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# Manipulation of a single qubit

Introduction to Quantum Computing

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Université de Montpellier

2022 – 2023

# Manipulation of a single qubit

- 1 Bloch sphere representation of a two-level system
- 2 Case of NMR: single qubit manipulation
- 3 Quantum gates and quantum circuits

# Manipulation of a single qubit

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# I. Bloch sphere representation of a two-level system

General expression of a quantum state  $|\psi\rangle$  of a two level quantum system

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

with  $(\alpha, \beta) \in \mathbb{C}^2$  and  $|\alpha|^2 + |\beta|^2 = 1$ . Coefficients  $(\alpha, \beta)$  might be expressed as follow

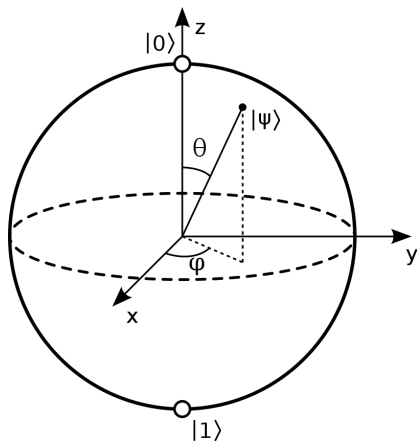
$$\alpha = \cos \frac{\theta}{2} \quad \text{and} \quad \beta = e^{i\varphi} \sin \frac{\theta}{2},$$

such that

$$|\psi\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\varphi} \sin \frac{\theta}{2} |1\rangle,$$

for  $\theta \in [0, 2\pi [$  and  $\varphi \in [0, 2\pi [$ . The parameters  $\theta$  and  $\varphi$  might be seen as the angle of the direction of the equivalent spin of the two level system.

# I. Bloch sphere representation of a two-level system



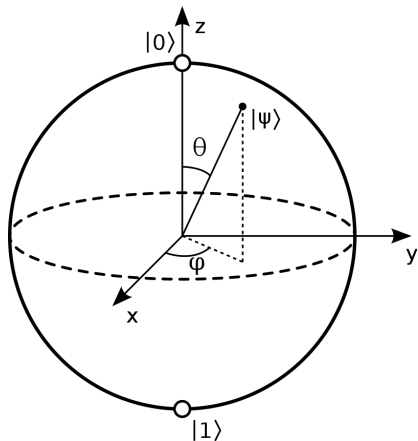
The geometrical representation of this direction on a unitary sphere is the **Bloch sphere** representation of the quantum state (Felix Bloch, Nobel Prize in 1952 for NMR). Any pure quantum state of a qubit can be visualized as a point on this unit sphere.

$$\theta = 0 \rightarrow |\psi\rangle = |0\rangle,$$

$$\theta = \pi \rightarrow |\psi\rangle = |1\rangle,$$

$$\theta = \frac{\pi}{2} \rightarrow |\psi\rangle = \frac{1}{\sqrt{2}} (|0\rangle + e^{i\varphi} |1\rangle).$$

# I. Bloch sphere representation of a two-level system



Any unitary operator  $\hat{U}$  might be seen as a rotation on the Bloch sphere.

Any unitary operator  $\hat{U}$  on a two-level system is a  $2 \times 2$  matrix, and might be expressed as a function of 4 basis operators. A commonly used basis consists in **Pauli's matrices**.

# I. Bloch sphere representation of a two-level system

**Pauli's matrices:**

$$\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

**Alternative notations:**

$$\hat{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \hat{Y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \hat{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

**Pauli's matrices are the generators of rotations for a two-level system.**



# I. Bloch sphere representation of a two-level system

## Rotation on the Bloch sphere.

Rotation of an angle  $\psi$  around the  $X$  axis

$$R_X(\psi) = \begin{bmatrix} \cos \frac{\psi}{2} & -i \sin \frac{\psi}{2} \\ -i \sin \frac{\psi}{2} & \cos \frac{\psi}{2} \end{bmatrix}.$$

Introducing Pauli's matrices

$$R_X(\psi) = \cos \left( \frac{\psi}{2} \right) \mathbb{I} - i \sin \left( \frac{\psi}{2} \right) \hat{X}.$$

## Pauli's matrices properties

$$\hat{X}^2 = \hat{Y}^2 = \hat{Z}^2 = \mathbb{I},$$

$$[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k \text{ and } \{\sigma_i, \sigma_j\} = 2\delta_{ij}\mathbb{I},$$

where  $\varepsilon_{ijk}$  is the Levi-Civita symbol and  $\delta_{ij}$  is the Kronecker symbol.

Consequently

$$\sigma_i\sigma_j = i\varepsilon_{ijk}\sigma_k + \delta_{ij}\mathbb{I}.$$

# I. Bloch sphere representation of a two-level system

Since  $\hat{X}^2 = \mathbb{I}$ ,

$$\hat{R}_X(\psi) = \cos\left(\frac{\psi}{2}\right) \mathbb{I} - i \sin\left(\frac{\psi}{2}\right) \hat{X} = \exp\left(-i\frac{\psi}{2} \hat{X}\right).$$

Similarly, one gets

$$\hat{R}_Y(\psi) = \cos\left(\frac{\psi}{2}\right) \mathbb{I} - i \sin\left(\frac{\psi}{2}\right) \hat{Y} = \exp\left(-i\frac{\psi}{2} \hat{Y}\right),$$

$$\hat{R}_Z(\psi) = \cos\left(\frac{\psi}{2}\right) \mathbb{I} - i \sin\left(\frac{\psi}{2}\right) \hat{Z} = \exp\left(-i\frac{\psi}{2} \hat{Z}\right).$$

# I. Bloch sphere representation of a two-level system

One may define the rotation around an arbitrary direction  $\vec{n}$

$$\vec{n} = \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}.$$

Let introduce the following operator

$$\hat{\sigma} = \begin{pmatrix} \hat{X} \\ \hat{Y} \\ \hat{Z} \end{pmatrix}.$$

Then,

$$\begin{aligned} \hat{R}_{\vec{n}}(\psi) &= \exp\left(-i\frac{\psi}{2}\vec{n} \cdot \hat{\sigma}\right) \\ &= \cos\left(\frac{\psi}{2}\right)\mathbb{I} - i\sin\left(\frac{\psi}{2}\right)\left(n_x\hat{X} + n_y\hat{Y} + n_z\hat{Z}\right) \end{aligned}$$

# I. Bloch sphere representation of a two-level system

How to perform such a rotation on a "real" system ?

*Let's consider the case of a spin 1/2 system in a magnetic field (NMR).*

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  - Qubit measurement
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## II.1. Nuclear spin in a static $\vec{B}$ field

Let consider a static magnetic field  $\vec{B}_0 = B_0 \vec{u}_z$ , so that  $z$  is the quantification axis. Let consider an atom with a nuclear spin  $\hat{I}$ , which is a spin  $1/2$ . It corresponds to a magnetic momentum  $\hat{M} = \gamma \hat{I}$ , where  $\gamma$  is the gyromagnetic factor (g-factor).

Magnetic interaction between the  $\vec{B}_0$  field and the magnetic momentum results in the following hamiltonian

$$\hat{H}_0 = -\hat{M} \cdot \vec{B}_0 = \gamma \hat{I} \cdot \vec{B}_0 = -\gamma \frac{\hbar}{2} B_0 \hat{Z}.$$

Introducing the **Larmor frequency**:  $\omega_0 = \gamma B_0$

$$\Rightarrow \hat{H}_0 = -\frac{1}{2} \hbar \omega_0 \hat{Z}.$$



## II.1. Nuclear spin in a static $\vec{B}$ field

$\hat{H}_0$  is time-independent, so

$$|\psi(t)\rangle = \exp\left(-i\frac{\hat{H}_0 t}{\hbar}\right) |\psi(0)\rangle,$$

then

$$|\psi(t)\rangle = \exp\left(i\frac{\omega_0 t}{2} \hat{Z}\right) |\psi(0)\rangle.$$

The evolution of the nuclear spin is a rotation along  $z$  axis at larmor frequency  $\omega_0$ .

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## 11.2. Static $\vec{B}_0$ field and RF $\vec{B}_{rf}$ field

Now adding a radio-frequency (RF) rotating field  $\vec{B}_{rf}$ , perpendicular to the static magnetic field  $\vec{B}_0$

$$\vec{B}_{rf} = B_1 (\cos(\omega_{rf}t + \phi) \vec{u}_x - \sin(\omega_{rf}t + \phi) \vec{u}_y).$$

One notes  $\omega_1 = \gamma B_1$ , such that the hamiltonian becomes

$$\hat{H} = -\frac{1}{2}\hbar\omega_0\hat{Z} - \frac{1}{2}\hbar\omega_1 \left( \cos(\omega_{rf}t + \phi) \hat{X} - \sin(\omega_{rf}t + \phi) \hat{Y} \right).$$

Considering the rotation frame at  $-\omega_{rf}$  around z, the state becomes

$$|\psi\rangle^{rot} = \exp\left(-\frac{i}{2}\omega_{rf}t\hat{Z}\right) |\psi\rangle.$$

*What is the expression of the hamiltonian in the rotating frame ?*

## 11.2. Static $\vec{B}_0$ field and RF $\vec{B}_{rf}$ field

Let consider a unitary transformation  $\hat{U}(t)$  on a state  $|\psi\rangle$

$$|\psi'\rangle = \hat{U}(t)|\psi\rangle \Leftrightarrow |\psi\rangle = \hat{U}^\dagger(t)|\psi'\rangle.$$

Then,

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = i\hbar \left( \frac{\partial \hat{U}^\dagger(t)}{\partial t} \right) |\psi'\rangle + i\hbar \hat{U}^\dagger(t) \frac{\partial |\psi'\rangle}{\partial t},$$

$$\hat{H}|\psi\rangle = \hat{H}\hat{U}^\dagger(t)\hat{U}(t)|\psi\rangle = \hat{H}\hat{U}^\dagger(t)|\psi'\rangle.$$

Therefore

$$i\hbar \left( \frac{\partial \hat{U}^\dagger(t)}{\partial t} \right) |\psi'\rangle + i\hbar \hat{U}^\dagger(t) \frac{\partial |\psi'\rangle}{\partial t} = \hat{H}\hat{U}^\dagger(t)|\psi'\rangle,$$

$$\Leftrightarrow i\hbar \frac{\partial |\psi'\rangle}{\partial t} = \left( -i\hbar \hat{U}(t) \frac{\partial \hat{U}^\dagger(t)}{\partial t} + \hat{U}(t) \hat{H} \hat{U}^\dagger(t) \right) |\psi'\rangle.$$

## 11.2. Static $\vec{B}_0$ field and RF $\vec{B}_{rf}$ field

Then, if states are transformed by a unitary operator  $\hat{U}(t)$ , the transformed state is governed by the transformed hamiltonian  $\hat{H}'$

$$\hat{H}' = \hat{U}(t)\hat{H}\hat{U}^\dagger(t) - i\hbar\hat{U}(t)\frac{\partial\hat{U}^\dagger(t)}{\partial t}.$$

For a rotation along  $z$  at  $\omega_{rf}$ ,

$$\hat{U}(t) = \exp\left(-i\frac{\omega_{rf}}{2}t\hat{Z}\right) \Rightarrow \hat{H}^{rot} = \frac{\hbar\omega_{rf}}{2}\hat{Z} + \hat{U}(t)\hat{H}\hat{U}^\dagger(t),$$

$$\begin{aligned}\hat{H}^{rot} &= -\frac{\hbar}{2}(\omega_0 - \omega_{rf})\hat{Z} \\ &\quad -\frac{\hbar}{2}\omega_1\left(\cos(\omega_{rf}t + \phi)\hat{U}(t)\hat{X}\hat{U}^\dagger(t)\right) \\ &\quad +\frac{\hbar}{2}\omega_1\left(\sin(\omega_{rf}t + \phi)\hat{U}(t)\hat{Y}\hat{U}^\dagger(t)\right)\end{aligned}$$

## II.2. Static $\vec{B}_0$ field and RF $\vec{B}_{rf}$ field

$$\Rightarrow \hat{U}(t)\hat{X}\hat{U}^\dagger(t) =? \quad \hat{U}(t)\hat{Y}\hat{U}^\dagger(t) =?$$

$$\begin{aligned}\hat{U}(t)\hat{X}\hat{U}^\dagger(t) &= \begin{pmatrix} e^{-i\omega_{rf}t/2} & 0 \\ 0 & e^{i\omega_{rf}t/2} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} e^{i\omega_{rf}t/2} & 0 \\ 0 & e^{-i\omega_{rf}t/2} \end{pmatrix}, \\ &= \begin{pmatrix} e^{-i\omega_{rf}t/2} & 0 \\ 0 & e^{i\omega_{rf}t/2} \end{pmatrix} \begin{pmatrix} 0 & e^{-i\omega_{rf}t/2} \\ e^{i\omega_{rf}t/2} & 0 \end{pmatrix}, \\ &= \begin{pmatrix} 0 & e^{-i\omega_{rf}t} \\ e^{i\omega_{rf}t} & 0 \end{pmatrix}.\end{aligned}$$

## II.2. Static $\vec{B}_0$ field and RF $\vec{B}_{rf}$ field

$$\begin{aligned}\hat{U}(t)\hat{Y}\hat{U}^\dagger(t) &= \begin{pmatrix} e^{-i\omega_{rf}t/2} & 0 \\ 0 & e^{i\omega_{rf}t/2} \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} e^{i\omega_{rf}t/2} & 0 \\ 0 & e^{-i\omega_{rf}t/2} \end{pmatrix}, \\ &= \begin{pmatrix} e^{-i\omega_{rf}t/2} & 0 \\ 0 & e^{i\omega_{rf}t/2} \end{pmatrix} \begin{pmatrix} 0 & -ie^{-i\omega_{rf}t/2} \\ ie^{i\omega_{rf}t/2} & 0 \end{pmatrix}, \\ &= \begin{pmatrix} 0 & -ie^{-i\omega_{rf}t} \\ ie^{i\omega_{rf}t} & 0 \end{pmatrix}.\end{aligned}$$

## II.2. Static $\vec{B}_0$ field and RF $\vec{B}_{rf}$ field

Consequently,

$$\hat{U}(t)\hat{X}\hat{U}^\dagger(t)\cos(\omega_{rf}t + \phi) = \frac{1}{2} \begin{pmatrix} 0 & e^{i\phi} + e^{-2i\omega_{rf}t}e^{-i\phi} \\ e^{-i\phi} + e^{2i\omega_{rf}t}e^{i\phi} & 0 \end{pmatrix},$$

and

$$\hat{U}(t)\hat{Y}\hat{U}^\dagger(t)\sin(\omega_{rf}t + \phi) = \frac{1}{2i} \begin{pmatrix} 0 & -ie^{i\phi} + ie^{-2i\omega_{rf}t}e^{-i\phi} \\ -ie^{-i\phi} + ie^{2i\omega_{rf}t}e^{i\phi} & 0 \end{pmatrix}.$$

The terms  $e^{-2i\omega_{rf}t}$  and  $e^{2i\omega_{rf}t}$  are fast rotation compared to the state dynamics. Their effect on the state dynamics is negligible. One then neglect those terms, which is the so-called **rotating wave approximation**.



## 11.2. Static $\vec{B}_0$ field and RF $\vec{B}_{rf}$ field

In the rotating wave approximation

$$\begin{aligned} & \hat{U}(t)\hat{X}\hat{U}^\dagger(t) \cos(\omega_{rf}t + \phi) - \hat{U}(t)\hat{Y}\hat{U}^\dagger(t) \sin(\omega_{rf}t + \phi) \\ & \approx \frac{1}{2} \begin{pmatrix} 0 & e^{i\phi} \\ e^{-i\phi} & 0 \end{pmatrix} - \frac{1}{2i} \begin{pmatrix} 0 & -ie^{i\phi} \\ -ie^{-i\phi} & 0 \end{pmatrix}, \\ & = \begin{pmatrix} 0 & e^{i\phi} \\ e^{-i\phi} & 0 \end{pmatrix}, \\ & = \begin{pmatrix} 0 & \cos\phi + i\sin\phi \\ \cos\phi - i\sin\phi & 0 \end{pmatrix}, \\ & = \underbrace{\cos\phi \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{=\hat{X}} - \underbrace{\sin\phi \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}}_{=\hat{Y}}, \end{aligned}$$

## 11.2. Static $\vec{B}_0$ field and RF $\vec{B}_{rf}$ field

In the rotating frame, in the rotating wave approximation, the hamiltonian becomes

$$\hat{H}^{rot} = -\frac{\hbar}{2}(\omega_0 - \omega_{rf})\hat{Z} - \frac{\hbar}{2}\omega_1(\cos\phi\hat{X} + \sin\phi\hat{Y}).$$

Introducing the detuning  $\delta$  between RF magnetic field frequency and Larmor frequency in the static field  $\delta = \omega_0 - \omega_{rf}$ , the hamiltonian reduces to

$$\hat{H}^{rot} = -\frac{\hbar\delta}{2}\hat{Z} - \frac{\hbar\omega_1}{2}(\cos\phi\hat{X} + \sin\phi\hat{Y}).$$

Any rotation of the state on the Bloch sphere is achievable, using the appropriate values of  $\delta$ ,  $\omega_1$  and  $\phi$  (detuning, amplitude and phase of the RF magnetic field).

It is that which is used in NMR sequences.

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3 Quantum gates and quantum circuits

## 11.3. Qubit measurement

Usually, the measurement of a qubit corresponds to the measurement of the observable  $\hat{Z}$ .

If a measurement of  $\hat{X}$  or  $\hat{Y}$  is required, one simply has to apply the appropriate rotation on the qubit to transform it as a  $\hat{Z}$  measurement after rotation.

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## 11.4. Few realization of qubits

- Nuclear spins in molecules;
- ions in an ion trap;
- quantum dots;
- **superconducting circuits** → Google, IBM, D-waves,...
- polarization states of photons;
- NV center in diamonds;
- ...

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  - Definitions
  - Single-qubit gates

# Manipulation of a single qubit

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## III.1. Definitions

In classical computing, algorithms are implemented by the mean of logical gates, acting on bits.

In quantum computing, quantum algorithm are implemented by the mean of **quantum gates**, acting on qubits.

A quantum gate is a unitary operator acting on several qubits.

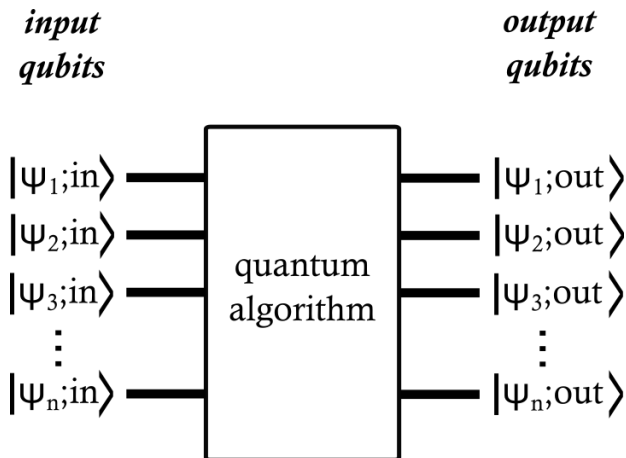
A single-qubit gate is a quantum gate acting on a single qubit.

Since it is unitary, a **single qubit gate is a rotation on the Bloch sphere.**

A gate is represented in the "**circuit model**" as a block with an input and an output. Gates are connected by "wires", representing the time evolution of qubits.

In the circuit model, a quantum algorithm is represented as a sequence of building blocks that carry out elementary computations (=gates) connected by wires.

## III.1. Definitions



## III.1. Definitions

In quantum computing, a **quantum register** is a system comprising multiple qubits. It's the quantum analog of the classical processor register.

Quantum computers perform calculations by manipulating qubits within a quantum register.

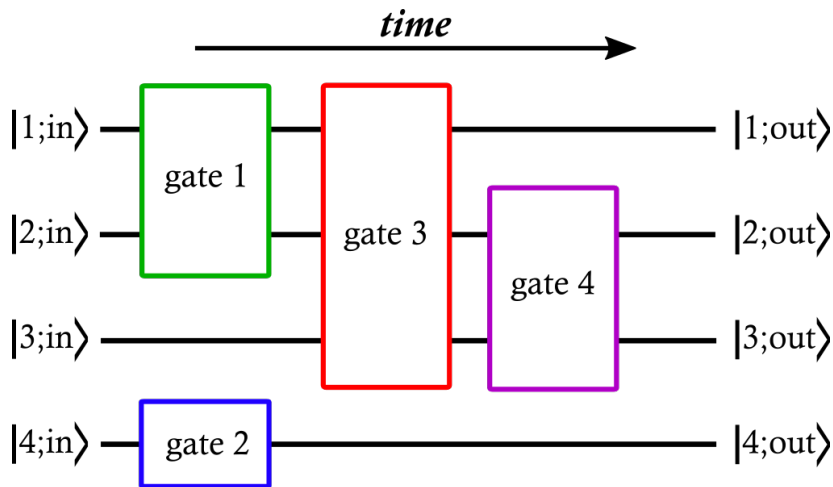
The size of a quantum register correspond to the number of qubits in it. The corresponding Hilbert space  $\mathcal{H}$  in which data of the quantum register are stored is the tensorial product of the Hilbert space of each qubit

$$\mathcal{H} = \mathcal{H}_n \otimes \mathcal{H}_{n-1} \otimes \mathcal{H}_{n-2} \otimes \cdots \mathcal{H}_1.$$

The size of  $\mathcal{H}$  is  $2^n \times 2^n$  where  $n$  is the size of the quantum register.

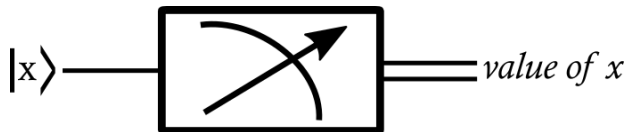
# III.1. Definitions

## Example of quantum circuit



## III.1. Definitions

To access to the result of a calculation, a measurement on at least one of the qubits of the quantum register has to be realized, with the following block representation

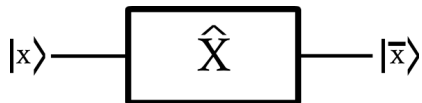


Note that it's not necessarily all the quantum register that has to be measured.

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## III.2. Single-qubit gates



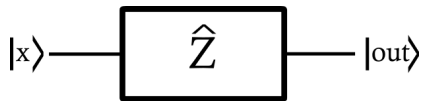
A **NOT gate** (bit flip) is a unitary operator that flips  $|0\rangle$  and  $|1\rangle$ , such that

$$\hat{U} = |0\rangle\langle 1| + |1\rangle\langle 0| \equiv \hat{X},$$

so that a NOT gate is actually an **X gate**.



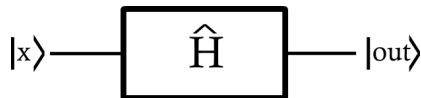
## III.2. Single-qubit gates



A **Z gate** (phase flip) is a unitary operator such that if the qubit is  $|1\rangle$ , its phase is shifted by  $\pi$ , and nothing if the qubit is  $|0\rangle$ .

$$\hat{U} = |0\rangle\langle 0| - |1\rangle\langle 1| \equiv \hat{Z}.$$

## III.2. Single-qubit gates



The Hadamard gate is one of the most important gates for quantum circuits.

$$\hat{H} \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Remark:

$$\hat{H} = \hat{R}_Y\left(\frac{\pi}{2}\right) \hat{Z}.$$

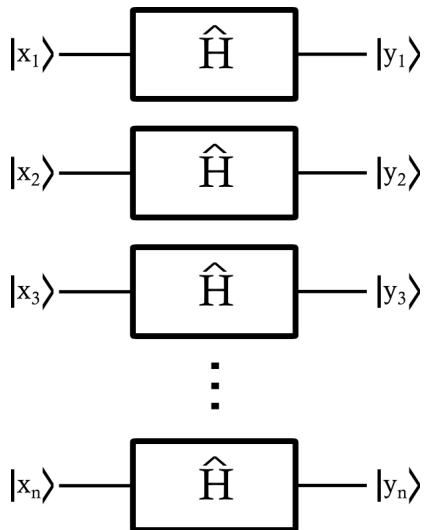
## III.2. Single-qubit gates

The Hadamard gate allows to transform a pure state ( $|0\rangle$  or  $|1\rangle$ ) into a superposition of states such as

$$\frac{1}{\sqrt{2}} (|0\rangle + |1\rangle), \quad \text{or} \quad \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle).$$

The Hadamard gate is a key gate to fully exploit quantum superposition.

## III.2. Single-qubit gates



Case of a quantum register:

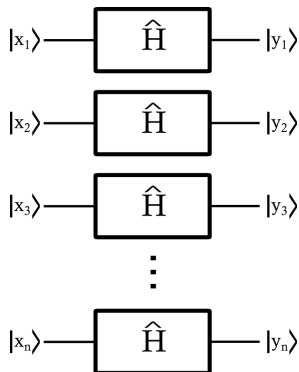
$$\begin{aligned} |x\rangle &= |x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_N\rangle \\ &= \bigotimes_{i=1}^N |x_i\rangle, \end{aligned}$$

$$\begin{aligned} |y\rangle &= |y_1\rangle \otimes |y_2\rangle \otimes \cdots \otimes |y_N\rangle \\ &= \bigotimes_{i=1}^N |y_i\rangle. \end{aligned}$$

$$\Rightarrow |y\rangle = \mathcal{H}^{\otimes n} |x\rangle = ?$$

## III.2. Single-qubit gates

If  $N = 1$



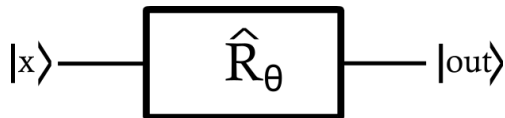
$$\begin{aligned}\hat{H}|x\rangle &= \frac{1}{\sqrt{2}} (|0\rangle + (-1)^x |1\rangle), \quad x \in \{0, 1\} \\ &= \frac{1}{\sqrt{2}} ((-1)^{0 \cdot x} |0\rangle + (-1)^{1 \cdot x} |1\rangle), \\ &= \frac{1}{\sqrt{2}} \sum_{K \in \{0,1\}} (-1)^{K \cdot x} |K\rangle.\end{aligned}$$

If  $N \in \mathbb{N}$

$$\hat{H}^{\otimes n} |x\rangle = \bigotimes_{i=1}^n \left( \frac{1}{\sqrt{2}} \sum_{K_i \in \{0,1\}} (-1)^{K_i \cdot x_i} |K_i\rangle \right),$$

$$\hat{H}^{\otimes n} |x\rangle = \frac{1}{\sqrt{2^n}} \sum_{K \in \{0,1\}^n} (-1)^{\langle K|x \rangle} |K\rangle.$$

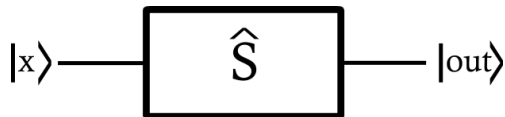
## III.2. Single-qubit gates



Phase gate

$$\hat{R}_\theta = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix} = |0\rangle\langle 0| + e^{i\theta} |1\rangle\langle 1|.$$

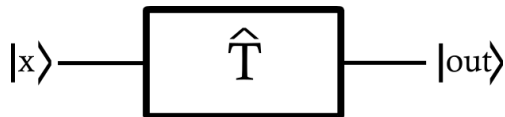
## III.2. Single-qubit gates



**S-gate** is a phase gate in the particular case where  $\theta = \pi/2$ .

$$\hat{S} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} = |0\rangle\langle 0| + i|1\rangle\langle 1|.$$

## III.2. Single-qubit gates



**T-gate** is a phase gate in the particular case where  $\theta = \frac{\pi}{4}$ .

$$\hat{T} = \begin{pmatrix} 1 & 0 \\ 0 & e^{j\frac{\pi}{4}} \end{pmatrix} = |0\rangle\langle 0| + e^{j\frac{\pi}{4}} |1\rangle\langle 1|.$$



## III.2. Quantum circuits and quantum algorithms

- 1 Initialization of qubits in a pure state (e.g.  $|0\rangle^{\otimes n} = |0\rangle \cdots |0\rangle$ ).
- 2 Set the system in a superposition of states.
- 3 Unitary manipulation of qubits.
- 4 Measurement of qubits.

These four steps are the main steps of a quantum algorithm.

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