Introduction of Quantum Computation and Information

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1 Introduction

Quantum mechanics, often simply referred to as "quantum physics," is one of the most profound and successful theories in the realm of physics. It is the fundamental framework that governs the behavior of particles and waves on the smallest scales of the universe, where classical physics breaks down and no longer applies. At this quantum level, the rules of the game are dramatically different, often described as "weird," "counterintuitive," and even "spooky."

Quantum mechanics delves into the subatomic world, exploring the behavior of electrons, photons, atoms, and molecules. It unveils the strange phenomena that underlie the very fabric of reality, from the superposition of particles in multiple states to the intriguing concept of entanglement, where particles separated by vast distances can instantaneously influence each other's properties. Quantum mechanics is the foundation upon which modern physics, chemistry, and even cutting-edge technologies like quantum computing and quantum cryptography are built.

At its core, quantum mechanics challenges classical physics' deterministic nature, introducing probabilistic principles into the mix. It relies on mathematical descriptions and complex wave functions to predict the outcomes of experiments, often with remarkable accuracy.

This theory has given us tremendous technological advances, such as lasers, transistors, and magnetic resonance imaging (MRI) machines. But perhaps its most famous advocate, Albert Einstein, once remarked that "God does not play dice with the universe" in response to the probabilistic nature of quantum mechanics. Yet, decades of experiments have validated these probabilistic predictions.

In this realm, particles can exist in multiple places at once, change behavior depending on whether they are observed or not, and become entangled with other particles in ways that seem to defy the classical notions of time and space.

Quantum mechanics is an exciting journey into the heart of nature's mysteries. It invites us to explore the foundations of reality, where the classical world we observe with our senses transforms into a realm of uncertainty, wonder, and infinite possibilities. It has shaped our understanding of the universe and continues to inspire generations of scientists and thinkers to probe the depths of existence and the true nature of reality.

2 Foundations of Quantum Mechanics

This section introduces the mathematical foundations of quantum mechanics. While it focuses on practical aspects rather than exhaustive mathematical rigor, we delve into key concepts relevant to quantum mechanics.

The Schrödinger equation, a linchpin of quantum theory, takes the form of a linear equation. Quantum mechanics formalism revolves around linear operators and abstract Hilbert spaces. Understanding the mathematical properties and structure of Hilbert spaces is crucial for grasping quantum mechanics. We'll briefly review Hilbert space properties and linear operators. We'll also explore Dirac's bra-ket notation.

Quantum mechanics emerged in two forms:

1. Schrödinger's wave mechanics for continuous systems

2. Heisenberg's matrix mechanics for discrete basis systems

Our journey will encompass the mathematics of representing kets, bras, bra-kets, and operators in both continuous and discrete bases.

2.1 Quantum Postulates

Quantum mechanics is founded on several postulates, which cannot be proven theoretically. They are justified only through an empirical fact that they are consistent with all the known experimental results. The choice of the postulates depends heavily on authors' taste. Here we give one that turns out to be the most convenient in the study of quantum information and computation.

The quantum mechanical counterparts to these concepts are defined by postulates, which allow us to comprehend:

- The mathematical description of a quantum state at a given time t.

- The computation of various physical properties from this quantum state.

- The means to determine the state of a system at any future time t, given its state at time t; in other words, how to depict the temporal evolution of a system.

The responses to these inquiries are furnished by the following set of five postulates.

Postulate 1: System State A pure state in quantum mechanics is represented in terms of a normalized vector $|\psi(t)\rangle$ in a Hilbert space $\mathcal{H}$ (a complex vector space with an inner product): $\langle\psi(t)|\psi(t)\rangle = 1$. Suppose two states $|\psi_1\rangle$ and $|\psi_2\rangle$ are physical states of the system. Then their linear superposition $c_1|\psi_1\rangle + c_1|\psi_1\rangle$ ($c_k \in \mathbb{C}$) is also a possible state of the same system. This is called the superposition principle.

The state of a physical system at time t is described by a state vector $|\psi(t)\rangle$ within a **Hilbert space** $\mathcal{H}$. This state vector $|\psi(t)\rangle$ encompasses and provides all the requisite details about the system. Moreover, any superposition of state vectors remains a valid state vector.

What is the Hilbert Space?(optional)

A Hilbert space $\mathcal{H}$ consists of a set of vectors $|\psi\rangle, |\phi\rangle, |\gamma\rangle, |\cdots\rangle, |\chi\rangle$, and a set of scalars $a, b, c, \ldots$, which satisfy the following four properties:

1. **$\mathcal{H}$ is a linear space**

2. **$\mathcal{H}$ has a defined scalar product that is strictly positive:**

   - The scalar product of an element $|\psi\rangle$ with another element $|\phi\rangle$ is in general a complex number, denoted by

   $$\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^* \in \mathbb{C} \tag{1}$$

   - The scalar product of $|\psi\rangle$ with $|\phi\rangle$ is linear with respect to the second factor if $|\phi\rangle = a|\phi_1\rangle + b|\phi_2\rangle$

   $$\langle\psi|a\phi_1 + b\phi_2\rangle = a\langle\psi|\phi_1\rangle + b\langle\psi|\phi_2\rangle \tag{2}$$

   and anti-linear with respect to the first factor if $|\psi\rangle = a|\psi_1\rangle + b|\psi_2\rangle$

   $$\langle a\psi_1 + b\psi_2|\phi\rangle = a^*\langle\psi_1|\phi\rangle + b\langle\psi_2|\phi\rangle \tag{3}$$

   - The scalar product of a vector $|\psi\rangle$ with itself is a positive real number:

   $$\langle\psi|\psi\rangle \geq 0 \tag{4}$$

   where the equality holds only for $|\psi\rangle = |O\rangle$ or ***null ket***.

   $$|O\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{5}$$

3. **$\mathcal{H}$ is separable:**
   There exists a Cauchy sequence $|\psi_n\rangle \in \mathcal{H}$ such that for every $|\psi\rangle$ of $\mathcal{H}$ and $\epsilon > 0$, there exists at least one $|\psi_n\rangle$ of the sequence for which

$$\||\psi - \psi_n\|| < \epsilon, \tag{6}$$

4. **$\mathcal{H}$ is complete:**

Every Cauchy sequence $\psi_n \in \mathcal{H}$ converges to an element of $\mathcal{H}$. That is, for any ψ_n, the relation

$$\lim_{n,m\to\infty} \|\psi_m - \psi_n\| = 0, \tag{7}$$

defines a unique limit ψ in $\mathcal{H}$ such that

$$\lim_{n\to\infty} \|\psi - \psi_n\| = 0, \tag{8}$$

Postulate 2: Quantum Measurement
For any physical quantity (i.e., observable) a, there exists a corresponding *Hermitian operator A* acting on the Hilbert space $\mathcal{H}$.

What is a Hermitian operator?
An operator A is said to be Hermitian if it is equal to its adjoint $A^{\dagger}$ [a].

$$A = A^{\dagger} \tag{9}$$

As an example consider the matrix A and B

$$A = \begin{pmatrix} 1 & i & 2 \\ -i & 3 & 1 \\ 2 & 1 & 4 \end{pmatrix}, \qquad B = \begin{pmatrix} 2 & 3 & 1 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix} \tag{10}$$

we can easily build transpose Conjugate of A and B:

$$A^{\dagger} = \begin{pmatrix} 1 & i & 2 \\ -i & 3 & 1 \\ 2 & 1 & 4 \end{pmatrix}, B^{\dagger} = \begin{pmatrix} 2 & 4 & 7 \\ 3 & 5 & 8 \\ 1 & 6 & 9 \end{pmatrix} \tag{11}$$

which we can easily see $A = A^{\dagger}$ and $B \neq B^{\dagger}$.

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[a] the symbol $\dagger$ means transpose conjugate.

When we make a measurement of a, we obtain one of the eigenvalues λ_j of the operator A. Let λ_1 and λ_2 be two eigenvalues of A:

$$A|\lambda_i\rangle = |\lambda_i\rangle \tag{12}$$

Suppose the system is in a superposition state $c_1|\lambda_1\rangle + c_2|\lambda_2\rangle$. If we measure a in this state, then the state undergoes an abrupt change to one of the eigenstates corresponding to the observed eigenvalue: If the observed eigenvalue is λ_1, the system undergoes a wave function collapse as follows:

$$c_1|\lambda_1\rangle + c_2|\lambda_2\rangle \longrightarrow |\lambda_1\rangle \tag{13}$$

and the state immediately after the measurement is $|\lambda_1\rangle$. Suppose we prepare many copies of the state $c_1|\lambda_1\rangle + c_2|\lambda_2\rangle$. The probability of collapsing to the state $|\lambda_k\rangle$ is given by

$$|c_k|^2. \tag{14}$$

In this sense, the complex coefficient c_i is called the ***probability amplitude***. It should be noted that a measurement produces one outcome λ_i and the probability of obtaining it is experimentally

evaluated only after repeating measurements with many copies of the same state. These statements are easily generalized to states in a superposition of more than two states. Suppose we would like to measure an observable a. Let $A = \sum_i \lambda_i \ket{\lambda_i} \bra{\lambda_i}$ be the corresponding operator, where

$$A \ket{\lambda_i} = \lambda_i \ket{\lambda_i}. \tag{15}$$

and we know

$$\sum_i \ket{\lambda_i} \bra{\lambda_i} = 1 \tag{16}$$

$$\braket{\lambda_i|\lambda_i} = \delta_{ij} \tag{17}$$

where $\delta_{ij} = 1$ for $i = j$ and is zero elsewhere. We can expand an arbitrary quantum state $\ket{\psi}$ in terms of $\ket{\lambda_i}$ as

$$\ket{\psi} = \sum_i c_i \ket{\lambda_i}, \qquad c_i \in \mathbb{C}. \tag{18}$$

Then we can find the probability of finding quantum state in the eigenstate $\ket{\lambda_i}$ of observable A with probability P_i

$$
\begin{aligned}
P_i &= |\braket{\lambda_i|\psi}|^2 \tag{19}\\
&= \left| \braket{\lambda_i | \sum_n c_n \lambda_n} \right|^2 = \left| \sum_n c_n \braket{\lambda_i|\lambda_n} \right|^2 \tag{20}\\
&= \left| \sum_n c_n \delta_{in} \right|^2 = |c_i|^2 = c_i^* c_i \tag{21}
\end{aligned}
$$

If the states $\ket{\psi}$ are mutually orthonormal,the probability will be equal to the sum of the individual probabilities and for physical normalized state it will be equal to one

$$P = \sum_i P_i = P_1 + P_2 + P_3 + \cdots = 1 \tag{22}$$

or

$$P = \sum_i |c_i|^2 = |c_1|^2 + |c_2|^2 + |c_3|^2 + \cdots = 1 \tag{23}$$

Expectation Value
The expectation value $\langle A \rangle$ of a after measurements with respect to many copies of a normalized state $\ket{\psi}$ is

$$\langle A \rangle = \braket{\psi|A|\psi} \tag{24}$$

to show the equivalence between two formalisms. According to the probability of observing λ_i upon measurement of a is $|c_i|^2$, and therefore the expectation value after many measurements is $\sum_i \lambda_i |c_i|^2$. We will obtain the same result since

$$
\begin{aligned}
\braket{\psi|A|\psi} &= \sum_{i,j} c_i c_j^* \braket{\lambda_j|A|\lambda_i} \tag{25}\\
&= \sum_{i,j} c_i c_j^* \lambda_i \delta_{ij} = \sum_i \lambda_i |c_i|^2 \tag{26}
\end{aligned}
$$

This measurement is called the **_projective measurement_**. Any particular outcome λ_i will be found with the probability

$$|c_i|^2 = \braket{\psi|M_i|\psi} \tag{27}$$

where $M_i = \ket{\lambda_i} \bra{\lambda_i}$ is the projection operator, and the state immediately after the measurement

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Some Examples:

Exp 1: Find the eigenvalues and the normalized eigenvectors of the matrix

$$A = \begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & -1 \end{pmatrix} \tag{29}$$

Solution:
To find the eigenvalues of A, we simply need to solve the secular equation $\det|A - aI| = 0$:

$$|A - aI| = \begin{vmatrix} (7-a) & 0 & 0 \\ 0 & (1-a) & -i \\ 0 & i & -(1+a) \end{vmatrix} = 0 \tag{30}$$

$$= (7-a)\Big[-(1-a)(1+a) + i^2\Big] = 0 \tag{31}$$

$$= (7-a)(a^2 - 2) = 0 \tag{32}$$

The eigenvalues of A are thus given by

$$a_1 = 7, \qquad a_2 = \sqrt{2}, \qquad a_3 = -\sqrt{2} \tag{33}$$

Let us now calculate the eigenvectors of A. To find the eigenvector corresponding to the first eigenvalue, $a_1 = 7$, we need to solve the matrix equation

$$\begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & -1 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = 7\begin{pmatrix} x \\ y \\ z \end{pmatrix} \Rightarrow \begin{matrix} 7x = 7x \\ y - iz = 7y \\ iy - z = 7z \end{matrix} \tag{34}$$

this yields $x = 1$ (because the eigenvector is normalized) and $y = z = 0$. So the eigenvector corresponding to $a_1 = 7$ is given by the column matrix

$$|a_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \tag{35}$$

This eigenvector is normalized since $\langle a_1|a_1\rangle = 1$. The eigenvector corresponding to the second eigenvalue, $a_{\sqrt{2}}$, can be obtained from the matrix equation

$$\begin{pmatrix} 7 & 0 & 0 \\ 0 & 1 & -i \\ 0 & i & -1 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \sqrt{2}\begin{pmatrix} x \\ y \\ z \end{pmatrix} \Rightarrow \begin{matrix} 7x = \sqrt{2}x \\ y - iz = \sqrt{2}y \\ iy - z = \sqrt{2}z \end{matrix} \Rightarrow \begin{matrix} (7-\sqrt{2})x = 0 \\ (1-\sqrt{2})y - iz = 0 \\ iy - (1+\sqrt{2})z = 0 \end{matrix} \tag{36}$$

this yields $x = 0$ and $z = i(\sqrt{2} - 1)y$. So the eigenvector corresponding to $a_2 = \sqrt{2}$ is given by the column matrix

$$|a_2\rangle = \begin{pmatrix} 0 \\ y \\ i(\sqrt{2} - 1)y \end{pmatrix} \tag{37}$$

The value of the variable y can be obtained from the normalization condition of $|a_2\rangle$:

$$1 = \langle a_2|a_2\rangle = \begin{pmatrix} 0 & y* & -i(\sqrt{2} - 1)y* \end{pmatrix}\begin{pmatrix} 0 \\ y \\ i(\sqrt{2} - 1)y \end{pmatrix} = 2(2 - \sqrt{2})|y|^2 \tag{38}$$

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Taking only the positive value of y (a similar calculation can be performed easily if one is interested in the negative value of y), we have $y = \dfrac{1}{2(2 - \sqrt{2})}$; hence the eigenvector $|a_2\rangle$ becomes

$$|a_2\rangle = \frac{1}{2(2 - \sqrt{2})} \begin{pmatrix} 0 \\ 1 \\ i(\sqrt{2} - 1) \end{pmatrix} \tag{39}$$

Following the same procedure that led to $|a_2\rangle$, we can show that the third eigenvector is given by

$$|a_3\rangle = \begin{pmatrix} 0 \\ y \\ -i(\sqrt{2} + 1)y \end{pmatrix} \tag{40}$$

its normalization leads to $y = \dfrac{1}{2(2 + \sqrt{2})}$ (we have considered only the positive value of y); hence

$$|a_3\rangle = \frac{1}{2(2 + \sqrt{2})} \begin{pmatrix} 0 \\ 1 \\ -i(\sqrt{2} + 1) \end{pmatrix} \tag{41}$$

Question: Check the two following conditions for these eigenstates

(a)
$$\langle a_i | a_j \rangle = 0, \qquad i, j \in \{1, 2, 3\}$$

(b)
$$\sum_{i=1}^{3} |a_i\rangle \langle a_i|$$

Exp 2: Consider a system whose state is given in terms of an orthonormal set of three vectors:

$$|\psi\rangle = \frac{\sqrt{3}}{3} |\phi_1\rangle + \frac{2}{3} |\phi_2\rangle + \frac{\sqrt{2}}{3} |\phi_3\rangle \tag{42}$$

(a) Verify that $|\psi\rangle$ is normalized. Then, calculate the probability of finding the system in any one of the states $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle$. Verify that the total probability is equal to one.

(b) Consider now an ensemble of 810 identical systems, each one of them in the state $|\psi\rangle$. If measurements are done on all of them, how many systems will be found in each of the states $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle$.

Solution:

(a) Using the orthonormality condition $\langle \phi_i | \phi_j \rangle = \delta_{ij}$ where $i, j \in \{1, 2, 3\}$, we can verify that $|\psi\rangle$ is normalized:

$$\langle \psi | \psi \rangle = \frac{3}{9} \langle \phi_1 | \phi \rangle + \frac{4}{9} \langle \phi_2 | \phi_2 \rangle + \frac{2}{9} \langle \phi_3 | \phi_3 \rangle \tag{43}$$

$$= \frac{3}{9} + \frac{4}{9} + \frac{2}{9} = 1 \tag{44}$$

Since $|\psi\rangle$ is normalized, the probability of finding the system in $|\phi_1\rangle$ is given by

$$P_1 = |\langle \phi_1 | \psi \rangle|^2 = \left| \frac{\sqrt{3}}{3} \langle \phi_1 | \phi_1 \rangle + \frac{2}{3} \langle \phi_1 | \phi_2 \rangle + \frac{\sqrt{2}}{3} \langle \phi_1 | \phi_3 \rangle \right|^2 = \frac{3}{9} = \frac{1}{3} \tag{45}$$

since $\langle \phi_1 | \phi_1 \rangle = 1$, $\langle \phi_1 | \phi_2 \rangle = 0$, and $\langle \phi_1 | \phi_3 \rangle = 0$. Similarly, from the relations $\langle \phi_2 | \phi_1 \rangle = 0$, $\langle \phi_2 | \phi_2 \rangle = 1$, and $\langle \phi_2 | \phi_3 \rangle = 0$, we obtain the probability of finding the system in $|\phi_2\rangle$:

$$P_2 = |\langle \phi_2 | \psi \rangle|^2 = \left| \frac{2}{3} \langle \phi_2 | \phi_2 \rangle \right|^2 = \frac{4}{9} \tag{46}$$

As for $\langle\phi_3|\phi_1\rangle = 0$, $\langle\phi_3|\phi_2\rangle = 0$, and $\langle\phi_3|\phi_3\rangle = 1$.

$$P_3 = |\langle\phi_3|\psi\rangle|^2 = \left|\frac{\sqrt{2}}{3}\langle\phi_3|\phi_3\rangle\right|^2 = \frac{2}{9} \tag{47}$$

As expected, the total probability is equal to one:

$$P = P_1 + P_2 + P_3\frac{3}{9} + \frac{4}{9} + \frac{2}{9} = 1 \tag{48}$$

(b) The number of systems that will be found in the state $|\phi_1\rangle$ is

$$N_1 = 810 \times P_1 = 270 \tag{49}$$

Likewise, the number of systems that will be found in states $|\phi_2\rangle$ and $|\phi_3\rangle$ are given, respectively, by

$$N_2 = 810 \times P_2 = 360, \qquad N_3 = 810 \times P_3 = 180 \tag{50}$$

Postulate 3: Evolution of a System

The time evolution of a quantum system is governed by the Schrödinger equation, which describes how the state vector $|\psi(t)\rangle$ changes over time. The Schrödinger equation is given by:

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \tag{51}$$

Where:

- i is the imaginary unit.

- $\hbar$ is the reduced Planck's constant.

- $\frac{d}{dt}$ represents the derivative with respect to time.

- $|\psi(t)\rangle$ is the state vector of the system at time t.

- $\hat{H}$ is the Hamiltonian operator, which represents the total energy operator for the system.

This postulate defines how the quantum state evolves over time under the influence of the Hamiltonian operator, which characterizes the system's energy. It is a fundamental principle in quantum mechanics that guides the dynamics of quantum systems.

But what is a linear space?

A linear vector space consists of two sets of elements and two algebraic rules:

1. A set of **vectors**

$$\{\psi, \phi, \gamma, \cdots, \chi\} \tag{52}$$

   and a set of **scalars**;

$$\{a, b, c, \ldots\} \tag{53}$$

2. a rule for **vector** *addition* and a rule for **scalar** multiplication

   (a) **Properties of the addition rule for vectors**
   - **Closure**:
     If ψ and ϕ are vectors (elements) of a space, their sum, $\psi + \phi$, is also a vector of the same space.
   - **Commutativity**:

     $$\psi + \phi = \phi + \psi \tag{54}$$

   - **Associativity**:

     $$(\psi + \phi) + \chi = \phi + (\psi + \chi) \tag{55}$$

   - **Existence of a zero or neutral vector**:
     for each vector O, there must exist a zero vector O such that:

     $$O + \psi = \psi + O = \psi \tag{56}$$

   - **Existence of a symmetric or inverse vector**:
     each vector ψ must have a symmetric vector $-\psi$

     $$-\psi + \psi = \psi - \psi = O \tag{57}$$

   (b) **Properties of the multiplication rule for scalars**
   The multiplication of vectors by scalars (scalars can be real or complex numbers) has these properties:
   - The product of a scalar with a vector gives another vector. In general, if ψ and ϕ are two vectors of the space, any linear combination $a\psi + b\phi$ is also a vector of the space, a and b being scalars.
   - **Distributivity with respect to addition:**

     $$a(\psi + \phi) = a\psi + a\phi, \tag{58}$$
     $$(a + b)\psi = a\psi + b\psi, \tag{59}$$

   - **Associativity with respect to multiplication of scalars**

     $$a(b\psi) = b(a\psi) \tag{60}$$

   - For each element ψ, there must exist a unitary scalar I and a zero scalar o such that:

     $$I\psi = \psi I = \psi \tag{61}$$
     $$o\psi = \psi o = o. \tag{62}$$