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UNIT-3
Quantum Mechanics & Quantum Computing
Physics of Semiconductor
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QUANTUM MECHANICS

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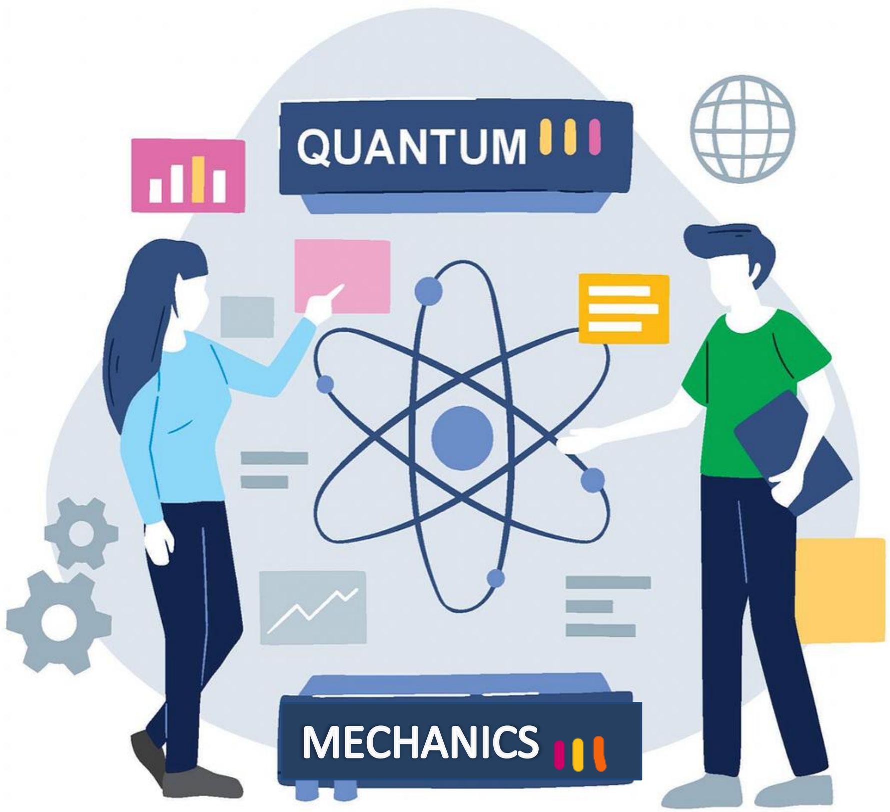
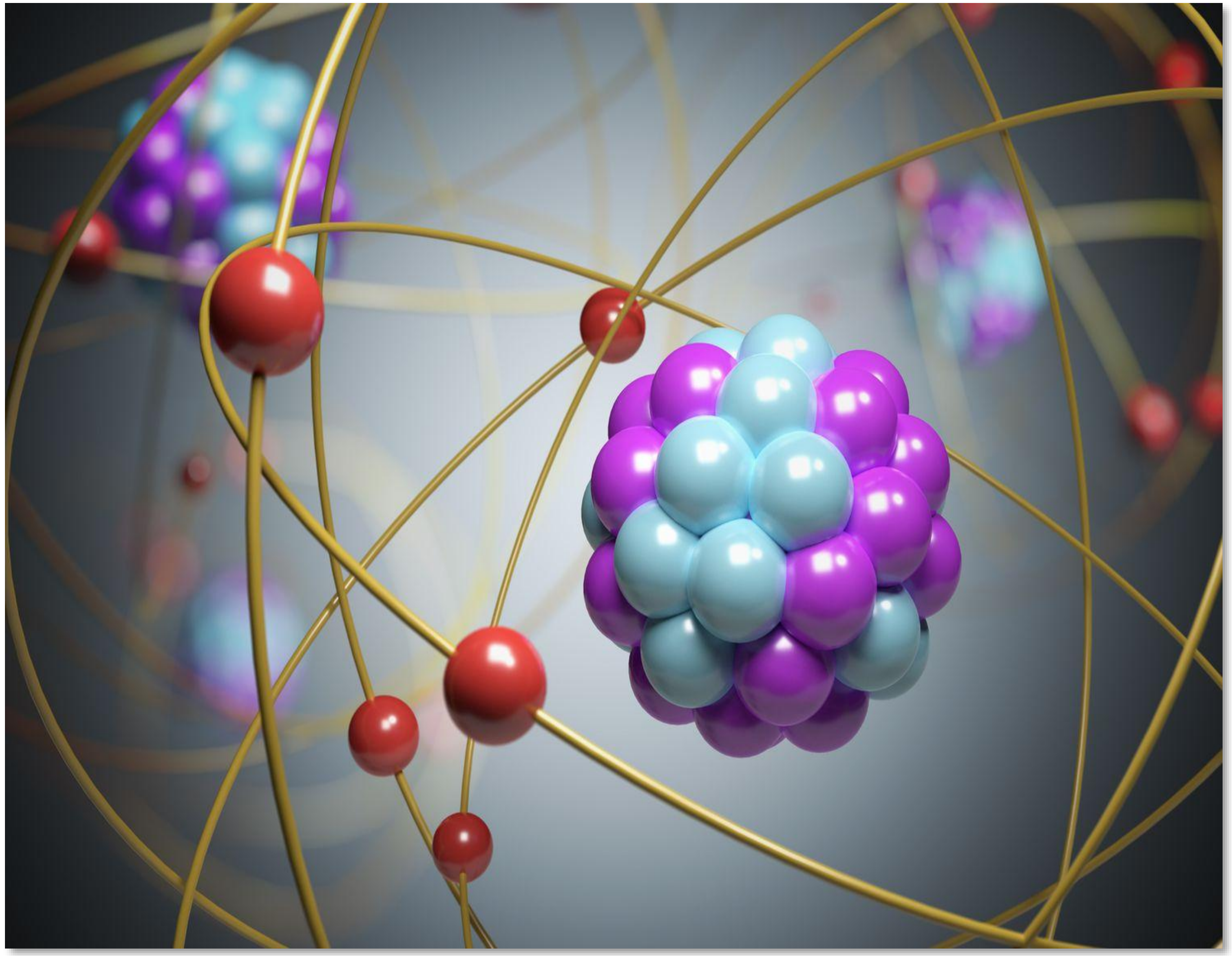
' * ' – only for knowledge, ' ** ' – conceptual base



INTRODUCTION

- Quantum Mechanics is a fundamental theory in physics that describes the behavior of matter and energy at very small scales such as atom and sub-atomic particles.

- In Quantum mechanics, the foundation of principles are purely probabilistic in nature as it is impossible to measure simultaneously the position of momentum of a particle at the sub-microscopic scale.



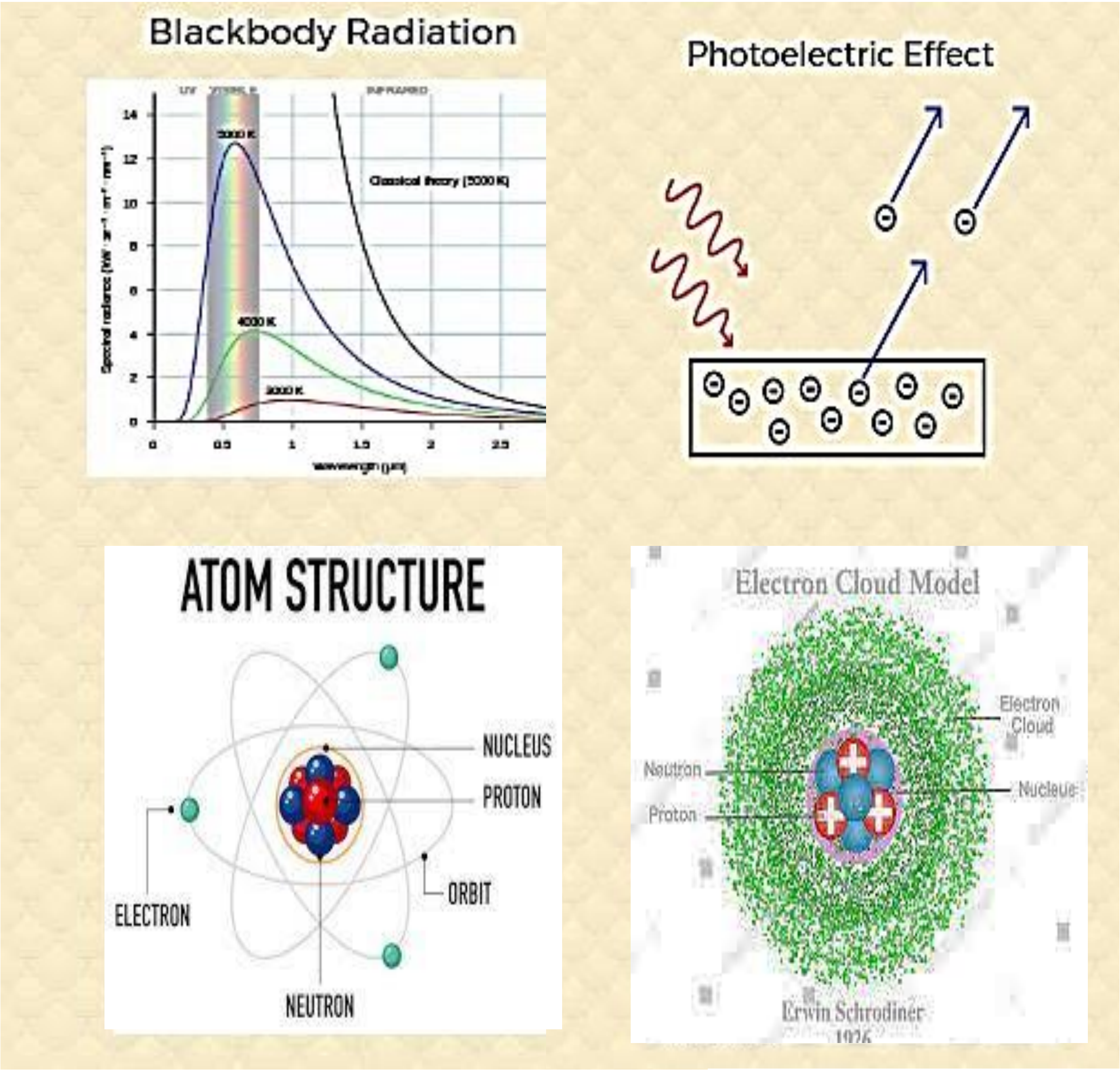
Failure of Classical Mechanics

- Classical Mechanics describes the motion of macroscopic objects. It provides extremely accurate results as long as the domain of the study is restricted to large objects and the speed involved does not approach the speed of light.

- Some unexplainable behavior (using classical theory) of phenomena at microscopic level gave birth to Quantum Mechanics or it was called as **Failure of Classical Physics** which could not explain the behavior of element / matter at microscopic level.

- **There are three failures of Classical Physics**

  1. **Black Body Radiation**
  2. **Structure/Stability of an Atom**
  3. **Photoelectric effect**



WAVE-PARTICLE DUALITY

For light: Diffraction, interference, and polarization display wave properties, while the photoelectric reveal particle-like behavior.

For matter (such as electrons): Electron diffraction (Davisson-Germer experiment) and interference show wave character, yet electrons are always detected as discrete point, revealing a particle aspect.

Louis De Broglie generalized this duality, proposed hypothesis, any particle, including an electron, exhibits both particle and wave characteristics, and the wavelength associated with the electron is:

$$\boxed{\lambda = \frac{h}{p}}$$

where, h is Planck's constant.

A moving particle is associated with a wave, called **De-Broglie wave** or **matter wave**.

Derivation steps:

For light (photons), energy is related to frequency ν by Planck's relation:

$$E = h\nu$$

Also, the wavelength and frequency relate by the speed of light c :

$$c = \lambda\nu \implies \nu = \frac{c}{\lambda}$$

Einstein's mass-energy relation:

$$E = mc^2 \longrightarrow$$ for photons $E = \mathrm{pc}$ where, p is momentum.

Equate Energy equations: $h\nu = \mathrm{pc} \quad \left(\frac{h}{p} = \frac{c}{\nu}\right) \longrightarrow \boxed{\lambda = \frac{h}{p} = \frac{h}{mv}}$

Equation represents general **De-Broglie equation** that can be applied for particles and waves.

HEISENBERG'S UNCERTAINTY PRINCIPLE

- **In classical mechanics,** position (x) and momentum (p) of macroscopic bodies can be precisely known simultaneously.

- **In quantum mechanics,** subatomic particles (like electrons) behave as wave packets spread over a region of space. This causes uncertainty in specifying the exact position of the particle. Since the wave packet contains multiple wavelengths, there is also uncertainty in the particle's momentum (from de Broglie relation).Therefore, position and momentum of a quantum particle cannot be measured simultaneously with perfect accuracy.

- Based on this, **Heisenberg (1927) stated the Uncertainty Principle:**

"It is impossible to determine both position and momentum of a quantum particle simultaneously with perfect precision."

Mathematically, Heisenberg Uncertainty Principle states that "the product of uncertainty in the simultaneous measurement of the position and momentum of a particle is equal to or greater than the $\hbar/2$ (=$h/4\pi$)", where h is the Planck's constant, i.e.

$$\Delta x \,.\, \Delta p \geq \hbar/2 \quad \text{OR} \quad \Delta x \,.\, \Delta p \geq h/4\pi$$

Δx= uncertainty in position, **Δp** = uncertainty in momentum, $\hbar$= reduced Planck's constant, **h** = Planck's constant.

$$\Delta E \cdot \Delta t \geq \hbar/2 \text{ or } h/4\pi$$

$$\Delta J \cdot \Delta \theta \geq \hbar/2 \text{ or } h/4\pi$$

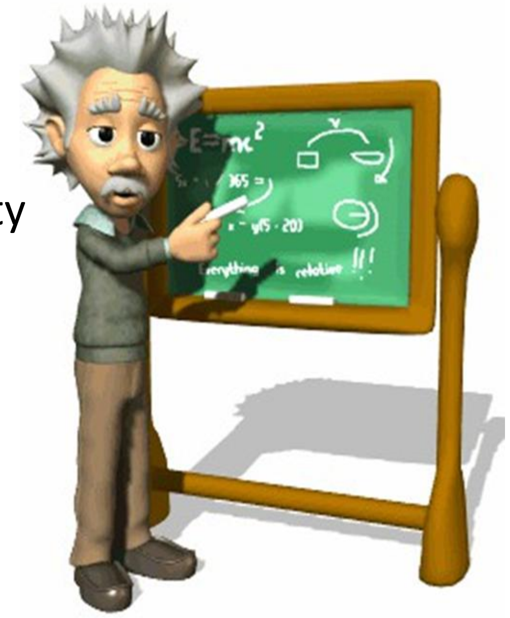
ΔE= uncertainty in energy, **Δt** = uncertainty in the time duration over which a quantum state exists

ΔJ= Uncertainty in angular momentum (which depends on angular velocity

$\Delta \theta$ = Uncertainty in angular position (angle)

Numerical Problems

1. An electron is moving with a velocity of 2×10^6m/s. Calculate its de Broglie wavelength.
2. A proton and an electron have the same kinetic energy of 1.5×10^{-18}J. Calculate and compare their de Broglie wavelengths. (Given: $m_e = 9.11 \times 10^{-31}$kg, $m_p = 1.67 \times 10^{-27}$kg, $h = 6.626 \times 10^{-34}$J·s)
3. Find the de Broglie wavelength of a ball with a mass of 0.15kg moving at 30m/s.
4. If uncertainty in the position of an electron is zero, the uncertainty in its momentum will be?
5. If the uncertainty in the velocities of two particles A and B with masses of 1.0 × 10^-27 kg and 1.0 × 10^-31 kg, respectively, is the same, what will be the ratio of uncertainty in their positions?
6. An electron is confined within a nucleus of radius 1×10^{-14}m. Estimate the minimum uncertainty in its momentum.
7. If the momentum of a particle is known with an uncertainty of 5×10^{-25}kg·m/s, what is the minimum uncertainty in its position according to the Heisenberg uncertainty principle?
8. Calculate the uncertainty in velocity of a proton if its position is known to within 1×10^{-10}m.



WAVE FUNCTION

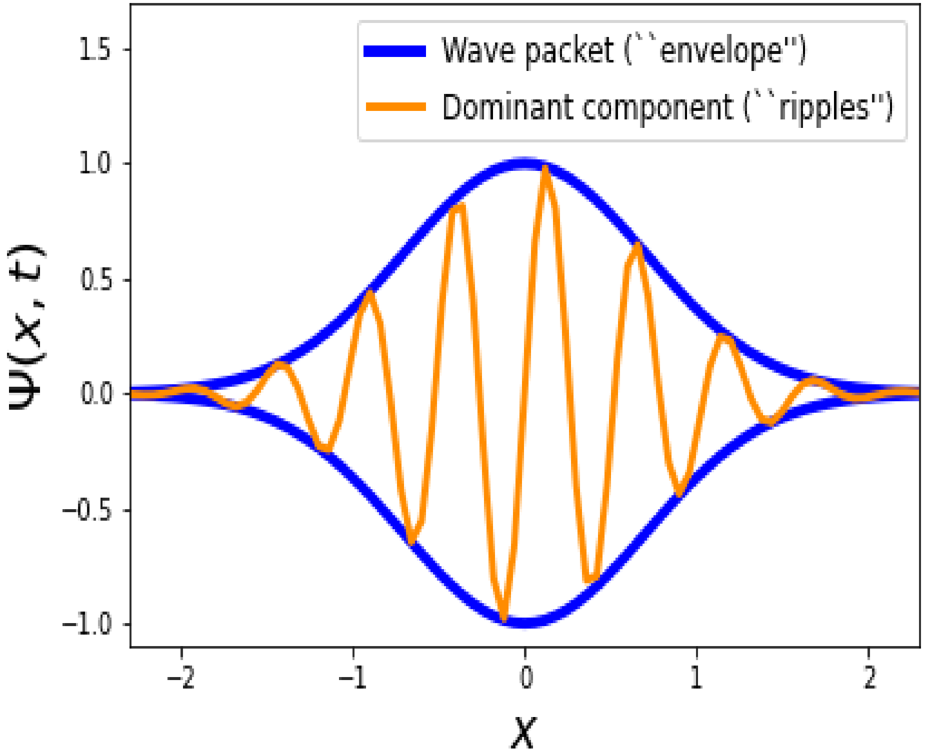
- From the analysis of electromagnetic waves, sound waves and other such waves, it has been observed that the waves are characterized by certain definite properties.
- In case of electromagnetic waves, electric and magnetic field vary periodically. In a similar way, in matter wave the quantity that varies is called the wave function denoted by Ψ.

- The space-time behavior of each moving quantum mechanical particle can be described by a function. This function is known as **wave function** and is generally denoted by Ψ (x, t) in 1-D or Ψ (r, t) in 3-D.

- It gives the probability of finding the particle at a certain position.

- **Ψ(r, t)** describes the full behavior of the particle over time.

- **Ψ(r)** represents a **stationary state** where the wave function does not change with time.



WAVE FUNCTION

WELL BEHAVED FUNCTIONS

The well-behaved wave function in quantum mechanics must satisfy these key conditions:

- **Single-valued:** The wave function $\Psi(r, t)$ must be single valued everywhere(no multiple values at the same position).
- **Finite:** The wave function $\Psi(r, t)$ must not be infinite anywhere; it should have finite values throughout space.
- **Continuous:** The wave function $\Psi(r, t)$ must be continuous without any sudden jumps or breaks over the entire region considered.
- **Continuous first derivative:** The first derivative of the wave function with respect to position must also be continuous (no abrupt changes in slope).
- **Square integrable (Normalizable):** The integral of the absolute square of the wave function over all space $\int|\psi|^2dv$ must be finite, so the total probability of finding the particle is **1**.
- **Boundary conditions:** The wave function usually goes to zero at infinity or at boundaries where the potential is infinitely large, ensuring the particle is localized.

WAVE FUNCTION

PROBABILITY DENSITY:

PROBABILITY DENSITY of a particle is the probability of finding the particle per unit volume of a given space at a particular time. Large $|\Psi|^2 \Rightarrow$ high probability; small $|\Psi|^2 \Rightarrow$ low probability.

It is generally expressed as the product of normalized wave function **Ψ** and its complex conjugate **Ψ*.**

The probability density, $P = |\psi(r, t)|^2 = \Psi^*(r, t)\Psi(r, t)$

Since the particle if existing somewhere in space, the total probability P to find the particle in space must be equal to 1.

Total Probability $P = \int |\psi(r, t)|^2\, dx = 1$

NORMALISED WAVE FUNCTION:

The process of integrating $|\psi|^2$ over all space to give unity is called **NORMALISATION**.

The normalization condition ensures that the total probability of finding the particle within all of space is 1, meaning the particle must exist somewhere.

A wave function is said to be normalised if $\int |\psi|^2 dv = 1$

OPERATORS IN QUANTUM MECHANICS

- An operator is a mathematical rule that changes a given function into a new function. If A is an operator, it is generally represented by **Â**.

- Mathematical operations in algebra and calculus like adding, subtracting, multiplying, dividing, finding the square root, differentiation or integration are represented by symbols like **+, -,×, ÷, √** can be considered as operators.
  Example: If **Â** is an operator and stands for **d/dx** (say),
  Then, when it operates on a function **x^2**, it gives **d/dx (x^2) = 2x**

- An operator in quantum mechanics is a mathematical rule or function that acts on a quantum state to produce another quantum state or extract physical information from it. Most quantum operators are linear, Hermitian (Self-adjoint), Non-commutative.

- Operators are often written with a "hat" symbol, such as $\hat{X}$ (position), $\hat{P}$ (momentum), or $\hat{H}$ (Hamiltonian/energy).

- **Example of quantum operators:** The linear **momentum operator** $\hat{P}$ when applied to the wave function ψ gives the corresponding observable quantity ' linear momentum' P and the **total energy operator** $\hat{H}$ when applied to ψ gives the corresponding observable quantity 'total energy' **E.**

OPERATORS IN QUANTUM MECHANICS

Momentum Operator

We know, $\Psi(x,\mathrm{t}) = \mathrm{A}\ e^{i(kx-\omega t)}$

Differentiating with respect to x

$$\therefore\ \frac{\partial\Psi(x,\mathrm{t})}{\partial x} = ik\Psi(x,\mathrm{t})$$

We know, $\mathrm{p} = \hbar\mathrm{k}$, $\quad k = \frac{\mathrm{p}}{\hbar}$

$$\frac{\partial\Psi(x,\mathrm{t})}{\partial\, x} = i\,\frac{p}{\hbar}\ \Psi(x,\mathrm{t})$$

$$\frac{\hbar}{i}\frac{\partial\Psi(x,\mathrm{t})}{\partial x} = p\Psi(x,\mathrm{t})$$

$$-i\hbar\ \frac{\partial\Psi(x,\mathrm{t})}{\partial x} = p\Psi(x,\mathrm{t})$$

The above equation represents ***momentum operator*** which operates on $\Psi(x)$.

For 1D, momentum operator is given by $\widehat{p_x} = -i\hbar\frac{\partial}{\partial x}$

For 3D, $\widehat{p} = -i\hbar\nabla$; where $\nabla = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$

Energy Operator

Let, the wave function of a free particle in positive X-direction is

$$\Psi(x, t) = Ae^{i(kx-\omega t)}$$

$$\therefore \qquad \frac{\partial \Psi}{\partial t} = -i\omega\Psi, \quad \text{where } \Psi = \Psi(x, t)$$

$$\text{or,} \qquad i\hbar\frac{\partial \Psi}{\partial t} = \hbar\omega\Psi \quad \text{or,} \quad i\hbar\frac{\partial \Psi}{\partial t} = E\Psi, \; [\because \; E = h\nu = \hbar\omega]$$

This equation implies the energy operator E denoted by $\hat{E}$ is given by

$$\boxed{\hat{E} = i\hbar\frac{\partial}{\partial t}}$$

EIGEN FUNCTION & EIGEN VALUE

- When an operator acting on a function always produce the same function multiplied by a constant factor, the function is called an **Eigen function** and the constant is known as **Eigen value** of the given operator.

- If Â is an operator that operates on a given function f(x), then,

$$\hat{A}\, f(x) = c\, f(x) \qquad \text{(c is a constant).}$$

- This equation is called **Eigen value equation;** the constant c is known as **Eigen value** and the function is known as **Eigen function** of the corresponding operator **Â.**

Problem 1: Why $\sin^2 x$ is not an eigen function of operator $\hat{A} = \left(\frac{d^2}{dx^2}\right)$?

Solution :

$\hat{A}\, f(x) = c\, f(x) = c$ = constant,

then f(x) is an eigen function and its eigen value is c.

Here, $f(x) = \sin^2 x$

$\hat{A}\, f(x) = \frac{d^2}{dx^2}(\sin^2 x\ )$

$= -\,2 \sin^2 x + 2 \cos^2 x$

$= 2 - 4 \sin^2 x$

So, $\sin^2 x$ is not an eigen function.

Problem 2: Which one of the following functions are eigen functions of the operator $\frac{d^2}{dx^2}$? Calculate also the eigen values where appropriate.

(i) Cos x (ii) sin 2x (iii) e^{4x} (iv) $(x^3 + 2x + 5)$

SCHRODINGER’S EQUATIONS (TDSE, TISE)

- The Schrödinger equation is a fundamental equation in quantum mechanics that describes how the quantum state (wave function) of a physical system changes over time or behaves spatially.

- Erwin Schrödinger worked extensively on wave mechanics, which used to deal with **the matter wave.** He gave two very important **equations for motion of matter waves**.

  1. Time Dependent Schrödinger Equation
  (The potential energy of a particle depends on time).

  2. Time Independent Schrödinger Equation
  (The potential energy of a particle does not depend on time).

- The Schrödinger equations may have many solutions out of these solutions; some are imaginary, which have no significance.
- The solutions which have significance for certain value are called the Eigen values.
- For each eigenvalue, there is a matching wave function Ψ called an eigenfunction.
- **A valid eigenfunction must:**

  (I) Be single-valued. (II) Be finite. (III) Be continuous everywhere in the region considered.

TIME DEPENDENT SCHRODINGER'S EQUATION

Case 1: FREE PARTICLE

Let us consider a free particle moving along x-direction. It can be described by a wave function,

$$\Psi(x, t) = A e^{i(kx-\omega t)} \quad \text{........(1)}$$

According to quantum theory,

Energy $E = \hbar\omega$ ....(2) **Momentum $p = \hbar k$ ....(3)**

The total energy of a free particle (of mass m) moving in x-direction

$$E = p^2/2m = (\hbar k)^2/2m \text{.........(4)}$$ **(P.E. = 0 for free particle)**

Differentiating equation (1) w.r.t time 't' once & space twice & comparing them we get one-dimensional (1D) time dependent Schrodinger wave equation for a free particle of mass m.

$$\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

(1D) - Time dependent Schrodinger wave equation for a free particle of mass m

TIME DEPENDENT SCHRODINGER'S EQUATION

Case 2: PARTICLE UNDER AN EXTERNAL FORCE FIELD

When a particle is moving under influence of external force it's potential energy will not be zero & hence total energy would be summation of the kinetic energy as well potential energy.

Time independent Schrodinger's wave equation for bound particle in one dimension which has mass 'm' can be given as:

$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]\Psi(x,t) = i\hbar\frac{\partial \Psi(x,t)}{\partial t}$$

(1D) - Time dependent Schrödinger wave equation

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(r,t)\right]\Psi(r,t) = i\hbar\frac{\partial \Psi(r,t)}{\partial t}$$

(3D) - Time dependent Schrödinger wave equation

TIME INDEPENDENT SCHRODINGER'S EQUATION

- When the potential energy V is independent of time, the Schrödinger equation can be separated into space and time parts.
- The spatial part leads to the **Time Independent Schrödinger Equation**, which describes stationary states with definite energy.

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\Psi(x) = E\,\Psi(x)$$

(1D) - Time Independent Schrödinger wave equation

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V(r)\right]\Psi(r) = E\,\Psi(r)$$

(3D) - Time Independent Schrödinger wave equation

POSTULATES OF QUANTUM MECHANICS

- Quantum mechanics is not derived from classical physics but is built upon a small set of fundamental postulates. These postulates define its mathematical and physical framework and are accepted as foundational truths based on extensive experimental observations.

- **THEY TELL US:**

  How to describe the state of a quantum system.
  How to represent and measure physical quantities.
  What results we might get from measurements.
  How the system changes over time when we are not measuring it.

POSTULATE 1 : STATE FUNCTION (WAVE FUNCTION)

The state of quantum mechanical system is completely described by a function $\psi(r,t)$ that depends on the co-ordinates of the particle and the time.

This function, called the wave function or the state function, contains all information that can be determined about the system.

POSTULATES OF QUANTUM MECHANICS

POSTULATE 2: OBSERVABLES AS OPERATORS

To every physical observable in classical mechanics there corresponds a linear Hermitian operator in quantum mechanics.

Observable means the quantity which can be experimentally measured. e.g position, momentum, energy etc.

POSTULATE 3: MEASUREMENT OUTCOMES (EIGENVALUE POSTULATE)

The only possible values of any observable of a system are given by the eigen value "a" in the operator equation $\hat{A}\psi = a\psi$,Where, $\hat{A}$ is the operator corresponding to the observable ψ is the eigen function and a is the eigenvalue.

POSTULATES OF QUANTUM MECHANICS

The operators corresponding to various observables (physical quantities) are given in the following table.

Name of Operator	Observables	Operators	Symbols
Position	Position with x coordinate	x	$\hat{X}$
Momentum	x component of momentum	$-i\hbar\frac{\partial}{\partial x}$	$\hat{p}_x$
Angular momentum	z component of angular momentum	$-i\hbar\frac{\partial}{\partial \phi}$	$\hat{L}_z$
K.E operator	Kinetic energy	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$	$\hat{T}$
P.E operator	Potential energy	$V_{(x)}$	$\hat{V}$
Total energy (E)	Hamiltonian operator (Time-independent)	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V_{(x)}$	$\hat{H}$
Total energy (E)	Hamiltonian operator (Time-dependent)	$-i\hbar\frac{\partial}{\partial t}$	$\hat{H}$

POSTULATE 4: PROBABILITY AND EXPECTATION VALUE (COLLAPSE POSTULATE)

- If a system is in a state described by a normalized wave function, the probability of measuring a specific eigenvalue is given by the squared amplitude of the coefficient in the expansion of the state in terms of the operator's eigenstates. Measurement also causes the wave function to "collapse" to the observed eigenstate.
- **The expectation value** represents the average result of repeated measurements of a physical quantity (an observable) on a quantum system.
- Calculated as **$\langle A \rangle = \langle \psi | A | \psi \rangle$,** it's the average outcome of an experiment, weighted by the probability of each possible result.

$$\boxed{\langle A \rangle = \int \psi^* \hat{A}\, \psi \, d\tau}$$

$\langle A \rangle$ is the expectation value of A
ψ^* is the complex conjugate of the wave function ψ
$\hat{A}$ is the operator corresponding to the observable A
$d\tau$ is the infinitesimal volume element

POSTULATE 5: TIME EVOLUTION (SCHRÖDINGER EQUATION)

- The time evolution of the quantum system is governed by the time-dependent Schrödinger equation:

$$\hat{H}\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi}{\partial t}$$

where, H is the Hamiltonian operator

- The time evolution of the quantum system is governed by the time-independent Schrödinger equation:

$$\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

PARTICLE IN A 1D INFINITE WELL/POTENTIAL BOX

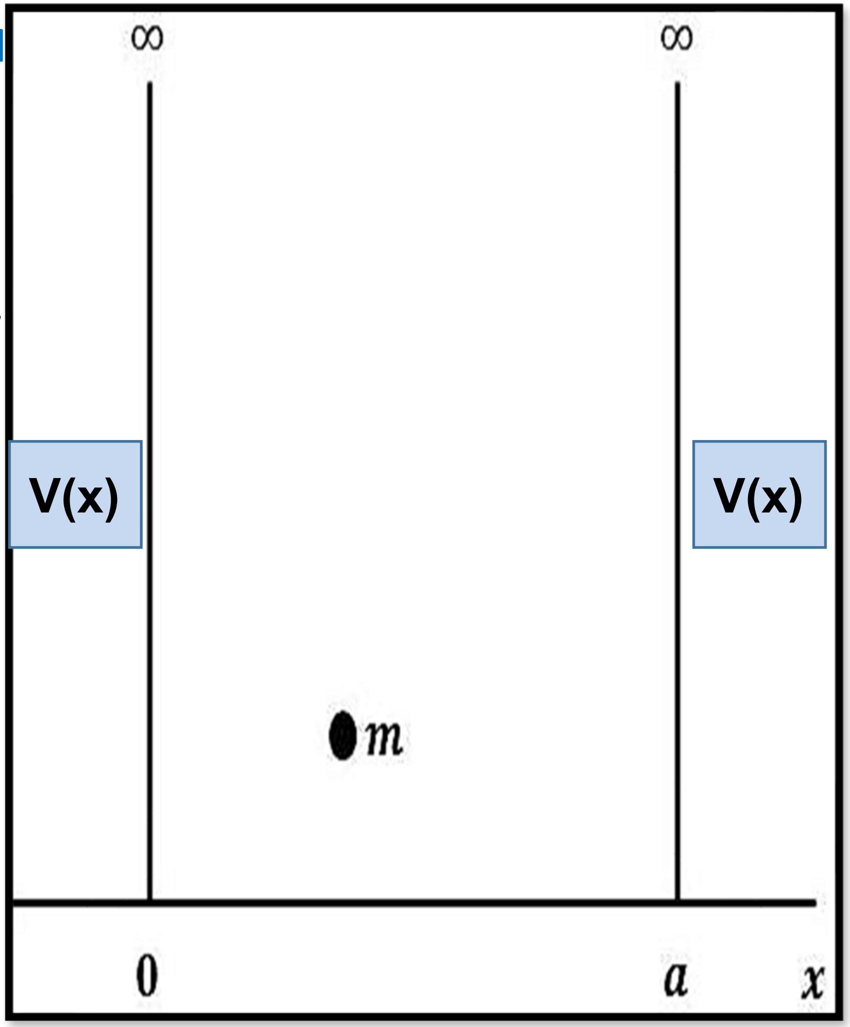
- **Consider, a particle of mass mm is inside a 1D box with infinite height and width a.**
- The particle can move only between x=0 and $x=a$.
- **Inside the box: Potential energy V=0** (free particle have zero potential energy), the particle moves freely inside the box.
- **Outside the walls: Potential energy V=∞,** the particle cannot escape from box.
- The particle is restricted to bounce back and forth inside the box.
- The walls are non-penetrable—the particle is trapped inside.

➢ **The particle cannot escape from the box,**

$$\mathbf{V = 0 \text{ for } 0 < x < a}$$
$$\mathbf{V = \infty \text{ for } 0 \geq x \geq a}$$

- **Since the particle cannot be present outside the box,**

$$\text{i.e. } |\Psi|^2 = 0 \text{ for } 0 \geq x \geq a$$



One-dimensional box (Infinite Potential Well)

PARTICLE IN A 1D INFINITE WELL/POTENTIAL BOX

Solution :

- The Schrödinger one – dimensional time independent equation is,

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\,\psi(x)$$

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad \ldots\ldots(1)$$

- For freely moving particle, $V(x) = 0$,

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0 \quad \ldots..(2)$$

Taking,

$$\frac{2mE}{\hbar^2} = k^2 \quad \ldots\ldots(3)$$

where k is known as wave vector, $k = 2\pi/\lambda$

- Equation (2) becomes,

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi\ x = 0 \quad \ldots..(4)$$

PARTICLE IN A 1D INFINITE WELL/POTENTIAL BOX

- **Solution of eq. (4) can be given by,**

$$\Psi\,(x) = A\sin kx + B\cos kx \;\; \ldots\ldots (5)$$

where A, B *and* k are unknown quantities and to calculate them it is necessary to construct boundary - conditions.

- **The boundary conditions are**

  (i) When $x = 0, \Psi\;x = 0$

  (ii) When $x = a, \Psi\;x = 0$

- **Putting Boundary Conditions (i) in eq. (5), we get**

$$\Psi\;(x) = 0 = A\sin 0 + B\cos 0$$

$$B = 0 \;\; \ldots\ldots (6)$$

- **Putting Boundary Conditions (ii) in eq. (5), we get**

$$\Psi\;(x) = 0 = A\sin ka + B\cos ka$$

- **But from eq. (6), put $B = 0$**

$$A\sin ka = 0\,,$$

But $A \neq 0$, so $\sin ka = 0$ $\longrightarrow$ $ka = n\pi$ or, $\boxed{k = \frac{n\pi}{a}}$ ….. (7) $where, n = 1,2,3 \ldots$

PARTICLE IN A 1D INFINITE WELL/POTENTIAL BOX

- Substituting equation (7) in equation (3)

$$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2}$$

$$\mathrm{E} = \frac{n^2\pi^2}{a^2}\frac{\hbar^2}{2m} \qquad (\hbar = \frac{h}{2\pi})$$

$$\mathrm{E} = \frac{n^2h^2}{8ma^2}$$

- In general, $\boxed{\mathrm{E} = \frac{n^2h^2}{8ma^2}}$ ..... (8) $where,$ **n = 1,2,3,4….**

- Equation (8) represents Eigen values of energy for different energy levels. This indicates discrete energy levels in quantum mechanics.
- Wave Function can be written as, (from equation (5) and (6))

$$\Psi\ (x) = A\sin kx$$

- Substitute equation (7), $\Psi(x) = A\sin\frac{n\pi x}{a}$ ……. (9)

PARTICLE IN A 1D INFINITE WELL/POTENTIAL BOX

- Let us find the value of A, if a particle is definitely present inside the box

$$P = \int_0^a |\Psi(x)^2| dx = 1$$

$$P = \int_0^a A^2 sin^2 \left(\frac{n\pi x}{a}\right) dx = 1 \quad \ldots .(from\, eq. 9)$$

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

Or, $\int_0^a \left\{\frac{1-\cos\frac{2n\pi x}{a}}{2}\right\} dx = \frac{1}{A^2}$

Or, $\int_0^a \left\{1 - cos\,\frac{2n\pi x}{a}\right\} dx = \frac{2}{A^2}$

Or, $(x)_0^a - \left(\frac{\sin\frac{2n\pi x}{a}}{2n\pi T_a}\right)_0^a = \frac{2}{A^2}$

Or, $(a - 0) - \left(\frac{sin\, 2n\pi - sin\, 0}{2n\pi T_a}\right) = \frac{2}{A^2}$

Thereby, $a = \frac{2}{A^2}$

$$A = \sqrt{\frac{2}{a}} \quad \ldots ..(10)$$

PARTICLE IN A 1D INFINITE WELL/POTENTIAL BOX

- **Substituting equation (10) into Eq. (9),we have**

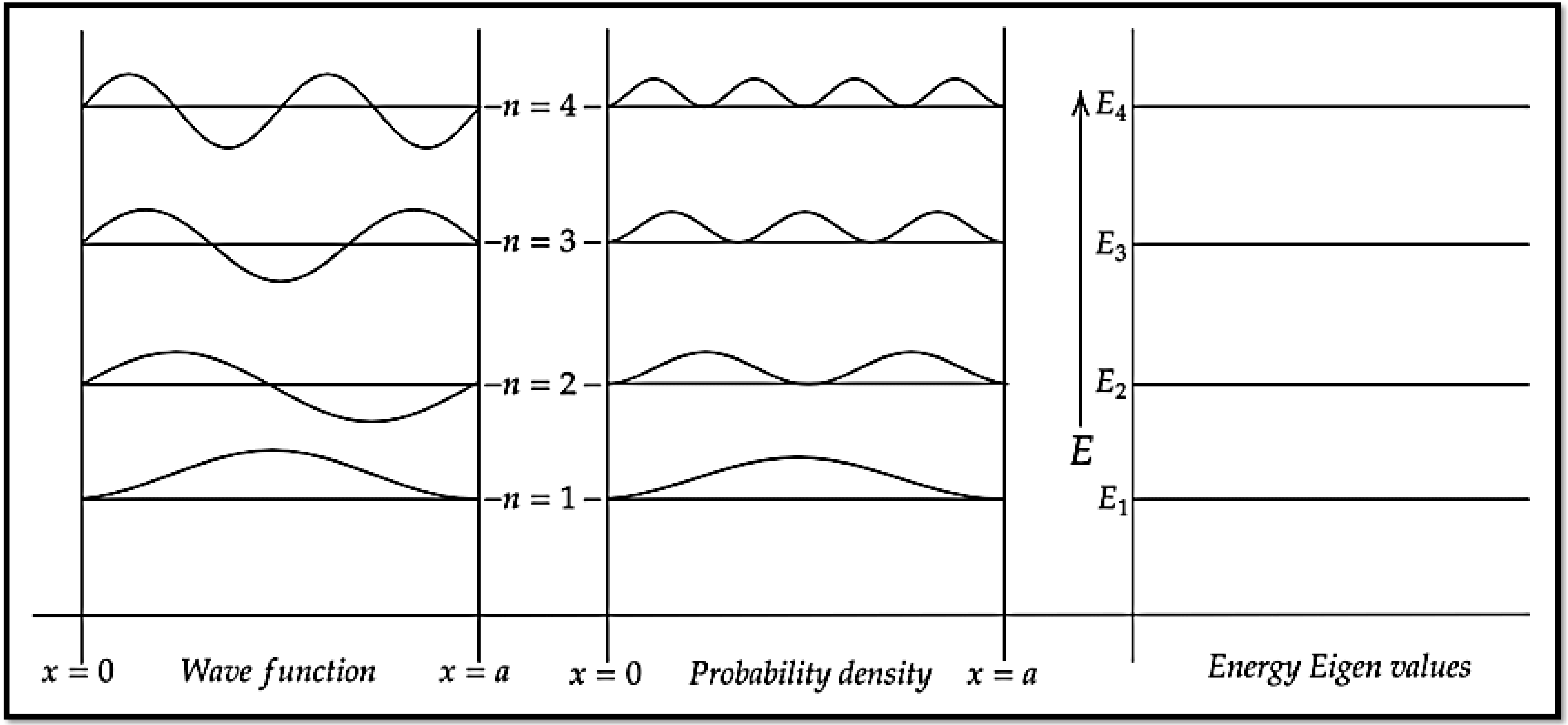
$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}} \qquad \ldots\ldots(11)$$

The wave function in n^{th} energy level is given in Equation (11).

- Therefore the particle in the box can have discrete values of energies. These values are quantized.
- **Note:** that according to classical mechanics, the particle in a box can have any energy value from 0 to infinity, but according to quantum mechanics only discrete values of energy are permissible. The particle cannot have zero energy. i.e. momentum and energy are quantized.
- The **Ψ_1, Ψ_2, Ψ_3** are normalized wave functions, given by equation (11).
- Each E_n value is known as **Eigen value** and the corresponding wave function is known as **Eigen function**.

- The wave function Ψ_1 has two nodes at $x = 0$ and $x = a$
- The wave function Ψ_2 has three nodes at $x = 0$, $x = a/2$ and $x = a$
- The wave function Ψ_3 has four nodes at $x = 0$, $x = a/3$, $x = 2a/3$ and $x = a$
- **The wave function Ψ_n has** $(\mathbf{n+1})$ nodes with boundary conditions.
- A node is the position of zero displacement.

PARTICLE IN A 1D INFINITE WELL/POTENTIAL BOX



Numerical Problems

1. Calculate the ground state energy of an electron in a 1-dimensional infinite potential well of length $L = 1$ nm.

2. Find the energy of the electron in the same 1 nm box at quantum number $n = 3$.

3. Determine the energy difference between 1st excited state and the ground state for an electron in a box of length L=2 nm.

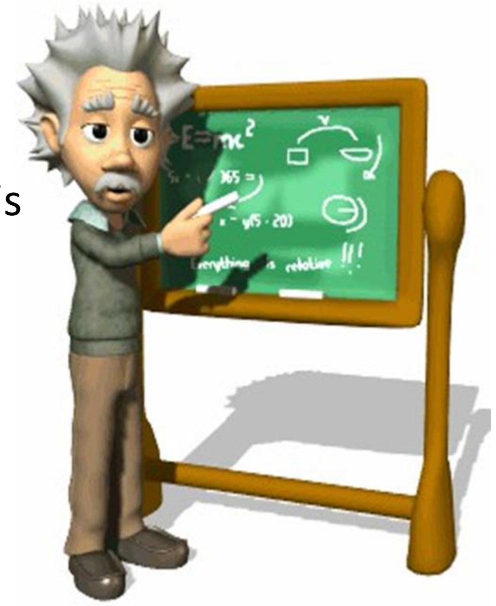
4. Calculate the wavelength of the photon emitted when an electron transitions from the first excited state to the ground state in a 2 nm long infinite potential well.

5. Find the required width L of an infinite potential well so that the ground state energy of an electron is 10 eV.

6. Find the probability of locating the particle in the middle half of the box (from L/4 to 3L/4) when it is in the ground state (n=1).

7. For a particle in a box in its ground state, calculate the expectation value of the position, the linear momentum, the kinetic energy, and the total energy.

8. A Quantum particle confined in 1D box of width 'a' is in its 1st excited state. Find the probability of locating the particle over an interval of (a/2) marked symmetrically at the center of box.

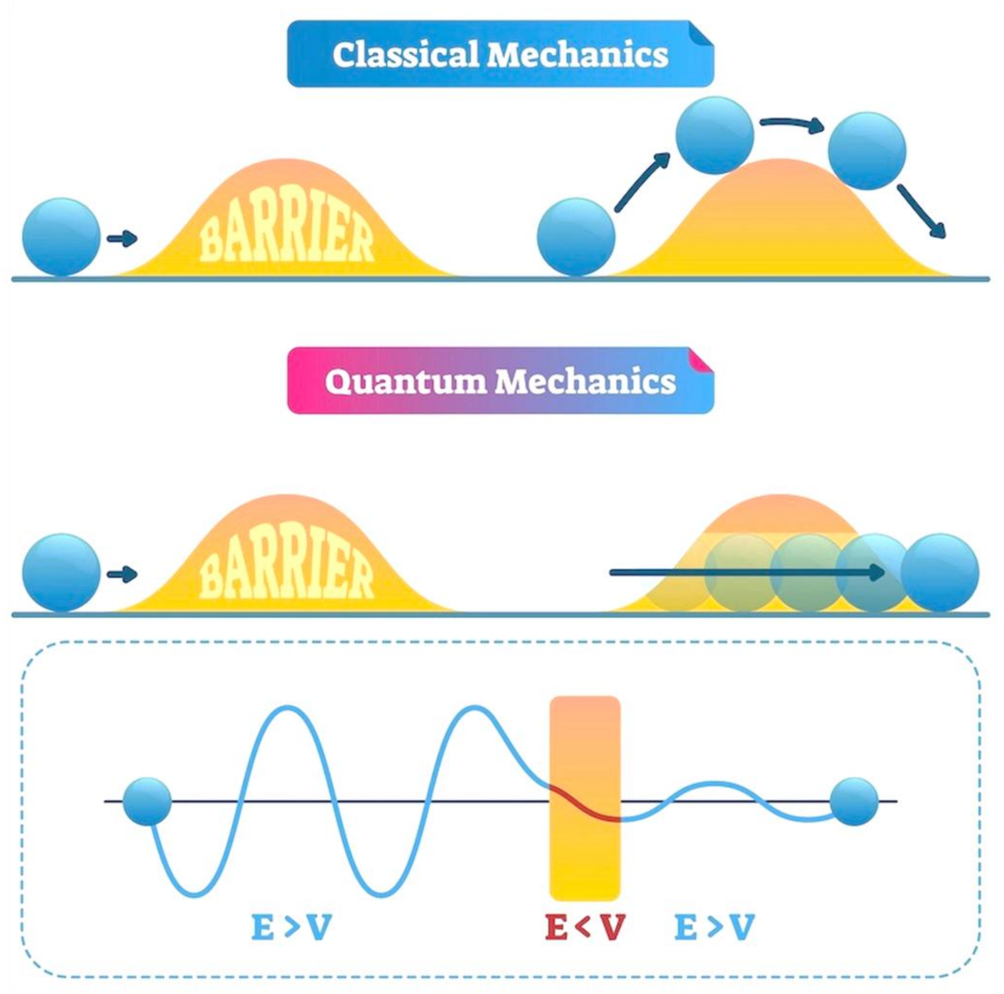


QUANTUM TUNNELLING

- **Quantum tunnelling** is a fundamental concept in quantum mechanics, describing **the ability of particles to penetrate energy barriers** that, according to classical physics, they should not be able to cross.

- **In classical physics**, particles encountering barriers with energy higher than their own kinetic energy are unable to pass through.

- **At the quantum level**, particles exhibit both particle-like and wave-like characteristics(de-Broglie hypothesis). This wave-particle duality enables them to exhibit tunnelling.



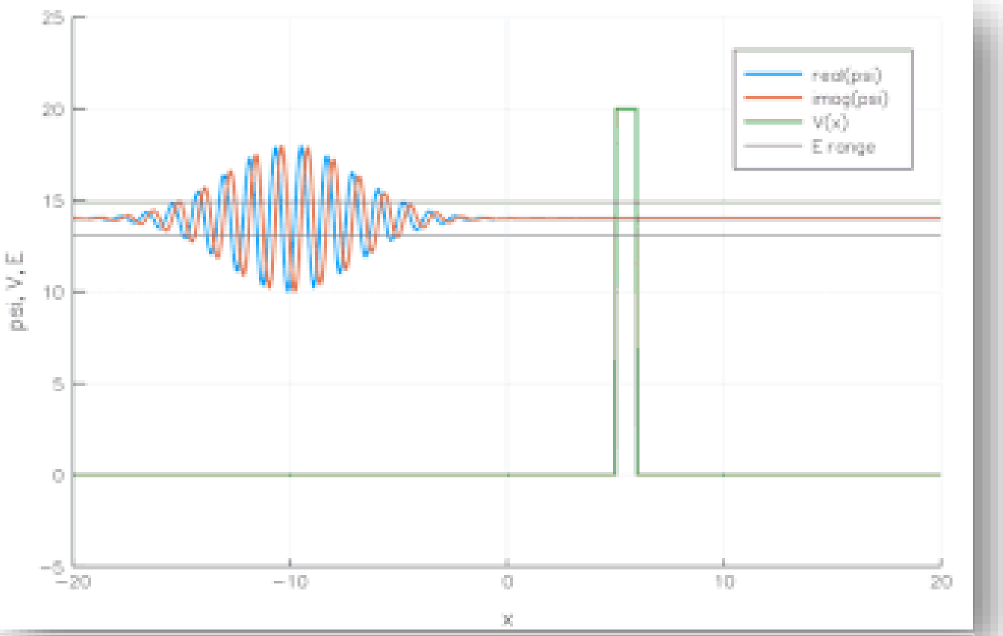
QUANTUM TUNNELLING

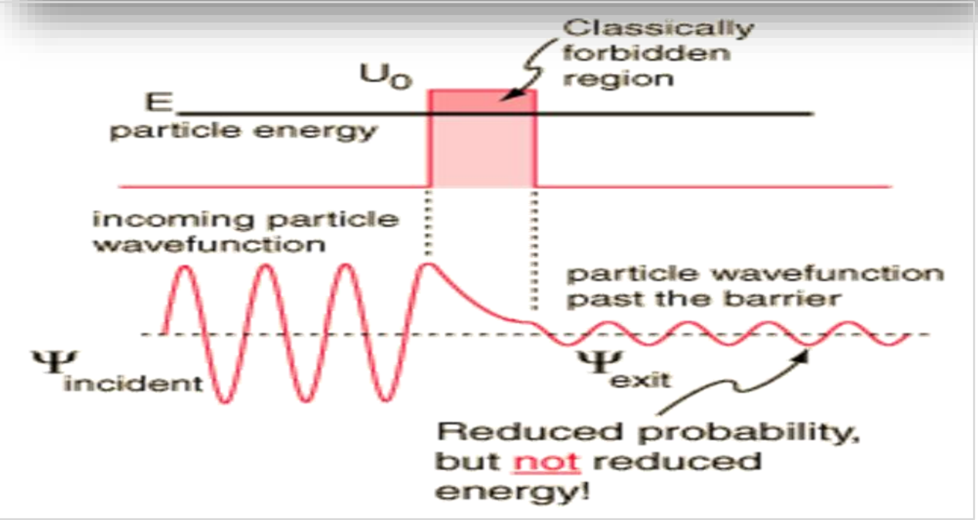
- When such particle of sufficiently less mass impinges on the barrier of finite potential, the solution of Schrodinger equation exists on the other side of the barrier even if energy of particle is less than barrier height. This gives a small probability that the particle may penetrate the barrier.

- **The probability** of a particle tunneling through a barrier decreases exponentially as the **barrier's height or width** increases, or as the **particle's mass** increases.

- **Electrons** can tunnel through barriers with thicknesses of about **1 to 3 nanometers (nm).**

- **Protons** can tunnel only through much thinner barriers, typically less than **0.1 nm.**

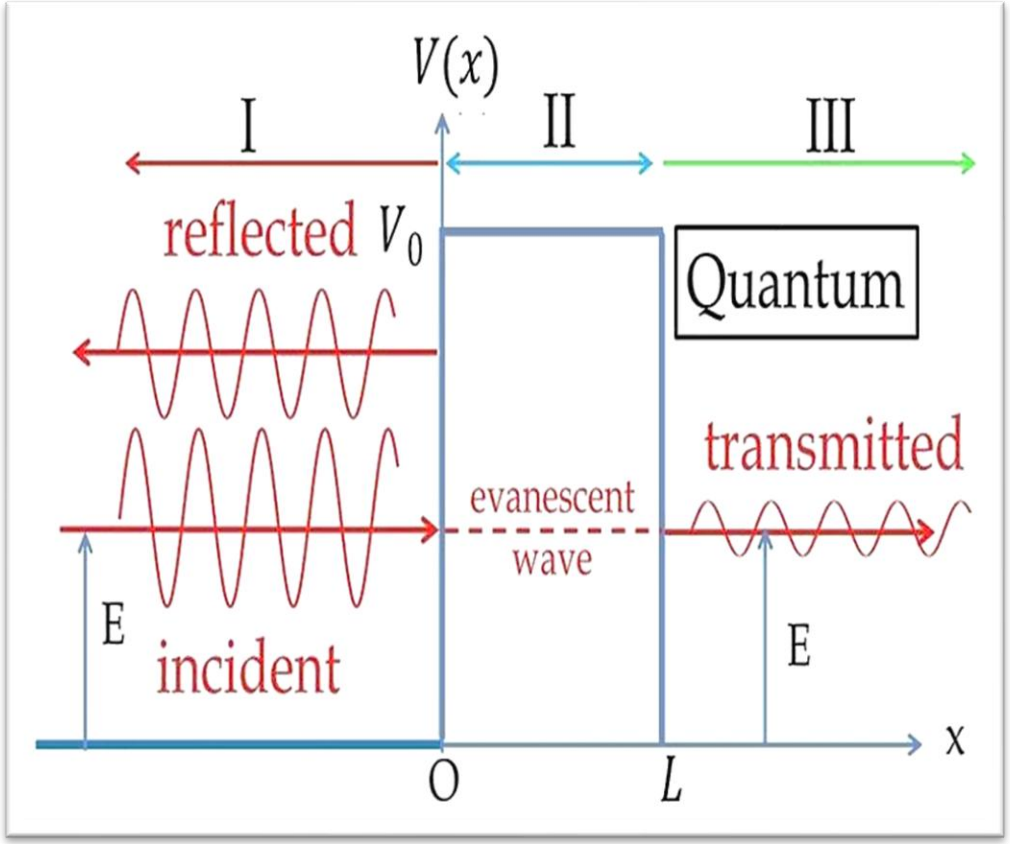




QUANTUM TUNNELLING

Potential barrier of finite height and width:

- Consider a particle of mass m incident on a potential barrier of height V_0 and width L.
- The energy of the particle is E and $E<V_0$.
- On both sides of the barrier V=0, which means that no forces act upon the particle in regions I and III.
- The barrier is represented by a potential of the form



$\boldsymbol{Region\ 1}$: $V(x) = 0$ **for $x < 0$**

$\boldsymbol{Region\ 2}$: $V(x) = V_0$ **for $0 \le x \le L$**

$\boldsymbol{Region\ 3}$: $V(x)=0$ **for $x>L$**

QUANTUM TUNNELLING

- From quantum mechanical calculations, the transmission probability T of a moving particle (wave) to cross the barrier is dependent on both

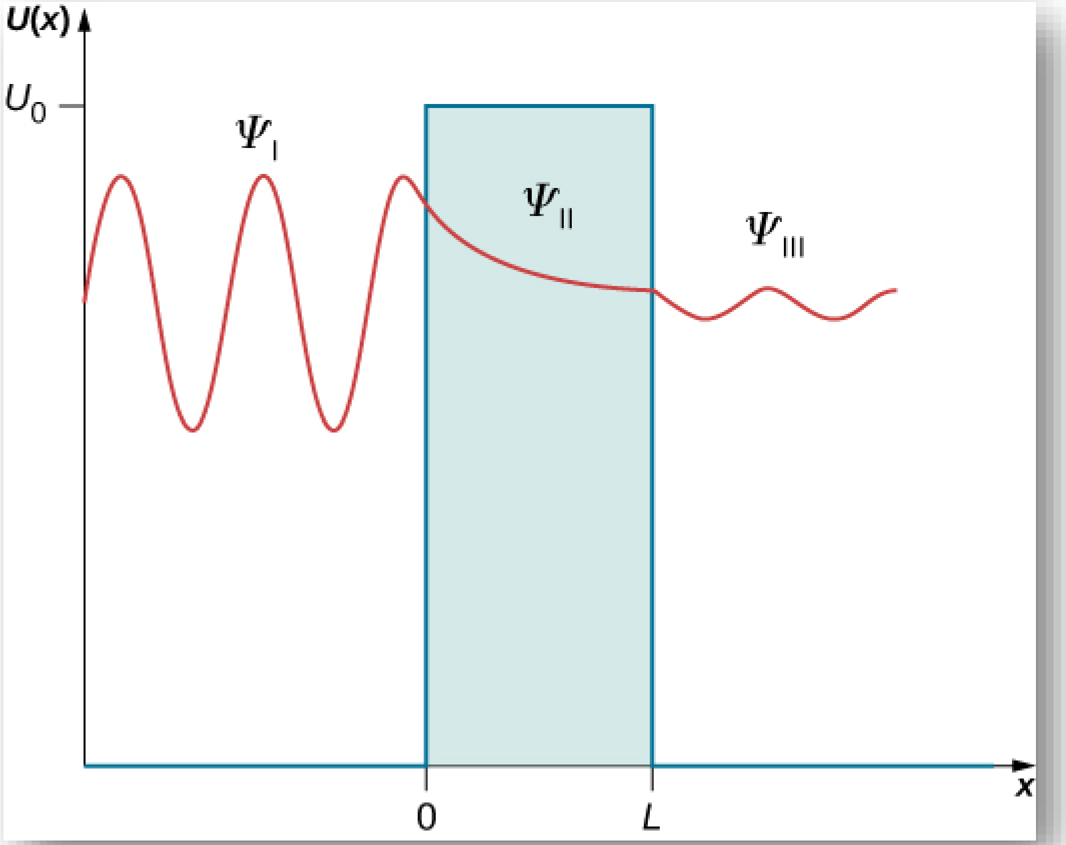
(I)Total energy of the particle, **E**
(II)The width of the barrier, **L**

and is approximately given by the equation below:

$$\mathbf{T} \approx \frac{16E}{V_0}\left(1 - \frac{E}{V_0}\right) e^{-2\alpha L}$$

Thus, there is higher probability of tunnelling out of the barrier when both **α and L are small**.

Here V_0 is the height of the barrier and $\alpha = \frac{2m}{\hbar^2}(V_0 - E)$



APPLICATION

- **Scanning Tunneling Microscope (STM):**

Uses quantum tunneling to image surfaces at the atomic level.

A sharp conducting tip is brought very close to the surface, allowing electrons to tunnel between the tip and the sample, producing a current that varies with distance and revealing atom-level details.

- **Tunnel Diodes and Electronics:**

Special electronic parts (like tunnel diodes) use tunneling for super-fast switching, making better and faster circuits.

Tunneling limits how small we can make computer chips, and helps in devices like flash memory and some types of transistors.

- **Flash Memory:**

Flash drives and memory cards work because electrons can tunnel through an insulating barrier, storing information even when the power is off.

APPLICATION

- **Quantum Computing:**

  Quantum computers use tunneling so that qubits can quickly solve problems by "shortcutting" through barriers. It also contributes to the implementation of quantum gates and the manipulation of quantum states in superconducting qubits.

- **Energy Storage and Fuel Cells:**

  Tunneling helps make tiny electrodes for batteries and supercapacitors, letting them charge faster and store more energy.

- **Nuclear Fusion:**

  In stars, tunneling allows particles to combine and create energy, even when they don't have enough energy to do it the classical way.

- **Quantum Biology:**

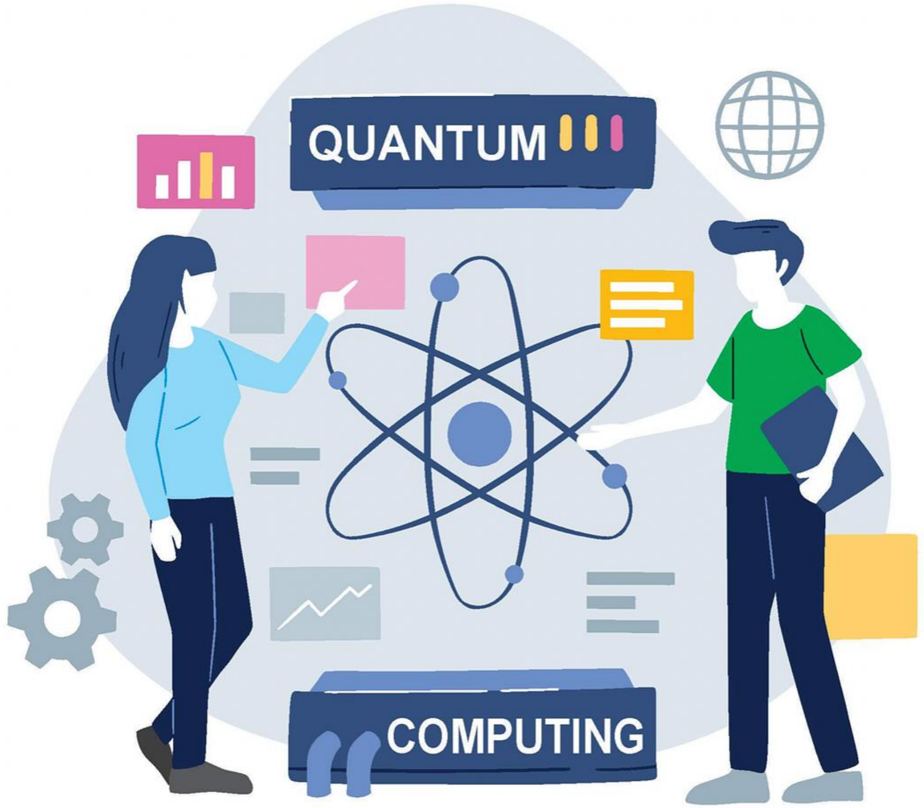
  Tunneling plays a role in biochemical processes such as enzyme activity, cellular respiration, photosynthesis, and even DNA mutation through proton and electron tunneling.

QUANTUM COMPUTING

CONTENT:

- CLASSICAL COMPUTING
- QUANTUM COMUTING
- QUBITS
- SUPERPOSITION
- ENTANGLEMENT
- MEASUREMENT
- QUANTUM GATES
- QUANTUM COMPUTER
- APPLICATION
- QUANTUM COMMUNICATION
- QUANTUM ALGORITHMS
- LIMITATION & CHALLENGES
- QUANTUM COMPUTING UPDATES*

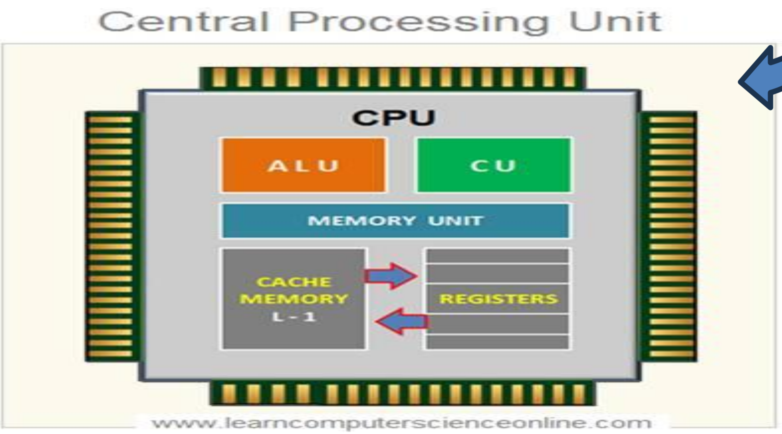
‘ * ‘ – only for knowledge, ‘ ** ‘ – conceptual base



CLASSICAL COMPUTING

- In classical computing processes information using bits—fundamental units that can exist only as 0 or 1.
- Classical computers operate sequentially, that it solve tasks by tackling one step at a time, like following instructions in a recipe one after another.
- For problems requiring exploration of many simultaneous possibilities—such as factoring large numbers or simulating molecular interactions—classical computers experience exponential slowdowns.

CLASSIAL COMPUTER



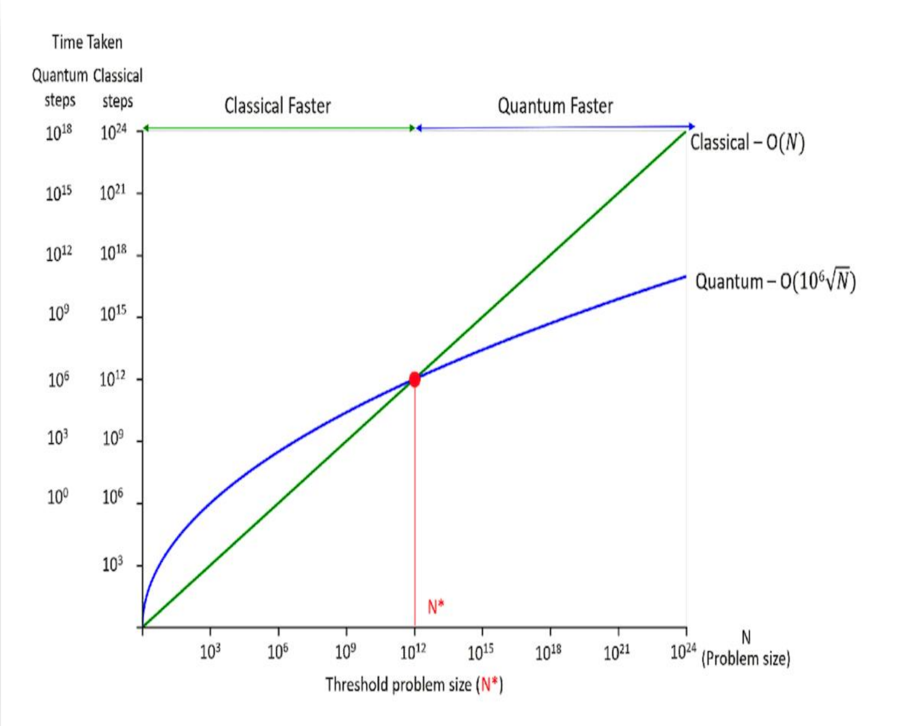
Complex problem solving in classical computer

Breaking Large Numbers (Factoring):

- When trying to find the factors of a huge number, a classical computer must check each possible divisor one by one.
- As the number gets bigger, the number of possibilities to check grows extremely fast—doubling, tripling, or worse with each extra digit.

For example:

- RSA-129 (129-digit number) was published in 1977 in Martin Gardner's "Mathematical Games" column in *Scientific American* as a challenge to the public to factor this number.
- It was estimated that factoring RSA-129 with available technology would take 40 quadrillion years.
- In 1994, a global effort involving about 1,600 computers coordinated via the Internet ultimately succeeded after several months.
- Today, with modern personal computers and advanced factorization software, factoring RSA-129 can be accomplished in about two and a half weeks on an average desktop PC.
- 2048-bit number using in cryptography.



LINEAR GROWTH IN OPERATION ITERATION

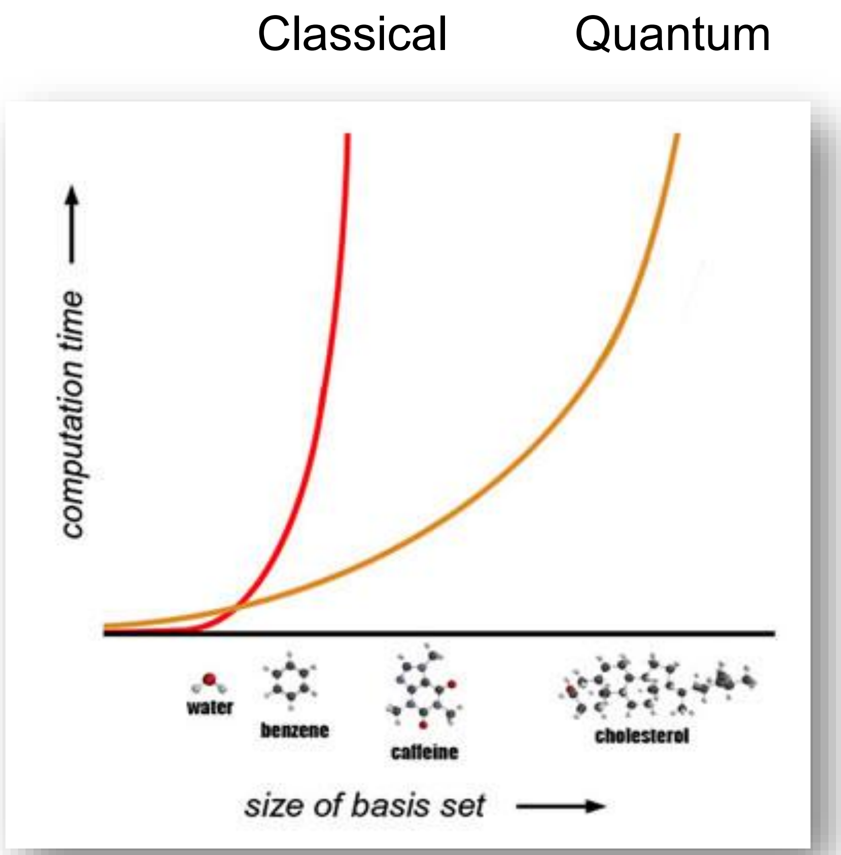
Complex problem solving in classical computer

Simulating Molecules:

- Molecules are made of atoms, and each atom adds more variables and states to consider during a simulation.
- The ways these atoms can interact multiply rapidly, and a classical computer must calculate the effect of each possible combination separately.

For example:

- ➢ The U.S. Department of Energy simulated 1,000 molybdenum atoms using the Blue Gene/L supercomputer. This system used 131,072 processors and performed 207 trillion calculations per second.
- ➢ Despite this massive computational power, simulating even 1,000 atoms at full quantum detail pushed classical computing limits.
- ➢ The main problem is that quantum complexity grows very fast as more atoms are added. This makes it nearly impossible for regular computers to simulate larger systems making it practically impossible to model larger systems precisely without approximations or quantum computing approaches.



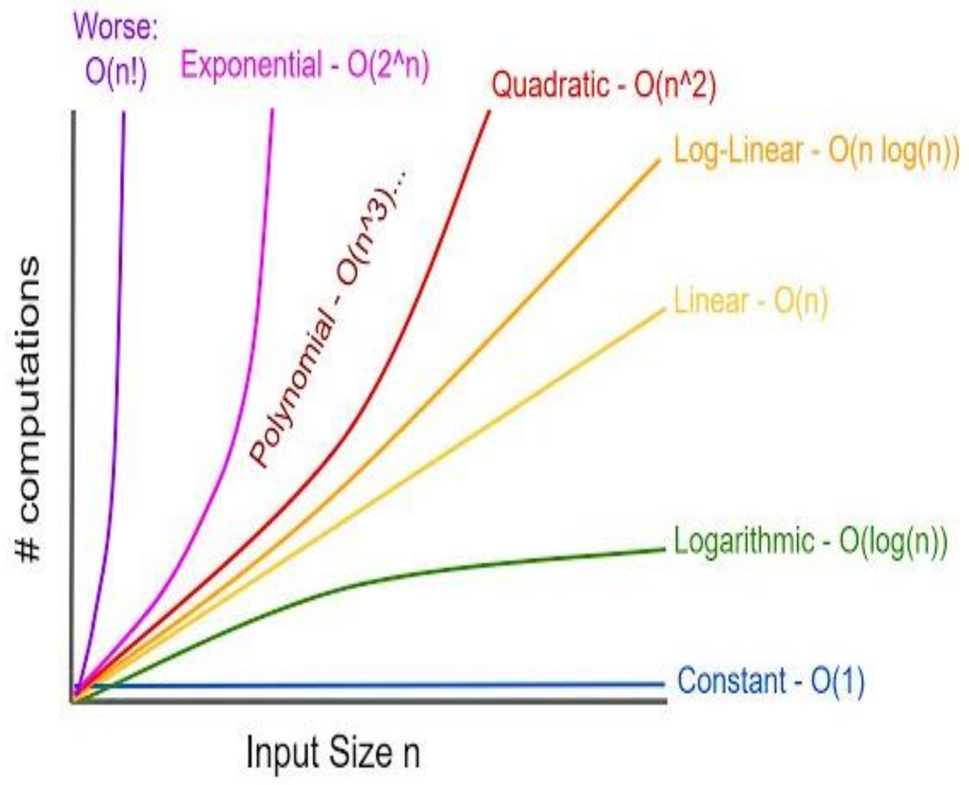
EXPONENTIAL GROWTH IN COMPUTATION TIME AS COMPLEXITY OF PROBLEM INCREASES

Complex problem solving in classical computer

- As linear growth in operation iteration, exponential growth in complexity of quantum system, and physical dimension limitation of making of microprocessor chips, that limits Moore's law, classical computers won't withstand the growing need of complex problem solving.

Moore's law:*

" The number of transistors on a microchip doubles approximately every two years, leading to exponential growth in computing power while the cost of these chips remains relatively low."

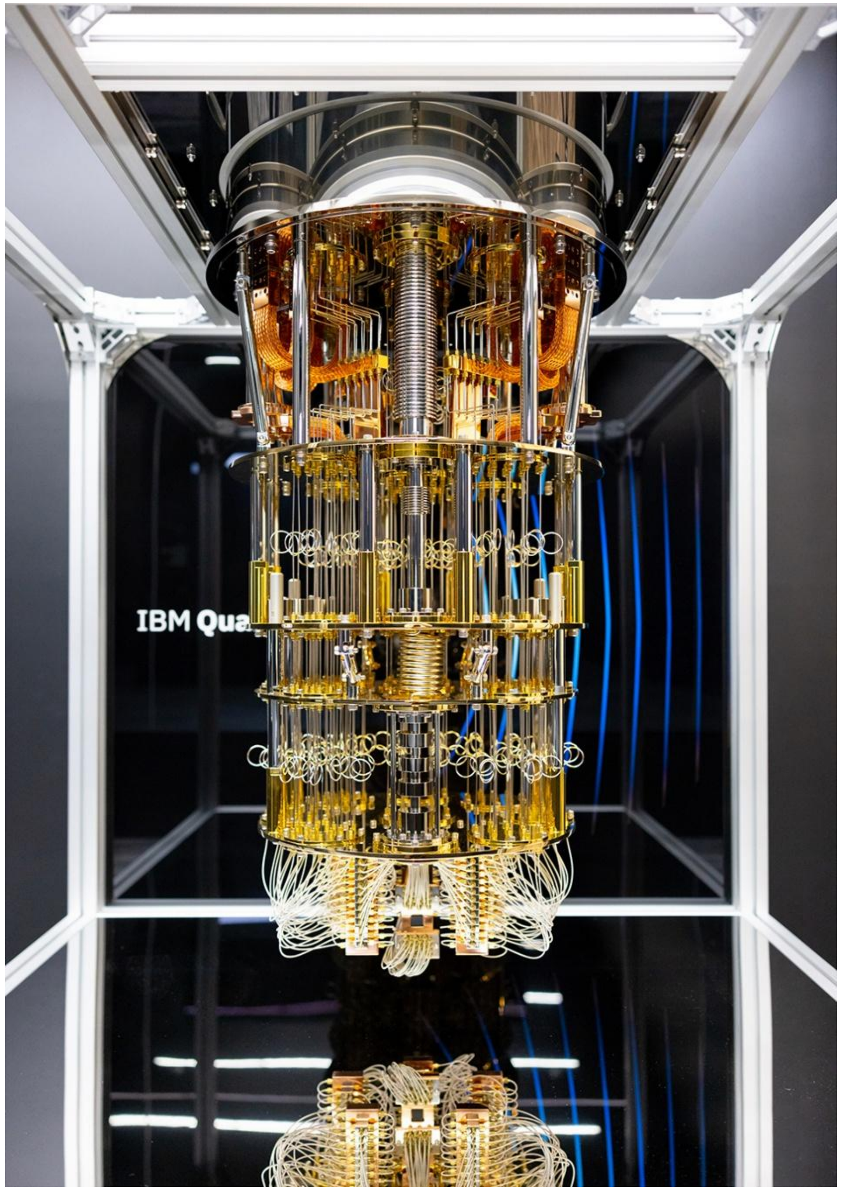


QUANTUM COMPUTING

Quantum computing operates on principles governing matter and energy at the atomic and subatomic levels, fundamentally different from classical physics.

Fundamental Principles:

- Quantum Superposition
- Quantum Entanglement
- Quantum Measurement

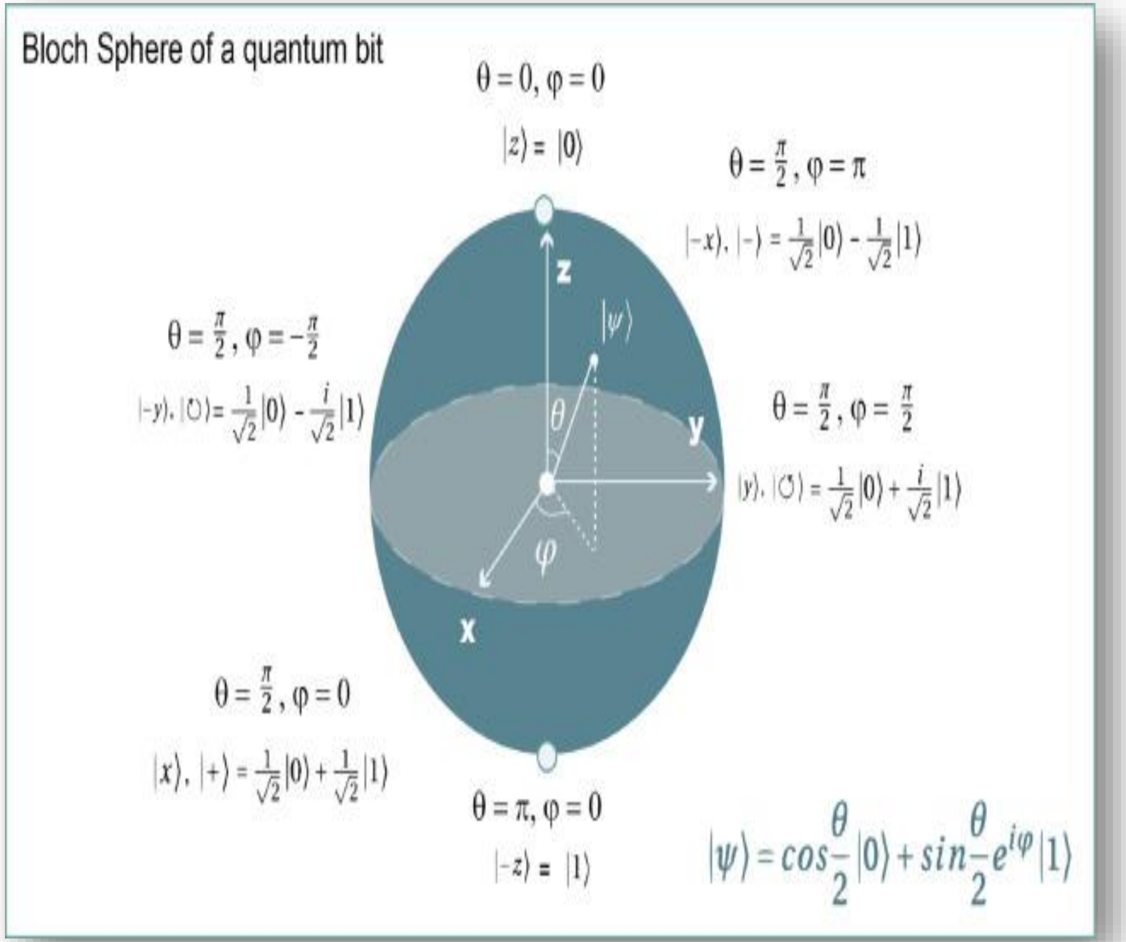


QUBITS

- A **qubit** is the **quantum version of a bit**.
- A qubit (short for quantum bit) is **the basic unit of information** in quantum computing, similar to a bit in classical computing.
- **Unlike a classical bit** which can be either 0 or 1, a qubit can exist in a state called superposition, where it can be both 0 and 1 simultaneously with certain probabilities.
- **Mathematically,** a qubit is represented as a **vector** in a two-dimensional complex vector space(Hilbert space), expressed as a linear superposition of two basis states $|0\rangle$ (spin up or $|\uparrow\rangle$) and $|1\rangle$ (spin down$|\downarrow\rangle$):

$$|\boldsymbol{\psi}\rangle = \boldsymbol{\alpha}|\mathbf{0}\rangle + \boldsymbol{\beta}|\mathbf{1}\rangle = \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{bmatrix}$$

where α and β are complex probability amplitudes satisfying the normalization condition $|\alpha|^2 + |\beta|^2 = 1$.
These coefficients represent the probabilities of finding the qubit in either state when measured.



- The basis states are usually represented as column vectors:

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

- For multiple qubits, the combined state is represented by the tensor (Kronecker) product of the individual qubit state spaces, resulting in a vector of dimension 2^n for n qubits. For example, two qubits live in a 4-dimensional space spanned by the basis:

$$|00\rangle = |0\rangle \otimes |0\rangle = \begin{bmatrix}1\\0\\0\\0\end{bmatrix}, |01\rangle = |0\rangle \otimes |1\rangle = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}, |10\rangle = |1\rangle \otimes |0\rangle = \begin{bmatrix}0\\0\\1\\0\end{bmatrix}, |11\rangle = |1\rangle \otimes |1\rangle = \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

- A general two-qubit state is written as:

$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

with complex amplitudes α_{ij} satisfying

$$|\alpha_{00}|^2 + |\alpha_{01}|^2 + |\alpha_{10}|^2 + |\alpha_{11}|^2 = 1$$

- Similarly, for n qubits, the state vector is a superposition over all $\boldsymbol{2^n}$ computational basis states:

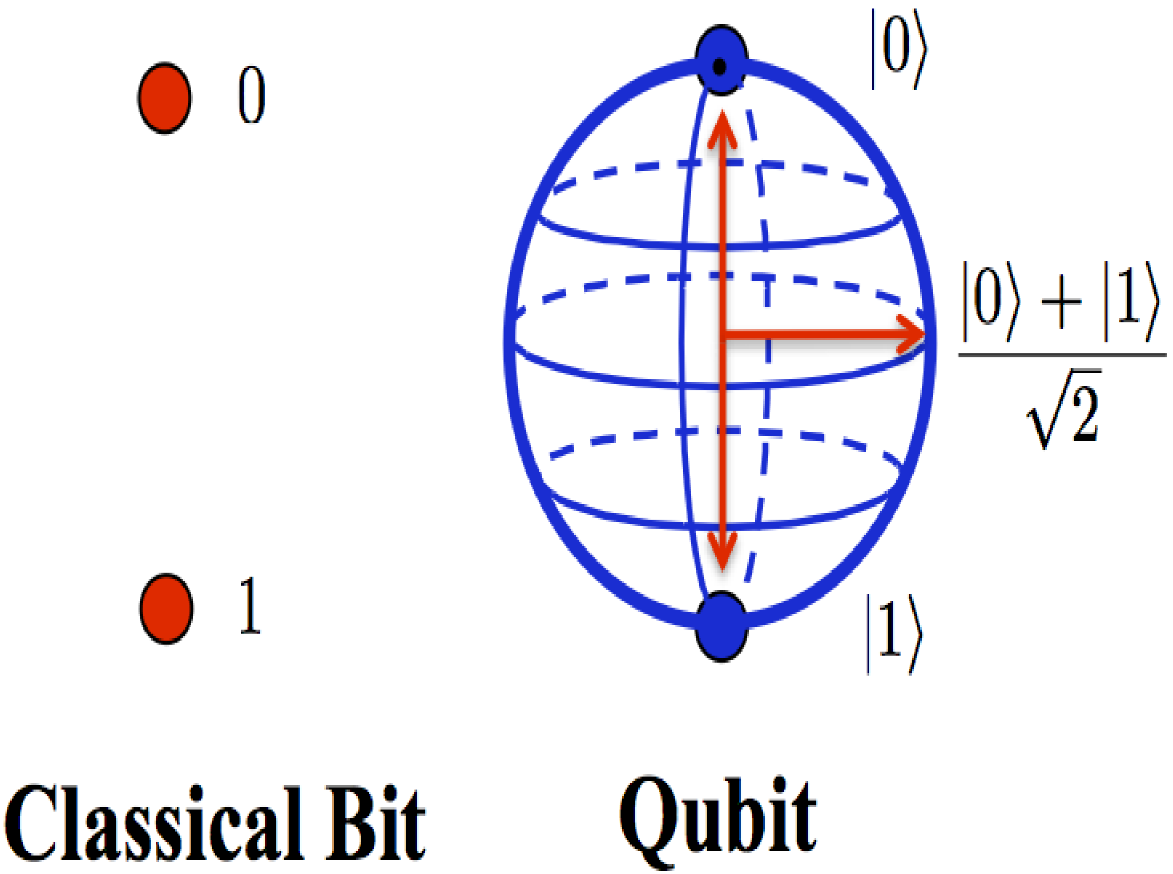
$$|\psi\rangle = \sum_{i=0}^{2^n-1} \alpha_i|i\rangle$$

where $|i\rangle$ represent the n-bit binary basis states and $\sum_i |\alpha_i|^2 = 1$

Bit vs Qubit

Classical bits: For a system of n bits, you can explicitly represent 1 out of 2^n possible states at any given time. If you want to use all combinations, you must enumerate them one by one. Classical computation is fundamentally sequential in this sense; a register of n bits can only be in one of those 2^n states at once.

Qubits: A register of n qubits can exist in a quantum superposition of all 2^n classical states at the same time. That means a quantum processor can, in principle, process information on all 2^n possible states simultaneously (before measurement collapses this outcome). This capability is often referred to as **"quantum parallelism."**



Numerical Problems

1. Given a qubit in state $|\psi\rangle=1/2|0\rangle+1/2|1\rangle$, what is the probability of measuring it as $|0\rangle$?

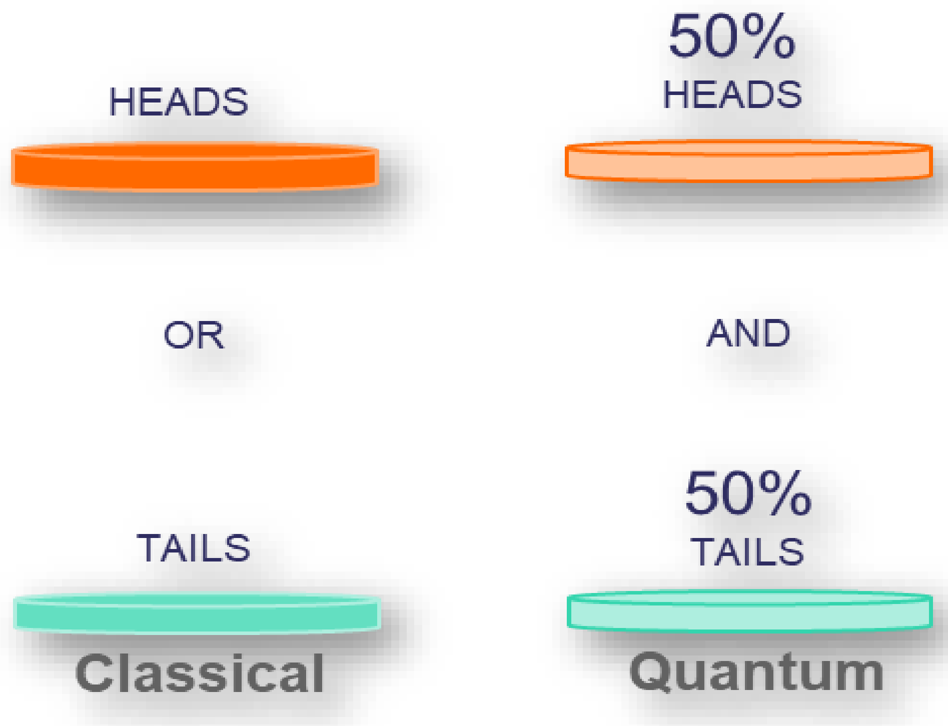
2. Given a qubit in state $|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$, what is the probability of measuring it as $|0\rangle$?

3. If a qubit state is $|\psi\rangle=\sqrt{0.3}|0\rangle+\sqrt{0.7}|1\rangle|\psi\rangle$, what is the probability of measuring $|1\rangle$?

QUANTUM SUPERPOSITION

- In a regular, or ‘classical’, computer, a **bit** (unit of information) can either be heads or tails. Whereas with a **qubit** (quantum bit), we can think of it as the state when the coin is flipped and is spinning around in the air.

- Prior to measurement, quantum state can be in a **superposition** of two or more classical states – so whilst a classical coin can only land on heads **or** tails, a quantum coin has a **probability** of being either heads or tails after measurement. While it is spinning around in the air, it is in an uncertain state, called **superposition**.

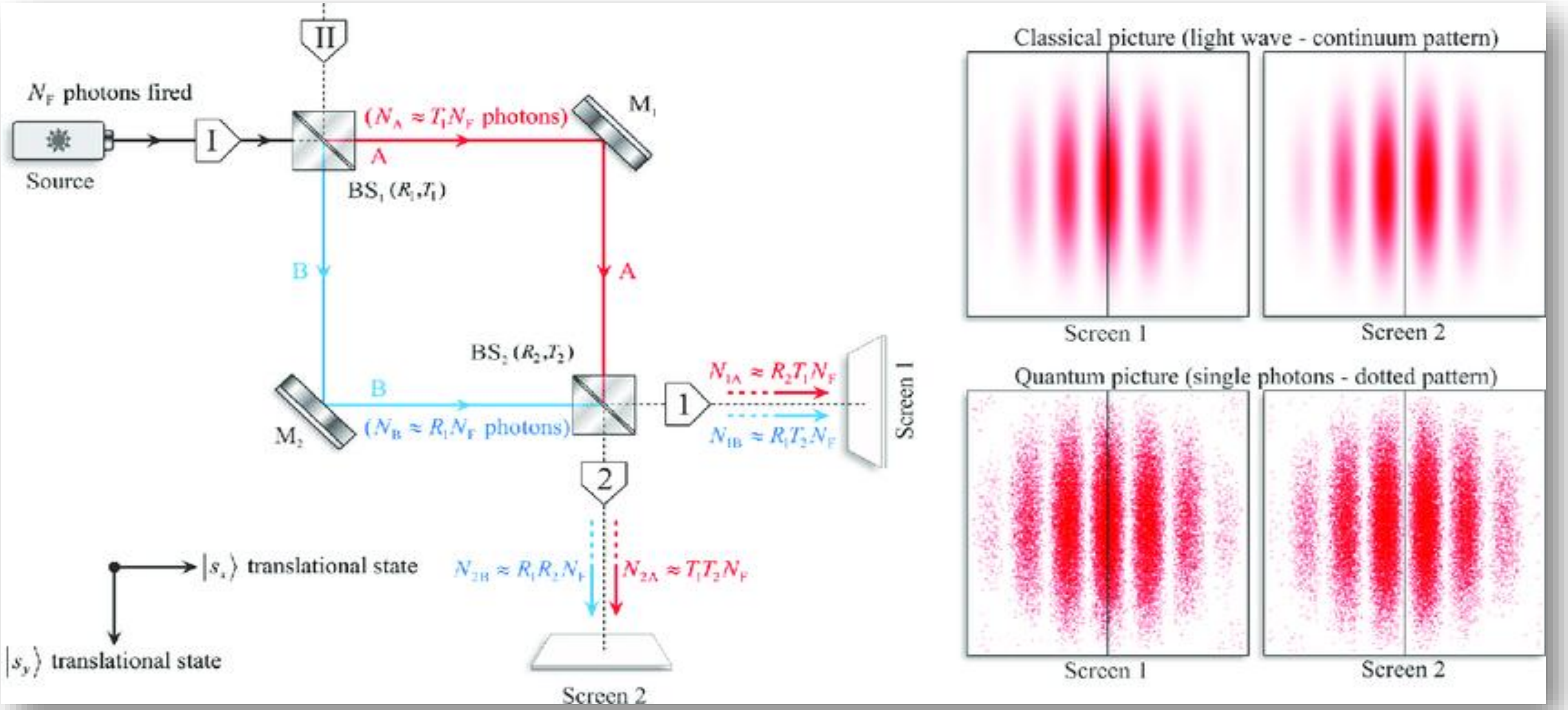


$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$$

$|0\rangle$ state with probability = $\left(\frac{1}{\sqrt{2}}\right)^2 = \left(\frac{1}{2}\right)$

$|1\rangle$ state with probability $\left(\frac{1}{\sqrt{2}}\right)^2 = \left(\frac{1}{2}\right)$

Mac Zehnder Interferometer **



Mac Zehnder Interferometer **

The Mach-Zehnder interferometer illustrates quantum superposition of photon paths by showing that a single photon, when entering the interferometer, can behave as though it travels both available paths simultaneously until it is measured.

Here's how it works:

•When a photon encounters the first beam splitter, its wavefunction is split: part of it travels along one path, and part along the other.

•Until a measurement is made, quantum theory describes the photon as being in a superposition state—taking both paths at once—not in a definite path.

•The two paths are then recombined at the second beam splitter. If no attempt is made to determine which path was taken (i.e., there's no "which-path" information), these path states interfere, leading to constructive or destructive interference at the detectors.

•The interference pattern observed at the output is direct evidence the photon was in a quantum superposition of both paths; such interference could not occur if the photon simply took one path or the other like a classical particle.

•However, if we try to detect which path the photon takes (by inserting detectors into the paths), the superposition collapses: the photon is forced into one path, and the interference pattern disappears.

In summary, in a Mach-Zehnder interferometer, the observed interference pattern arises because the photon exists in a superposition of both paths until measured, vividly demonstrating core principles of quantum mechanics.

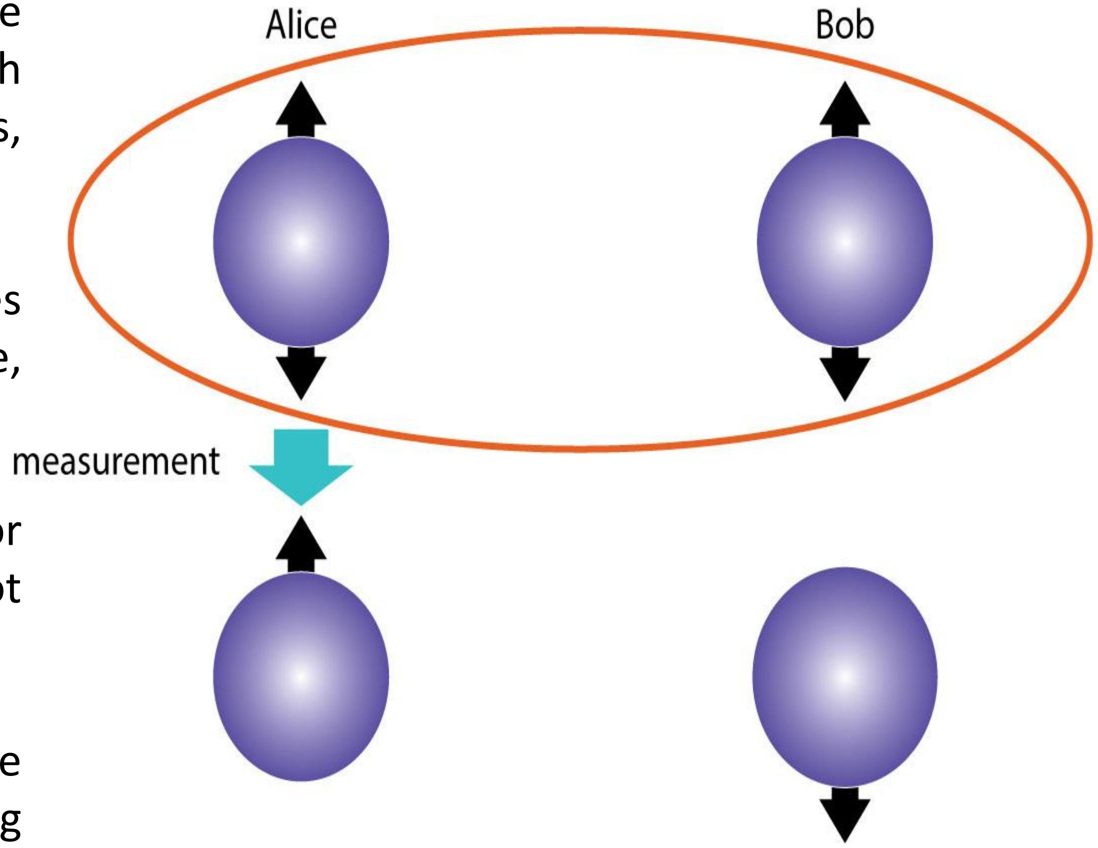
QUANTUM ENTANGLEMENT

- **Quantum entanglement** is a fundamental quantum phenomenon where **the quantum states** of two or more particles become **interconnected** such that the state of each particle cannot be described independently of the others, even when the particles are separated by large distances.

- This shared state means the properties of the particles remain deeply correlated no matter how far apart they are, an effect called ***non-locality***.

- The instantaneous correlation does not involve any signal or information traveling between the particles, so it does not violate the speed of light limit in relativity.

- Instead, the entangled system must be considered as one **unified quantum object** with a collective state extending across space.



Bell's State

- Bell states represent fundamental examples of quantum entanglement. They are four special maximally entangled states of two qubits.

- A simple example of Bell-state measurement outcomes is:

- When measuring the Bell state

$$|\Phi^{+}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

the result **always** indicates that the two qubits are either both 0 or both 1. If you find one qubit in state 0, the other will also be 0, and similarly for 1.

For $$|\Psi^{+}\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$$

the measurement outcome shows that the qubits are always opposite: if one is 0, the other is 1, and vice versa.

This means measuring one Bell state reveals a **perfect correlation or anti-correlation** between the two qubits, confirming their entanglement.

$$|\Phi^{+}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

$$|\Phi^{-}\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}}$$

$$|\Psi^{+}\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}$$

$$|\Psi^{-}\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}$$

Four Bell States

QUANTUM MEASUREMENT

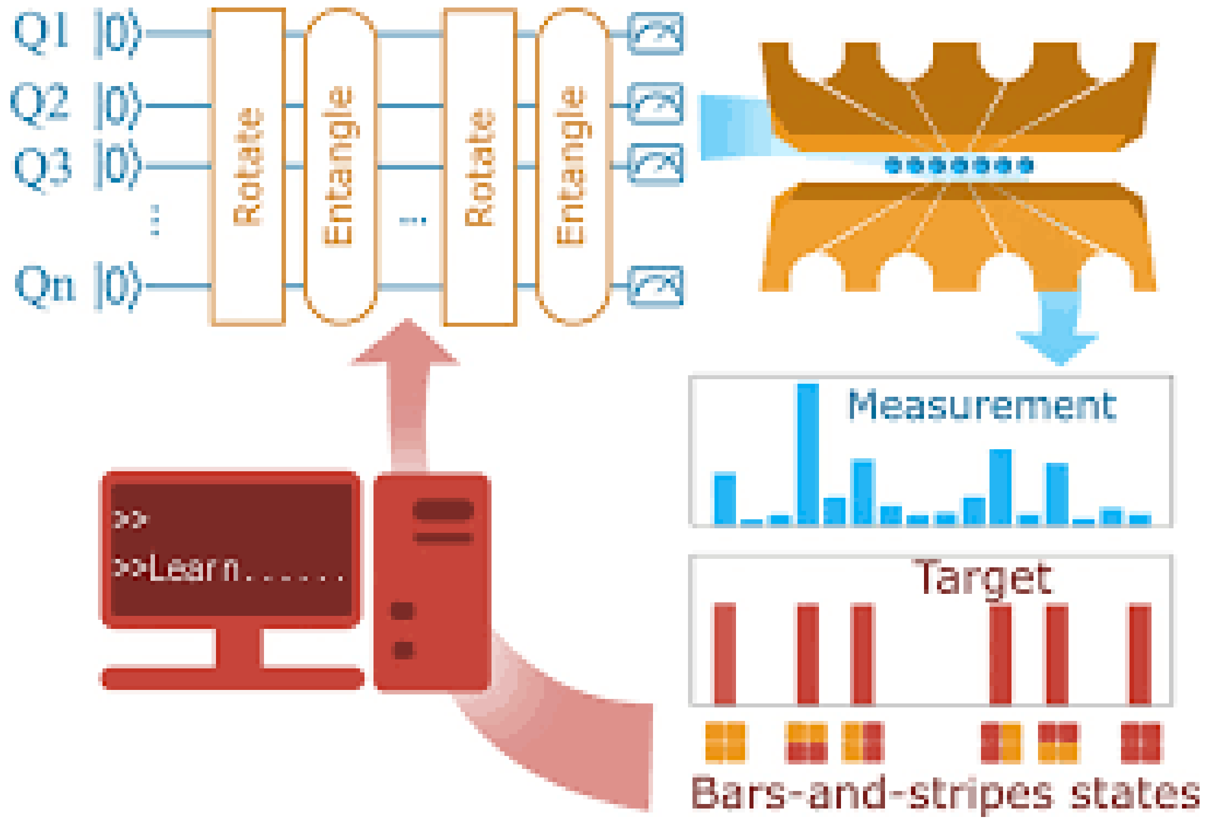
•**Quantum measurement** is the process where observing a quantum system forces it into one definite state from a range of possible superposed states.

•Before measurement, a quantum system (like a qubit) can exist in a superposition—a mix—of several possible outcomes.

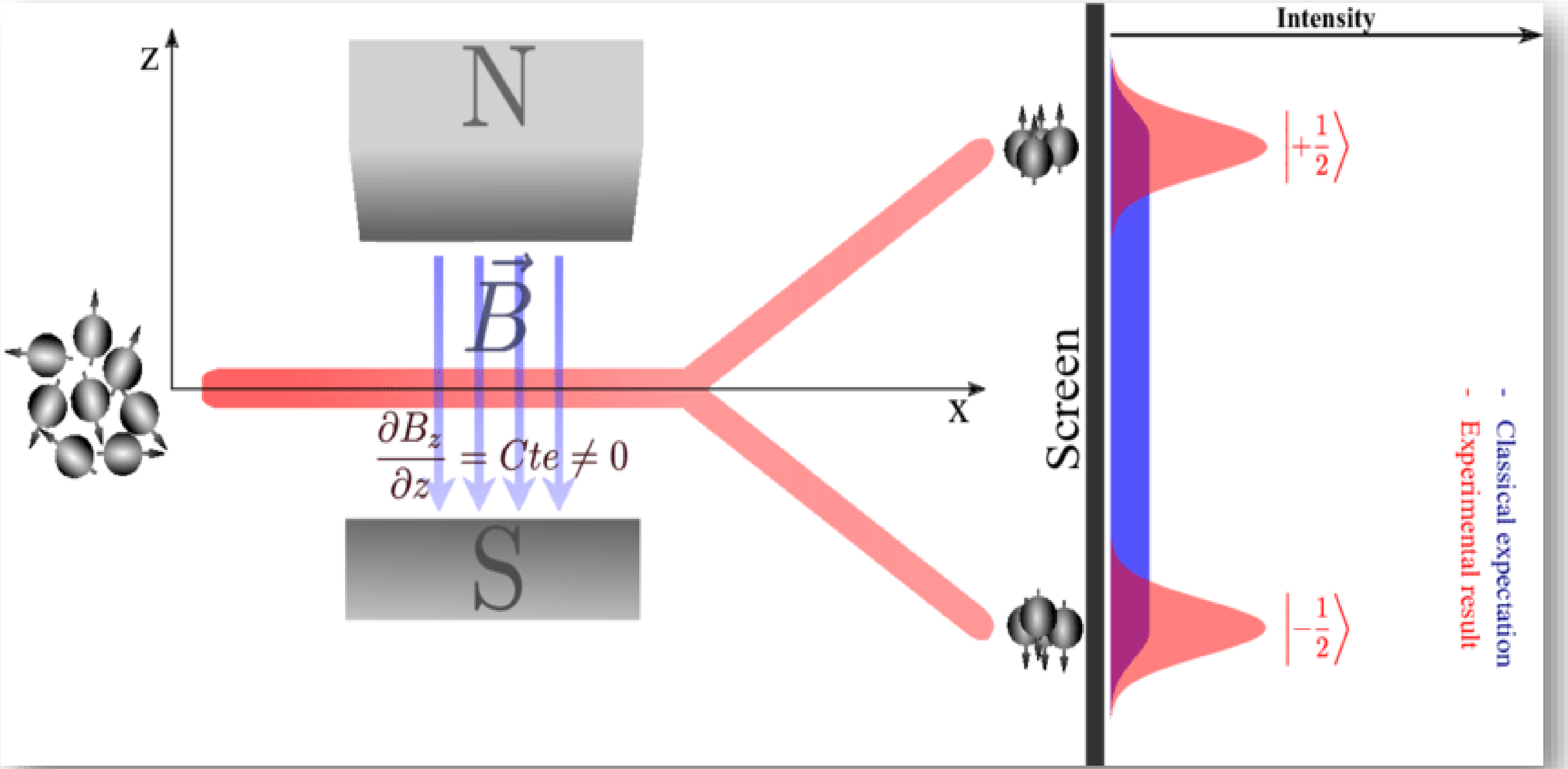
•The act of measurement “collapses” the superposition to a single value (e.g., spin up or down), and the original quantum state is irreversibly lost.

•**Measurement is probabilistic:** you cannot predict the exact outcome of a single measurement, only the probabilities for each possible result.

•This collapse is fundamental and distinguishes quantum from classical measurements; it’s also central to quantum computing, where measurements extract classical information from qubits.



Stern-Gerlach Experiment **



Stern-Gerlach Experiment **

The Stern–Gerlach experiment explanation relates quantum measurement:

1.Superposition Before Measurement

Each atom's spin is both "up" and "down" before measurement.

2.Measurement Causes Collapse

Passing through the magnetic field makes the spin pick either "up" or "down" — the superposition ends.

3.Two Distinct Outcomes

Atoms hit the detector at just two spots, showing only two possible spin values.

4.Outcome Depends on Measurement Direction

Changing the measurement axis changes the possible outcomes, i.e., spin measured along different directions gives different results.

5.Quantum to Classical Link

The magnetic field connects spin (quantum) with position (classical), so the detector can see the result.

6.Random but Predictable Statistics

Each atom's outcome is random, but many atoms together show a clear pattern, like half "up" and half "down."

The experiment shows that measuring a quantum property forces it into one definite state, gives only certain outcomes, depends on how you measure it, and turns quantum behavior into a clear classical result.

Numerical Problems

1. Given qubit state $|\psi\rangle = \frac{3}{5}|0\rangle + \frac{4}{5}|1\rangle$, find the probability of measuring $|0\rangle$.

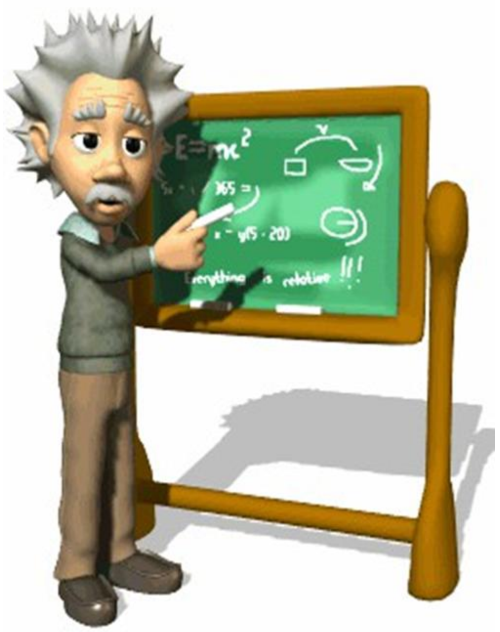
2. If a qubit is in the state $|\psi\rangle = \frac{1}{\sqrt{3}}|0\rangle + \sqrt{\frac{2}{3}}|1\rangle$, what is the probability of measuring $|1\rangle$?

3. For the superposition $|\psi\rangle = \frac{1}{2}|0\rangle + \sqrt{\frac{3}{4}}|1\rangle$, calculate the probability of $|0\rangle$ measurement.

4. Consider Bell state $1/\sqrt{2}(|00\rangle+|11\rangle)$. On measuring the first qubit to be $|0\rangle$, what is the probability the second qubit is $|1\rangle$?

5. For the entangled state $1/\sqrt{2}(|01\rangle-|10\rangle)$, what is the probability of measuring both qubits as $|0\rangle$?

6. Given an entangled state $1/2|00\rangle+1/2|01\rangle+1/2|10\rangle-1/2|11\rangle$, what is the probability both qubits are measured as $|0\rangle$?



Numerical Problems

7. A qubit in state |ψ⟩=1/√2(|0⟩+|1⟩) is measured in the computational basis. What are the probabilities for outcomes |0⟩ and |1⟩?

8. Qubit in state: |ψ⟩=a|0⟩+b|1⟩, where a=cosπ/6, b=sinπ/6.

   Find the probability of measuring |1⟩.

9. Two paths of a quantum particle interfere with amplitudes $\psi_1 = \sqrt{0.4}$ and $\psi_2 = \sqrt{0.6}e^{i\pi/3}$. Find the total probability.

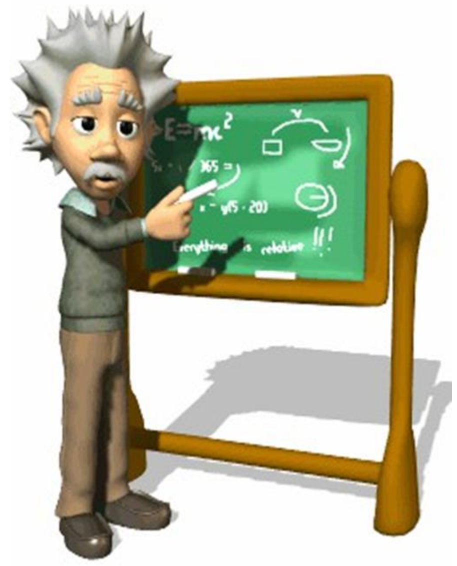
10. Two photon paths interfere with amplitudes $\frac{1}{2}$ and $\frac{1}{2}e^{i\pi}$. What is the probability of detection?

11. Two paths with amplitudes $\frac{1}{\sqrt{3}}$ and $\frac{\sqrt{2}}{\sqrt{3}}e^{i\phi}$. For $\phi = 0$, find probability.

12. An unknown 2-qubit state is

$$|\psi\rangle=\alpha\_00\ |00\rangle+\alpha\_01\ |01\rangle+\alpha\_10\ |10\rangle+\alpha\_11\ |11\rangle,$$

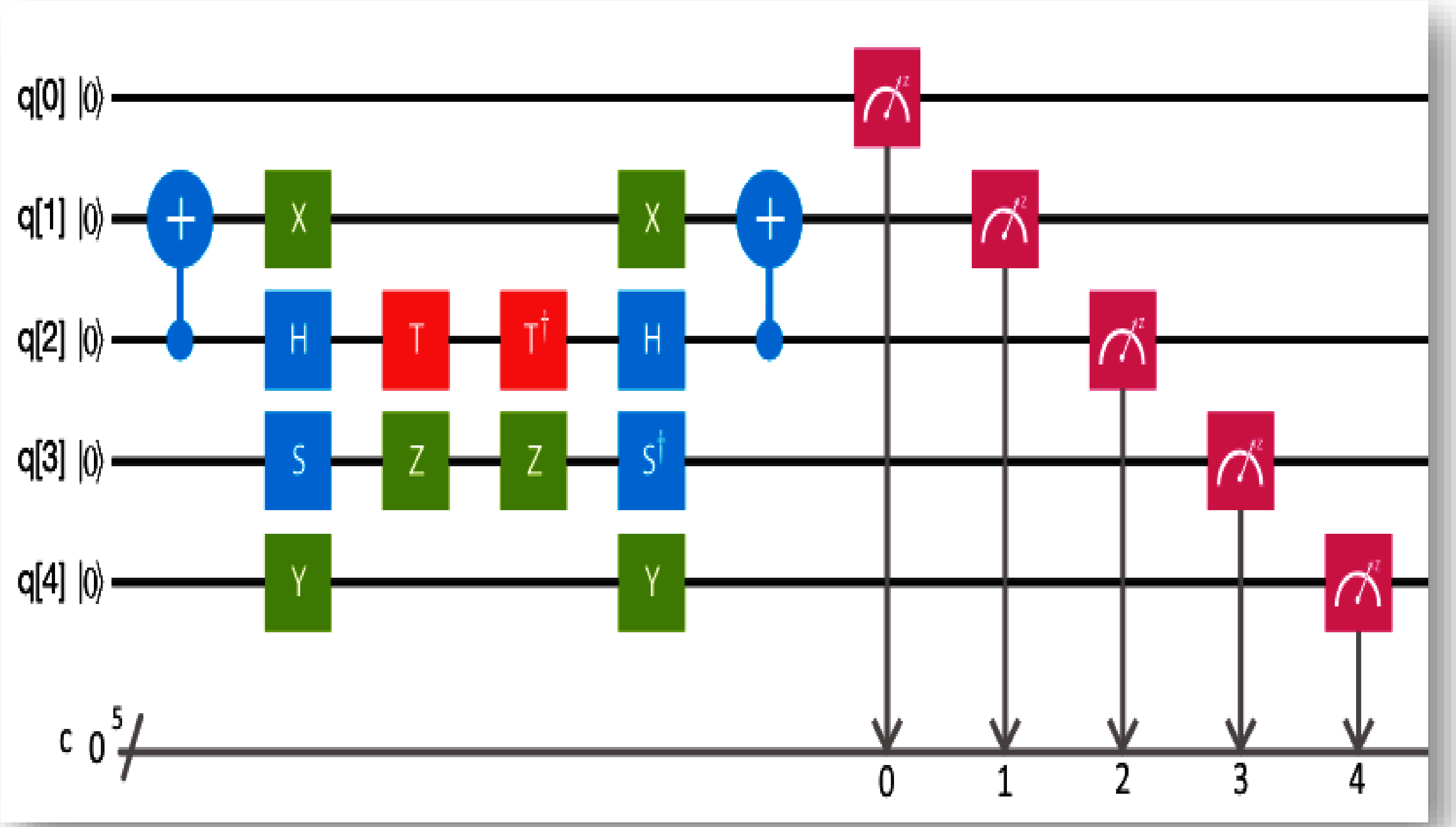
   with normalization $|\alpha\_00\ |\hat{}2+|\alpha\_01\ |\hat{}2+|\alpha\_10\ |\hat{}2+|\alpha\_11\ |\hat{}2=1$.
   (a) What is the probability of measuring the first qubit as “1”?
   (b) If that outcome occurs, what is the normalized post-measurement state of the two qubits?



QUANTUM GATES

- Quantum gates are the fundamental operations that manipulate qubits their amplitudes and phases to perform computation in quantum computing.

- They are the quantum analogs of classical logic gates but act on quantum states, which can be superpositions of classical states.



QUANTUM GATES

- Quantum gates are the basic building blocks of quantum circuits.
- All quantum gates are represented by unitary matrices (their inverse is equal to their conjugate transpose), ensuring reversibility and no information loss.

Properties and Importance:

- Quantum gates are reversible, meaning their operations can be undone, unlike many classical logic gates.
- The set of these gates is universal, i.e., any quantum computation can be built from combinations of these gates.
- Quantum gates handle the complex phenomena of superposition and entanglement, enabling the exponential computational possibilities unique to quantum computers.

Single-Qubit Gates

Gate	Symbol	Matrix Representation	Action on Basis States
Pauli-X	X	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$X\|0\rangle = \|1\rangle, X\|1\rangle = \|0\rangle$
Pauli-Y	Y	$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$	Bit+phase flip
Pauli-Z	Z	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$Z\|0\rangle = \|0\rangle, Z\|1\rangle = -\|1\rangle$
Hadamard	H	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$	Creates superposition: $H\|0\rangle = \frac{\|0\rangle+\|1\rangle}{\sqrt{2}}$
Phase (S)	S	$\begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$	Adds 90° phase to $\|1\rangle$
T-gate	T	$\begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$	Adds 45° phase to $\|1\rangle$

Multiple-Qubit Gates

Gate	Function	Circuit Symbol	Matrix	Example Input → Output
Controlled-NOT (CNOT)	Flips the target qubit if the control qubit is $\|1\rangle$.	●—⊕	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\|10\rangle \rightarrow \|11\rangle$; $\|00\rangle \rightarrow \|00\rangle$
Controlled-Z (CZ)	Applies a phase-flip (Z) to the target when the control is $\|1\rangle$.	●—⊕ (with ⊕ replaced by "Z")	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$	$\|11\rangle \rightarrow -\|11\rangle$; $\|01\rangle \rightarrow \|01\rangle$
SWAP	Swaps the states of two qubits.	×—×	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$\|01\rangle \rightarrow \|10\rangle$; $\|10\rangle \rightarrow \|01\rangle$

Numerical Problems

1. A qubit is initialized to $|0\rangle$.What is the resulting state after applying a Hadamard (H) gate, followed by a Pauli-X (NOT) gate?

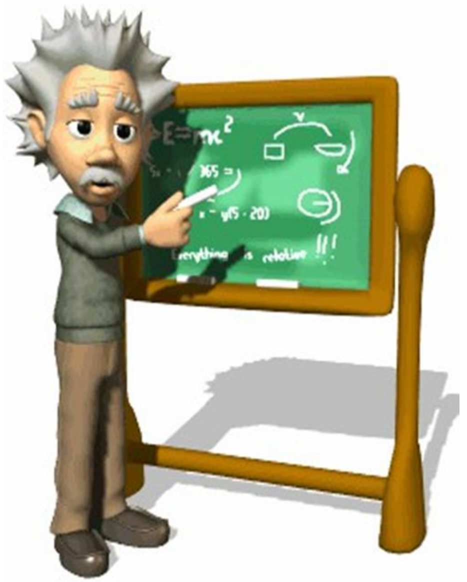
2. Two qubits start in $|00\rangle$. Apply a Hadamard on the first qubit, then a CNOT with control on the first and target on the second. What is the final state?

3. For a two-qubit system, if you apply (in order) an X on the first qubit and a CNOT, what is the overall matrix?

4. Consider a two-qubit system initialized in the state $|\,00\rangle$ .A Hadamard gate H is applied only on the first qubit, while the second qubit remains unchanged.
   a) Write down the matrix representation of the combined operation $H \otimes I$, where I is the identity operation on the second qubit.
   b) Calculate the resulting state vector after applying $H \otimes I$ on $|\,00\rangle$.
5. Consider a two-qubit system in the state:

$$|\,\psi\rangle = \frac{|\,00\rangle + |\,10\rangle}{\sqrt{2}}$$

   where the first qubit is in a superposition and the second qubit is $|\,0\rangle$. After applying a CNOT gate write down physical significance of the resulting state.

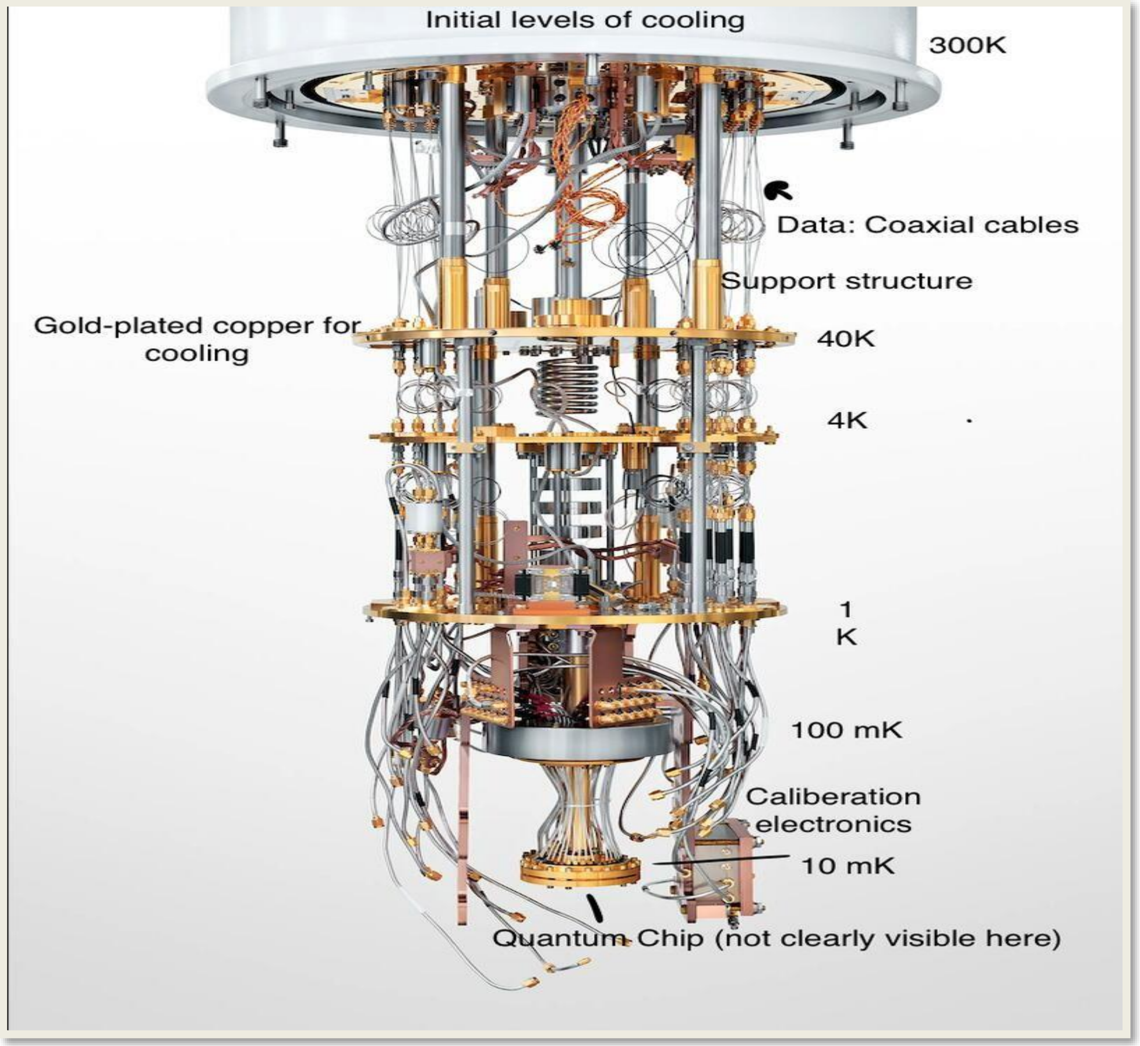


Key Differences Between Quantum and Classical Computing

Aspect	Classical Computing	Quantum Computing
Basic unit	Bit: 0 or 1	Qubit: 0, 1, or both (superposition)
Data processing	Deterministic; each step is predictable	Probabilistic; outcomes have associated probabilities
Computation model	Boolean algebra, sequential or limited parallelism	Linear algebra & quantum mechanics; massive parallelism via superposition and entanglement
Scalability	Linear with number of bits	Exponential with qubits (2N states for N qubits)
Gate operations	On/off logic gates	Quantum gates manipulate probability amplitudes
Reversibility	Usually not reversible	All operations must be reversible
Common use today	Universal—everyday computing tasks	Early, specialized use (optimization, simulation, cryptography)

QUANTUM COMPUTER

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



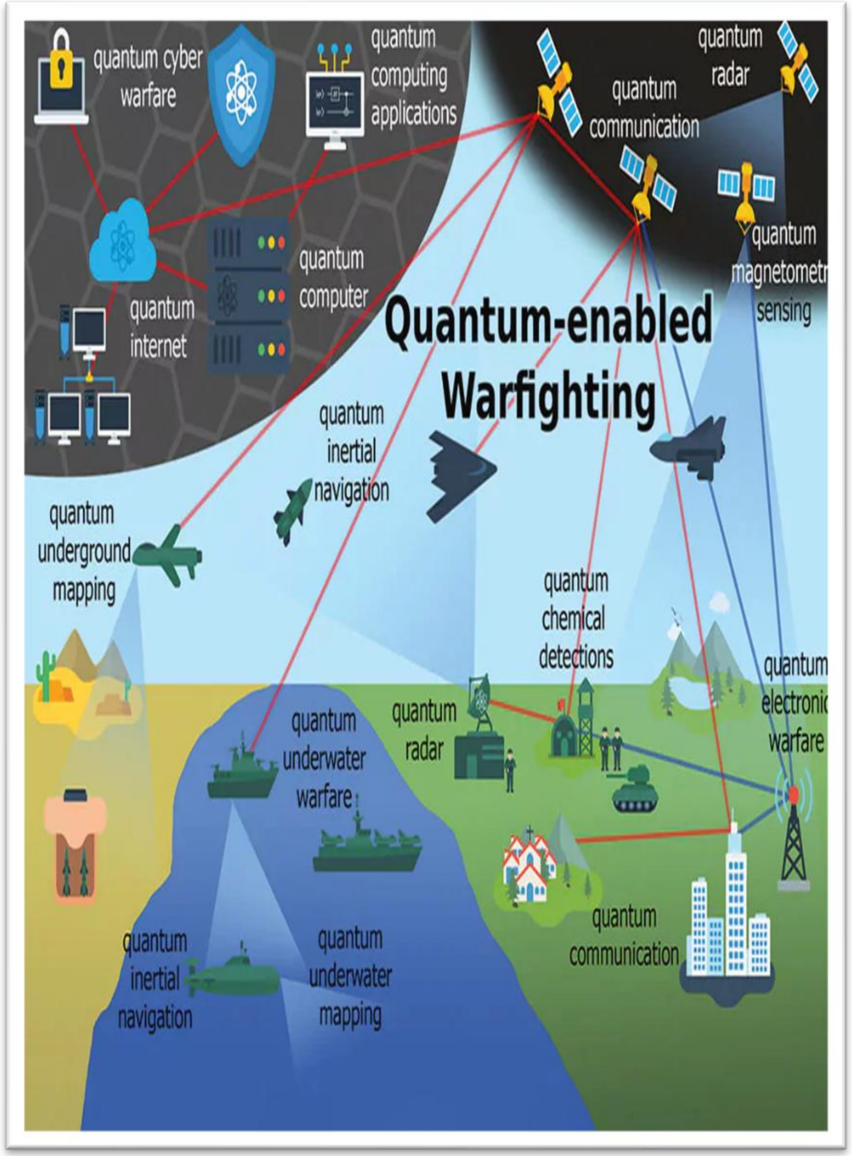
- Quantum computers are designed with several layers, each with a specific job to make quantum computing work.

1. **Physical Layer:** This is where the qubits live. These qubits are kept super cold (near absolute zero) so they don’t lose their quantum nature.
2. **Control & Measurement Layer:** Special electronics send signals (like microwaves or lasers) to control the qubits or to measure what information they hold. This lets the system read and write quantum information.
3. **Classical Control Processor:** This is a regular computer that turns instructions from software into signals for the quantum hardware. It keeps everything in sync, making sure the quantum operations happen at the right time.
4. **Quantum Error Correction:** Quantum info is fragile and can be wiped out by errors. Error correction spreads information across multiple qubits, so mistakes can be detected and fixed, keeping calculations reliable.
5. **Compiler & Software:** High-level quantum programs are translated into simple quantum “gates” the hardware understands. Special software frameworks help write and optimize these programs.
6. **Host Processor & Application:** This is the interface for the user. It manages jobs, stores results, and connects quantum computing to regular computers for practical tasks like optimization, cryptography, and more.

APPLICATION

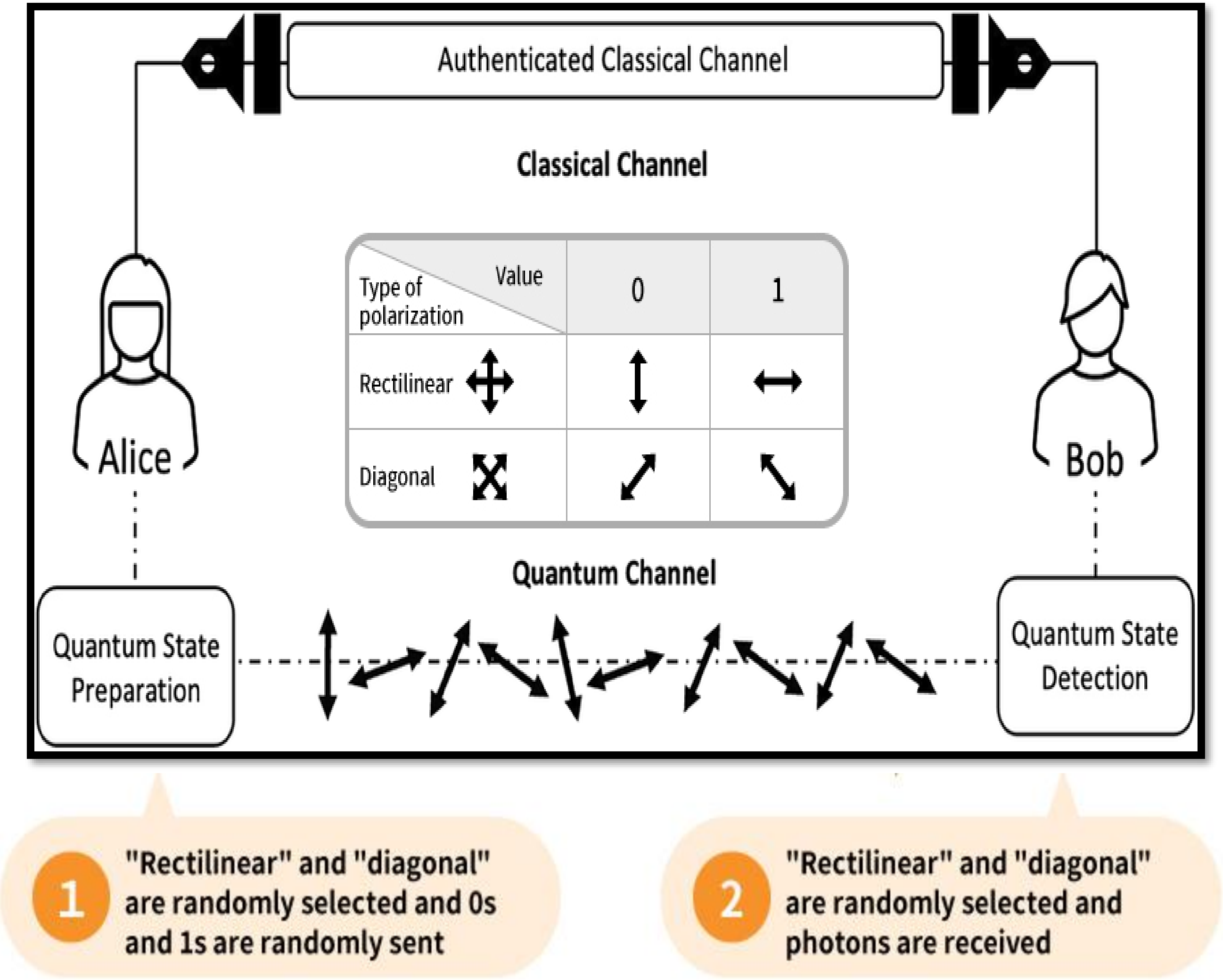
Possible practical applications of quantum computing across various industries:

- **Drug discovery:** Speeds up designing treatments by simulating complex molecules.
- **Materials science:** Develops advanced materials for energy and electronics.
- **Finance:** Optimizes portfolios, risk analysis, and fraud detection.
- **Logistics:** Improves routing and resource management for efficiency.
- **AI:** Enhances training and pattern recognition on big data.
- **Cybersecurity:** Breaks classical encryption while enabling quantum-safe security.
- **Climate modeling:** Provides detailed environmental simulations.
- **Manufacturing:** Optimizes processes and defect detection.
- **Quantum sensing:** Delivers ultra-precise measurements for navigation and diagnostics.



QUANTUM COMMUNICATION

- **Quantum communication** is a way of sending information that uses superposition, Entanglement.
- **Classical communication** sends bits as strings of 0s and 1s using many particles (electrons or photons) per bit.
- **In quantum communication**, the information is encoded in the special "quantum state" of a single particle, such as a photon.
- Quantum communication uses **polarization** to encode information, an oscillation in one direction can be 1 and another 0.
- Two sets of polarizer are commonly used, **rectilinear** and **diagonal**.
- In order to receive the data, **the polarization of the filter must match with the photons**.



QUANTUM COMMUNICATION

Suppose Alice wants to send a short, plain message (like a string of bits: 1101) to Bob using a quantum channel

Step 1: Alice Encodes the Message in Quantum States

Alice has a message, e.g., **1101**.

She decides how to encode each bit:

- **0:** Prepare a photon in the horizontal polarization state $|0\rangle$.
- **1:** Prepare a photon in the vertical polarization state $|1\rangle$.

Step 2: Alice Sends the Qubits to Bob

Alice sends the four photons, each representing one bit, over the quantum channel to Bob.

Step 3: Bob Measures Each Received Photon

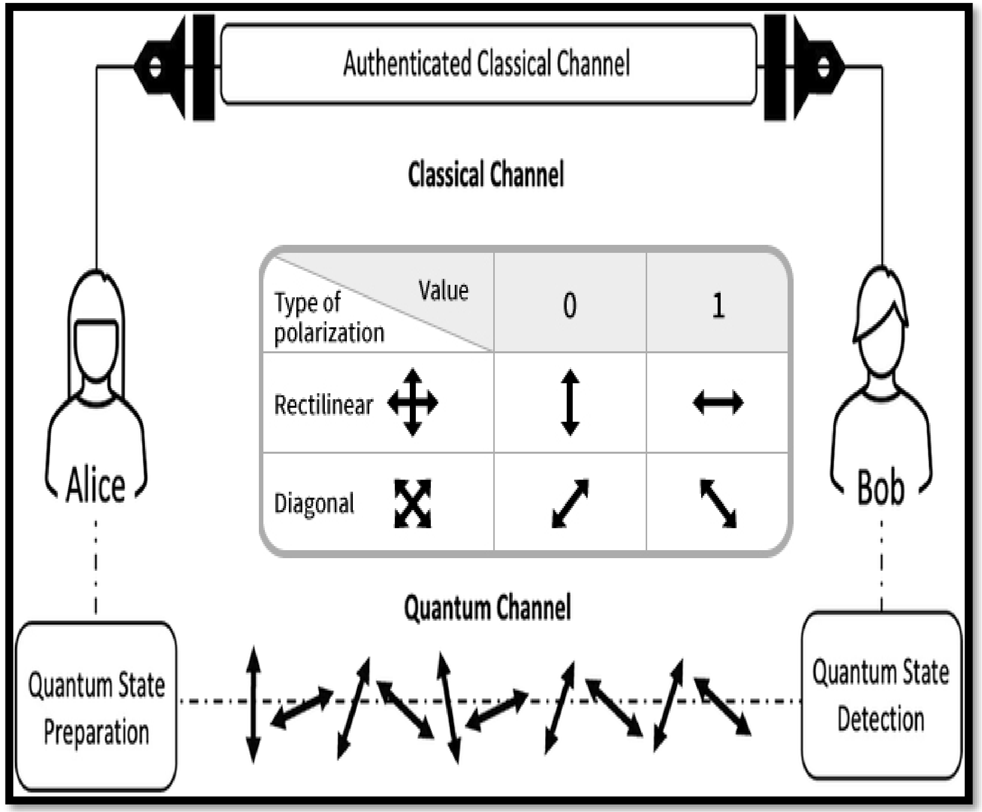
Knowing the encoding (horizontal = 0, vertical = 1), Bob measures each photon's polarization using the rectilinear basis.

Step 4: Bob Recovers the Message

From his measurements, Bob reconstructs the bit string:

- Vertical photon $|1\rangle$ maps to bit 1
- Horizontal photon $|0\rangle$ maps to bit 0

Bob thus retrieves the message **1101** exactly.



1 "Rectilinear" and "diagonal" are randomly selected and 0s and 1s are randomly sent

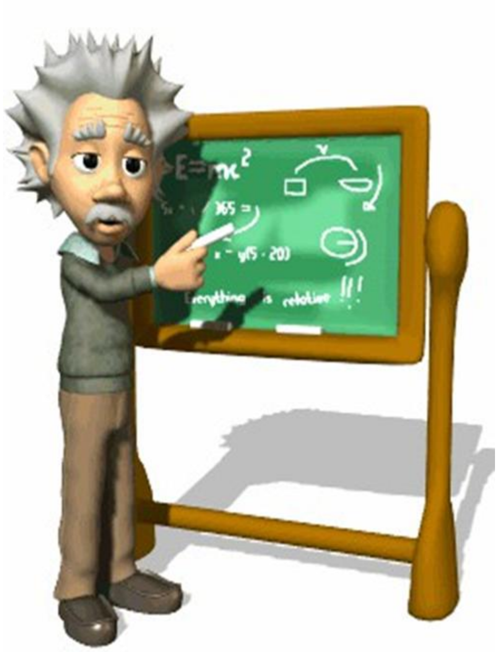
2 "Rectilinear" and "diagonal" are randomly selected and photons are received

Numerical Problems

1. In a QKD system, what is the minimum number of photons Alice and Bob need to exchange to generate a secure key of 128 bits considering a 10% photon loss?

2. In a quantum communication protocol, what is the minimum number of photons Alice should prepare to achieve an average of 500 detected photons at Bob’s end over a channel with 3% detection efficiency?

3. A secret key length of 256 bits is generated using QKD. On average, 2 photons are needed to securely transmit one bit. Calculate the total photons sent.



QUANTUM ALGORTITHM

- Quantum algorithm is a finite sequence of quantum operations (gates and measurements) on qubits that uses superposition, entanglement, and interference to solve certain computational problems faster than any classical algorithm.

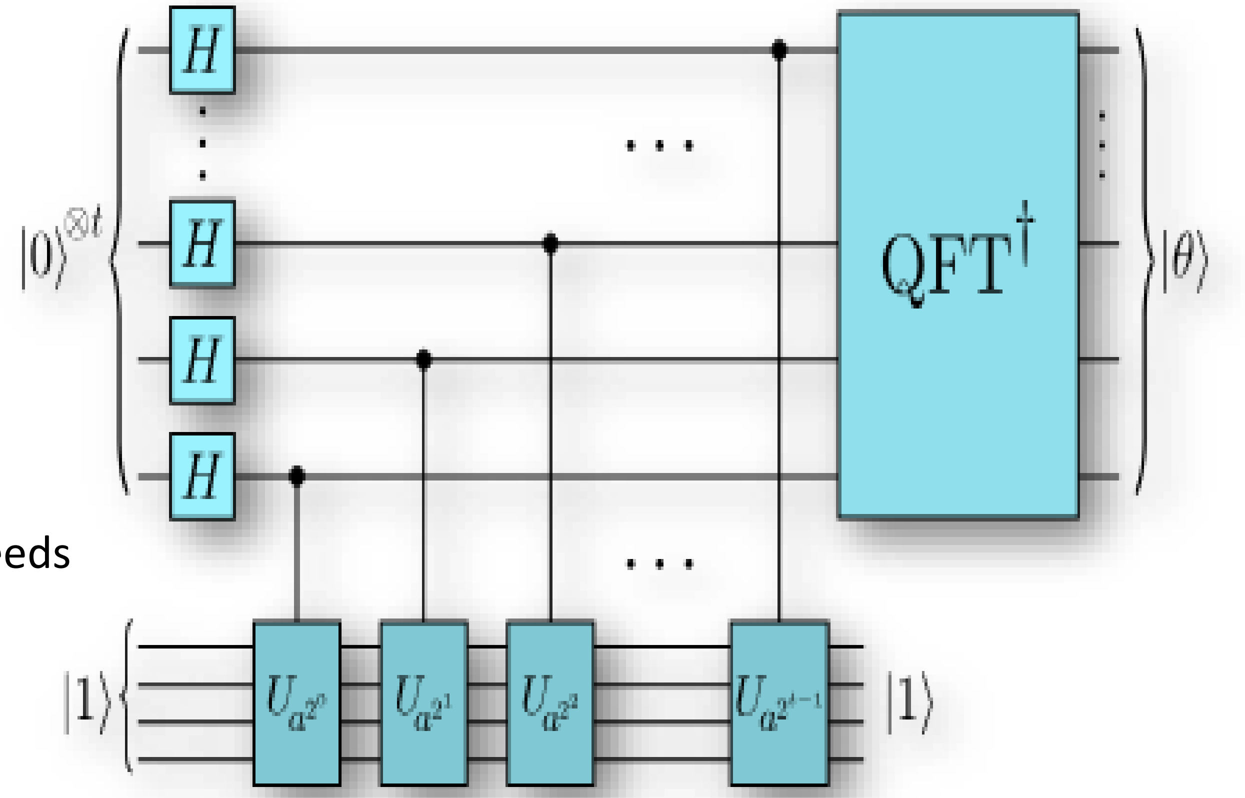
- ## Practical Considerations:

Error Correction: Real devices are noisy; fault-tolerance demands massive qubit overhead.

Resource Scaling: Shor's factoring at cryptographic sizes needs thousands of qubits and deep circuits.

Hybrid Approaches: Variational algorithms (QAOA, VQE) tolerate noise but lack provable asymptotic speedups.

Undecidable Problems: Quantum computers cannot tackle classically undecidable tasks.



Common Quantum Algorithms

Algorithm	Use Case	Speedup Over Classical
Shor’s	Breaking codes	Exponential
Grover’s	Search	Quadratic
QFT	Signal/period analysis	Exponential
Phase Estimation	Quantum chemistry/simulation	Polynomial–exponential
VQE, QAOA	Optimization, chemistry	Heuristic (practical)
Simon–Deutsch-Jozsa	Demonstration/education	Exponential (in theory)

LIMITATIONS & CHALLENGES:

- **Fragility:** Qubits are highly susceptible to noise and environmental interference, making them hard to scale.
- **Error Rates:** High error rates and short coherence times remain technological barriers.
- **Resource and Operational Challenges:** High energy and maintenance needs (especially for cooling),Error correction increases hardware demands, Very expensive and not widely accessible.
- **Practical Use:** Most quantum computers today are in the experimental stage and only outperform classical ones for a narrow range of problems(e.g., factoring, unstructured search, quantum simulation).
- **Security & Ethical Challenges :** Can break current encryption, Risk of misuse for harmful purposes.
- **Not a Classical Computer Replacement:** Quantum computers will not replace classical computers for everyday tasks—they excel at certain, highly complex problems.

QUANTUM COMPUTING TODAY:

- Latest quantum simulators and software:

IBM Quantum Experience (Qiskit): Online simulator with visual circuit builder and Python integration for easy quantum circuit simulation and prototyping on classical computers.

Microsoft Azure Quantum: Cloud platform supporting Q# language and classical simulators, integrated with machine learning and HPC for business readiness.

Google Quantum AI (Cirq): Open-source framework with high-performance simulators accessible via Google Collab for rapid experimentation and research.

Quantinuum InQuanto: High-fidelity simulators focused on industrial quantum chemistry applications with enterprise solutions.

QuTiP: Open-source tool for advanced simulation of quantum optics and open quantum systems used in research and education.

QUANTUM COMPUTING TODAY:

- IBM is making a new quantum processor called Nighthawk with 120 qubits. It can run complex circuits with 5,000 two-qubit gates. IBM is also working on quantum error correction and linking quantum computing with classical supercomputers to get better results on early quantum systems.

- Microsoft has made progress with 24 logical qubits and started the Quantum Ready program to help businesses prepare for quantum computing. They focus on training, hybrid apps, and quantum-safe security. Microsoft is also developing topological quantum computers with stable qubits. Their Majorana 1 chip aims for up to one million qubits.

- Google's latest quantum chip the Willow, which reduces errors exponentially and performs task in 5 minutes that would take classical supercomputers 10 septillion years.

- India has achieved a significant breakthrough in quantum communication by successfully demonstrating secure quantum communication using quantum entanglement over a distance of more than one kilometer in free space. This experiment was conducted on the IIT Delhi campus by a team from the Defense Research and Development Organization (DRDO) and IIT Delhi.

REFFERENCES BOOKS