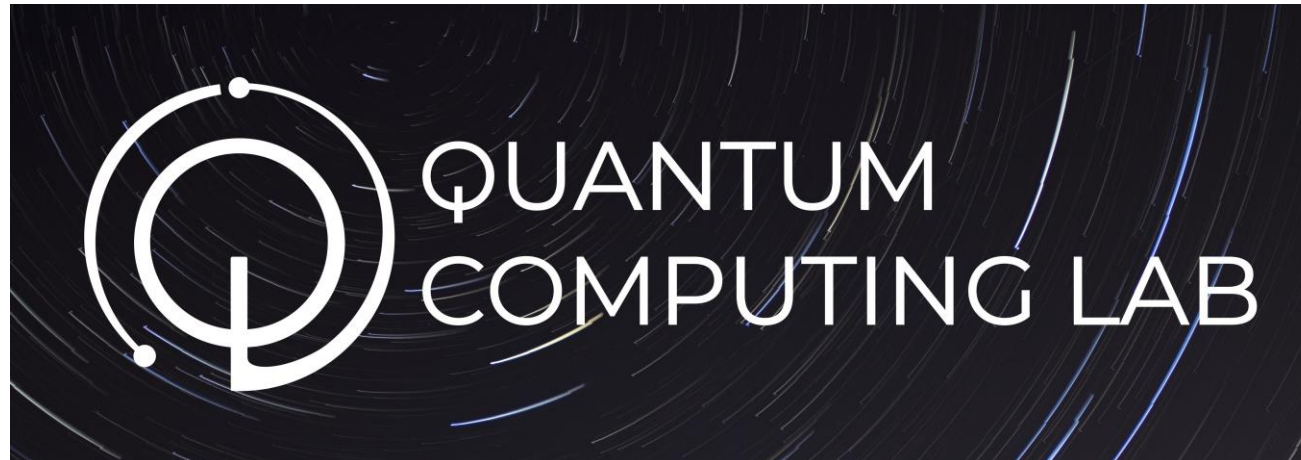
CINECA Quantum Computing Lab:

- Research with Universities, Industries and QC startups
- Internship programs, Courses and Conference (HPCQC)

<https://www.quantumcomputinglab.cineca.it>



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Recap of Quantum Computing

Vectors

Ket: $|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix}$ $\psi_i \in \mathbb{C}$
Complex Number

Bra: $\langle\psi| = (\psi_1^* \ \psi_2^* \ \dots \ \psi_n^*)$ ψ_i^* Complex Conjugate

Scalar Product

$$\langle \phi | \psi \rangle = \begin{pmatrix} \phi_1^* & \phi_2^* & \dots & \phi_n^* \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix}$$

$$\langle \phi | \psi \rangle \in \mathbb{C}$$

Complex Number

Scalar Product

$$\langle \phi | \psi \rangle = \begin{pmatrix} \phi_1^* & \phi_2^* & \dots & \phi_n^* \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix}$$

$$\langle \phi | \psi \rangle \in \mathbb{C}$$

Complex Number

The scalar product induces a **norm**

$$\| |\psi\rangle \| = \sqrt{\langle \psi | \psi \rangle}$$

Outer Product

$$|\psi\rangle\langle\phi| = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix} \begin{pmatrix} \phi_1^* & \phi_2^* & \dots & \phi_n^* \end{pmatrix} = \begin{pmatrix} \psi_1\phi_1^* & \psi_1\phi_2^* & \dots & \psi_1\phi_n^* \\ \psi_2\phi_1^* & \psi_2\phi_2^* & \dots & \psi_2\phi_n^* \\ \vdots & \vdots & \ddots & \vdots \\ \psi_n\phi_1^* & \psi_n\phi_2^* & \dots & \psi_n\phi_n^* \end{pmatrix}$$

Dimension = $n \times n$

Tensor Product

$$|\phi\rangle \otimes |\psi\rangle =$$

$$\begin{pmatrix} \phi_1 \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix} \\ \phi_2 \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix} \\ \vdots \\ \phi_n \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix} \end{pmatrix}$$

$$\text{Dimension} = n^2$$

Tensor Product

$$|\phi\rangle \otimes |\psi\rangle =$$

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$$\text{Dimension} = n^2$$

Compact form:

$$|\psi\rangle \otimes |\phi\rangle = |\psi\rangle |\phi\rangle = |\psi \phi\rangle$$

1. Unit of Information

Classically

Unit of classical information is the bit

State of a bit:

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

Quantumly

To a closed quantum system is associated a space of states H which is a Hilbert space. The pure state of the system is then represented by a unit norm vector on such Hilbert space.

The unit of quantum information is the quantum bit a.k.a. Qubit

State of a qubit:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Postulates of Quantum Computing (1)

Space of states: $\mathcal{H} \simeq \mathbb{C}^2$

State of a qubit:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$\alpha, \beta \in \mathbb{C} \quad |\alpha|^2 + |\beta|^2 = 1$$

Postulates of Quantum Computing (1)

Space of states: $\mathcal{H} \simeq \mathbb{C}^2$

State of a qubit:

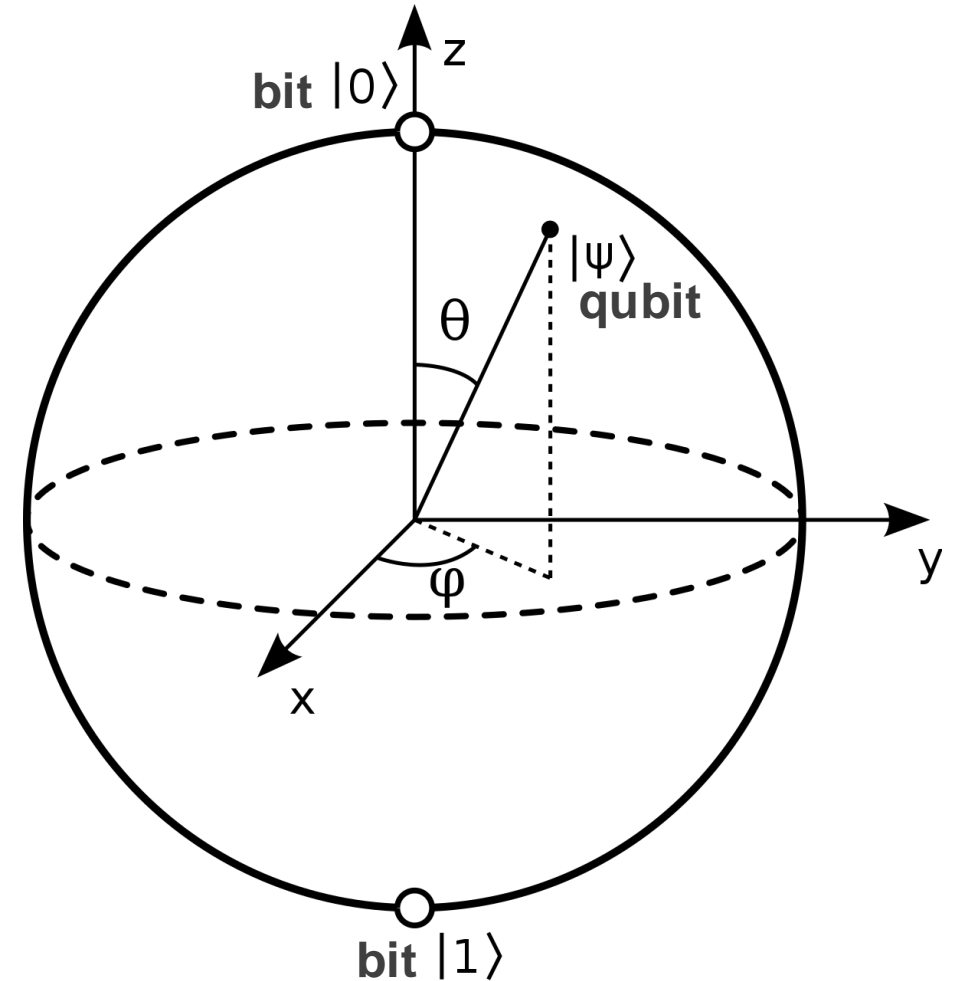
$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$\alpha, \beta \in \mathbb{C} \quad |\alpha|^2 + |\beta|^2 = 1$$

Can be parametrized as:

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

$$\theta \in [0, \pi] \quad \phi \in [0, 2\pi]$$



2. Composite systems

Classically

State of N bits:

$$|000\dots 0\rangle, |100\dots 0\rangle, |010\dots 0\rangle \dots |111\dots 1\rangle$$

Postulates of Quantum Computing (2)

Quantumly

The space of states of a composite system is the tensor product of the spaces of the subsystems

$$\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \dots \otimes \mathbb{C}^2$$

State of N qubits:

$$\alpha_1 |000\dots 0\rangle + \alpha_2 |100\dots 0\rangle + \alpha_3 |010\dots 0\rangle + \dots \alpha_n |111\dots 1\rangle$$

$$\alpha_i \in \mathbb{C} \quad \sum_i |\alpha_i|^2 = 1$$

Quantum Entanglement

States that can be written as tensor product

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes \dots \otimes |\psi_N\rangle$$

are called **factorable or product states**

Quantum Entanglement

States that **can NOT** be written as tensor product

$$|\psi\rangle \neq |\psi_1\rangle \otimes |\psi_2\rangle \otimes \dots \otimes |\psi_N\rangle$$

are called **entangled states**

Quantum Entangled Bell's states

$$\frac{1}{\sqrt{2}} \left(|00\rangle + |11\rangle \right)$$

$$\frac{1}{\sqrt{2}} \left(|01\rangle + |10\rangle \right)$$







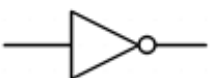
$$\frac{1}{\sqrt{2}} \left(|00\rangle - |11\rangle \right)$$

$$\frac{1}{\sqrt{2}} \left(|01\rangle - |10\rangle \right)$$

3. State Change

Postulates of Quantum Computing (3)

Classically: logic gates

Logic Gate	Symbol	Description	Boolean
AND		Output is at logic 1 when, and only when all its inputs are at logic 1, otherwise the output is at logic 0.	$X = A \cdot B$
OR		Output is at logic 1 when one or more are at logic 1. If all inputs are at logic 0, output is at logic 0.	$X = A + B$
NAND		Output is at logic 0 when, and only when all its inputs are at logic 1, otherwise the output is at logic 1	$X = \overline{A \cdot B}$
NOR		Output is at logic 0 when one or more of its inputs are at logic 1. If all the inputs are at logic 0, the output is at logic 1.	$X = \overline{A + B}$
XOR		Output is at logic 1 when one and Only one of its inputs is at logic 1. Otherwise is it logic 0.	$X = A \oplus B$
XNOR		Output is at logic 0 when one and only one of its inputs is at logic 1. Otherwise it is logic 1. Similar to XOR but inverted.	$X = \overline{A \oplus B}$
NOT		Output is at logic 0 when its only input is at logic 1, and at logic 1 when its only input is at logic 0. That's why it is called and INVERTER	$X = \overline{A}$

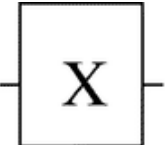
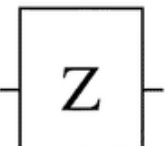
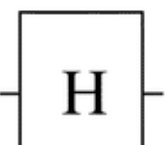
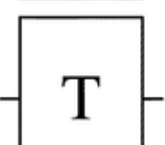
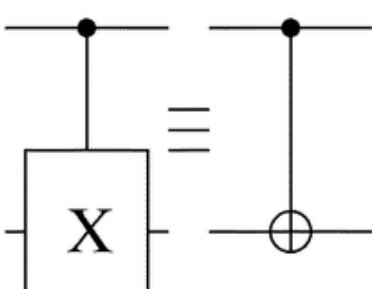
Quantumly

The state change of a closed quantum system is described by a unitary operator

$$i \frac{d|\psi\rangle}{dt} = H|\psi\rangle \quad \Rightarrow \quad |\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle$$
$$U = e^{-iHt}$$

Schrodinger Equation

Quantumly: Quantum Gates

X Gate Bit-flip, Not		\equiv	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \beta 0\rangle + \alpha 1\rangle$
Z Gate Phase-flip		\equiv	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha 0\rangle - \beta 1\rangle$
H Gate Hadamard		$\equiv \frac{1}{\sqrt{2}}$	$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \frac{\alpha + \beta 0\rangle + \alpha - \beta 1\rangle}{\sqrt{2}}$
T Gate		\equiv	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha 0\rangle + e^{i\pi/4}\beta 1\rangle$
Controlled Not Controlled X CNot		\equiv	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = a 00\rangle + b 01\rangle + d 10\rangle + c 11\rangle$

4. Measurement

Classically

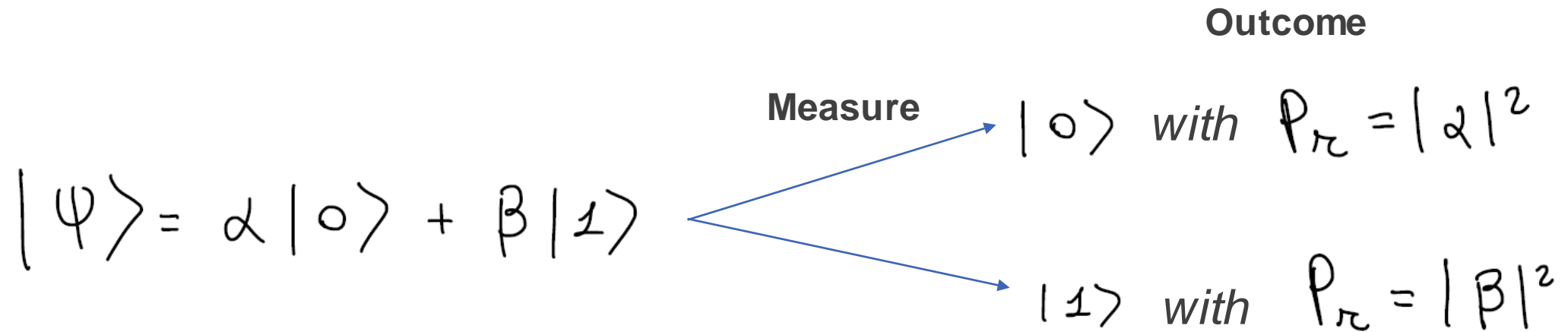
Measuring returns the state of a bit with certainty



Measurements do not affect the state of a bit

Quantumly

Measuring returns the bit state with some probability



Measurement affects the state of a qubit

Quantumly

- To **any observable** physical quantity is associated an **hermitian operator** O

$$O |\sigma_i\rangle = \sigma_i |\sigma_i\rangle$$

- A **measurement** outcomes are the **possible eigenvalues** $\{\sigma_i\}$.
- The **probability of obtaining** σ_i as a result of the measurement is

$$P_{\psi}(\sigma_i) = |\langle \psi | \sigma_i \rangle|^2$$

- The effect of the **measure** is to **change the state** $|\psi\rangle$ **into the eigenvector** of O

$$|\psi\rangle \rightarrow |\sigma_i\rangle$$

Quantum Algorithms

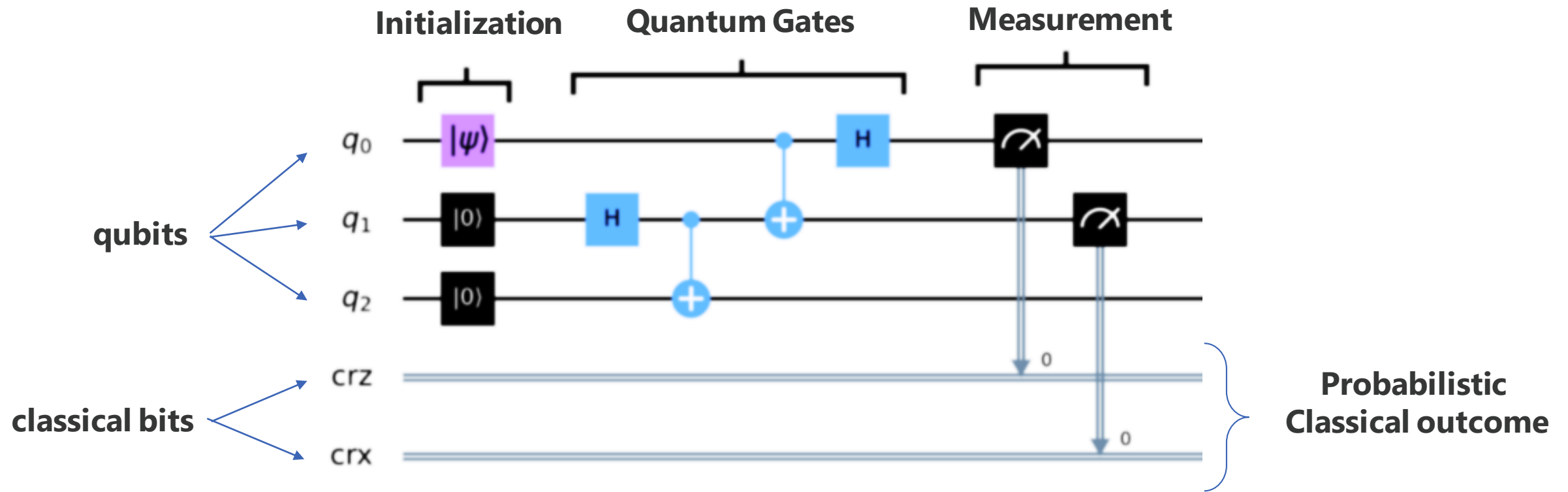
Quantum Algorithm = Quantum Circuit

A quantum circuit with n input qubits and n output qubits is defined by a unitary transformation

$$U \in U(2^n)$$

$$\left[\begin{array}{l} U^\dagger U = U U^\dagger = I \\ U^{-1} = U^\dagger \end{array} \right]$$

Quantum Algorithms



Quantum Algorithms: Gates

Single Qubit Gates

Generic single qubit rotation:

$$R_{\vec{n}}(\theta) = \cos\left(\frac{\theta}{2}\right) \mathbb{I} - i \sin\left(\frac{\theta}{2}\right) \vec{n} \cdot \vec{\sigma}$$

Pauli matrices:

$$\sigma_x = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Identity: $\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Single Qubit Gates: Hadamard

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



$$H|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) = |+\rangle$$

$$H|1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) = |-\rangle$$

Single Qubit Gates: Phase

$$U_\phi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$$

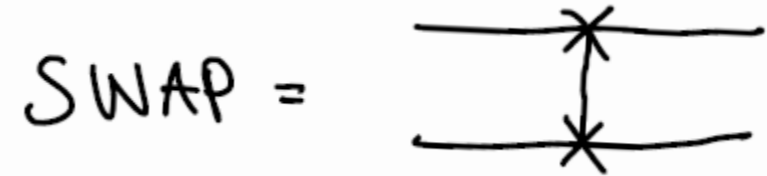
$$U_\phi |0\rangle = |0\rangle$$

$$U_\phi |1\rangle = e^{i\phi} |1\rangle$$

Two Qubit Gates: SWAP

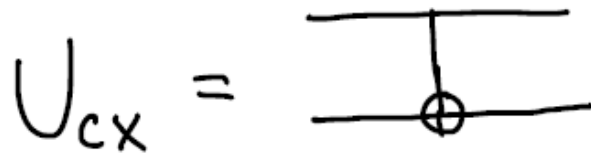
$$U_{\text{SWAP}} |z_1\rangle |z_2\rangle = |z_2\rangle |z_1\rangle \quad z_1, z_2 \in \{0, 1\}$$

$$U_{\text{SWAP}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$



Two Qubit Gates: Control Not

$$U_{CX} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$



$$U_{CX} |z_1\rangle |z_2\rangle = |z_1\rangle X^{z_1} |z_2\rangle$$

$$U_{CX} |00\rangle = |00\rangle$$

$$U_{CX} |10\rangle = |11\rangle$$

$$U_{CX} |01\rangle = |01\rangle$$

$$U_{CX} |11\rangle = |10\rangle$$

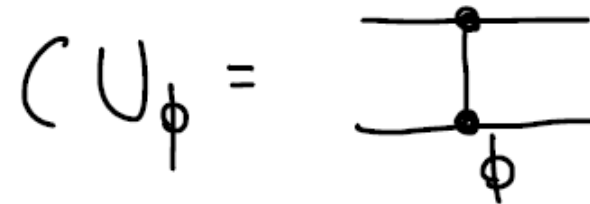
Two Qubit Gates: Control Unitary

$$(U |z_1\rangle |z_2\rangle = |z_1\rangle U^{z_1} |z_2\rangle$$

Control Phase

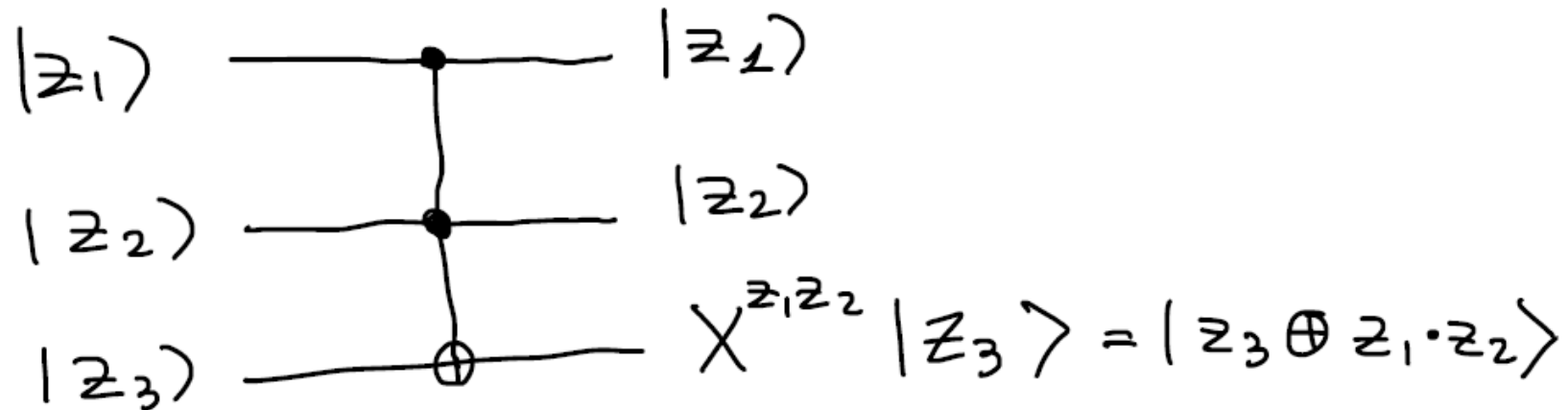
$$(U_\phi |z_1\rangle |z_2\rangle = |z_1\rangle U_\phi^{z_1} |z_2\rangle$$

$$CU_\phi = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{pmatrix}$$



Three Qubit Gates: Toffoli

$$U_{C_2X} |z_1 z_2 z_3\rangle = |z_1 z_2\rangle X^{z_1 z_2} |z_3\rangle$$



Quantum Algorithms: Universality

Universal set of Quantum Gates

We can exactly build any unitary $U \in U(2^n)$ on n qubits
by means of single qubit gates and Control-Not

$$G_{ex} = \left\{ U \in U(2) ; U_{cx} \right\}$$

Universal set of Quantum Gates

We can exactly build any unitary $U \in U(2^n)$ on n qubits by means of single qubit gates and Control-Not

$$G_{ex} = \left\{ U \in U(2) ; U_{cx} \right\}$$

$$R_{\vec{n}}(\theta) = \cos\left(\frac{\theta}{2}\right) \mathbb{I} - i \sin\left(\frac{\theta}{2}\right) \vec{n} \cdot \vec{\sigma}$$

$$U_{cx} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Universal set of Quantum Gates

Given $U, U' \in \mathcal{U}(2^n)$, U' approximates U within ε ($\varepsilon > 0$) if $d(U, U') < \varepsilon$

Universal set of Quantum Gates

Given $U, U' \in \mathcal{U}(2^n)$, U' approximates U within ε ($\varepsilon > 0$) if $d(U, U') < \varepsilon$

where $d(U, U') = \max_{|\psi\rangle} \|(U - U')|\psi\rangle\|$

and $\| |\psi\rangle \| = \sqrt{\langle \psi | \psi \rangle}$

Universal set of Quantum Gates

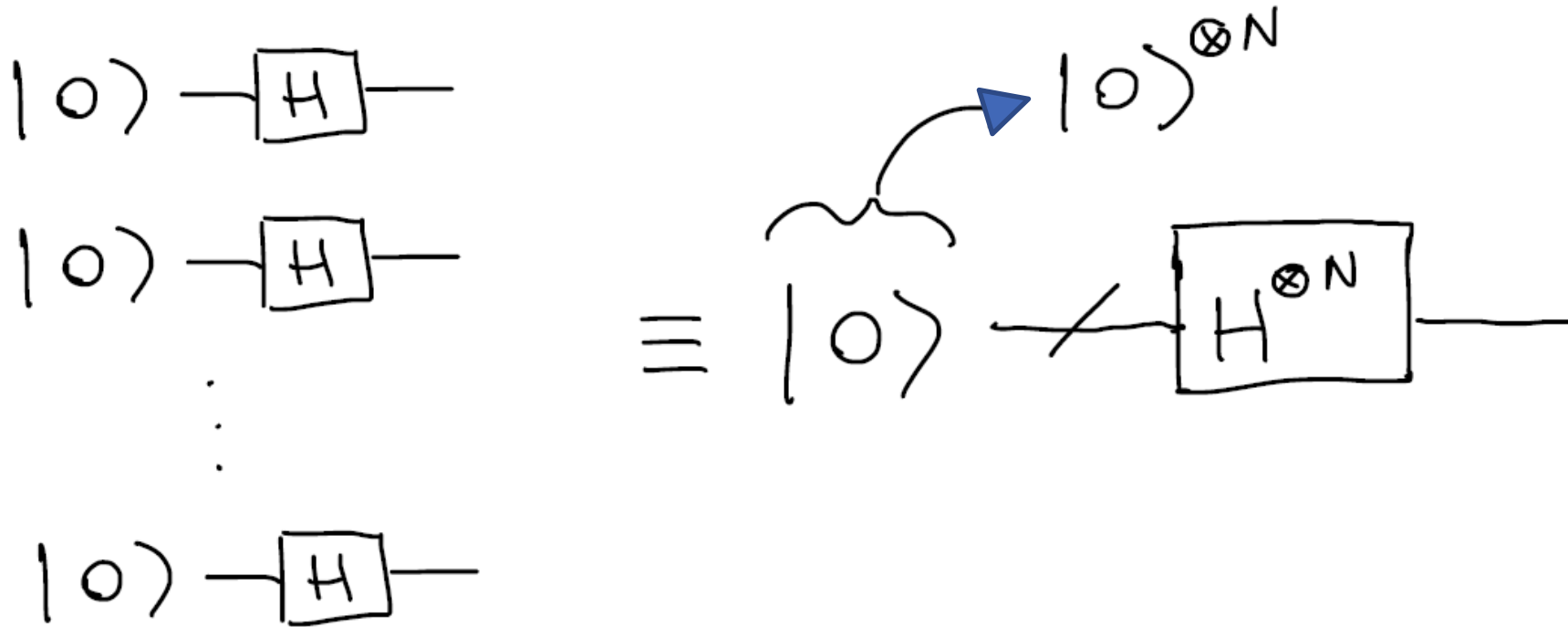
We can approximate any unitary $U \in U(2^n)$ on n qubits
by means of the following gates

$$\{H, S, T, U_{CX}\}$$

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \quad T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$$

Quantum Algorithms: basics

Multiple Hadamard gates



Single Qubit Gates: Hadamard

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

$$H = \text{---} \boxed{H} \text{---}$$

$$H|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) = |+\rangle$$

$$H|1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) = |-\rangle$$

Multiple Hadamard gates



$$\Rightarrow H = \frac{1}{\sqrt{2}} \left(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| - |1\rangle\langle 1| \right)$$



$$\Rightarrow H^{\otimes N} = \frac{1}{\sqrt{2^N}} \sum_{x,y \in \{0,1\}^N} (-1)^{x \cdot y} |x\rangle\langle y|$$

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