Quantum Mechanics postulates

Introduction to Quantum Computing

Kenneth MAUSSANG

Université de Montpellier

Ecole Centrale Casablanca

2020 – 2021

Quantum Mechanics postulates

1 Quantum states

2 Classical bits VS quantum bits

Quantum Mechanics postulates

1 Quantum states
- Hilbert space
- Multiparticule quantum states
- Measurements

2 Classical bits VS quantum bits

1. Quantum states
   - Hilbert space
   - Multiparticule quantum states
   - Measurements

2. Classical bits VS quantum bits

I.1. Hilbert space

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

Dirac notation : 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 $\mathcal{H}$.

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

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

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

I.1. Hilbert space

A braket is a scalar product of two vectors

$$\textbf{braket} : \langle b|a\rangle = a_1 b_1^* + \cdots + a_d b_d^* = \langle a|b\rangle^* \in \mathbb{C}.$$

Particular case

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

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

$$\boxed{\langle\psi|\psi\rangle = 1}.$$

All quantum states are normalized.

I.1. Hilbert space

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

$$\forall |\psi\rangle \in \mathcal{H}, \exists (a_1, \cdots, a_d) \text{ such that}$$

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

$P = |\langle\alpha_i|\psi\rangle|^2 = |a_i|^2$ 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 $\hat{H}$ ($\Leftrightarrow$ energy);
- orbital momentum $\hat{\vec{L}} = (\hat{L}_X, \hat{L}_Y, \hat{L}_Z)$;
- spin momentum $\hat{\vec{S}} = (\hat{S}_X, \hat{S}_Y, \hat{S}_Z)$;

ket-bra:

$$|a\rangle\langle b| = \begin{pmatrix} a_1 b_1^* & a_1 b_2^* & \cdots & a_1 b_d^* \\ a_2 b_1^* & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ a_d b_1^* & \cdots & \cdots & a_d b_d^* \end{pmatrix}.$$

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

Examples:

- Projector on a state $|\psi\rangle$

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

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

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

Quantum Mechanics postulates

1 Quantum states
- Hilbert space
- Multiparticule quantum states
- Measurements

2 Classical bits VS quantum bits

We use tensor product to describe multiple particle states

$$|a\rangle \otimes |b\rangle = \begin{pmatrix} a_1 \\ \vdots \\ a_d \end{pmatrix} \otimes \begin{pmatrix} b_1 \\ \vdots \\ b_d \end{pmatrix} = \begin{pmatrix} a_1 b_1 \\ a_1 b_2 \\ \vdots \\ a_2 b_1 \\ \vdots \\ a_d b_d \end{pmatrix}.$$

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

$$|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle,$$

sometimes noted

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

I.2. Multiparticule quantum states

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,

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

is entangled.

But the following state is **not entangled**

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

1 Quantum states
- Hilbert space
- Multiparticule quantum states
- Measurements

2 Classical bits VS quantum bits

I.3. 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 λ_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 λ_i, the state $|\psi\rangle$ collapses after measurement on state $|\alpha_i\rangle$.

It's a so-called **projective measurement.**

1 Quantum states

2 Classical bits VS quantum bits
- Classical information
- Digitization
- Classical logical gates
- Classical computng circuit
- Notion of qubit
- Dynamics of a qubit
- Manipulation of a qubit
- Exponential operator

1 Quantum states

2 Classical bits VS quantum bits
- Classical information
- Digitization
- Classical logical gates
- Classical computng circuit
- Notion of qubit
- Dynamics of a qubit
- Manipulation of a qubit
- Exponential operator

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.

$$11 \times 2 = 22 \text{ in decimal system;}$$

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

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

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

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

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

II.1. Classical information

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 ($2^3 = 8$).

$$1 \text{ octet} = 8 \text{ bits} = 2^8 = 256 \text{ numbers encoded.}$$

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

$$0, 1, \cdots, 9, A, B, C, D, E \text{ and } F.$$

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:

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

II.1. Classical information

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,...

1 Quantum states

2 Classical bits VS quantum bits
- Classical information
- Digitization
- Classical logical gates
- Classical computng circuit
- Notion of qubit
- Dynamics of a qubit
- Manipulation of a qubit
- Exponential operator

II.2. Digitization

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.

$$1 = 0 \times 2^3 + 0 \times 2^2 + 0 \times 2^1 + 1 \times 2^0 \quad \leftrightarrow \quad 0001,$$
$$2 = 0 \times 2^3 + 0 \times 2^2 + 1 \times 2^1 + 0 \times 2^0 \quad \leftrightarrow \quad 0010,$$
$$3 = 0 \times 2^3 + 0 \times 2^2 + 1 \times 2^1 + 1 \times 2^0 \quad \leftrightarrow \quad 0011,$$
$$4 = 0 \times 2^3 + 1 \times 2^2 + 0 \times 2^1 + 0 \times 2^0 \quad \leftrightarrow \quad 0100.$$

Only positive integers might be converted to binaries.

II.2. Digitization

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

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

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)

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

Coding in 16 bits

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

Color scales Gray scales: 8 bits $\rightarrow$ 256 values.

II.2. Digitization

Color coding Red, Green, Blue: **RGB coding**.

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

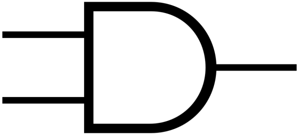
$8 \times 3 = 24$ bits for color coding.

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

1 Quantum states

2 Classical bits VS quantum bits
- Classical information
- Digitization
- Classical logical gates
- Classical computng circuit
- Notion of qubit
- Dynamics of a qubit
- Manipulation of a qubit
- Exponential operator

AND gate

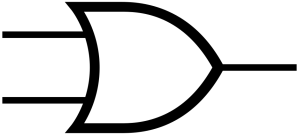


$$A \cdot B$$

Truth table

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

OR gate

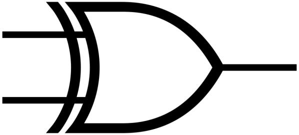


$$A + B$$

Truth table

A	B	$A + B$
0	0	0
0	1	1
1	0	1
1	1	1

XOR gate

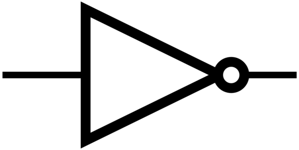


$$A \oplus B$$

Truth table

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

NOT gate

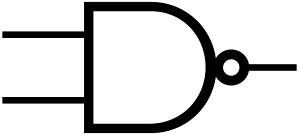


$\bar{A}$

Truth table

A	$\bar{A}$
0	1
1	0

NAND gate

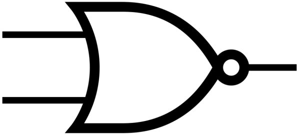


$$\overline{A \cdot B}$$

Truth table

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

NOR gate

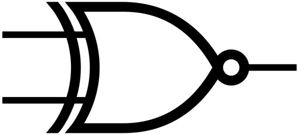


$$\overline{A+B}$$

Truth table

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

XNOR gate



$$A \odot B$$

Truth table

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

1 Quantum states

2 Classical bits VS quantum bits
- Classical information
- Digitization
- Classical logical gates
- Classical computng circuit
- Notion of qubit
- Dynamics of a qubit
- Manipulation of a qubit
- Exponential operator

II.4. Classical logical gates

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 ?
  $\Longrightarrow$ **changing radically the vision of computing!**

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

1 Quantum states

2 Classical bits VS quantum bits
- Classical information
- Digitization
- Classical logical gates
- Classical computng circuit
- Notion of qubit
- Dynamics of a qubit
- Manipulation of a qubit
- Exponential operator

II.5. Notion of qubit

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 2×2, 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.

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

Classical bit	**Qubit**
0 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 $|1\rangle$

$$\Rightarrow \boxed{\text{quantum parallelism}}.$$

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.

Quantum Mechanics postulates

1 Quantum states

2 Classical bits VS quantum bits
- Classical information
- Digitization
- Classical logical gates
- Classical computng circuit
- Notion of qubit
- Dynamics of a qubit
- Manipulation of a qubit
- Exponential operator

II.6. Dynamics of a qubit

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

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\,|\psi(t)\rangle = \hat{H}(t)\,|\psi(t)\rangle,$$

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

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

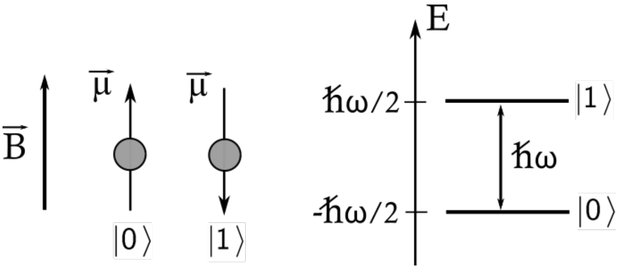
Spectral decomposition of $\hat{H}$

$$\hat{H} = \sum_i E_i\,|\psi_i\rangle\langle\psi_i|,$$

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).



$$\hat{H} = -\frac{\hbar\omega}{2}\left(|0\rangle\langle 0| - |1\rangle\langle 1|\right).$$

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

$$\begin{aligned} |\psi(t)\rangle &= \alpha e^{i\frac{\omega t}{2}}\,|0\rangle + \beta e^{-i\frac{\omega t}{2}}\,|1\rangle, \\ &= e^{i\frac{\omega t}{2}}\left(\alpha\,|0\rangle + \beta e^{-i\omega t}\,|1\rangle\right). \end{aligned}$$

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

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

1 Quantum states

2 Classical bits VS quantum bits
- Classical information
- Digitization
- Classical logical gates
- Classical computng circuit
- Notion of qubit
- Dynamics of a qubit
- Manipulation of a qubit
- Exponential operator

II.7. Manipulation of a qubit

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

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

And the probability is conserved

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

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

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

Let note α 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: $|\alpha| = 1$.

Quantum Mechanics postulates

1 Quantum states

2 Classical bits VS quantum bits
- Classical information
- Digitization
- Classical logical gates
- Classical computng circuit
- Notion of qubit
- Dynamics of a qubit
- Manipulation of a qubit
- Exponential operator

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

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

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

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