

## Quantum Mechanics postulates

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## Quantum Mechanics postulates

Introduction to Quantum Computing

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2 Classical bits VS quantum bits



- Hilbert space
- Multiparticule quantum states
- Measurements





#### Hilbert space

Multiparticule quantum states

Measurements

2 Classical bits VS quantum bits



A quantum system is described by a quantum state, formally a vector of a Hilbert space  $\mathcal{H}$ .

<u>Dirac notation</u> : used to describe quantum states of a system. Let  $(a, b) \in \mathbb{C}^d$  and an Hilbert space of dimension  $d \times d$ , noted  $\mathcal{H}$ .

$$\mathsf{ket}: \ |a\rangle = \begin{pmatrix} a_1 \\ \vdots \\ a_d \end{pmatrix} \in \mathcal{H},$$

A bra is the complex conjugated and transposed of a ket.

bra : 
$$\langle b| = |b\rangle^{\dagger} = \begin{pmatrix} b_1 \\ \vdots \\ b_d \end{pmatrix}^{\dagger} = \begin{pmatrix} b_1^* & \dots & b_d^* \end{pmatrix}.$$



A braket is a scalar product of two vectors

$$\mathbf{braket}: \langle b|a\rangle = a_1b_1^* + \dots + a_db_d^* = \langle a|b\rangle \ ^* \in \mathbb{C}.$$

Particular case

 $\langle a | a \rangle = \| | a \rangle \|^2 \in \mathbb{R}^+$  is the norm of the state  $| a \rangle$ .

If a ket describes a physical state, the conservation of probability imposes

$$\langle \psi | \psi 
angle \; = 1$$
 .

All quantum states are normalized.



Let  $\{|\alpha_1\rangle, \cdots, |\alpha_d\rangle\}$  a basis of  $\mathcal{H}$  and eigenvectors of an observable  $\hat{A}$ .

$$egin{array}{l} eta \mid \psi 
ightarrow \in \mathcal{H}, \exists (a_1, \cdots, a_d) ext{ such that } \end{array}$$

$$|\psi\rangle = a_1 |\alpha_1\rangle + \cdots + a_d |\alpha_d\rangle = \sum_{i=1}^d a_i |\alpha_i\rangle.$$

 $P = |\langle \alpha_i | \psi \rangle |^2 = |a_i|^2$  is the probability that a measurement of  $\hat{A}$  of the quantum state  $|\psi \rangle$  gives  $|\alpha_i \rangle$  as result.



#### Example of observables:

- position  $\hat{\vec{R}} = (\hat{X}, \hat{Y}, \hat{Z});$ impulsion  $\hat{\vec{P}} = (\hat{P}_X, \hat{P}_Y, \hat{P}_Z);$ hamiltonian  $\hat{H} \iff \text{energy};$ orbital momentum  $\hat{\vec{L}} = (\hat{L}_X, \hat{L}_Y, \hat{L}_Z);$ 
  - spin momentum  $\hat{\vec{S}} = (\hat{S}_X, \hat{S}_Y, \hat{S}_Z);$



### I.1. Hilbert space

ket-bra:

$$|a\rangle\langle b| = egin{pmatrix} a_1b_1^* & a_1b_2^* & \cdots & a_1b_d^* \ a_2b_1^* & \ddots & \ddots & \vdots \ \vdots & \ddots & \ddots & \vdots \ a_db_1^* & \cdots & \cdots & a_db_d^* \end{pmatrix}.$$

A  $d \times d$  matrix is an operator on  $\mathcal{H}$ .

Examples:

 $\blacksquare$  Projector on a state  $|\psi\,\rangle$ 

$$P_{|\psi\rangle} = |\psi\rangle \langle \psi|.$$

Projector on a subspace defined by a basis  $\{|\beta_1\rangle, \cdots, |\beta_p\rangle\}$ 

$$P = \sum_{i=1}^{p} |\beta_i\rangle\langle\beta_i|.$$



Hilbert space

#### Multiparticule quantum states

Measurements





### I.2. Multiparticule quantum states

We use tensor product to describe multiple particle states

$$|a\rangle \otimes |b\rangle = \begin{pmatrix} a_1 \\ \vdots \\ a_d \end{pmatrix} \otimes \begin{pmatrix} b_1 \\ \vdots \\ b_d \end{pmatrix} = \begin{pmatrix} a_1b_1 \\ a_1b_2 \\ \vdots \\ a_2b_1 \\ \vdots \\ a_db_d \end{pmatrix}$$

**Example:** system A is in state  $|\psi_A\rangle$ , system B is in state  $|\psi_B\rangle$ . The total system  $\{A \bigcup B\}$  is

$$|\psi\rangle = |\psi_{\mathsf{A}}\rangle \otimes |\psi_{\mathsf{B}}\rangle,$$

sometimes noted

$$|\psi\rangle = |\psi_A\psi_B\rangle = |\psi_A\rangle |\psi_B\rangle.$$



A state  $|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$  is a state of the total system but a state of  $\{A \bigcup B\}$  might not necessarily be written as a tensor product of two states of A and B. In the latter case, particules are so-called **entangled**.

#### Example:

- $|\psi_{A,1}\rangle$  and  $|\psi_{A,2}\rangle$  two states of A;
- $|\psi_{B,1}\rangle$  and  $|\psi_{B,2}\rangle$  two states of *B*;

then,

$$\left|\psi\right\rangle = \frac{1}{\sqrt{2}} \left(\left|\psi_{A,1}\right\rangle \left|\psi_{B,1}\right\rangle + \left|\psi_{A,2}\right\rangle \left|\psi_{B,2}\right\rangle\right),$$

is entangled.



#### But the following state is not entangled

$$\begin{aligned} |\psi\rangle &= \frac{1}{2} \left( |\psi_{A,1}\rangle + |\psi_{A,2}\rangle \right) \otimes \left( |\psi_{B,1}\rangle + |\psi_{B,2}\rangle \right), \\ &= \frac{1}{2} \left( |\psi_{A,1}\rangle |\psi_{B,1}\rangle + |\psi_{A,1}\rangle |\psi_{B,2}\rangle \right. \\ &+ \left|\psi_{A,2}\rangle |\psi_{B,1}\rangle + \left|\psi_{A,2}\rangle |\psi_{B,2}\rangle \right). \end{aligned}$$



- Hilbert space
- Multiparticule quantum states
- Measurements





A measurement is performed by a detector sensitive to an observable. We choose orthogonal bases states to describe and measure quantum states. Let's consider an observable  $\hat{A}$  used for measurements, of eigenvectors  $\{|\alpha_1\rangle, \cdots, |\alpha_d\rangle\}$ . The probability to measure the eigenvalue  $\lambda_i$  of the eigenvector  $|\alpha_1\rangle$  for a state  $|\psi\rangle$  is

$$P_i = |\langle \alpha_i | \psi \rangle |^2$$
.

If the measurement of  $\hat{A}$  provides the value  $\lambda_i$ , the state  $|\psi\rangle$  collapses after measurement on state  $|\alpha_i\rangle$ .

It's a so-called projective measurement.



#### 2 Classical bits VS quantum bits

- Classical information
- Digitization
- Classical logical gates
- Classical computing circuit
- Notion of qubit
- Dynamics of a qubit
- Manipulation of a qubit
- Exponential operator



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## II.1. Classical information

Classical information is encoded in bits. Instead of using a decimal system, computers are using binary system for calculation due to its simplicity.

Multiplying by 2 is performed by adding a 0.

 $11 \times 2 = 22$  in decimal system;

 $11_{10} = 1011_2$  and  $22_{10} = 10110_2$ ;

 $\Rightarrow$  1011  $\times$  10 = 10110 in binary system.

 Dividing by 2 is performed by removing the last number corresponding to the rest of the division

 $11 \div 2 = 5$  rest 1 in decimal system;

 $1011 \div 10 = 101$  rest 1 in binary system.

In classical information, a bit is a unit of a binary number : 0110101...

In the hardware, it might correspond to the state of a transistor, a voltage, or a flux of photons in an optic fiber. It might take only two values: either 1 or 0.

Usually, information is encoded on 8 bits, so-called an octet. It's related to base 3  $(2^3 = 8)$ .

1 octet = 8 bits =  $2^8 = 256$  numbers encoded.

Hexadecimal is often used to have a more compact description of binary numbers. It's a base  $16 = 2^4$ , noted

$$0, 1, \dots, 9, A, B, C, D, E$$
 and  $F$ .



Each batch of 4 bits is a binary representation of a number in base 16.

$$\begin{array}{ll} A_{16} = 10_{10} = 1010_2 & D_{16} = 13_{10} = 1101_2 \\ B_{16} = 11_{10} = 1011_2 & E_{16} = 14_{10} = 1110_2 \\ C_{16} = 12_{10} = 1100_2 & F_{16} = 15_{10} = 1111_2 \end{array}$$

Example:

$$10101101110_2 = \underbrace{101}_{5} \vdots \underbrace{0110}_{6} \vdots \underbrace{1110}_{E} = 56E_{16} = 1390_{10}.$$



A bit might take only two values : 0 or 1.

An ensemble of bits permits to encode an integer number.

Information is stored as a succession of bits: 011001010...

1 and 0 might be seen as logical values : TRUE or FALSE.

A classical numerical calculation is performed by the mean of **logic** gates: NOT, OR, XOR, C-NOT,...



### 2 Classical bits VS quantum bits

Classical information

#### Digitization

- Classical logical gates
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Digitization corresponds to the process that convert a decimal number into a digital number (binary).

Let  $(n, N) \in \{0, 1\}^N$  such that

$$n=\sum_{i=0}^N a_i\times 2^i,$$

where  $\{a_i\}$  is then the digital number corresponding to n

$$n \leftrightarrow a_N a_{N-1} a_{N-2} \cdots a_2 a_1 a_0.$$

With N bits, one might encode  $2^N$  integer numbers.



Example: coding on 4 bits.

$$\begin{split} 1 &= 0 \times 2^3 + 0 \times 2^2 + 0 \times 2^1 + 1 \times 2^0 &\leftrightarrow \quad 0001, \\ 2 &= 0 \times 2^3 + 0 \times 2^2 + 1 \times 2^1 + 0 \times 2^0 &\leftrightarrow \quad 0010, \\ 3 &= 0 \times 2^3 + 0 \times 2^2 + 1 \times 2^1 + 1 \times 2^0 &\leftrightarrow \quad 0011, \\ 4 &= 0 \times 2^3 + 1 \times 2^2 + 0 \times 2^1 + 0 \times 2^0 &\leftrightarrow \quad 0100. \end{split}$$

Only positive integers might be converted to binaries.



For a real number (a "floating" number), one converts it as an integer and the power of 10 corresponding. For example

$$1.321 = \underbrace{1321}_{\text{integer}} \cdot 10^{-3} \nwarrow_{\text{signe + integer}} .$$

The larger is the precision on the number, the larger the number of coding bits required will be. The choice of the number of bits coding is a compromise between the precision required, the memory available, the fastness of acquisition or the fastness of calculation.

Precise calculations are "slow" and requires memory.



#### Examples

Coding in 8 bits (1 octet)

$$n_{max} = 2^8 - 1 = 255 \rightarrow \text{coding } n \in [0, 255].$$

Coding in 16 bits

 $n_{max} = 2^{16} - 1 = 65535 \text{ values} \rightarrow \text{ coding } n \in [0, 65535].$ 

<u>Color scales</u> Gray scales: 8 bits  $\rightarrow$  256 values.



Color coding Red, Green, Blue: RGB coding.

8 bits for red R, 8 bits for green G, 8 bits for blue B.

 $8 \times 3 = 24$  bits for color coding.

 $n_{max} = 2^{24} - 1 = 16777216 \approx 16$  millions of color available.



#### 2 Classical bits VS quantum bits

- Classical information
- Digitization

#### Classical logical gates

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## AND gate



A	В	$A \cdot B$
0	0	0
0	1	0
1	0	0
1	1	1



# OR gate







## XOR gate



A	В	$A \oplus B$
0	0	0
0	1	1
1	0	1
1	1	0



# NOT gate







## NAND gate



A	В	$\overline{A \cdot B}$
0	0	1
0	1	1
1	0	1
1	1	0



# NOR gate



Α	В	$\overline{A+B}$
0	0	1
0	1	0
1	0	0
1	1	0



## XNOR gate



A	В	$A \odot B$
0	0	1
0	1	0
1	0	0
1	1	1



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Logic gate and more generally electronical circuit are made from basic elements like capacitor or transistor: classical physics, no quantum effects, no state superposition.

Moors's law: downsizing the key element of a processor, the transistor.

On chip, density of transistors doubles each 18 months.

Intel Core i7 8th generation (2017): 14nm transistors!



IBM has announced in 2017 being able to produce chips with 5nm transistors!

#### IBM roadmap 2014:

- quantum effects are no longer negligeable;
- new materials ? (post-silicon era);
- toward quantum computing ? ⇒ changing radically the vision of computing!

Instead of dealing with quantum effects, exploiting them for calculation: **new vision of computing!** 



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The simplest quantum system is a two-state system (so-called two-level system).

E.g.: spin 1/2 in a  $\vec{B}$  field, polarization of a photon,...

Let consider the case of a spin 1/2 in a  $\vec{B}$  field. The Hlbert space associated if of dimension  $2 \times 2$ , of the following basis

 $\mathcal{B}=\{|\!\uparrow\rangle,|\!\downarrow\rangle\}.$ 

In the context of quantum information, those two states are labelled as  $|0\rangle$  and  $|1\rangle$  (e.g.  $|\uparrow\rangle = |1\rangle$  and  $|\downarrow\rangle = |0\rangle$ ) and are the quantum equivalent of the classical bits 0 and 1.



## II.5. Notion of qubit

What is the main difference between a classical bit and a quantum qubit ?

Classical bitQubit0 or 1 $|0\rangle$  or  $|1\rangle$ OR $\alpha |0\rangle + \beta |1\rangle$ 

The huge difference with a qubit is the possibility to be a superposition of  $|0\,\rangle$  and  $|1\,\rangle$ 

 $\Rightarrow$  quantum parallelism .

It's the key point that will permit to a quantum computer to speed up calculations compared to a classical computer.



Quantum superpositions allow to perform calculation on many states **at the same time**.

 $\rightarrow$  Quantum algorithms with exponential speed-up.

**BUT** once we measure the superposition of states, it collapses to one of its states. Therefore, we can only get one "answer" and not all answers to all states in the superposition.

Then, it is not that easy to design quantum algorithms, but we can use interference effects.



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The time evolution of a state  $|\psi\rangle$  of a closed quantum system is described by the Schrödinger equation

$$i\hbar rac{\mathrm{d}}{\mathrm{d}t} \ket{\psi(t)} = \hat{H}(t) \ket{\psi(t)},$$

where  $\hat{H}(t)$  is the hamiltonian. A closed quantum system does not interact with any other systems. When  $\hat{H}(t) = \hat{H}$  is not time dependent, the general solution is

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



### $\hat{H}$ is hermitian

$$\hat{H}^{\dagger} = \hat{H} \Rightarrow \left(\hat{H} |\psi\rangle\right)^{\dagger} = \langle \psi | \hat{H}.$$

Spectral decomposition of  $\hat{H}$ 

$$\hat{H} = \sum_{i} E_{i} |\psi_{i}\rangle \langle \psi_{i}|,$$

with eigenvalues  $E_i$  and eigenvectors  $|\psi_i\rangle$ .

The smallest value of  $E_i = E_0$  is the ground state energy with the corresponding eigenstate  $|\psi_0\rangle$ .



Example: two-level system (e.g. electron spin in a B field).





### II.6. Dynamics of a qubit

$$\begin{array}{l} \text{If } |\psi(0)\rangle = |0\rangle \Rightarrow |\psi(t)\rangle = e^{i\frac{\omega t}{2}}|0\rangle; \\ \text{If } |\psi(0)\rangle = |1\rangle \Rightarrow |\psi(t)\rangle = e^{-i\frac{\omega t}{2}}|1\rangle; \\ \text{If } |\psi(0)\rangle = \alpha |0\rangle + \beta |1\rangle, \ |\alpha|^2 + |\beta|^2 = 1, \text{ then} \\ |\psi(t)\rangle = \alpha e^{i\frac{\omega t}{2}}|0\rangle + \beta e^{-i\frac{\omega t}{2}}|1\rangle, \\ = e^{i\frac{\omega t}{2}}(\alpha |0\rangle + \beta e^{-i\omega t}|1\rangle). \end{array}$$

The global phase of a quantum state is not relevant for the final probability of a measurement (equivalent to a choice of energies' origine). So it is equivalent to the following state

$$|\psi(t)\rangle = \alpha |0\rangle + \beta e^{-i\omega t} |1\rangle$$



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A two level state might be manipulated by applying external operation on it. The total probability is conserved. Let call  $\hat{U}$  the operator applied

$$|\psi'\rangle = \hat{U}|\psi\rangle.$$

And the probability is conserved

$$\langle \psi' | \psi' \rangle = \langle \psi | \psi \rangle \Rightarrow \langle \psi | \hat{U}^{\dagger} \hat{U} | \psi \rangle = \langle \psi | \psi \rangle.$$

The operator  $\hat{U}$  preserves the norm of a vector: it is a unitary opertor properties.

$$\hat{U}$$
 is unitary  $\Leftrightarrow \ \hat{U}^\dagger \hat{U} = \hat{U} \hat{U}^\dagger = \mathbb{I}.$ 



Let note  $\alpha$  an eigenvalue of  $\hat{U}$ 

$$\hat{U} | \alpha \rangle = \alpha | \alpha \rangle,$$
  
 $\Rightarrow \langle \alpha | \hat{U}^{\dagger} \hat{U} | \alpha \rangle = | \alpha |^{2} = 1.$ 

Then,

$$\alpha = e^{j\theta_{\alpha}}, \ \theta_{\alpha} \in \mathbb{R}.$$

Eigenvalues of  $\hat{U}$  are complexe values with a unitary modulus:  $|\alpha| = 1$ .



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### II.8. Exponential operator

Let  $\hat{A}$  being an operator on a quantum system. The exponential operator is defined as follow

$$\exp\left(i\hat{A}x\right) = \sum_{n=0}^{+\infty} \frac{\left(i\hat{A}x\right)^n}{n!}, \text{ with } x \in \mathbb{R}.$$

In the particular case where  $\hat{A}^2 = \mathbb{I}$ , then

$$\exp\left(i\hat{A}x\right) = \sum_{p=0}^{+\infty} \frac{\left(i\hat{A}x\right)^{2p}}{2p!} + \sum_{p=0}^{+\infty} \frac{\left(i\hat{A}x\right)^{2p+1}}{(2p+1)!},$$
$$= \sum_{p=0}^{+\infty} \frac{(ix)^{2p}}{2p!} + \sum_{p=0}^{+\infty} \frac{(ix)^{2p+1}}{(2p+1)!}\hat{A}.$$

Then,  $orall \hat{A}$  such that  $\hat{A}^2 = \mathbb{I}$ ,

$$\exp\left(i\hat{A}x\right) = \cos x + i\sin x\hat{A}.$$



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