

MODULE – 5: Introduction to Quantum Mechanics & Quantum Computing

Quantum Mechanics: Heisenberg Uncertainty Principle and Significance, Application: Spectral line broadening, Wave Function: Significance, Born Interpretation, Dirac Notation and Normalization of Wave Function, Time Independent Schrodinger Wave Equation, Application of Schrödinger Wave Equation for a Particle in 1-D infinite Height Potential Well: Eigen States and Eigenvalues.

Principles of Quantum Information & Quantum Computing: Introduction, Qubit and its Properties, Representation of a Qubit as a Bloch sphere, Quantum Gates: Pauli Gates, Hadamard Gate and CNOT Gate.

QUANTUM MECHANICS

Quantum mechanics is the branch of physics that deals with the description of the physical properties of nature at the scale of atoms and subatomic particles incorporating the concepts of quantization of energy, wave-particle duality, and the uncertainty principle. It differs from classical physics in that energy, momentum, and other quantities of a bound system are restricted to discrete values (quantization), objects have characteristics of both particles and waves (wave-particle duality); and there are limits to how accurately the value of a physical quantity can be predicted before its measurement, given a complete set of initial conditions (the uncertainty principle). It is the foundation of all quantum physics including quantum chemistry, quantum field theory, quantum technology, quantum information science, and quantum computing.

Failure of Classical Physics:

Classical physics, which is based mainly on Newtonian mechanics, Maxwell's electromagnetic theory, and classical thermodynamics, successfully explains the motion of macroscopic objects and many everyday physical phenomena. However, it fails to explain several observations at the atomic and subatomic scales. Classical physics could not adequately explain **blackbody radiation**, as the classical theory predicted an infinite amount of energy at high frequencies, leading to the ultraviolet catastrophe. It also failed to explain the **photoelectric effect**, particularly the existence of a threshold frequency and the dependence of electron kinetic energy on the frequency of incident light. Similarly, the **stability of atoms** could not be

MODULE – 5: Introduction to Quantum Mechanics & Quantum Computing

explained using classical electrodynamics, since an orbiting electron should continuously radiate energy and eventually collapse into the nucleus. Classical theories also failed to correctly describe **atomic and molecular spectra**, where discrete rather than continuous energy levels are observed. Phenomena such as **Compton scattering, electron diffraction, specific heat of solids at low temperatures, and the wave-particle duality of matter and radiation** further demonstrated the inadequacy of classical concepts. These limitations led to the development of **quantum mechanics**, which provides a more appropriate framework for describing microscopic systems and their interactions.

Heisenberg Uncertainty principle:

According to de-Broglie, a moving material particle is associated with a wave packet, which has a small spread in the space. This wave nature implies that there are fundamental limits to the accuracy with which we can measure particle properties such as position and momentum.

Consider the wave group shown below fig (a). The particle corresponding to this wave group may be located anywhere within the group at a given time. The narrower its wave group, the more precisely a particles position can be specified (fig (b)). But the wavelength λ of the waves in a narrow wave packet is not well defined. This means that, since $\lambda = h/p$, the particle's momentum is not a precise quantity.

On the other hand, a wide wave packet (fig (a)) has a clearly defined wavelength. The momentum that corresponds to this wavelength is therefore a precise quantity. But the width of the group is too large for us to be able to say exactly where the particle is at a given time. Thus, we have the uncertainty principle given by Heisenberg.

Position-Momentum Uncertainty principle:

“It is impossible to know both the exact position and exact momentum of an object at the same time.”

$$\text{Mathematically } \Delta x \cdot \Delta p \geq \frac{h}{4\pi}$$

Where Δx is the uncertainty in the measurement of position and Δp is the uncertainty in the

measurement of momentum.

If we arrange matter, so that Δx is small, corresponding to narrow wave group then Δp will be large. If we reduce Δp in some way, a broad wave group is inevitable and Δx will be large.

Energy-Time uncertainty principle:

It states that “**It is impossible to measure both the exact energy and exact time in a physical process at the same time**”

$$\text{i.e., } \Delta E \cdot \Delta t \geq \frac{h}{4\pi}$$

Where ΔE is the uncertainty in the measurement of energy, Δt is the uncertainty in the measurements of time

Angular displacement and Angular momentum uncertainty principle:

It states that “**It states that “It is impossible to measure both the exact angular displacement and exact angular momentum in a physical process at the same time”**”

$$\text{i.e., } \Delta L \cdot \Delta \theta \geq \frac{h}{4\pi}$$

where ΔL is uncertainty in the measurement of momentum and $\Delta \theta$ is uncertainty in the measurement of displacement.

Physical Significance:

The physical significance of the Heisenberg’s uncertainty principle is that one should not think of the exact position or an accurate value for momentum of a particle. Instead, one should think of the probability of finding the particle at a certain position or of the most probable value for the momentum of the particle. Similar interpretation is made for the conjugate pair ΔE and Δt and ΔL and $\Delta \theta$.

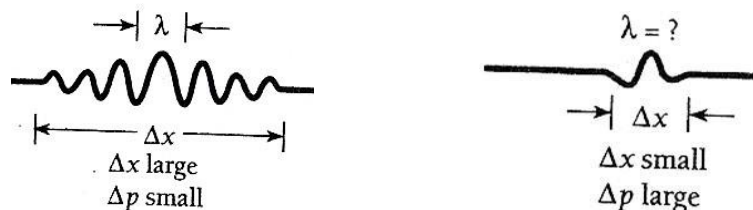


Fig. a

Application: Spectral Line Broadening:

One important application of the energy–time uncertainty principle is the explanation of natural broadening of spectral lines.

When an atom is in an excited state, it does not remain there indefinitely. The excited state has a finite lifetime Δt . According to the uncertainty principle,

$$\Delta E \cdot \Delta t \geq \frac{h}{4\pi}$$

Therefore, a state with a finite lifetime cannot have an exactly defined energy. There is an inherent uncertainty ΔE in the energy of the state.

For an atomic transition,

$$E = h\nu$$

and hence

$$\Delta E = h\Delta\nu$$

Substituting into the uncertainty relation,

$$h\Delta\nu \cdot \Delta t \geq \frac{h}{4\pi}$$

Canceling from both sides,

$$\Delta\nu \geq \frac{h}{4\pi \cdot \Delta t}$$

Thus, because an excited atomic state has a **finite lifetime**, its energy cannot have an exactly definite value. Consequently, the emitted radiation has a small range of frequencies rather than a single frequency. This produces **natural broadening of spectral lines**.

Wave function- its significance:

Quantity whose variations make up matter waves is called the wave function. Exhibits

MODULE – 5: Introduction to Quantum Mechanics & Quantum Computing

wave-like properties of a particle and contain all possible information about the state of the system. The value of ψ associated with a moving body at x, y, z in space at the time 't' is related to the likelihood of finding the body there at that time. It is complex number with both real and imaginary parts.

Physical significance of Wave function

Probability of occurrence is a real and a positive quantity. Since ψ is complex, it has no attributable physical significance.

But the square of the absolute value of the wave function is always positive and real and is known as **probability density**.

It is given by $|\psi|^2 = \psi \cdot \psi^*$

where ψ^* is the complex conjugate of ψ .

The probability of finding particle at certain place at given time must be in between **0 and 1**. ex:

0.3 means probability of finding particle is 30% similarly -0.2 means meaningless. "The probability of experimentally finding a particle is proportional to the value of $|\psi|^2$ there at 't'. Large value of $|\psi|^2$ means the strong possibility of the body's presence, while a small value of means the slight-possibility of its presence.

Dirac notation

Dirac notation, also called bra-ket notation, is a compact notation used to represent quantum states.

It was introduced by physicist Paul Dirac.

There are two fundamental forms: $|\psi\rangle$ and $\langle\psi|$ where $|\psi\rangle$ is Ket notation and $\langle\psi|$ Bra notation.

They are given as

$$|\psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

and

$$\langle \psi | = (a^* \quad b^*)$$

Normalization of Wave function

If ψ is the wave function associated with a particle, then the probability of **finding the particle in a volume dV is $|\psi|^2 dV$** . If the particle is present somewhere in a particular region, the integral of $|\psi|^2$ over all the space must be finite. If the particle is certainly to be found in certain region of space then

$$\int_{-\infty}^{+\infty} |\psi|^2 dV = 1$$

Any wave function satisfying the above equation is said to be **normalized wave function**. Often ψ is not a normalized wave function and have some constants. The process to determine that constant value and equate to ψ for unity is known as normalization

Eigen functions

Wave functions which are single-valued with finite value everywhere and also their first derivatives with respect to their variables are continuous everywhere are known as **Eigen functions**

Eigen Values

The values of a physical observable such as energy, momentum etc for which Schrödinger's wave equation can be solved are called **Eigen values**.

Time-independent Schrödinger wave equation:

Consider a particle, moving freely in the positive x-direction in a stationary potential field. The wavelength of the associated deBroglie wave is given by

$$\lambda = \frac{h}{p} \quad \rightarrow *$$

The wave equation for de-Broglie wave associated with such a particle can be written in complex notation as

$$\psi = Ae^{-i(\omega t - kx)} \quad A \rightarrow \text{Amplitude of the wave}$$

$$\psi = Ae^{+i(kx - \omega t)} \rightarrow (1)$$

Since the particle is moving in a stationary or steady field, the potential energy of the particle does not depend on time but it varies only with the position of the particle.

Differentiating (1) w.r.t x twice we get

$$\frac{d\psi}{dx} = Ae^{i(kx - \omega t)}(ik)$$

$$\frac{d^2\psi}{dx^2} = Ae^{i(kx - \omega t)}(ik)^2$$

$$= -k^2\psi$$

But $k = \frac{2\pi}{\lambda}$, substituting in the above equation we get

$$\frac{d^2\psi}{dx^2} = -\frac{4\pi^2\psi}{\lambda^2}$$

$$\text{Or } \frac{1}{\lambda^2} = -\frac{1}{4\pi^2\psi} \cdot \frac{d^2\psi}{dx^2} \quad \text{----- (2)}$$

If 'm' is the mass of the particle moving with a velocity 'v' then K.E is

$$\text{K.E} = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{p^2}{2m} \quad \text{----- (3)}$$

Where $p = mv$, momentum of the particle. But $p = \frac{h}{\lambda}$; from (*)

$$\therefore \text{K.E} = \frac{h^2}{\lambda^2 \cdot 2m} = \frac{h^2}{2m} \cdot \frac{1}{\lambda^2}$$

$$= \frac{h^2}{2m} \times -\frac{1}{4\pi^2\psi} \cdot \frac{d^2\psi}{dx^2}$$

$$\text{K.E} = -\frac{h^2}{8\pi^2m\psi} \cdot \frac{d^2\psi}{dx^2} \text{-----} (4)$$

Let ‘V’ be the potential energy of the particle which depends on the position of the particle in the field. Then total energy ‘E’ of the particle is

$$E = \text{K.E} + \text{P.E}$$

$$E = -\frac{h^2}{8\pi^2m\psi} \times \frac{d^2\psi}{dx^2} + V$$

$$\text{ie } \frac{d^2\psi}{dx^2} = -\frac{8\pi^2m}{h^2}(E - V)\psi$$

$$\text{or } \boxed{\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2}(E - V)\psi = 0}$$

This is the time independent Schrödinger’s wave equation in one dimension.

For two dimensions,

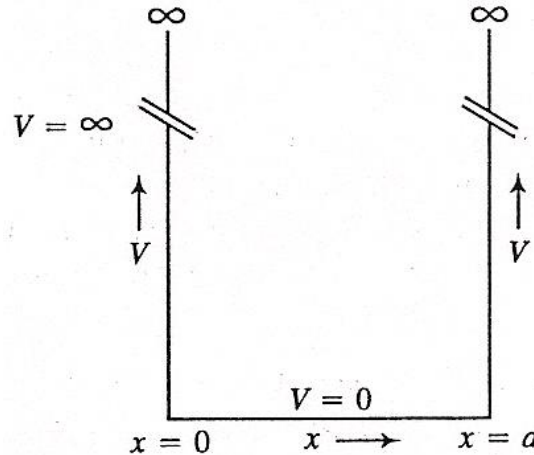
$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{8\pi^2m}{h^2}(E - V)\psi = 0$$

In three dimensions, it becomes

$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \frac{8\pi^2m}{h^2}(E - V)\psi = 0$$

Applications of Schrodinger's wave equation:

Energy Eigen values of a particle in one-dimensional, infinite potential well (particle in a box):



Consider a particle, which is free to move in the x-direction only in the region $x = 0$ and $x = L$. Outside this region the potential energy is taken to be infinite and within this region it is zero ie $V = 0$ for $0 < x < L$ and $V = \infty$ for $x \geq \infty$ and $x \leq 0$

We have the Schrödinger's time independent wave equation in one dimension

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2}(E - V)\psi = 0 \quad \text{----- (1)}$$

Outside the well, the equation (1) becomes

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2}(E - \infty)\psi = 0 \quad \text{Since } V = \infty$$

This equation holds good only if $\psi = 0$ for all points outside the well, ie $|\psi|^2 = 0$ which means that the particle cannot be found at all outside the well.

Inside the well, equation (1) becomes

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2}E\psi = 0 \quad (\text{Since } V = 0)$$

MODULE – 5: Introduction to Quantum Mechanics & Quantum Computing

$$\text{Let } \frac{8\pi^2 m}{h^2} E = k^2 \quad \text{-----} \quad (2)$$

Then;

$$\frac{d^2 \psi}{dx^2} + k^2 \psi = 0 \quad \text{-----} \quad (3)$$

The solution for the above equation is

$$\psi = A \sin kx + B \cos kx \quad \text{-----} \quad (4)$$

At $x = 0$, $\psi = 0$, substituting in (4) we get

$$0 = A \sin 0 + B \cos 0$$

$$\Rightarrow B = 0$$

At $x=L$, $\psi = 0$ and equation (4) becomes

$$0 = A \sin kL + B \cos kL$$

$$\Rightarrow A \sin kL = 0 \quad (\text{Since } B=0)$$

Here 'A' need not be zero

$$\therefore \sin kL = 0$$

i.e. $kL = n\pi$, where $n=0, 1, 2, 3, \dots$ is an integer called quantum number.

$$\therefore k = \frac{n\pi}{L}$$

Substituting the values of B and k in (4)

$$\boxed{\psi_n = A \sin \frac{n\pi}{L} x} \quad \text{-----} \quad (5)$$

which represents the permitted solutions. Since there is only one particle and at any time it is present somewhere inside the well only, the integral of the wave function over the entire space in the well must be equal to unity.

$$\text{i.e. } \int_0^L |\psi_n|^2 dx = 1$$

$$\int_0^L \left| A \sin \frac{n\pi}{L} x \right|^2 dx = 1$$

$$\int_0^L A^2 \sin^2 \left(\frac{n\pi x}{L} \right) dx = 1$$

$$A^2 \left[\frac{1}{2} \int_0^L dx - \frac{1}{2} \int_0^L \cos \frac{2n\pi}{L} x dx \right] = 1 \quad \left[\int_0^{\theta} \sin^2 \theta = \frac{1}{2} (1 - \cos 2\theta) \right]$$

$$\text{Or } \frac{A^2}{2} \left[x - \frac{L}{2n\pi} \sin \left(\frac{2n\pi}{L} x \right) \right]_0^L = 1$$

$$\text{Or } \frac{A^2}{2} \left[L - \frac{L}{2n\pi} \sin(2n\pi) - 0 \right] = 1$$

$$\Rightarrow \frac{A^2 L}{2} = 1$$

$$\Rightarrow \boxed{A = \sqrt{\frac{2}{L}}}$$

Substituting in (5) we get

$$\boxed{\psi_n = \sqrt{\frac{2}{L}} \sin \left(\frac{n\pi}{L} \right) x} \quad \text{----- (6)}$$

which are the normalized wave functions of a particle in a one-dimensional infinite potential well.

Energy Eigen Value

From eqn. (2)

$$\frac{8\pi^2 m}{h^2} E = k^2$$

Since $k = \frac{n\pi}{L}$

Substituting the value of k in eqn. (2) we get

$$E_n = \frac{n^2 h^2}{8mL^2}$$

Zero-point energy:

The lowest acceptable value for n=1. Because for n=0, $\psi_n = 0$ (from equation (5)), which means that the particle is not present inside the well which is not true.

The lowest energy corresponding to n=1 is called zero-point energy and it is given by

$$E_o = \frac{h^2}{8mL^2}$$

The lowest permitted state of energy is referred to as ground state energy. The energy state for n>1 is called excited states.

Solved Numerical Problems:

1. An electron is confined within a region of 1 Å. Calculate the minimum uncertainty in its momentum.

Soln: According to Heisenberg's uncertainty principle,

$$\Delta p = \frac{h}{4\pi \Delta x}$$

Since $\Delta x = 1 \times 10^{-10} \text{ m}$

$$\Delta p = \frac{6.626 \times 10^{-34}}{4\pi(1.0 \times 10^{-10})}$$

$$\Delta p = 5.28 \times 10^{-25} \text{ kg m/s}$$

2. The uncertainty in the momentum of an electron is $2 \times 10^{-24} \text{ kg m/sec}$. Calculate the minimum uncertainty in its position.

Soln: According to Heisenberg's uncertainty principle,

$$\Delta x = \frac{h}{4\pi\Delta p}$$

$$\Delta x = \frac{6.626 \times 10^{-34}}{4\pi(2.0 \times 10^{-24})}$$

$$\Delta x = 2.64 \times 10^{-11} \text{ m}$$

3. A particle is described by the normalized wave function

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right), \quad 0 < x < L$$

Calculate the probability of finding the particle between $x=0$ and $x=L/2$.

Soln: According to Born's interpretation,

$$P = \int_a^b |\psi(x)|^2 dx$$

Therefore,

$$P = \int_0^{L/2} \left| \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) \right|^2 dx$$
$$P = \frac{2}{L} \int_0^{L/2} \sin^2\left(\frac{\pi x}{L}\right) dx$$

Using

$$\int \sin^2(ax) dx = \frac{x}{2} - \frac{\sin(2ax)}{4a}$$

we get

$$P = \frac{2}{L} \left[\frac{x}{2} - \frac{L}{4\pi} \sin\left(\frac{2\pi x}{L}\right) \right]_0^{L/2}$$

At $x=L/2$,

$$\sin(\pi) = 0$$

Hence,

$$P = \frac{2}{L} \left(\frac{L}{4} \right)$$

$$\boxed{P = \frac{1}{2}}$$

Therefore, $P = 0.5 = 50\%$

4. An electron is confined in a one-dimensional infinite potential well of width 1nm. Calculate its ground-state energy.

Soln: For a particle in a box,

$$E_n = \frac{n^2 h^2}{8mL^2}$$

For ground state, $n=1$

$$E_1 = \frac{(1)^2 (6.626 \times 10^{-34})^2}{8(9.109 \times 10^{-31})(1 \times 10^{-9})^2}$$
$$E_1 = 6.02 \times 10^{-20} \text{ J}$$

$$E_1 = \frac{6.02 \times 10^{-20}}{1.602 \times 10^{-19}}$$

$$E_1 = 0.376 \text{ eV}$$

5. An electron is confined in a one-dimensional infinite potential well of width 2nm. Calculate the energy corresponding to the second energy level.

Soln: W.K.T

$$E_n = \frac{n^2 h^2}{8mL^2}$$

For ground state, n=2,

$$E_2 = \frac{(2)^2 (6.626 \times 10^{-34})^2}{8(9.109 \times 10^{-31})(2 \times 10^{-9})^2}$$

$$E_2 = 6.02 \times 10^{-20} \text{ J}$$

$$E_2 = 0.376 \text{ eV}$$

Sample Questions:

1. Apply Heisenberg's uncertainty principle to explain the origin of spectral line broadening. (L2)
2. State and Explain Heisenberg's uncertainty principle in all three forms. Discuss their physical significance. (L2)
3. State and explain the Heisenberg Uncertainty Principle. Discuss its physical significance and why it is important for microscopic particles. (L2)
4. Explain the Heisenberg Uncertainty Principle with its mathematical expression and discuss its significance in quantum mechanics. (L2)
5. Explain the origin of spectral line broadening using the Heisenberg Uncertainty Principle. (L2)

MODULE – 5: Introduction to Quantum Mechanics & Quantum Computing

6. Derive the one-dimensional time-independent Schrödinger equation for a particle of mass m confined to one dimension. (L2)
7. Assuming the Schrödinger wave equation, find the energy Eigen values of a particle in an infinite potential well. (L2)
8. State and explain Heisenberg's uncertainty principle. Give its physical significance. (L2)
9. Describe the physical significance of a wave function in respect of probability density. Mention the properties of a wave function.
10. Describe the wave function and explain its physical significance and the properties of a physically acceptable wave function.
11. Explain the concept of a wave function and discuss its physical significance along with the essential properties of a valid wave function.

Principles of Quantum Information & Quantum Computing

Introduction:

Quantum computing is a type of computation whose operations can harness the phenomena of quantum mechanics, such as superposition, interference, and entanglement. Devices that perform quantum computations are known as **quantum computers**. Developing Computing methods based on the principles of Quantum theory Quantum computers stores the information in a quantum system in the form of Qubits. In quantum computing, electrons or photons can be considered as qubits. Instead of 0 and 1, It can choose two electronics states of an atom or two different polarization orientations of light for the two states. But as per quantum mechanics the atom can also be prepared in the state in which is said to be a coherent superposition of both the states to represent zero and one Using quantum computing, quicker computation could be achieved and small-size computer can be obtained through Quantum computing concepts

Concept of Qubit and its properties:

Concept of Qubit

- ❖ In quantum computing, a **qubit** or **quantum bit** is a basic unit of quantum information
- ❖ A quantum system like atom or electrons can exist in states as 0 and 1 or simultaneously both as 0 and 1.
- ❖ It will not be known definitely, in which states they would be.
- ❖ But the number called probability factors associated with the corresponding state provide the probability of the atoms/electron's existence in each of these states.
- ❖ Since, they follow the quantum principles; it becomes a quantum system and called as quantum bits or Qubit.
- ❖ Similarly in case of light, a Qubit may correspond to superposed state of horizontal and vertical polarization of photons apart from two individual states.

Properties of Qubits

A Qubit can be physically implemented by the two states of an electron or horizontal and vertical polarizations of photons as $|\downarrow\rangle$ and $|\uparrow\rangle$

Superposition

A Qubit can be in a superposed state of the two states $|0\rangle$ and $|1\rangle$ (**Ket notation**). If measurements are carried out with a qubit in superposed state, then the results that we get will be probabilistic

It is represented as $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

Where α and β are complex numbers and $|\alpha|^2 + |\beta|^2 = 1$

No Cloning Theorem

The Qubit changes its state once it is subjected to the measurement. It means, one cannot copy the information from the qubit the way we do it in classical computers, as there will be no similarity between the copy and the original. This is known as “**no cloning principle**”

Entanglement

Two Qubits can strongly correlate with each other. Changing state of one of the qubits will instantaneously change the state of the other one in predictable way. This happens even if they are separated by very long distances.

Representation of Qubits by Bloch Sphere

- ❖ The pure state space qubits (Two Level Quantum Mechanical Systems) can be visualized using an imaginary sphere called Bloch Sphere. It has a unit radius
- ❖ This Bloch sphere picture is elegant and powerful for the single qubit.
- ❖ The Arrow on the sphere represents the state of the Qubit. The north and south poles are used to represent the basis states $|0\rangle$ and $|1\rangle$ respectively. The other locations on the bloch sphere represents the superposition state i.e $|0\rangle$ and $|1\rangle$ states and represented by $\alpha|0\rangle + \beta|1\rangle$ with $|\alpha|^2 + |\beta|^2 = 1$. Thus a Qubit can be any point on the Bloch Sphere.

MODULE – 5: Introduction to Quantum Mechanics & Quantum Computing

- ❖ The Bloch sphere allows the state of the qubit to be represented in unit spherical coordinates. They are the polar angle θ and the azimuth angle ϕ . The Bloch sphere is represented by the equation

$$|\psi\rangle = \cos \theta/2 |0\rangle + e^{i\phi} \sin \theta/2 |1\rangle$$

here $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$. The normalization constraint is given by

$$|\cos \theta/2|^2 + |\sin \theta/2|^2 = 1$$

- ❖ For any Gate operation, taking an initial state to the final state of the single-qubit, is equivalent to a composition of one or more simple rotations on the Bloch sphere.

Single qubit

A Single Qubit has two computational basis states $|0\rangle$ and $|1\rangle$. In single qubit the state of qubit will be either in $|0\rangle$ and $|1\rangle$ where

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Above basis vectors are written as column matrix in the form of identity matrix

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

which represents the single qubit state. The pictorial representation of the single qubit is as follows. $\alpha |0\rangle + \beta |1\rangle$

Two qubit

A two-qubit system has 4 computational basis states denoted as $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$. The matrix representation of two qubit state is

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

The pictorial representation of two qubit is as follows. $\alpha |00\rangle + \beta |01\rangle + \gamma |10\rangle + \delta |11\rangle$

Transformation operation of single and two qubit system **Pauli X-Gate:**

In Quantum Computing the Pauli X-gate is also referred as quantum NOT gate. Here qubits takes the state $|0\rangle$ to $|1\rangle$ and vice versa. It is analogous to the classical not gate.

The Matrix representation of Quantum Not Gate is given by

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$X|0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle$$

$$X|1\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle$$

A Quantum State is given by $\alpha |0\rangle + \beta |1\rangle$ and its matrix representation is given by

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Hence the operation of Quantum Not Gate on quantum state is given by

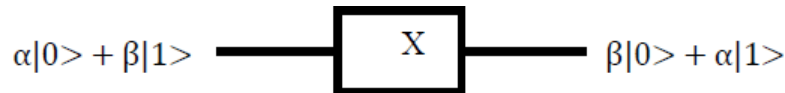
$$X \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \beta \\ \alpha \end{pmatrix}$$

Thus the quantum state becomes $\alpha |1\rangle + \beta |0\rangle$. Similarly, the input $\alpha |1\rangle + \beta |0\rangle$ to the quantum not gates changes the state to $\alpha |0\rangle + \beta |1\rangle$. The quantum not gate circuit and the truth table are as shown below.

Truth table

Input	Output
$ 0\rangle$	$ 1\rangle$
$ 1\rangle$	$ 0\rangle$
$\alpha 0\rangle + \beta 1\rangle$	$\beta 0\rangle + \alpha 1\rangle$

Symbol



Hadamard Gate:

The Hadamard gate is a single-qubit operation that maps basis state $|0\rangle$ and $|1\rangle$ to

$\frac{|0\rangle + |1\rangle}{\sqrt{2}}$ and $\frac{|0\rangle - |1\rangle}{\sqrt{2}}$ states respectively

Matrix representation

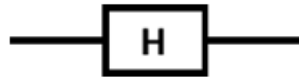
$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Operation of Hadamard Gate

$$H|0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$H|1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

Symbol



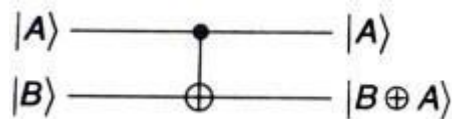
Truth table

Input	Output
$ 0\rangle$	$\frac{ 0\rangle + 1\rangle}{\sqrt{2}}$
$ 1\rangle$	$\frac{ 0\rangle - 1\rangle}{\sqrt{2}}$

Controlled Not Gate or CNOT Gate

The CNOT gate is a typical multi-qubit logic gate. The CNOT gate operates on a quantum register that consists of 2 qubits. The CNOT gate flips the second qubit (the target qubit) if and only if the first qubit (the control qubit) is $|1\rangle$ and the circuit is as follows.

Symbol



The Matrix representation of CNOT Gate is given by

$$U_{CN} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

The Transformation could be expressed as

$$|A, B\rangle \rightarrow |A, B \oplus A\rangle$$

Consider the operations of CNOT gate on the four inputs $|00\rangle, |01\rangle, |10\rangle$ and $|11\rangle$.

Operation of CNOT Gate for input $|00\rangle$

$$UCN|00\rangle = |00\rangle$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Here in the inputs to the CNOT Gate the control qubit is $|0\rangle$. Hence no change in the state of Target qubit $|0\rangle$

$$|00\rangle \rightarrow |00\rangle$$

Operation of CNOT Gate for input $|01\rangle$

$$UCN|01\rangle = |01\rangle$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

Here in the inputs to the CNOT Gate the control qubit is $|0\rangle$. Hence no change in the state of Target qubit $|1\rangle$

$$|01\rangle \rightarrow |01\rangle$$

Operation of CNOT Gate for input $|10\rangle$

$$UCN|10\rangle = |11\rangle$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Here in the inputs to the CNOT Gate the control qubit is $|1\rangle$. Hence the state of Target qubit flips from $|0\rangle$ to $|1\rangle$.

$$|10\rangle \rightarrow |11\rangle$$

Operation of CNOT Gate for input $|11\rangle$

$$UCN|11\rangle = |10\rangle$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

Here in the inputs to the CNOT Gate the control qubit is $|1\rangle$. Hence the state of Target qubit flips from $|1\rangle$ to $|0\rangle$.

$$|11\rangle \rightarrow |10\rangle$$

Truth table

Input	Output
$ 00\rangle$	$ 00\rangle$
$ 01\rangle$	$ 01\rangle$
$ 10\rangle$	$ 11\rangle$
$ 11\rangle$	$ 10\rangle$

Sample Questions:

1. Explain the Bloch sphere representation of a qubit and describe how the quantum state of a qubit is represented on the Bloch sphere.
2. Explain the properties of a qubit and describe how a qubit differs from a classical bit.
3. Apply the Pauli-X, Hadamard, and CNOT gates to given single-qubit and two-qubit input states and predict the corresponding output states.
4. Apply the Pauli-X gate to the states $|0\rangle$ and $|1\rangle$, and determine the corresponding output states.
5. Apply the Hadamard gate to the states $|0\rangle$ and $|1\rangle$, and determine the resulting superposition states.
6. Apply a CNOT gate to the two-qubit states $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$ and predict the corresponding output states.