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

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

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:

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

where $2\pi\hbar = h = 6.63\cdot10^{-34}\ Js$ 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:

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

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 $\hat{x}\cdot\hat{p}\ f(x,t) - \hat{p}\cdot\hat{x}\ f(x,t) = ihf(x,t)$. Thus

$$\hat{x}\cdot\hat{p} - \hat{p}\cdot\hat{x} = ih. \tag{4}$$

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

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

Then (2) can be expressed as

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

The previous relation suggests the definition of another operator

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

so that the Schrödinger equation (2) becomes

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

The operator $\widehat{H}$ is the Hamiltonian of the system. Comparing (1) and (7), it appears that $\widehat{H}$ 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 linear operators, and thus so is $\widehat{H}$.

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 linear combinations of functions

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

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

$$E_l = \hbar\omega_l \tag{10}$$

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

$$\psi(x,t) = \sum_l c_l\,\psi_l(x,t), \tag{11}$$

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

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

Thus, according to (8),

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

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

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

It consists of all linear combinations

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

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 linear combination of other functions $\psi_k(x,t)$ as all angular frequencies ω_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

$$|c_0|^2 + |c_1|^2 + \cdots + |c_{d-1}|^2 = 1, \tag{15}$$

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 linear operators over V are represented by $d\times d$ matrices over C.

In base S, the k-th component of the vector $|\psi_l\rangle$ 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

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

Once the base B has been chosen, any linear 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, … , E_{d-1} (real numbers). Let $|u_0\rangle$, $|u_1\rangle$, …, $|u_{d-1}\rangle$ be the corresponding normalized eigenvectors ($\langle u_l|u_l\rangle = 1$). According to a classical property of linear algebra, H has a spectral decomposition

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

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 Δt. According to (9), with $E_l = \hbar\omega_l$,

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

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:

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

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

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

that is, complex numbers with modules equal to 1, and the eigenfunctions are the same as those of $\widehat{H}$. 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

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

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 C. The evolution of the particle state, over a time interval Δt, is defined by a unitary operator $\widehat{U}$ that can be derived from the Hamiltonian operator $\widehat{H}$. Using the matrix representation of those operators, (20) is deduced from (17) by replacing E_l by

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

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

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

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

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

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

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

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

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

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:

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

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

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

is a base of V. If the vector space dimensions are respectively equal to d_1, $d_2, \ldots, d_m$, the dimension of V is equal to $D = d_1 \cdot d_2 \cdot \ldots \cdot d_m$. 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 Halmitonian 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 $|v_l\rangle$, 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

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