

## Summary of Chapter 2

This note is a summary of Chapter 2 of [1]. It is a short introduction to Quantum Mechanics that aims at understanding some of the theoretical foundations of Quantum Computation.

Consider a particle of mass  $m$  moving within a 1-dimensional space. Then, according to the classical Newtonian Mechanics, its energy can be expressed as

$$E = \frac{p^2}{2m} + V(x) , \quad (1)$$

where  $p = mv$  is the momentum and  $V$  the potential energy. The latter is the work done on the particle to move it from its initial position to its current position.

Quantum Mechanics associates a wave function to the particle and substitutes the concepts of momentum and potential energy by operators acting on the wave function.

### 1. Wave function and Schrödinger equation

According to quantum mechanics, all particles can be represented by a wave function  $\psi(x,t)$ , that is, a complex function of two real variables (1-dimensional case), namely the coordinate  $x$  and the time  $t$ . The physical meaning of  $\psi(x,t)$  is the following: at any time  $t$ , the module  $|\psi(x,t)|$  of the wave function is the square root of the probability that the particle coordinate is equal to  $x$ . In particular, integrating  $|\psi(x,t)|^2$  all along the particle domain, the result should be equal to 1.

The wave function  $\psi(x,t)$  must satisfy the Schrödinger equation:

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x) \psi(x,t) \quad (2)$$

where  $2\pi\hbar = h = 6.63 \cdot 10^{-34} \text{ Js}$  is the Planck constant.

## 2. Hamiltonian

Define two operators,  $\hat{p}$  and  $\hat{x}$ , that operate on the set of complex functions of real variables  $x$  and  $t$ :

$$f(x,t) \xrightarrow{\hat{p}} -i\hbar \frac{\partial f(x,t)}{\partial x}, f(x,t) \xrightarrow{\hat{x}} xf(x,t). \quad (3)$$

They are non-commutative operators as  $\hat{x} \cdot \hat{p} \neq \hat{p} \cdot \hat{x}$ . Given a function  $f(x,t)$ , simple derivative calculus show that  $\hat{x} \cdot \hat{p} f(x,t) - \hat{p} \cdot \hat{x} f(x,t) = i\hbar f(x,t)$ . Thus

$$\hat{x} \cdot \hat{p} - \hat{p} \cdot \hat{x} = i\hbar. \quad (4)$$

Operators that are functions of the operator  $\hat{x}$  can be defined: if  $g$  is a complex function of a real variable  $x$ , then  $g(\hat{x})$  is an operator that executes the operation

$$f(x,t) \xrightarrow{g(\hat{x})} g(x)f(x,t). \quad (5)$$

Then (2) can be expressed as

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \left( \frac{\hat{p}^2}{2m} + V(\hat{x}) \right) \psi(x,t). \quad (6)$$

The previous relation suggests the definition of another operator

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}), \quad (7)$$

so that the Schrödinger equation (2) becomes

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \hat{H} \psi(x,t). \quad (8)$$

The operator  $\hat{H}$  is the Hamiltonian of the system. Comparing (1) and (7), it appears that  $\hat{H}$  is derived from the system energy, as calculated in classical mechanics, by substituting the momentum  $p$  and the potential energy  $V(x)$  by operators  $\hat{p}$  and  $V(\hat{x})$ .

Observe that  $\hat{p}$  and  $V(\hat{x})$  are lineal operators, and thus so is  $\hat{H}$ .

### 3. Solutions of the Schrödinger equation

One of the principles of quantum mechanics (de Broglie's hypothesis) is that all particles are associated with waves, and that the energy of a photon is proportional to the wave frequency, namely  $E = hf = \hbar\omega$ . For that reason, the solutions of (8) are assumed to be lineal combinations of functions

$$\psi_l(x, t) = e^{-i\omega_l t} \psi_l(x), \quad (9)$$

with  $\omega_0 < \omega_1 < \omega_2 \dots$ , and to every particular solution (9) corresponds a value

$$E_l = \hbar\omega_l \quad (10)$$

of the particle energy. As already mentioned above, the integral of  $|\psi(x)|^2$  along the particle domain, must be equal to 1. Thus, the general form of a solution is

$$\psi(x, t) = \sum_l c_l \psi_l(x, t), \quad (11)$$

where the coefficients  $c_l$  are complex numbers whose modules  $|c_l|$  are equal to the square root of the probability that the particle energy is equal to  $E_l$ .

From (9), (10) and (11), a simple derivative calculus shows that

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = \sum_l c_l E_l \psi_l(x, t). \quad (12)$$

Thus, according to (8),

$$\hat{H} \psi(x, t) = \sum_l c_l E_l \psi_l(x, t).$$

This relation demonstrates the fundamental property of the Hamiltonian operator: the values of the particle energy are the eigenvalues of the Hamiltonian, and the corresponding eigenfunctions are the functions  $\psi_l(x, t)$ .

#### 4. Vector space

The expression (11) suggests the definition of a vector space  $V$  over the field  $C$  of complex numbers. In order to simplify the presentation assume that the possible values of the particle energy belong to a finite set  $\{E_0, E_1, \dots, E_{d-1}\}$ . Within the frame of quantum computation this is an assumable assumption. It means that  $|c_l|^2 \cong 0$  if  $l \geq d$ . Then define the space vector  $V$  over  $C$  generated by the set

$$S = \{\psi_0(x,t), \psi_1(x,t), \dots, \psi_{d-1}(x,t)\}. \quad (13)$$

It consists of all lineal combinations

$$\psi(x,t) = \sum_{l=0}^{d-1} c_l \psi_l(x,t). \quad (14)$$

The vector addition and the scalar multiplication are trivially defined as they amount to operations over the complex field. Furthermore, according to definition (9), none of the functions  $\psi_l(x,t)$  could be expressed as a lineal combination of other functions  $\psi_k(x,t)$  as all angular frequencies  $\omega_l$  are different. So, the spanning set  $S$  is a base of  $V$  and the dimension of  $V$  is  $d$ .

From the probabilistic interpretation of the wave function, it is assumed that if  $\psi(x,t)$  is a solution of (8), then the coefficients  $c_l$  in (14) satisfy the condition

$$|c_0|^2 + |c_1|^2 + \dots + |c_{d-1}|^2 = 1, \quad (15)$$

and that  $|c_l|^2$  is the probability that the particle energy is equal to  $E_l$ . Thus, the solutions of (8) are represented by unitary elements of  $V$ .

Consider the natural base  $S$  of  $V$ . Every function  $\psi(x,t)$  of  $V$  can be represented by a column vector, denoted by the symbol  $|\psi\rangle$ . Its components are the coefficients  $c_l$  of the representation of  $\psi(x,t)$  in base  $S$ . The adjoint row vector, composed of the complex conjugates  $c_l^*$  of the components of  $|\psi\rangle$ , is denoted by the symbol  $\langle\psi|$ . In particular, the norm

of  $|\psi\rangle$  is equal to the inner product  $\langle\psi|\psi\rangle = \langle\psi|\cdot|\psi\rangle$ , and the lineal operators over  $V$  are represented by  $d\times d$  matrices over  $C$ .

In base  $S$ , the  $k$ -th component of the vector  $|\psi\rangle$  that corresponds to the particular solutions  $\psi_l(x,t)$  is equal to 1 if  $k = l$ , and to 0 if  $k \neq l$ . So,  $S$  is an orthonormal base:  $\langle\psi_l|\psi_l\rangle = 1$ ,  $\langle\psi_l|\psi_k\rangle = 0$  if  $k \neq l$ . Obviously, any other base could be used to represent the elements of  $V$ , but preferably an orthonormal base

$$B = \{|v_0\rangle, |v_1\rangle, \dots, |v_{d-1}\rangle\}, \langle v_l|v_l\rangle = 1, \langle v_l|v_k\rangle = 0 \text{ if } k \neq l. \quad (16)$$

Once the base  $B$  has been chosen, any lineal operator  $\hat{A}$  over  $V$  can be defined by a matrix  $A$  over the complex field. Let  $H$  be the matrix representation of the Hamiltonian operator. It can be proven that  $H$  is hermitian ( $H = H^+$ ). According to the fundamental property of the Hamiltonian, the eigenvalues of  $H$  are the particle energy values  $E_0, E_1, \dots, E_{d-1}$  (real numbers). Let  $|u_0\rangle, |u_1\rangle, \dots, |u_{d-1}\rangle$  be the corresponding normalized eigenvectors ( $\langle u_l|u_l\rangle = 1$ ). According to a classical property of lineal algebra,  $H$  has a spectral decomposition

$$H = \sum_{l=0}^{d-1} E_l |u_l\rangle\langle u_l|. \quad (17)$$

Observe that the product of a  $d$ -component column vector  $|u_l\rangle$  by a  $d$ -component row vector  $\langle u_l|$  is a  $d\times d$  matrix.

## 5. Evolution

The relations (9) and (11) permit to calculate the wave function evolution during a time interval  $\Delta t$ . According to (9), with  $E_l = \hbar\omega_l$ ,

$$\psi_l(x, t+\Delta t) = e^{-i\frac{E_l}{\hbar}\Delta t} \psi_l(x, t). \quad (18)$$

The evolution of the wave function between times  $t$  and  $t+\Delta t$  can be described by an operator  $\hat{U}$  that executes the following operation:

$$\psi(x, t) = \sum_{l=0}^{d-1} c_l \psi_l(x, t) \xrightarrow{\hat{U}} \sum_{l=0}^{d-1} c_l e^{-i\frac{E_l}{\hbar}\Delta t} \psi_l(x, t). \quad (19)$$

Thus, the eigenvalues of  $\hat{U}$  are

$$e^{-i\frac{E_l}{\hbar}\Delta t}, l = 0, 1, \dots, d-1,$$

that is, complex numbers with modules equal to 1, and the eigenfunctions are the same as those of  $\hat{H}$ . Using the matrix representation  $U$ , with the same base  $B$  of  $V$  as before, it can be proven that  $U$  is unitary ( $UU^* = U^*U = I$ ) and has a spectral decomposition

$$U = \sum_{l=0}^{d-1} e^{-i\frac{E_l}{\hbar}\Delta t} |u_l\rangle\langle u_l|. \quad (20)$$

In conclusion, the quantum state of a particle can be represented by a unitary vector belonging to a vectorial space  $V$  over the complex field  $\mathbb{C}$ . The evolution of the particle state, over a time interval  $\Delta t$ , is defined by a unitary operator  $\hat{U}$  that can be derived from the Hamiltonian operator  $\hat{H}$ . Using the matrix representation of those operators, (20) is deduced from (17) by replacing  $E_l$  by

$$e^{-i\frac{E_l}{\hbar}\Delta t}, l = 0, 1, \dots, d-1.$$

Inversely, given a unitary operator  $\hat{U}$  over  $V$ , whose eigenvalues are complex numbers  $e^{-i\varphi_l}$ , where  $\varphi_l$  is a real number, and whose corresponding normalized eigenvectors in base  $B$  are  $|u_0\rangle, |u_1\rangle, \dots, |u_{d-1}\rangle$ , so that, in matrix form,

$$U = \sum_{l=0}^{d-1} e^{-i\varphi_l} |u_l\rangle\langle u_l|, \quad (21)$$

then, an operator  $\hat{H}$  can be defined. In matrix form

$$H = \sum_{l=0}^{d-1} \hbar\varphi_l |u_l\rangle\langle u_l|. \quad (22)$$

The problem of defining a physical configuration, such that the particle behavior is defined by a unitary matrix (21), amounts to finding a configuration such that the corresponding Hamiltonian is (22), generally not an easy task.

## 6. Measurement

Choosing a base  $B$  of  $V$  as before, the quantum state of the particle can be represented as

$$|\psi\rangle = c_0|v_0\rangle + c_1|v_1\rangle + \dots + c_{d-1}|v_{d-1}\rangle, |c_0|^2 + |c_1|^2 + \dots + |c_{d-1}|^2 = 1. \quad (23)$$

A measurement operator  $M$ , in base  $B$ , associates to  $|\psi\rangle$  a natural  $l \in \{0, 1, \dots, d-1\}$  and a new state vector  $|\psi'\rangle$ . It is a non-deterministic operator that works as follows:

$$M|\psi\rangle = (l, |v_l\rangle) \text{ with a probability equal to } |c_l|^2, l = 0, 1, \dots, d-1.$$

This means that a measurement operator does not give a complete description of the current quantum state. It generates the identifier of one of the vectors of  $B$ , with some associated probability. Furthermore, it collapses the particle state: if the measurement result is  $l$ , the new particle state is  $|\psi'\rangle = |v_l\rangle$ .

## 7. Systems consisting of several particles

The theory can be extended to the case of systems that are made up of several particles. Then, the quantum states are unitary vectors of a vectorial space  $V$  that, in turn, is the tensor product of  $m$  vector spaces:

$$V = V_1 \times V_2 \times \dots \times V_m.$$

If  $B_1, B_2, \dots, B_m$  are the chosen bases for spaces  $V_1, V_2, \dots, V_m$ , then the set

$$B = \{|v_1\rangle \times |v_2\rangle \times \dots \times |v_m\rangle, |v_1\rangle \in B_1, |v_2\rangle \in B_2, \dots, |v_m\rangle \in B_m\},$$

is a base of  $V$ . If the vector space dimensions are respectively equal to  $d_1, d_2, \dots, d_m$ , the dimension of  $V$  is equal to  $D = d_1 \cdot d_2 \cdot \dots \cdot d_m$ . The conclusions are qualitatively the same as in the case of a single particle. The system evolution is defined by a  $D \times D$  unitary matrix  $U$  that is derived from a  $D \times D$  hermitian matrix  $H$  (the Hamiltonian operator). The eigenvalues of  $H$  are real numbers, the eigenvalues of  $U$  are complex numbers whose norm is equal to 1, and those matrices are related by (17) and (20).

## 8. Comments

Observe that the vector space model includes two fundamental aspects of quantum mechanics: superposition and entanglement.

- According to (20), a quantum state  $|\psi\rangle$  is a superposition of quantum states  $|v_i\rangle$ , each of them with a certain probability of being identified by a measurement operation.
- According to the definition of  $V$  in the case of a system consisting of two particles, the following unitary vector

$$\frac{1}{\sqrt{2}}(|v_1\rangle \times |v_2\rangle) + \frac{1}{\sqrt{2}}(|w_1\rangle \times |w_2\rangle), |v_1\rangle \text{ and } |w_1\rangle \in B_1, |v_2\rangle \text{ and } |w_2\rangle \in B_2, (24)$$

define a quantum state in which the individual particle states are not independent: as an example, if the first particle state is  $|v_1\rangle$ , then the second particle state must be  $|v_2\rangle$  and could not be  $|w_2\rangle$ . This is because a compound state such as (24) is not necessarily the product of two individual states such as  $\frac{1}{\sqrt{2}}(|v_1\rangle + |w_1\rangle)$  and  $\frac{1}{\sqrt{2}}(|v_2\rangle + |w_2\rangle)$ , whose product is  $\frac{1}{2}(|v_1\rangle \times |v_2\rangle) + \frac{1}{2}(|v_1\rangle \times |w_2\rangle) + \frac{1}{2}(|w_1\rangle \times |v_2\rangle) + \frac{1}{2}(|w_1\rangle \times |w_2\rangle)$ .

## Reference

[1] J.P.Deschamps, Computación Cuántica, Marcombo, Barcelona, 2023.