# **Unit IV- QUANTUM COMPUTING**

#### **Stern-Gerlach Experiment:**

This experiment demonstrates the spin states possessed by electrons in an atom.

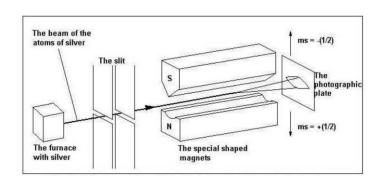
#### **Principle:**

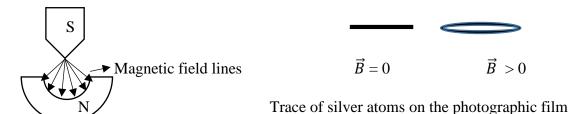
An electron revolving around a nucleus results in orbital magnetic moment  $(m_l)$  and the spin of an electron results in spin magnetic moment  $(m_s)$ . An atom with an unpaired electron, behaves like a bar magnet. When a bar magnet is placed in an inhomogeneous magnet field, it experiences a resultant force. The magnitude and direction of the resultant force depend on the orientation of the axis of the bar magnet relative to the magnetic field. This force causes deflection of the bar magnet.

A silver atom is a monovalent element and it has an unpaired electron in 5s orbital. This unpaired electron results in spin magnetic moment of the atom. Therefore, a silver atom behaves like a bar magnet. The spin magnetic moment of an electron can have only two possible orientations in an external magnetic field — one with spin up and the other one with spin down, with respect to the magnetic field. When the silver atoms are passed through an inhomogeneous magnetic field, if the atoms with spin up electrons are deflected upwards, the atoms with spin down electrons are deflected downwards by the inhomogeneous magnetic field.

#### **Construction:**

In Stern-Gerlach experiment, silver atoms are produced by heating silver in a small electric oven. An inhomogeneous magnetic field is produced by having a knife edged and a cylindrically grooved magnetic poles as shown in the figure. The intensity of magnetic field is greatest at the knife edge and decreases towards the cylindrical pole. The silver atoms are passed through a series of slits to make a thin beam of atoms. Then, they are passed through the inhomogeneous magnetic field. Trace of the silver atoms is recorded on a photographic film. The entire set up is enclosed in a vacuum chamber to avoid collision of silver atoms with air molecules.





Inhomogeneous magnetic field

#### **Result and Discussion:**

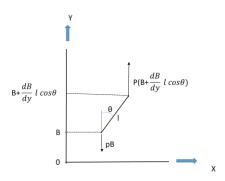
In the absence of magnetic field, the trace of the silver atoms on the photographic film is a horizontal straight line. In the presence of the inhomogeneous magnetic field the silver atom beam splits into two components and the trace is as shown in the figure.

The angular momentum J of silver atoms is entirely due to spin of its valence electron. The spin angular momentum is given by

$$S = \sqrt{s(s+1)} \, \frac{h}{2\pi}$$

Where,  $s = \frac{1}{2}$ .

The number of orientations of the angular momentum with respect to an external magnetic field is given by (2s+1) = [2(1/2) + 1] = 2. Therefore, the spin magnetic moment can have only two orientations with respect to the magnetic field.



Suppose, the magnetic field is inhomogeneous along Y-direction. The field gradient is  $\frac{dB}{dy}$ . Let the atomic magnet with magnetic moment M, pole strength p and length 1 inclined at an angle  $\theta$  with the

field direction is placed in such a field as shown in the figure. If the field strength at one pole is B then the field strength at the other pole is  $B + \frac{dB}{dy}lcos\theta$ . Force on one pole of the atomic magnet is pB and on the other pole is  $p \left(B + \frac{dB}{dy}lcos\theta\right)$ . The extra force  $p\left(\frac{dB}{dy}lcos\theta\right)$  on one pole displaces the atom as a whole. The force  $F_y$  is given by

$$F_y = p.l \cos\theta \left(\frac{dB}{dy}\right) = M \cos\theta \left(\frac{dB}{dy}\right).$$

Where, pl = M is the magnetic moment.

Due to this force, the atomic magnet will be displaced from its straight path in the field direction. The splitting of silver atom beam into two components in an inhomogeneous magnetic field verifies the existence of some silver atoms with spin up electrons and some silver atoms with spin down electrons.

#### **Polarization of Light:**

**Light wave**: Light wave is a transverse electromagnetic wave. A light wave consists of electric and magnetic fields vibrating perpendicular to each other and to the direction of propagation. It is the electric vector which is more effective in a light wave. Therefore, the plane in which the electric vector oscillates is important.

**Unpolarised light**: A light wave which has its electric vector oscillating in all possible directions perpendicular to the direction of propagation of light is called an unpolarised light.

**Polarised light**: A light wave which has its electric vector oscillating geometrically restricted is called an unpolarised light.

**Linearly polarised light**: A light wave whose electric vector is restricted to a plane perpendicular to the direction of propagation of light is called a linearly polarised light or plane polarised light.

**Circularly polarised light**: A light wave whose tip of electric vector traces a circle perpendicular to the direction of propagation is called a circularly polarised light.

**Elliptically polarised light**: A light wave whose tip of electric vector traces an ellipse perpendicular to the direction of propagation is called an elliptically polarised light.

A plane polarised light can be converted into either a circularly or an elliptically polarised light by suitable methods.

Production of plane polarised light: Plane polarised light can be produced by,

- (i) Reflection
- (ii) Refraction
- (iii) Scattering
- (iv) Selective absorption
- (v) Double refraction

**Polariser**: A polariser is an optical device that transforms unpolarised light into polarised light.

**Analyser**: An analyser is an optical device which is used to identify the plane of vibration of a polarised light.

**Half wave plate:** A half wave plate is a thin birefringent crystal of right thickness that introduces a path difference of  $\frac{\lambda}{2}$  between two orthogonal electric vibrations one making  $0^{\circ}$  and the other one making  $90^{\circ}$  with the optic axis of the half wave plate.

Quarter wave plate: A quarter wave plate is a thin birefringent crystal of right thickness that introduces a path difference of  $\frac{\lambda}{4}$  between two orthogonal electric vibrations one making  $0^{\circ}$  and the other one making  $90^{\circ}$  with its optic axis.

#### **Production of plane polarised light:**

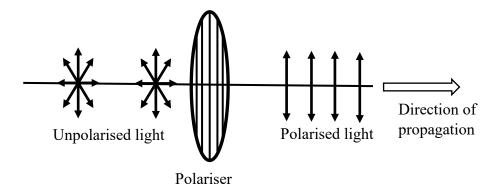


Fig.1 Production of plane polarised light.

An unpolarised light which has the electric field vector oscillating in all possible directions is passed through a polariser. The polariser allows only that part of light whose electric vector vibration is restricted to only one plane and blocks all other vibrations. A linearly polarised light is obtained on the other side of the polariser as shown in Fig.1.

#### **Detection of plane polarised light:**

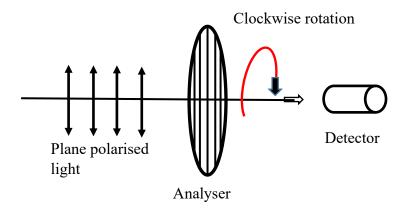


Fig. 2 Detection of plane polarised light

An analyser is introduced in the path of light as shown in Fig.2. The analyser is rotated through one full circle either clockwise or anticlockwise. If the intensity of transmitted light is zero twice, then the light is plane polarised.

#### **Production of circularly polarised light:**

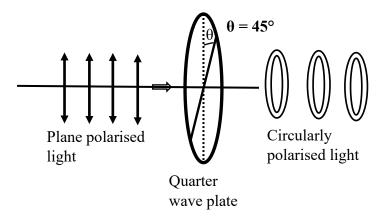


Fig.3 Production of circularly polarised light.

A beam of plane polarised light is incident on a quarter wave plate such that the electric vector makes an angle  $\theta = 45^{\circ}$  with the optic axis of the quarter wave plate as shown in Fig.3. The resultant light is a circularly polarised light.

#### **Detection of circularly polarised light:**

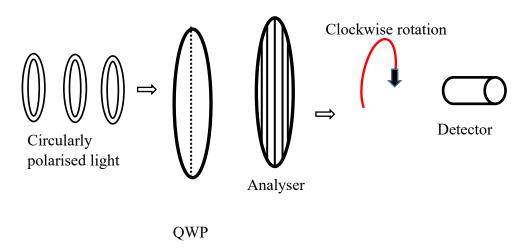


Fig. 4 Detection of circularly polarised light

An analyser is introduced in the path of light as shown in Fig.4. The quarter wave plate (QWP) converts light into plane polarised light if it is circularly polarised. The analyser is rotated through one full circle either clockwise or anticlockwise. If the intensity of transmitted light is zero twice, then the light is circularly polarised.

#### **Production of elliptically polarised light:**

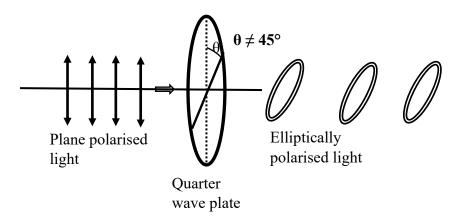


Fig.5 Production of circularly polarised light.

A beam of plane polarised light is incident on a quarter wave plate such that the electric vector makes an angle  $\theta \neq 45^{\circ}$  with the optic axis of the quarter wave plate as shown in Fig.5. The resultant light is an elliptically polarised light.

#### **Detection of elliptically polarised light:**

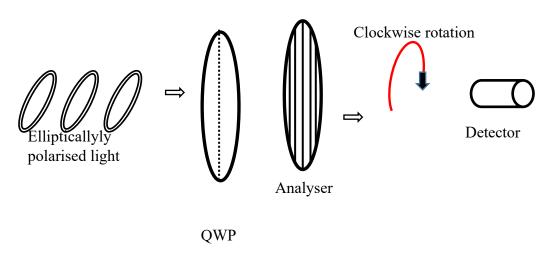


Fig. 6 Detection of elliptically polarised light

A quarter wave plate and an analyser are introduced in the path of light as shown in Fig.6. The quarter wave plate (QWP) converts light into a plane polarised light if it is elliptically polarised. The analyser is rotated through one full circle either clockwise or anticlockwise. If the intensity of transmitted light is zero twice, then the light is elliptically polarised.

#### **Classical Computing:**

The principles of classical physics and mathematical reasoning form the foundation of classical computing.

Traditional computer software is designed for serial computation. It indicates that one task must be finished before starting another.

Parallel computing is possible on a computer with multiple processors. It means it can work on multiple tasks at the same time, and the results should be integrated.

#### Moore's Law:

Moore's law is not a natural law. It is an observation did by Gordon G. Moore.

# It states that the number of transistors on a computer chip and, thus its power doubles every 2 years.

Computer hardware is getting smaller, cheaper and faster. This has been possible because of the miniaturization in ICs (integrated circuits). It means the spacing between the transistors and other components keeps on decreasing.

#### Is Moore's law still holding?

Although Moore's law trend continued for more than 50 years, the transistor counts doubled after 3 years, not 24 months.

# Need for quantum computing:

There are two problems associated with miniaturization.

- 1) When the separation between the components is of the order of atomic dimensions, the uncertainty principle and other quantum mechanical laws become prominent. In other words, the computation based on classical physics will no longer be reliable.
- 2) The heat produced by one component will affect the performance of another component. The present day computers generate a lot of heat.

#### **Quantum computing:**

A quantum computer is a machine that performs calculations based on the laws of quantum mechanics, which is the behaviour of particles at the sub-atomic level.

The fundamental concept of classical computation and information is a "bit". The data is stored in a bit. The bit can take the value 0 or 1.

The corresponding parameter in a quantum computer is a quantum bit or qubit.

#### Single particle quantum interference

A laser that emits one photon at a time is used in the experimental setup (Fig. a). This can be accomplished by employing a set of attenuators, which can filter out laser light and ensure that only one photon emerges at a time. This photon is then split by a beam splitter. The beam splitter reflects half of the light that strikes it and allows the other half to pass through. Photon detectors A and B detect the photon with equal probabilities. Hence it can be concluded that during any one run the photon has traveled one of the paths since it cannot be split into two. *However, this assumption is not true*.

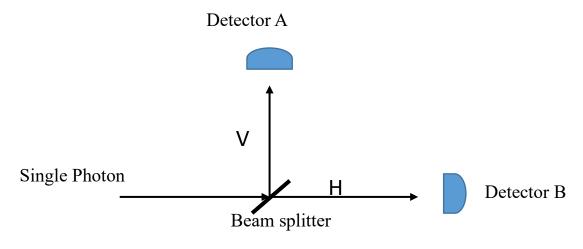
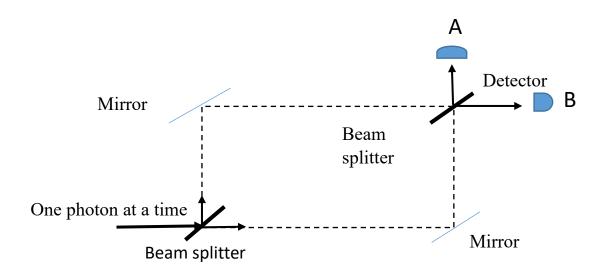


Fig. (a)

Now experimental set up is changed as shown in Fig. (b). A single photon may travel horizontally, gets deflected by a mirror, and reaches the detector. Another possibility is that it passes vertically, gets deflected by a mirror, and reaches the detector. Hence if the photon really takes a single path through the apparatus, both detectors would detect it with equal probabilities. However, this does not happen. The photon always strikes detector A and never detector B. If we change the path length by introducing a glass plate in one of the paths (say vertical one), the photon is detected by detector B and never by detector A. It means that the photon was in a superposition state, and it travelled through both paths simultaneously. At the second beam splitter, both the components interfered, constructively or destructively, and get detected by one of the detectors.



**Fig.** (b)

# Difference between classical computing and quantum computing:

Classical Computing	Quantum Computing		
Conventional computing is based on the classical phenomenon of electrical circuits being in a single state at a given time, either on or off.	Quantum computing is based on the phenomenon of Quantum Mechanics, such as superposition and entanglement, the phenomenon where it is possible to be in more than one state at a time.		
Information storage and manipulation are based on "bit", which is based on voltage or charge; low is 0 and high is 1.	Information storage and manipulation are based on Quantum Bit or "qubit", which is based on the spin of an electron or polarization of a single photon.		
The circuit behaviour is governed by classical physics.	The circuit behaviour is governed by quantum mechanics.		
Conventional computing uses binary codes i.e. bits 0 or 1 to represent information.	Quantum computing uses Qubits i.e.  0>,  1> and the superposition state of both  0> and  1> to represent information.		
Transistors are the basic building blocks of conventional computers.	Superconducting Quantum Interference Devices (SQUID) or Quantum Transistors are the basic building blocks of quantum computers.		
In conventional computers, data processing is done in the Central Processing Unit or CPU, which consists of an Arithmetic and Logic Unit (ALU), processor registers and a control unit.	In quantum computers, data processing is done in a Quantum Processing Unit or QPU, which consists of several interconnected qubits.		

#### Comparison of classical and quantum information

- ➤ Information, either classical or quantum, is physical.
- ➤ It is transmitted by physical means.
- ➤ It is stored in physical system.

Quantum information	Classical information		
It is encoded to some property of a	It is encoded to some property of a		
quantum system like the polarization of a	physical system obeying the laws of		
photon or spin of an electron.	classical physics.		
It is processed using quantum gates.	It is processed using classical gates.		
The fundamental unit of information is a	The fundamental unit of information is a		
qubit.	bit.		
It is difficult to store, transmit and	It is easy to store, transmit and process.		
process.			
There is no way to copy unknown	It is easy to make copies of classical		
information.	information.		
In general, the measurement of	It can be measured without disturbing it.		
information destroys it.			

#### **Quantum Superposition**

Quantum superposition is a phenomenon associated with quantum systems such as nuclei, electrons and photons, for which wave-particle duality and other non-classical effects are observed. A quantum system can exist in more than one state at the same time. The result of the measurement is the observation of some definite state with a given probability.

Quantum superposition is easily demonstrated using a coin. A coin has a 50/50 probability of landing as either heads or tails while flipped in the air.

#### What state is the coin in while it is in the air? Is it heads or tails?

We can say that the coin is in a superposition of both heads and tails. When it lands, it has a definite state, either heads or tails. The word "state" means any particular way that a system can possibly be described. For example, the coin can be either heads, or tails, or a combination of heads or tails while flipped in the air. All of these cases are called states of the coin system. The measurement destroys the superposition.

#### Qubit:

A qubit, like a bit, also makes use of two states  $|0\rangle$  and  $|1\rangle$  to hold information.

Mathematically, qubits  $|0\rangle$  and  $|1\rangle$  can be represented as column matrices:

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

However, unlike classical bits, a qubit,  $|\Psi\rangle$  can also be in a superposition state of  $|0\rangle$  and  $|1\rangle$  states.

It can be written as  $|\Psi\rangle = \alpha |0\rangle + \beta |1\rangle$ 

where  $\alpha$  and  $\beta$  are generally complex numbers which represent the probability amplitudes of the states.

When a qubit is measured, it only results in either  $|0\rangle$  or  $|1\rangle$ .

## Summation of probabilities

The probability of measuring the qubit in state  $|0\rangle$  is  $|\alpha|^2$ , and the probability of measuring the qubit in state  $|1\rangle$  is  $|\beta|^2$ .

Since the total probability of observing all the states of the quantum system must add up to 100%, the amplitudes must follow this rule:

$$|\alpha|^2 + |\beta|^2 = 1$$

This is called a normalization rule.

#### **Physical Realization of Qubits:**

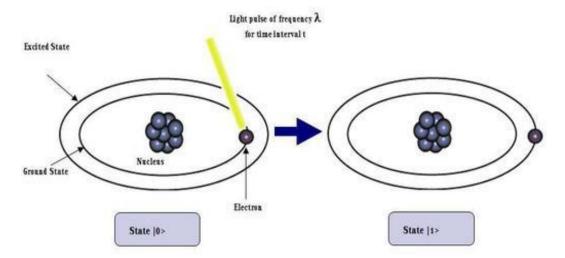
In a classical computer, the 0- and 1-bit mathematically represent the two allowed voltages across a wire in a classical circuit. Semiconductor devices called transistors are used to control what happens to these voltages.

#### "What is a qubit made out of?"

Energy levels of an atom: Consider the electron in a hydrogen atom. It can be in its ground state (i.e. an s orbital) or in an excited state. So we can also store a qubit of information in the quantum state of the electron, i.e., in the superposition.

Ground state |0>

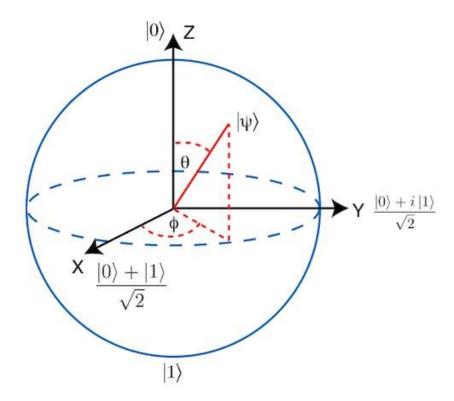
Excited state |1>



- > Spin: Elementary particles like electrons and protons carry an intrinsic angular momentum called spin. Their spins can be used as qubits with  $|0>=|\uparrow>$ ,  $|1>=|\downarrow>$
- ➤ **Polarization of Photon:** A linearly polarized photon can be either horizontally or vertically polarized with respect to some direction in which the photon is moving. Quantum researchers can create photons one at a time and encode qubits of information into their polarization.

#### Bloch Sphere Representation

Bloch sphere is a physical representation of all possible qubit states. It is a sphere of unit radius and the state of a qubit can be represented by a vector in this sphere. |0> is at the north pole, |1> is at the south pole, as shown in Figure.



Using the spherical coordinate system, an arbitrary position of the state vector of a qubit can be written in terms of the angles  $\theta$  (elevation, the state vector makes from the z-axis) and  $\phi$  (azimuth, the angle of projection of the state vector in the x-y plane from the x-axis) it makes in the Bloch sphere as:

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right) |0\rangle + e^{i\phi} \sin\left(\frac{\theta}{2}\right) |1\rangle = \begin{bmatrix} \cos\left(\frac{\theta}{2}\right) \\ e^{i\phi} \sin\left(\frac{\theta}{2}\right) \end{bmatrix}$$

#### Note:

- For  $\varphi = 0$  and  $\theta = 0$ , the state  $|\psi\rangle$  corresponds to  $|0\rangle$  and is along +z-axis.
- For  $\varphi = 0$  and  $\theta = 180^{\circ}$  the state  $|\psi\rangle$  corresponds to  $|1\rangle$  and is along -z-axis.
- When  $\theta = 90^{\circ}$ ,  $|\psi\rangle$  is in the x-y plane.

For 
$$\varphi = 90^{\circ}$$
,  $|\psi\rangle = \frac{1}{\sqrt{2}}$  ( $|0\rangle + i|1\rangle$ ), is a superposition state along +y-axis.

For 
$$\varphi = -90^{\circ}$$
,  $|\psi\rangle = \frac{1}{\sqrt{2}}$  ( $|0\rangle - i|1\rangle$ ), is a superposition state along the -y-axis.

For 
$$\varphi = 0^{\circ}$$
,  $|\psi\rangle = \frac{1}{\sqrt{2}}$  ( $|0\rangle + |1\rangle$ ), is a superposition state along the +x-axis.

For 
$$\varphi = 180^{\circ}$$
,  $|\psi\rangle = \frac{1}{\sqrt{2}}$  ( $|0\rangle - |1\rangle$ ), is a superposition state along the -x-axis.

For a classical computer, the two logical states 0 and 1 are represented by the poles of a sphere.

In contrast, the state of a qubit can be represented by any point on the sphere. Since there are infinite points on the sphere, a qubit in principle has more capacity to store information compared to a classical bit.

**Note:** Bloch sphere represents the state of only one qubit. There is no generalization of the Bloch sphere for multiple qubits.

#### Difference between classical "bits" and "qubits":

A fundamental difference between classical bits and qubits is the way they operate.

The classical bits can be deterministically set in a "0" or a "1" state.

It is read (or measured) any number of times as long as it is powered.

Reading a classical bit does not destroy its state. A bit retains its state as long as it is powered.

The qubits are probabilistic.

They are in a superposition state of  $|0\rangle$  and  $|1\rangle$  with different probabilities.

They possess characteristics of both states simultaneously, at all times, until measured.

The qubits lose their internal state when they are measured.

#### The framework of quantum mechanics for quantum computing:

#### **Wave function in Dirac notation:**

A wave function (say  $\psi$ ) represents the physical state of a system.

According to Paul Dirac, the state of a system is described by a vector, called a state vector, in Hilbert space  $\mathcal{H}$ . Depending on the degree of freedom (i.e. the type of state) of the system being considered,  $\mathcal{H}$  may have infinite-dimensional.

[<u>Hilbert space  $\mathcal{H}$ </u>: It is a complex vector space. It has all the properties of linear vector space like vector addition and scalar multiplication. In addition, it satisfies inner product operation.

An inner product is a generalization of the dot product It is a method of multiplying vectors together in a vector space, with the result being a scalar.]

If  $\psi$  is a wavefunction, then in Dirac notation  $\psi$  is represented as  $|\psi\rangle$ , which is called a **ket vector**.

**Example**: Suppose  $\psi = A e^{-i k x}$ 

Dirac notation  $| \psi \rangle = A e^{-i k x}$ 

**Note:** Only the notation of  $\psi$  is changed. The form of the wave function remains unchanged.

If  $\psi^*$  is the complex conjugate of  $\psi$ , then  $\psi^*$  is represented as  $<\psi|$ , which is called a **bra vector** Hence,

$$<\psi|=A^*e^{ikx}$$

**Basis:** In quantum mechanics, the "basis vectors" can be thought of as a set of mutually perpendicular vectors, one for each "dimension" of the space in which the state vector is expressed. The magnitude of a basis vector is one. There is a one-to-one correspondence between basis vectors and dimensions of the space.

#### **Matrix form of a wave function:**

Consider a discrete and complete basis that is made up of an infinite set of kets  $|\phi_1\rangle$ ,  $|\phi_2\rangle$ ,  $|\phi_3\rangle$  ··· etc.

The state vector  $|\psi\rangle$  can be written as a linear combination of kets  $|\phi_1\rangle$ ,  $|\phi_2\rangle$ ,  $|\phi_3\rangle$  ··· etc as follows:

$$|\psi>=a_1|\phi_1>+a_2|\phi_2>+a_3|\phi_3>+\cdots+a_n|\phi_n>=\sum_{n=1}^{\infty}a_n|\phi_n>$$

Where the coefficients  $a_1$ ,  $a_2$ ,  $a_3$ ....  $a_n$ , represent the projection of  $|\psi\rangle$  onto  $|\phi_n\rangle$ .  $a_n$  is the component of  $|\psi\rangle$  along the vector  $|\phi_n\rangle$ .

Hence,  $|\psi\rangle$  can be represented as a **column vector** (**column matrix**) given by

$$|\psi\rangle \rightarrow \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_n \end{bmatrix}$$

[A **column matrix** is a matrix having all its elements in a single column. The elements are arranged in a vertical manner. The order of a column matrix having n elements is n x 1]

The bra vector  $\langle \psi |$  can be represented by a **row vector** (**row matrix**) :

$$<\psi| \to [a_1^* \ a_2^* \ a_3^* \ \dots \dots a_n^*]$$

[A **row matrix** is a matrix having all its elements in a single row. The elements are arranged in a horizontal manner. The order of a row matrix having n elements is  $1 \times n$ ]

#### Remark:

A ket  $|\psi\rangle$  is normalized if  $\langle\psi|\psi\rangle=\sum_n |a_n|^2=1$ 

If  $|\psi>$  is not normalized, we can multiply it by a constant 'a' so that

$$< a \psi | a \psi > = |a|^2 < \psi | \psi > = 1$$

Hence, the normalization constant 'a' =  $1/\sqrt{\langle \psi | \psi \rangle}$ 

#### **Inner product:**

If  $\psi = \psi(x)$  and  $\phi = \phi(x)$  are two wavefunctions, then their inner product can be defined as

$$(\psi,\phi) = \int \psi^*(x) \, \phi(x) dx$$

In Dirac notation  $(\psi, \phi)$  is written as  $<\psi|\phi>$ .

Since the inner product (scalar product) is a complex number in quantum mechanics,

$$<\psi|\phi>=<\phi|\psi>^*$$

This property can be demonstrated as follows:

$$<\phi|\psi>^* = (\int \phi^*(x)\psi(x)dx)^* = \int \psi^*(x)\phi(x)dx = <\psi|\phi>$$

For any state vector  $|\psi\rangle$ ,  $\langle\psi|\psi\rangle$  is real and positive.

If the state  $|\psi\rangle$  is normalized,  $\langle\psi|\psi\rangle=1$ 

Therefore,  $\langle \psi | \psi \rangle = 0$  only if  $| \psi \rangle = 0$ .

#### **Matrix form of inner product:**

Let 
$$|\psi\rangle = a_1 |\phi_1\rangle + a_2 |\phi_2\rangle + a_3 |\phi_3\rangle + \cdots + a_n |\phi_n\rangle$$

$$= \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_n \end{bmatrix}$$

$$|\Phi> = b_1 | \phi_1> + b_2 | \phi_2> + b_3 | \phi_3> + \cdots + b_n | \phi_n>$$

$$=egin{bmatrix} b_1 \ b_2 \ b_3 \ \vdots \ b_n \end{bmatrix}$$

$$<\psi|\phi>=[\ a_{1}^{*}\ a_{2}^{*}\ a_{3}^{*}\ \dots\dots a_{n}^{*}]egin{bmatrix} b_{1}\ b_{2}\ b_{3}\ \vdots\ b_{n} \end{bmatrix}$$

$$= a_1^*b_1 + a_2^*b_2 + a_3^*b_3 + \dots + a_n^*b_n$$

#### **Condition for orthogonality:**

Two ket vectors  $|\psi\rangle$  and  $|\phi\rangle$ , are said to be orthogonal if their inner product is zero.

i.e. 
$$\langle \psi | \phi \rangle = 0$$

#### **Condition for orthnormality:**

Two ket vectors  $|\psi\rangle$  and  $|\phi\rangle$ , are said to be orthonormal if they are orthogonal and if each of them is normalized.

i.e. 
$$\langle \psi | \phi \rangle = 0$$
,  $\langle \psi | \psi \rangle = 1$ ,  $\langle \phi | \phi \rangle = 1$ 

#### **Operator:**

An operator  $\hat{A}$  is a mathematical rule that when applied to a ket vector  $|\psi\rangle$  transforms it to another ket vector  $|\phi\rangle$  of the same space and when it acts on a bra vector  $|\psi\rangle$  transforms it to another bra vector  $|\psi\rangle$ .

i.e. 
$$\hat{A} \mid \psi \rangle = |\phi \rangle$$
,  $\hat{A} \langle \psi | = \langle \phi |$ 

Linear operators can be represented as square matrices in quantum mechanics.

**Unity operator** ( $\hat{I}$ ): It leaves any ket vector unchanged.

i.e. 
$$\hat{I} \mid \psi > = \mid \psi >$$

#### **Identity matrix(I):**

An identity matrix is a square matrix in which all the elements of principal diagonals are one, and all other elements are zeros. If any matrix is multiplied by the identity matrix, the result will be given a matrix.

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

Example: The matrix form of ket vectors  $|0\rangle$  and  $|1\rangle$  can be written as:

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$
 and  $|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ , then

$$I \mid 0 \rangle = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1x1 + 0x0 \\ 0x1 + 1x0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$I \mid 1 \rangle = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1x0 + 0x1 \\ 0x0 + 1x1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

#### **Hermitian matrix:**

A Hermitian matrix is a square matrix composed of complex numbers, and it is equal to its conjugate transpose.

Example: 
$$M = \begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix}$$

The conjugate transpose of the matrix is  $M^H$  or  $M^{\dagger} = \begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix}$ 

Here, 
$$M = M^{\dagger}$$

Hence M is a Hermitian matrix.

#### **Unitary matrix:**

Unitary Matrix is a square matrix of complex numbers. The product of the conjugate transpose of a unitary matrix, with the unitary matrix itself, gives an identity matrix.

Example:

$$U = \frac{1}{3} \begin{bmatrix} 2 & -2+i \\ 2+i & 2 \end{bmatrix}$$

Taking conjugate 
$$\overline{U} = \frac{1}{3} \begin{bmatrix} 2 & -2 - i \\ 2 - i & 2 \end{bmatrix}$$

If we take the transpose of the above matrix, it is called a Hermitian matrix.

$$U^{\dagger} = \frac{1}{3} \begin{bmatrix} 2 & 2 - i \\ -2 - i & 2 \end{bmatrix}$$

$$\therefore U^{\dagger}.U = \frac{1}{3} \begin{bmatrix} 2 & 2 - i \\ -2 - i & 2 \end{bmatrix} \frac{1}{3} \begin{bmatrix} 2 & -2 + i \\ 2 + i & 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I$$
Similarly,  $U.U^{\dagger} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I$ 

Hence, U is a unitary matrix.

## Pauli matrices:

The Pauli matrices are a set of four 2x2 complex matrices. They are used to represent spin angular momentum. These matrices are Hermitian and Unitary.

These matrices are very powerful in quantum computing as they can be used to represent quantum logic gates. They can set the rotational parameters for qubits. These matrices go by a variety of notations.

$$\sigma_1 \equiv \sigma_x \equiv X \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \sigma_2 \equiv \sigma_y \equiv Y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\sigma_3 \equiv \sigma_z \equiv Z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

#### **Quantum Gates:**

Classical computer circuits consist of wires and logic gates. The wires carry information around the circuit, while the logic gates manipulate information, converting it from one to another. Classical computers manipulate bits using classical logic gates, such as OR, AND, NOT, NAND, etc.

Similarly, quantum computers manipulate qubits using quantum gates which are usually represented as unitary matrices. A gate which acts on k qubits is represented by a 2k X 2k unitary matrix. The number of qubits in the input and output of the gate has to be equal. The action of the quantum gate is found by multiplying the matrix representing the gate with the vector which represents the quantum state.

#### **Single qubit gates:**

#### Pauli-X gate

In classical computers, the NOT gate takes one input and reverses its value. For example, it changes the 0 bit to a 1 bit or changes a 1 bit to a 0 bit. It is like a light switch flipping a light from ON to OFF, or from OFF to ON.

Pauli-X gate is a quantum analogue of the classical NOT gate.

- The application of this gate rotates the qubit by  $180^{\circ}$  along the x-axis. It transforms  $|0\rangle$  to  $|1\rangle$  and vice versa.
- The matrix form of X-gate is obtained as follows

$$X = |0 > < 1| + |1 > < 0|$$

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

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

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

Circuit representation

• Dirac notation

$$X |0\rangle = |1\rangle$$

$$X |1\rangle = |0\rangle$$

• When the qubit is in a superposition state  $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ , then

$$X |\psi\rangle = \alpha |1\rangle + \beta |0\rangle$$

• In matrix form  $|\psi\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ 

Then the action of X gate is

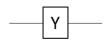
$$X \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \beta \\ \alpha \end{bmatrix}$$

## Pauli -Y gate

- The application of this gate rotates the qubit by 180° along the y-axis.
- It transforms  $|0\rangle$  to  $i|1\rangle$  and  $|1\rangle$  to  $-i|0\rangle$ .
- Matrix for of Y-gate

$$Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

• Circuit representation



• Dirac notation

$$Y |0\rangle = i |1\rangle$$

$$Y |1\rangle = -i |0\rangle$$

# Pauli - Z gate

- $\bullet$  The application of this gate rotates the qubit by  $180^{\circ}$  along the z-axis.
- It leaves  $|0\rangle$  unchanged and flips the sign of  $|1\rangle$  to  $|1\rangle$ .
- Matrix for of Z-gate

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

• Circuit representation



• Dirac notation

$$Z|0\rangle = |0\rangle$$

$$Z|1\rangle = -|1\rangle$$

#### Hadamard gate

- It is one of the most important gates for quantum computing. If the qubit starts in a definite |0>
   or |1> state, the Hadamard gate puts each into a superposition of |0> and |1> states.
- Matrix representation  $H \equiv \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
- Circuit representation

• Dirac notation

$$H|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$$

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

#### **Multiple qubits gates:**

#### **CNOT** gate:

- It is a Controlled NOT (CNOT) gate.
- It acts on two qubits.
- It performs the NOT operation on the second qubit only when the first qubit is |1> otherwise leaves it unchanged.
- Matrix representation

$$CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \qquad \begin{vmatrix} a \rangle \\ |b \rangle \qquad \qquad \begin{vmatrix} a \oplus b \end{vmatrix}$$

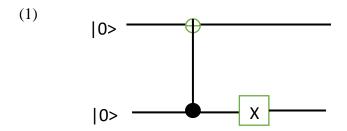
Dirac notation

$$CNOT |00\rangle = |00\rangle$$
;  $CNOT |01\rangle = |01\rangle$ 

CNOT 
$$|10\rangle = |11\rangle$$
; CNOT  $|11\rangle = |10\rangle$ 

#### **Quantum circuits:**

A quantum circuit is required to carry out computations on a quantum computer. It consists of a series of operations referred to as quantum gates. These quantum gates, which are assigned to certain qubits, change the quantum states of some of the qubits, causing those qubits to perform the calculations required to solve a problem.

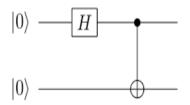


CNOT gate leaves it unchanged as the first qubit is |0>.

In the second step, X-gate flips the second qubit to |1>.

Hence the output is |01>.

(2)



The states change from the start to the end after every gate:

The Hadamard gate changes  $|0\rangle$  to  $\frac{1}{\sqrt{2}}$  ( $|0\rangle + |1\rangle$ ).

Therefore,

$$|00> \rightarrow \frac{1}{\sqrt{2}} (|0>+|1>) |0> \rightarrow \frac{1}{\sqrt{2}} (|00>+|10>).$$

In the last step, the first qubit is the control qubit.

Case 1: |00>

The control qubit is |0>, so the target qubit remains unchanged.

Case 2: |10>

The control qubit is  $|1\rangle$ , so the target qubit flips from  $|0\rangle$  to  $|1\rangle$ .

Hence the output is  $\frac{1}{\sqrt{2}}$  (|00>+|11>).

#### Accounting for the extra-ordinary capability of quantum computing:

The main advantage that a quantum computer has over a classical computer is **parallelism.** A quantum computer can perform operations on all of the states simultaneously because qubits can be in a superposition of states.

Let us consider two systems.

**System 1**: With 2 bits

This can represent 4 different values.

Possible states are [00, 01, 10, 11]

Particular state-value  $\in \{0,1,2,3\}$ , one of the 4 possible values

#### System 2: With 2 qubits

This can represent infinite different values (vector space) formed from 4 different basis state,

$$00 \equiv |00\rangle, 01 \equiv |01\rangle, 10 \equiv |10\rangle, 11 \equiv |11\rangle$$

Possible states: Infinite

particular state-value:  $\alpha |00\rangle + \beta |01\rangle + \gamma |10\rangle + \delta |11\rangle$ 

such that  $|\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 = 1$ 

Hence, an n-bit classical system can be in **one of the 2<sup>n</sup> possible states at a time**, and all it needs is the value of these **n-bits to be fully recognized.** 

An n-qubit system can be in a superposition of all of those states  $2^n$  states at a given time and needs the value of coefficients of all of the  $2^n$ -1 states (considering that summation is 1) basis to be fully recognized.

Consequently, a quantum computer can compute with 2<sup>n</sup> values in a single step. This enormous parallelism is one reason why quantum computers are so powerful

Operator	Gate(s)		Matrix
Pauli-X (X)	$-\mathbf{x}$	-	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	$- \boxed{\mathbf{Y}} -$		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	$- \boxed{\mathbf{z}} -$		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	$-\!$		$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	$-\!\!\left[\mathbf{S}\right]\!\!-\!\!$		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8~(\mathrm{T})$	$- \boxed{\mathbf{T}} -$		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP		<del></del>	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)			$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0$