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MODERN COLLEGE OF ENGINEERING

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Engineering Physics

Semester – I/II

Unit – 3: Quantum Mechanics

Importance of Quantum Mechanics in Engineering

Quantum mechanics drives innovation in various engineering fields and computer science, enabling cutting-edge technologies. Across disciplines, quantum principles unlock new possibilities. In electrical engineering, quantum mechanics informs transistor design, while materials scientists leverage it to reveal atomic-level properties. Mechanical engineers apply quantum principles to nanoscale systems, aerospace engineers utilize quantum-inspired materials, and chemical engineers rely on quantum mechanics for catalyst design. Nuclear engineers harness its power for energy applications, biomedical engineers for medical imaging, and optical engineers for laser advancements. In computer science, quantum mechanics fuels breakthroughs in quantum computing, information processing, algorithms, cryptography, artificial intelligence, data science, and software engineering. These applications transform industries, yielding improved efficiency, precision, miniaturization, and security. Research focuses on quantum computing, algorithms, error correction, and materials science. Studying quantum mechanics is crucial for engineering students, providing a fundamental understanding of matter and energy at the atomic and subatomic level. This knowledge is essential for designing and optimizing electronic devices, materials, and systems. Quantum mechanics underlies modern technologies like transistors, lasers, and MRI. By grasping quantum principles, engineers develop innovative solutions, materials, and devices, tackling complex problems in energy, nanotechnology, and biomedicine. Moreover, studying quantum mechanics cultivates valuable skills: problem-solving, mathematical modeling, and computational thinking. As industry leaders like Google, IBM, and Microsoft invest in quantum technologies, the demand for quantum-educated engineers grows, making this field exciting and rewarding to explore.

Subtopics in Unit – 3

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Quantum Mechanics

3.1. Why Quantum Theory

There are two main reasons to study quantum mechanics: it's fascinating and it's practical.

Quantum mechanics is fascinating because it's weirder than anything imagined by science fiction. Particles can act like waves! Measurement results are unpredictable! Energies can only take on specific discrete values! Events in distant locations can exhibit strange correlations! In many ways, no one fully "understands" quantum mechanics, yet it operates with a clear logic, expressed through some of the most beautiful mathematics ever created.

On the practical side, quantum mechanics governs the fundamental structure of all matter and interactions. It explains why atoms are stable, why certain nuclei undergo radioactive decay, and why carbon dioxide contributes to the greenhouse effect. Quantum mechanics forms the foundation of chemistry, materials science, and subatomic physics. We can apply quantum theory to develop technologies like microscopes, lasers, solar cells, nuclear reactors, and secure methods for transmitting encrypted information. Researchers worldwide continue to uncover new applications for quantum mechanics.

3.2. de Broglie Hypothesis

The de Broglie hypothesis, proposed by French physicist Louis de Broglie in 1924, is a groundbreaking concept in quantum mechanics that suggests particles of matter (such as electrons, protons, and even larger particles) exhibit wave-like properties. Prior to this, it was widely believed that waves were a property of light, while matter was treated as discrete particles. de Broglie unified these concepts by proposing that matter could also have wave characteristics.

Wave-Particle Duality: De Broglie extended the idea of wave-particle duality, which had already been established for light (as evidenced by Einstein's explanation of the photoelectric effect), to all particles of matter. According to this hypothesis, particles like electrons, which were traditionally viewed as solid, localized particles, also exhibit wave-like behaviors under certain conditions.

Wavelength of Matter Waves:

Statement: The de Broglie hypothesis states that all matter exhibits wave-like properties, and the wavelength (λ) associated with a moving particle is inversely proportional to its momentum.

The mathematical expression for de Broglie wavelength is:

$$\lambda = h/p$$

Where:

h is Planck's constant (6.626×10^{-34} Js)

p is the momentum of the particle, which is the product of its mass and velocity ($p=mv$).

This formula shows that the wavelength of a particle is smaller for more massive or faster-moving particles. Particles such as electrons, protons, and even larger objects can display wave-like behavior under certain conditions.

Experimental Confirmation: The de Broglie hypothesis was confirmed experimentally by Davisson and Germer in 1927. They observed that when electrons were directed at a crystal, they produced diffraction patterns, similar to those produced by light waves. This diffraction phenomenon is characteristic of waves and provided strong evidence for the wave-like nature of electrons.

Implications in Quantum Mechanics: De Broglie's hypothesis laid the foundation for the development of wave mechanics and the Schrödinger equation. The idea that particles could exhibit wave-like properties helped physicists understand the behavior of particles at the quantum level, where classical mechanics no longer applied.

Electron Waves in Atoms: De Broglie's work also led to the concept that electrons in atoms exist in quantized states because the electron's de Broglie wavelength must fit an integer number of wavelengths into the orbit of the atom. This idea was critical to the development of the Bohr model of the atom and later the quantum mechanical model of the atom.

Significance: The de Broglie hypothesis was a pivotal concept in the evolution of quantum mechanics. It provided a new understanding of the nature of particles, leading to the development of modern physics, including the study of quantum fields and particle-wave duality. It also had profound implications in fields like electron microscopy, where the wave nature of electrons allows them to resolve much smaller structures than light microscopes can.

We can arrive at the expression of de Broglie wavelength by:

- Analogy with radiation
- Relativistic considerations (kinetic energy of the particle, and potential difference)

3.2.1. de Broglie Wavelength by Analogy with Radiation

To derive the de Broglie wavelength using an analogy with radiation, we start by recognizing the similarities between matter and light waves. The key analogy is based on the fact that both light and matter exhibit wave-particle duality, meaning that light, typically considered as a wave, can also behave like a particle (photon), and similarly, matter particles (such as electrons) can exhibit wave-like behavior.

Derivation:

Energy of a Photon: The energy of a photon (light particle) is given by Einstein's relation:

$$E = h\nu$$

where:

E is the energy of the photon,

h is Planck's constant,

ν is the frequency of the photon (number of oscillations per second)

Wave-like nature: Light also behaves like a wave, with its wavelength λ related to its frequency by the equation:

$$c=\lambda\nu$$

where c is the speed of light in a vacuum.

Photon Momentum: The momentum of a photon is related to its energy and wavelength. Using the relation $E = pc$, where c is the speed of light, we can express the momentum as:

$$E = pc$$

Combining this with E=hν and c=λν, we get:

$$h\nu = pc$$

Since c=λν, we rearrange to find λ in terms of p:

$$\lambda = h/p$$

This relation shows that the wavelength of a photon is inversely proportional to its momentum.

3.2.2. de Broglie Wavelength in terms of K. E. of the Particle

The de Broglie wavelength λ of a particle is given by:

$$\lambda = h/p$$

where *h* is Planck's constant and *p* is the momentum of the particle.

For a particle with mass m moving with velocity *v*, the momentum *p* is:

$$p = mv$$

The kinetic energy (K.E.) of the particle is given by:

$$K.E. = 1\,(mv^2)/2$$

From this equation, we can solve for v in terms of K.E.:

$$v = \sqrt{(2\,K.E./m)}$$

Now, substitute this expression for v back into the formula for momentum:

$$p = m.\sqrt{2\ K.E./m} = \sqrt{2\ m\ K.E.}$$

Now that we have $p=\sqrt{2\ m\ K.E.}$, we can substitute this into the de Broglie wavelength formula:

$$\lambda = h/p = h/\sqrt{2\ m\ K.E.}$$

Thus, the de Broglie wavelength λ in terms of the **kinetic energy** of the particle is:

$$\lambda = h/\sqrt{2\ m\ K.E.}$$

3.2.3. de Broglie Wavelength for an electron in Terms of Potential Difference

When an electron is accelerated through a potential difference V, it gains **kinetic energy** equal to the work done by the electric field:

$$K.E. = eV$$

where:

- e is the **charge of the electron** ($e \approx 1.6\times10^{-19}$ C),
- V is the **potential difference** through which the electron is accelerated.

The kinetic energy K.E. of an electron with mass m and velocity v is also given by:

$$K.E. = 1\ (mv^2)/2$$

Equating these two expressions for kinetic energy, we get:

$$eV = 1\ (mv^2)/2$$

Solving for v, the velocity of the electron:

$$v = \sqrt{2\ eV/m}$$

The momentum p of the electron is given by:

$$p = mv$$

Substituting $v = \sqrt{2eV/m}$ from the previous step:

$$p = m \cdot \sqrt{2eV/m} = \sqrt{2eV.m}$$

Now, using de Broglie's formula for wavelength λ:

$$\lambda = h/p$$

Substitute **p** = $\sqrt{2eV.m}$:

$$\lambda = h/\sqrt{2eV.m}$$

Thus, the de Broglie wavelength λ of an electron accelerated through a potential difference V is:

$$\lambda = h/\sqrt{2eV.m}$$

This formula shows that the de Broglie wavelength of an electron decreases as the accelerating potential difference V increases.

Substituting values of h, e, mass of electron (m) (all in SI Units), we get:

$$\lambda = \frac{12.27}{\sqrt{V}}$$

Properties of Matter Waves:

1. The wavelength of a matter wave is inversely related to its particles momentum.
2. Matter wave can be reflected, refracted, diffracted and undergo interference.
3. The position and momentum of the material particles cannot be determined accurately and simultaneously.

4. The amplitude of the matter waves at a particular region and time depends on the probability of finding the particle at the same region and time.

Numericals: Example and Practice Problems: de Broglie Wavelength

Example: What is the de Broglie wavelength of an electron when accelerated through a potential difference of 10000 volts?

Sol: Given: V= 10000 volts

Formula: $\lambda = \frac{12.27}{\sqrt{V}}$

Solution: $\lambda = \frac{12.27}{\sqrt{10000}} = 0.1227\ \text{Å}$

Problems:

3.1. The energy of photon is 5.28 x 10^{-19} eV. Calculate frequency and wavelength. (Ans: ν= 1.278×10^{15}Hz, λ=235 nm)

3.2. Find the De-Broglie wavelength of 10 KeV electrons. (Ans: 0.123 nm)

3.3. An electron has kinetic energy equal to its rest mass energy. Calculate De-Broglie's wavelength associated with it. (Ans: 1.717 × 10^{-2} Å)

3.4. Which has a shorter wavelength 1 eV photon or 1 eV electron? Calculate the value. (Ans: Wavelength of 1 eV Photon: 1240.82 nm; Wavelength of 1 eV Electron: 1.23 nm)

3.5. Determine the velocity and kinetic energy of a neutron having De-Broglie wavelength 1 Å. Mass of neutron is 1.67×10^{-27} Kg (Ans: Velocity: 3.97×10^{3} m/s; Kinetic Energy: 1.32×10^{-20} J)

3.6. Find the de Broglie wavelength of:

a) An electron accelerated through a potential difference of 182 volts. (Ans: 0.91 Å)

b) 1 kg object moving with a speed of 1m/s. (Ans: 6.63 × 10^{-24} Å)

3.7. If electron had existed inside the nucleus, then its de Broglie wavelength would be roughly of order of nuclear distance, ie. 10^{-14} m. How much momentum corresponds to this

wavelength? How much energy corresponds to this momentum ? Express this energy in MeV and explain how this result proves that the cannot exist inside the nucleus. (The maximum nuclear binding energy is 8.8 MeV per nuclear particle). (Ans: 15093.75 MeV)

3.9. An electron initially at rest is accelerated through a potential difference of 3000 V. Calculate for the electron wave the following parameters:

a) the de Broglie Wavelength (Ans: 0.224 Å)

b) the momentum (Ans: 2.96×10^{-23} kgm/s)

3.10. An electron is accelerated through a potential difference of 10 kV. Calculate the de Broglie wavelength and momentum of electron. (Ans: λ=0.1227 Å, p= 5.403×10^{-23} kg.m/s)

3.11. An electron has K.E. equal to its rest mass energy. Calculate the de Broglie wavelength associated with it. (Ans: 1.717×10^{-2} Å)

3.12. Calculate de Broglie Wavelength of 10 keV protons in Å. (Ans: 2.868×10^{-3} Å)

3.13. At what K.E. an electron will have a wavelength of 5000 Å? (Ans: 6.038×10^{-3} eV)

3.14. Calculate the de Broglie wavelength for a proton moving with velocity 1% of velocity of light. (Ans: 1.32×10^{13} m)

3.15. An electron beam is accelerated from rest through a potential difference of 200 V. Calculate the associated wavelength. (Ans: 0.868 Å)

3.16. Calculate the energy (in eV) with which a proton has to acquire de Broglie wavelength of 0.1 Å. (Ans: 8.2 eV)

3.17. Calculate the de Broglie wavelength of electron having K.E. 1 keV. (Ans: 0.39 Å)

3.18. Compute the wavelength of the de Broglie waves associated with a proton moving with 5% of the velocity of light. Proton has 1836 times the mass of one electron. (Ans: 2.65×10^{-13} m)

3.19. Proton and alpha particles are accelerated through some potential difference \. Compute the ratio of their de Broglie Wavelength. (Ans: $1/\sqrt{8}$)

3.3. Wave Function

In quantum mechanics, the wave function (ψ) is a mathematical function that provides a complete description of the quantum state of a system. It encapsulates all the information about a particle, such as its position, momentum, and energy.

Water waves → height of water surfaces varies

Light waves → electric & magnetic fields vary

Matter waves → wave function (ψ)

ψ is related to the probability of finding the particle. Max Born put these ideas forward for the first time.

In general, the wave function is a complex quantity and can be written as,

$$\Psi=A+iB$$

Where, A and B are real.

Complex conjugate of ψ is:

$$\Psi^*=A-iB$$

The product $\Psi\ \Psi^* = |\Psi|^2 = A^2+B^2$ is a real and positive quantity. Although $|\Psi|^2$ is a positive and real quantity, it need not be less than 1. Hence, we still cannot say that the probability of finding the particle is equal to $|\Psi|^2$. We can only say that the probability is proportional to $|\Psi|^2$.

3.3.1 Physical Significance of the Wave Function ψ

The physical significance of the wave function ψ in quantum mechanics lies primarily in its ability to describe the probabilistic nature of particles and their observable properties.

1. Probability Density Interpretation

The reason why ψ itself cannot be directly interpreted in terms of experimental outcomes is straightforward. The probability of finding an object at a particular location and time must fall between 0 and 1, with 0 indicating the object is certainly not there, and 1 indicating it is certainly there. Intermediate probabilities, like 0.2, mean there is a 20% chance of finding the object in that location. However, wave amplitudes can be positive or negative, and a negative probability, such as -0.2, is nonsensical. Therefore, ψ cannot serve as an observable quantity on its own. For this reason, the square of the absolute value of the wave function ψ, denoted $|\psi|^2$, is used instead and is known as the **probability density**. The probability of experimentally detecting the particle described by ψ at a point (x,y,z) at time t is proportional to $|\psi|^2$.

The most important physical significance of the wave function ψ is given by the Born interpretation, which states:

- The square of the modulus of the wave function, $|\psi(x,t)|^2$, represents the probability density of finding a particle at a specific position x and time t.
- This means that: $|\psi(x,t)|^2$=Probability density at position x and time t. In three dimensions, the probability density is $|\psi(r,t)|^2$, where r represents the position vector.
- Small value of $|\psi^2$ →Less possibility of presence. As long as $|\psi|^2$ is not exactly zero at a particular location, there is always a finite, albeit small, chance of detecting the particle there.

2. Normalization

The wave function must be normalizable, meaning the total probability of finding the particle somewhere in space is finite and equal to 1:

$$\int_{-\infty}^{\infty} |\ \psi(\mathrm{x},\mathrm{t})|^2 dx = 1$$

For a three-dimensional wave function:

$$\int_{-\infty}^{\infty} |\ \psi(\mathrm{x},\mathrm{t})|^2 d^3r = 1$$

This ensures that $|\psi|^2$, interpreted as a probability density, is meaningful.

3. Probability Amplitude (ψ)

The wave function **ψ** itself is known as the probability amplitude**,** which is a complex-valued function. While $|\psi|^2|$ provides the probability density, ψ contains more information:

- **Magnitude (|ψ|)**: Related to the probability density.
- **Phase (θ)**: Plays a critical role in quantum interference and superposition.

For example, if two wave functions ψ_1 and ψ_2 are superimposed, the resulting wave function is:

$$\psi_{total}=\psi_1+\psi_2$$

The probabilities depend on the relative phase of ψ_1 and ψ_2, leading to constructive or destructive interference.

4. Charge Density (ρ_q)

For a charged particle (like an electron with charge $q=-e$), the wave function also relates to the charge density ρ_q. The charge density is given by:

$$\rho_q(r,t)=q|\psi(r,t)|^2$$

- Here, q is the charge of the particle.
- $|\psi(r,t)|^2$ gives the probability density, and multiplying it by q provides the charge distribution over space.

This is particularly important in systems where the spatial distribution of charge, such as in electronic clouds in atoms or molecules, influences physical properties like electric fields and potentials.

5. Phase and Interference

The wave function, often complex-valued, has a phase component that plays a crucial role in interference and superposition phenomena:

- The phase of the wave function determines how wave functions interact with each other.
- For instance, if two wave functions interfere constructively (in phase), they reinforce each other, increasing the probability density. If they interfere destructively (out of phase), they cancel each other, reducing the probability density.

5. Evolution of the Wave Function

The Schrödinger equation governs how ψ evolves over time, and thus indirectly describes the evolution of probability and charge densities. For example, in a time-dependent system:

$$\mathbf{i}\hbar\frac{\partial\boldsymbol{\psi}}{\partial\mathbf{t}} = \hat{\mathrm{H}}\boldsymbol{\psi}$$

where H^ is the Hamiltonian operator. Solving this equation yields the time-dependent wave function ψ(r,t), and from it, $|\psi|^2$ and ρ_q can be computed at any moment.

3.3.2 Properties of a Wave Function ψ

A well-behaved wave function in quantum mechanics satisfies certain mathematical and physical conditions to ensure it provides a meaningful and consistent description of a quantum system. These properties are essential for the wave function ψ(x,t) to describe the state of a particle in a way that aligns with the principles of quantum mechanics.

1. Normalization

The wave function must be normalizable, meaning the total probability of finding the particle somewhere in space is finite and equal to 1:

$$\int_{-\infty}^{\infty} |\,\psi(\mathrm{x},\mathrm{t})|^2 dx = 1$$

For a three-dimensional wave function:

$$\int_{-\infty}^{\infty} |\,\psi(\mathrm{x},\mathrm{t})|^2 d^3r = 1$$

This ensures that $|\psi|^2$, interpreted as a probability density, is meaningful.

2. Continuity

The wave function $\psi(x,t)$ and its derivatives must be continuous across its domain. Discontinuities in would imply undefined probabilities, which is not physically meaningful.

3. Single-Valued

The wave function must be single-valued at every point in space. At a given position x, there must be only one value of $\psi(x,t)$. A multi-valued wave function would lead to ambiguity in the probability density.

4. Differentiability

The wave function must be differentiable (at least once). This is required because:

- The Schrödinger equation involves the derivative of ψ.
- Observables like momentum involve derivatives of the wave function (e.g., $\hat{p}=-i\hbar\partial/\partial x$).

Exceptions can occur at points where the potential is infinite (e.g., at a hard boundary), but even in such cases, ψ must remain piecewise differentiable.

5. Finite Value

The wave function must be finite everywhere:

$$|\psi(x,t)| < \infty \text{ for all } x \text{ and } t$$

An infinite wave function is not physical, as it would lead to undefined or infinite probabilities.

6. Square Integrability

The wave function must satisfy the condition of square integrability**:**

$$\int_{-\infty}^{\infty} |\ \psi(\mathrm{x},\mathrm{t})|^2 dx < \infty$$

This ensures that the total probability of finding the particle is finite.

7. Boundary Conditions

The wave function must satisfy appropriate **boundary conditions**, which depend on the physical system:

- For an infinite potential well, ψ(x) = 0 at the boundaries.
- For free particles, ψ(x) should approach 0 as x → ±∞.

3.4. Schrödinger's Time-Independent Wave Equation

The Schrödinger Wave Equation is a foundational equation in quantum mechanics. It describes how the quantum state of a physical system changes with time and space. It provides a mathematical framework for studying the behavior of microscopic particles, such as electrons, atoms, and molecules.

Types of Schrödinger Wave Equations

There are two primary forms of the Schrödinger equation:

1. **Time-Dependent Schrödinger Wave Equation:** This equation describes the evolution of the wave function in both time and space:

$$\frac{\mathrm{i}\hbar}{2m}\frac{\partial\psi(\mathrm{x},\mathrm{t})}{\partial\mathrm{t}} = \hat{\mathrm{H}}\psi(\mathrm{x},\mathrm{t})$$

where:

- ψ(x,t) is the wave function, which depends on position x and time t,
- $\hbar$ is the reduced Planck's constant ($\hbar$=h/2π),
- I is the imaginary unit,

- $\hat{H}$ is the Hamiltonian operator, representing the total energy of the system.

2. **Time-Independent Schrödinger Wave Equation:** This equation applies to systems where the potential energy V(x) does not change with time. It describes stationary states (states with definite energy):

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

where:

- $\psi(x)$ is the spatial part of the wave function,
- E is the total energy of the particle.

Schrödinger's Time-Independent Wave Equation

Schrödinger's Time-Independent Wave Equation is based on principles of wave mechanics and quantum mechanics. It provides a mathematical description of a quantum system, particularly for particles moving under the influence of a potential V(x).

The Time-Independent Schrödinger Equation is derived from the Time-Dependent Schrödinger Equation, assuming that the potential energy V(x) does not vary with time. This derivation uses the method of separation of variables.

The time-dependent Schrödinger equation for a three-dimensional wave is given by:

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

where:

- $\psi(r,t)$ is the wave function, a function of position (x,y,z) and time t,
- i is the imaginary unit ($i^2=-1$),
- $\hbar$ is the reduced Planck's constant ($\hbar$=h2π),
- $\hat{H}$ Hamiltonian operator.

The Hamiltonian operator $\hat{\mathrm{H}}$ is expressed as:

$$\hat{\mathrm{H}} = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$

Here: $\frac{\partial^2}{\partial \mathrm{x}^2}$

- ∇^2 is the Laplacian operator, $\nabla^2 = \frac{\partial^2}{\partial \mathrm{x}^2} + \frac{\partial^2}{\partial \mathrm{y}^2} + \frac{\partial^2}{\partial \mathrm{z}^2}$
- $-\frac{\hbar^2}{2\mathrm{m}}\nabla^2$ is the kinetic energy operator,
- V(x) is the potential energy, which is a function of position.

Substituting $\hat{\mathrm{H}}$ into the Time-Dependent Schrödinger Equation:

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

Assume that the wave function ψ(r,t) can be written as a product of two independent functions:

$$\psi(\mathrm{r},\mathrm{t}) = \psi(\mathrm{r})\varphi(\mathrm{t})$$

where:

- ψ(r) is the spatial part of the wave function, depending on (x,y,z),
- φ(t) is the time-dependent part of the wave function, depending only on t.

Substitute ψ(r,t)=ψ(r)φ(t) into the Time-Dependent Schrödinger Equation:

$$\mathrm{i}\hbar\frac{\partial}{\partial \mathrm{t}}[\psi(\mathrm{r})\phi(\mathrm{t})] = \hat{\mathrm{H}}[\psi(\mathrm{r})\phi(\mathrm{t})]$$

Since ψ(r) depends only on r and φ(t) depends only on t, we can rewrite the derivatives using the product rule for derivatives:

$$\psi(\mathrm{r}).\,\mathrm{i}\hbar\frac{\partial\phi(\mathrm{t})}{\partial \mathrm{t}} = \phi(\mathrm{t}).\left(-\frac{\hbar^2}{2m}\nabla^2\psi(\mathrm{r}) + V(r)\psi(\mathrm{r})\right)$$

Divide through by ψ(r)φ(t) to separate the variable:

$$\frac{i\hbar}{\phi(t)}.\frac{\partial\phi(t)}{\partial t}=\frac{-\frac{\hbar^2}{2m}\nabla^2\psi(r)+V(r)\psi(r)}{\psi(r)}$$

The left side depends only on t, and the right side depends only on r. Thus, both sides must equal a constant, which we call E (the total energy):

$$\frac{i\hbar}{\phi(t)}.\frac{\partial\phi(t)}{\partial t}=E$$

And

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r)+V(r)\psi(r)=E\psi(r)$$

From the temporal part:

$$i\hbar\frac{\partial\phi(t)}{\partial t}=E\phi(t)$$

This is a first-order differential equation whose solution is:

$$\phi(t)=e^{-\frac{iEt}{\hbar}}$$

The spatial part of the wave function satisfies:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r)+V(r)\psi(r)=E\psi(r)$$

Rearranging:

$$(-\frac{\hbar^2}{2m}\nabla^2+V(r))\psi(r)=E\psi(r)$$

This is the **time-independent Schrödinger wave equation** in three dimensions:

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

OR

The general differential equation for a wave with wave function ψ travelling with velocity u in three dimension is

$$\frac{\partial^2\psi}{\partial t^2} = u^2\left[\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right]$$

i.e $\frac{\partial^2\psi}{\partial t^2} = u^2\nabla^2\psi$ ------- [1]

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is called as Laplace operator.

The general solution for equation [1] is

$$\psi(x, y, z, t) = \psi_0(x, y, z)e^{-i\omega t} - - - - - [2]$$

We have $\psi_0(x, y, z)$ as the amplitude of wave at point(x, y, z).

The above equation can also be written as

$$\psi(\vec{r}, t) = \psi_o(\vec{r})e^{-i\omega t}\text{-------}[3]$$

Where

$\vec{r} = (x\hat{\imath} + y\hat{\jmath} + z\hat{k}) is\ the\ position\ vector\ of\ point\ (x, y, z)$

Differentiating [3] partially twice with respect to time is

$$\frac{\partial\psi}{\partial t} = -i\omega\varphi_0 e^{-i\omega t}$$

$$\frac{\partial^2\psi}{\partial t^2} = (-i\omega) - i\omega\varphi_0 e^{-i\omega t}$$

$$\frac{\partial^2\psi}{\partial t^2} = -\omega^2\psi_0 e^{-i\omega t}\text{--------}[4]$$

But we know that $\psi = \psi_0 e^{-i\omega t}$-----------[5]

Therefore, eq. [4] will become

$$\frac{\partial^2\psi}{\partial t^2} = -\omega^2\psi - - - - - - [6]$$

Substituting eq. [6] in eq. [1] we get

$$-\omega^2\psi = u^2\nabla^2\psi$$

$$\Rightarrow u^2\nabla^2\psi + \omega^2\psi = 0$$

$$\nabla^2\psi + \frac{\omega^2}{u^2}\psi = 0\text{---------}[7]$$

We know that angular frequency $\omega = 2\pi\gamma$-----[8]

We also know that $\gamma = \frac{u}{\lambda}$ $\quad where\ u = velocity$

[Ref: we know E= h$\nu = h\frac{c}{\lambda}$ $where\ c\ is\ nothing\ but\ velocity$]

Therefore eq [8] will become as

$$\omega = 2\pi\frac{u}{\lambda}\text{---------}[9]$$

$$\frac{\omega}{u} = \frac{2\pi}{\lambda}$$

$$\frac{\omega^2}{u^2} = \frac{4\pi^2}{\lambda^2}\text{---------}[10]$$

From De Broglie equation we have

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

$$\lambda^2 = \frac{h^2}{p^2} - - - - - - - [11]$$

We know that the total energy of the particle is the sum of kinetic energy and potential energy.

$$E = \frac{1}{2}mv^2 + V\text{------}[12]$$

$$E = \frac{m^2v^2}{2m} + V\text{--------}[13]$$

$$E = \frac{p^2}{2m} + V$$

$$2m(E - V) = p^2 ------ [14]$$

Substitute p^2 $from\ eq\ [14]\ in\ Eq\ [11]$

$$\lambda^2 = \frac{h^2}{2m(E - V)} ------ [15]$$

Now substitute λ^2 $from\ Eq\ [15]\ in\ Eq\ [10]$

$$\frac{\omega^2}{u^2} = \frac{4\pi^2}{\frac{h^2}{2m(E-V)}} ----- [16]$$

$$\Rightarrow \quad \frac{\omega^2}{u^2} = \frac{8m\pi^2(E-V)}{h^2} \text{-----}[17]$$

Substituting $\frac{\omega^2}{u^2}$ $from\ Eq\ [17] in\ Eq\ [7]\ we\ get$

$$\nabla^2\psi + \frac{8m\pi^2(E-V)}{h^2}\psi = 0\text{--------}[18]$$

$$\nabla^2\psi + \frac{2m(E-V)}{\hbar^2}\psi = 0\text{--------}[19]$$

($\hbar$ is the reduced Planck's constant. Has the value $h/2\pi$ (where h is Planck's constant))
Equation [19] is Schrödinger's time-independent wave equation.

3.5 Operators

In quantum mechanics, operators are mathematical entities corresponding to physical observables (e.g., position, momentum, energy). They act on wave functions to extract measurable properties or describe the evolution of a quantum system.

3.5.1 Definition of an Operator

An operator $\hat{O}$ is a rule that maps one function to another:

$$\hat{O}\psi(x)=f(x)$$

Operators act on wave functions to provide measurable outcomes or new states.

3.5.2 Types of an Operator

Quantum mechanical operators can be classified as follows:

a. Linear Operators

An operator $\hat{O}$ is linear if it satisfies:

$$\hat{O}(a\psi_1+b\psi_2)=a\hat{O}\psi_1+b\hat{O}\psi_2$$

where a and b are constants, and ψ1, ψ2 are wave functions.

b. Hermitian Operators

Hermitian operators are associated with measurable quantities (observables). They satisfy:

$$\int \psi_1^*(\hat{O}\,\psi_2)dx = \int \psi_2(\hat{O}\,\psi_1)dx$$

where ψ_1^* is the complex conjugate of ψ_1

Properties:

1. Their eigenvalues are real.
2. Their eigenfunctions corresponding to different eigenvalues are orthogonal.

Examples: Position ($\hat{x}$), momentum ($\hat{p}$), and Hamiltonian ($\hat{H}$) operators.

Common Operators in Quantum Mechanics

a. Position Operator ($\hat{x}$)

The position operator represents the position of a particle. In one dimension:

$$\hat{x}\,\psi(x)=x\psi(x)$$

b. Momentum Operator ($\hat{p}$)

The momentum operator is given by:

$$\hat{p} = -i\hbar\partial/\partial x$$

Action: acts as a derivative operator

$$\hat{p}\psi(x) = -i\hbar\partial\psi(x)/\partial x$$

c. Hamiltonian Operator ($\widehat{H}$) or energy operator

The energy operator in quantum mechanics is the operator associated with the total energy of a system. It is commonly called the Hamiltonian operator and is denoted by $\widehat{H}$. The Hamiltonian plays a central role in the formulation of quantum mechanics, particularly in the Schrödinger equation.

The energy operator $\widehat{H}$ is defined based on the physical system and its total energy, which includes both kinetic and potential energy:

$$\widehat{H}=\widehat{K}+\widehat{V}$$

where:

- $\widehat{K}$ is the kinetic energy operator.
- $\widehat{V}$ is the potential energy operator.

Time-Independent Schrödinger Equation

The energy operator appears in the time-independent Schrödinger equation as:

$$\widehat{H}\psi=E\psi,$$

where:

- ψ is the wavefunction of the system,
- E is the energy eigenvalue.

d. Eigenvalues and Eigenfunctions

If ψ is an eigenfunction of an operator $\hat{O}$ with eigenvalue o, then:

$$\hat{O}\psi=o\psi$$

Properties:

1. Observables are represented by Hermitian operators; their eigenvalues are real.
2. The eigenfunctions of Hermitian operators form a complete orthonormal set.

e. Operator Algebra

Operators follow rules similar to algebra, but they may not commute:

- Addition: $(\hat{A}+\hat{B})\psi=\hat{A}\psi+\hat{B}\psi$
- Multiplication: $(\hat{A}\hat{B})\psi=\hat{A}\,(\hat{B}\psi)$

3.6 Applications of Schrödinger's Time-independent Wave Equation

The Schrödinger Time-Independent Wave Equation is a cornerstone of quantum mechanics, used to describe the stationary states of a quantum system. It has numerous applications across various fields of physics, chemistry, and materials science. Here are the main applications:

1. Energy Levels of Atomic Systems

- The equation is used to calculate the quantized energy levels of atoms.
- Example: Solving the equation for the hydrogen atom gives the exact energy levels of its electron, matching experimental spectra.

2. Quantum Harmonic Oscillator

- It describes systems with quadratic potential, such as vibrations in molecules or lattice vibrations (phonons) in solids.
- The solutions are crucial in understanding quantum phenomena like zero-point energy.

3. Particle in a Potential Well

- The equation is used to model particles trapped in finite or infinite potential wells, such as electrons in a quantum dot or neutrons in a nucleus.
- Applications include understanding quantum confinement in semiconductors and nanostructures.

4. Chemical Bonding

- The equation explains how electrons behave in molecules, leading to the formation of chemical bonds.

- It is fundamental to molecular orbital theory and valence bond theory, predicting molecular structure and stability.

5. Solid-State Physics

- The wave equation is applied to electrons in crystalline solids, leading to concepts like energy bands, band gaps, and conductors/semiconductors/insulators.
- It underpins the operation of devices such as transistors, diodes, and solar cells.

6. Quantum Tunneling

- The equation describes tunneling phenomena where particles pass through energy barriers they classically shouldn't.
- Applications include:
  - Operation of tunnel diodes and scanning tunneling microscopes.
  - Understanding nuclear fusion in stars.

7. Spectroscopy

- Solving the equation helps predict spectral lines for various atoms and molecules.
- It forms the theoretical basis for techniques like infrared (IR), nuclear magnetic resonance (NMR), and ultraviolet-visible (UV-Vis) spectroscopy.

8. Nanotechnology

- The equation is key in designing quantum dots, nanowires, and other nanoscale devices, where quantum effects dominate.

9. Nuclear Physics

- It is used to study the behavior of nucleons (protons and neutrons) within the nucleus, explaining nuclear structure and reactions.

10. Optical and Laser Physics

- Solving the equation explains the behavior of photons in quantum systems, including the operation of lasers and quantum optics experiments.

11. Astrophysics

- The Schrödinger equation models quantum states in white dwarfs, neutron stars, and other high-density astrophysical objects.
-

3.6.1 Particle in a Rigid Box (Infinite Potential Well)

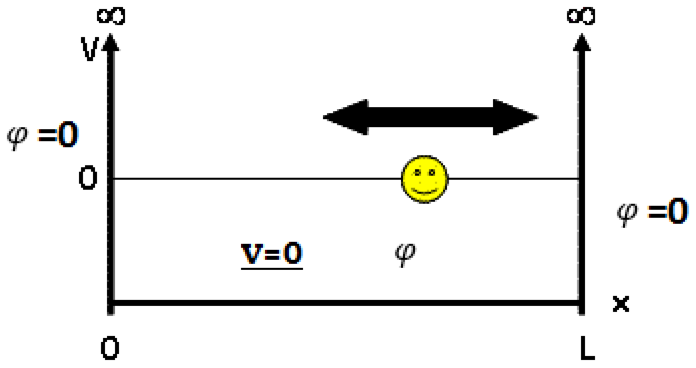


Figure 3.1. Infinite potential well.

The particle in a box problem is a common application of a quantum mechanical model to a simplified system consisting of a particle moving horizontally within an infinitely deep well from which it cannot escape.

The solutions to the problem give possible values of E and φ that the particle can possess. E represents allowed energy values and ψ (x) is a wavefunction, which when squared gives us the probability of locating the particle at a certain position within the box at a given energy level.

The potential energy is *0 inside the box* $\mathrm{V} = \infty$ for $\mathrm{x} < 0$ or $\mathrm{x} > \mathrm{L}$ and *goes to infinity at the walls of the box*

i.e , V=0 for x>0 or x<L and V=∞ for x<0 or x>L).

We assume the walls have infinite potential energy to ensure that the particle has zero probability of being at the walls or outside the box.

Doing so significantly simplifies our later mathematical calculations as we employ these ***boundary conditions*** *when solving the Schrödinger Equation*

The potential energy distribution is shown in the figure.

The particle does not exist in the walls and beyond them.

$$\psi = 0 \; for \; x \leq 0 \; and \; x \geq L$$

The wave function φ exists only for 0 < x > L. that is with in the box

We have Schrödinger's time independent wave equation as

$$\nabla^2\psi + \frac{8m\pi^2(E-V)}{h^2}\psi = 0\text{----- [1]}$$

Since here we have one dimensional case we can replace $\nabla^2\psi$ by $\frac{\partial^2\psi}{\partial x^2}$ as φ is the function of only x.

Also substituting. V=0 for x>0 or x<L,

Schrödinger's time independent wave equation will become as

$$\frac{\partial^2\psi}{\partial x^2} + \frac{8m\pi^2(E)}{h^2}\psi = 0\text{----- [2]}$$

Let $K^2 = \frac{8m\pi^2(E)}{h^2}$ ----- [3]

Therefore equation [2] will become as

$$\frac{\partial^2\psi}{\partial x^2} + K^2\varphi = 0\text{----- [4]}$$

The general solution for equation [3] is

$$\psi = AsinKx + BcosKx\text{--------[5]}$$

where A, B, and K are constants which can be determined by using boundary conditions.

The solution to the Schrödinger equation we found above is the general solution for a 1-dimensional system.

We now need to apply our boundary conditions to find the solution to our particular system.

According to our boundary conditions, the probability of finding the particle at x=0 or x=L is zero.

When x=0 , sin(0)=0 , and cos(0)=1 ;

Therefore, B in equation [4] must equal 0 to fulfill this boundary condition giving:

$$\psi = AsinKx\text{-------[6]}$$

The second boundary condition is

$\psi = 0\, for\;\; x \geq L$

Therefore equation [5] will become,

$$0 = AsinKL \text{ -----} \quad [7]$$

$$\Rightarrow \qquad sinKL = 0$$

$$\Rightarrow \qquad KL = 0$$

$$\Rightarrow\; K = n\pi;\;\; n = 1,2,3.....$$

$$\Rightarrow K = \frac{n\pi}{L} \text{ -------}[8]$$

Form equation [3] we have

$$K^2 = \frac{8m\pi^2(E)}{h^2}$$

Therefore equation [8] will become,

$$\frac{8m\pi^2(E)}{h^2} = \frac{n^2\pi^2}{L^2} \text{ -----}[9]$$

Therefore $E = \frac{n^2h^2}{8mL^2}$ -------[10]

Where n =1,2,3…..

This is an important result that tells us:

- The energy of a particle is quantized and
- The lowest possible energy of a particle is NOT zero.
- This is called the zero-point energy and means the particle can never be at rest because it always has some kinetic energy.
- This is also consistent with the Heisenberg Uncertainty Principle: if the particle had zero energy, we would know where it was in both space and time.
- Also, these values are discrete. They are not continuous as expected from classical mechanics.

- Thus according to quantum mechanics, particle inside the box cannot have all values of energy but only those desecrate values, given by equation [10]
- These energy values are known as **Energy Eigen** values.

Numericals: Example and Practice Problems: Particle in a Rigid Box

Example: An electron is bound by a potential which closely approaches an infinite square well of width 2.5 Å. Calculate the lowest three permissible quantum energies the electron can have.

Sol: Given:

n=1,2,3

L=2.5 Å = $2.5 \times 10^{-10}\ m$

m=9.109×10^{-31} kg

Formula:

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

Solution:

1 eV=1.602×10^{-19} J

h = $6.626 \times 10^{-34}\ J.s = 4.134 \text{ x } 10^{15}$ eV

Substitute the constants into the formula:

$$E_n = \frac{n^2(4.391 \times 10^{-67})\ (\mathrm{J.s})^2}{4.555 \times 10^{-49}\ \mathrm{kg.m}^2} = n^2\ \left(9.641 \times 10^{-19}\ J\right) = n^2\ (6.02\ eV)$$

(As 1 kg.m^2/s^2=1 J)

For, n=1,

$$E_1 = 6.02\ eV$$

For n=2,

$$E_2 = 4 \times 6.02\ eV = 24.07eV$$

For n=3,

$$E_2 = 9 \times 6.02\ eV = 54.16\ eV$$

Problems:

3.20. Lowest energy of an electron trapped in a potential well is 38 eV. Calculate the width of the well. (e=1.6x10^{-19} C, h=6.63x10^{-34} J-sec, me=9.1x10^{-31} kg). (Ans: L= 0.9965 Å)

3.21. A neutron is trapped in an infinite potential well of width 10^{-14} m. Calculate its first energy eigen value in eV. (Mass of neutron =1.67 x 10^{-27} kg). (Ans: E_1= 2.05 x10^{6} eV)

3.22. Calculate the energy difference between the ground state and the first excited state of an electron in the rigid box length 1 Å. (Ans: 113.21 eV)

3.23. Compare the lowest three energy states for (i) an electron confined in a potential well of width 10 Å and (ii) a grain of dust mass 10^{-6} gm in an infinite potential well of width 0.1 mm. What can you conclude from this comparison? (Ans: E_1= 3.434 x10^{-34} eV, E_2= 1.37 x10^{-31} eV, E_3= 3.09 x10^{-31} eV)

3.24. An electron is bound by a potential which closely approaches an infinite square well of width 1 Å. Calculate the lowest three permissible quantum energies the electron can have. (Ans: E_1= 37.74 eV, E_2= 150.96 eV, E_3= 339.66 eV)

3.25. A electron is trapped in a rigid box of width 2 Å. Calculate its lowest energy and momentum. Hence, find energy of the third energy level. (Ans: E_1= 9.434 eV, p_1=1.66 x10^{-24} kg.m/s, E_1= 84.906 eV)

3.26. Lowest energy of an electron trapped in a rigid box is 4.19 eV. Calculate the width of the box. (Ans: L= 3 Å)

3.27. Calculate the energy required to excite the electron from its ground state to fourth excited state in a rigid box of length 0.1 mm. (Ans: 113.125 eV)

3.28. A neutron is trapped in an infinite potential well of width 10^{-10} m. Calculate the values of energy and momentum in its ground state. (Ans: E= 3.28 x 10^{-21} J, p= 3.313 x 10^{-24} kg.m/s)

3.7 Quantum Tunneling

3.7.1 Tunneling Effect

The tunneling effect is a quantum mechanical phenomenon where a particle passes through a potential energy barrier that it classically should not be able to cross. This occurs because, in quantum mechanics, particles exhibit wave-like properties, and their wavefunctions extend into and across potential barriers, allowing for a finite probability of transmission through the barrier.

3.7.2 Tunneling of an Electron in a Non-Rigid Box

The concept of an electron tunneling in a non-rigid box can be understood by comparing classical physics and quantum physics:

1. Classical Physics Perspective

In classical physics, a particle (such as an electron) confined within a box experiences boundaries that it cannot cross if it lacks sufficient energy. In this case, the "walls" of the box are not infinitely high but finite. This implies that the electron might "attempt" to escape, but only if its energy exceeds the potential energy of the wall. If the electron's energy E is less than the height of the potential barrier V_0, it cannot escape the box. The particle is strictly confined within the box.

2. Quantum Physics Perspective

In quantum physics, the behavior of particles like electrons is governed by the **Schrödinger equation**. Unlike classical particles, quantum particles exhibit wave-like behavior, leading to the phenomenon of **quantum tunneling**.

- **Finite Potential Barrier (Non-Rigid Box):**
    - The electron has a non-zero probability of penetrating and passing through the potential barrier, even if its energy E is less than the height of the barrier V_0.
    - This is because the wavefunction ψ, which describes the electron's state, extends into the barrier and does not abruptly drop to zero.
- **Tunneling Mechanism:**

- When the wavefunction reaches the barrier, it decays exponentially within the barrier region.
- If the barrier is thin enough or of moderate height, the wavefunction may reappear on the other side of the barrier, indicating a probability for the electron to "tunnel through." The electron is no longer strictly confined within the box, and tunneling allows it to escape, even if its classical energy is insufficient to overcome the barrier.

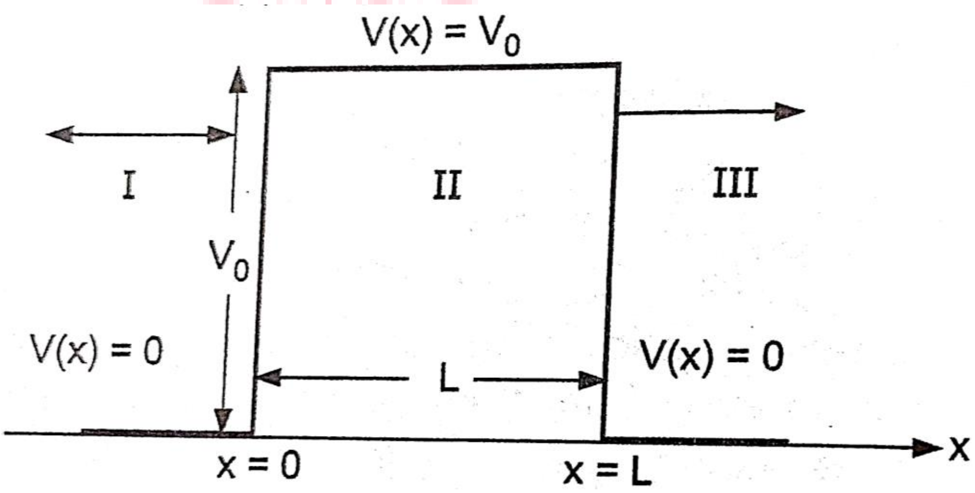


Figure 3.2. Illustration of quantum tunneling phenomenon.

Table 3.1. Key differences between tunneling of electron in a non-rigid box on the basis of classical physics and quantum physics

Aspect	*Classical Physics*	*Quantum Physics*
Escape Condition	The electron must have energy $E \geq V_0$ to escape the box.	The electron can tunnel through the barrier even if $E < V_0$.
Probability	The escape probability is zero if $E < V_0$	There is a non-zero probability of tunneling through the barrier for $E < V_0$.
Wave Nature	Not considered; the electron is treated as a particle only.	Wave-particle duality allows the wavefunction to penetrate the barrier.

Application	Cannot explain phenomena like tunneling diodes or radioactive decay.	Accurately explains quantum tunneling phenomena observed in devices and nature.

3.8 Quantum Computing

3.8.1 Qubits (Quantum Bits)

A qubit (quantum bit) is the fundamental unit of quantum information, analogous to the classical bit in conventional computing. However, unlike a classical bit, which can be in one of two states (0 or 1), a qubit can exist in a superposition of both states simultaneously, making it far more powerful for certain types of computation.

Properties of Qubits

1. **Superposition:**
   - A qubit can be in a state that is a combination of $|0\rangle$ and $|1\rangle$:

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

     where:

     - α and β are complex numbers representing the probability amplitudes.
     - $|\alpha|^2$ and $|\beta|^2$ are the probabilities of measuring the qubit in $|0\rangle$ and $|1\rangle$, respectively.
     - $|\alpha|^2+|\beta|^2=1$ (normalization condition).
2. **Entanglement:**
   - Qubits can become entangled, meaning the state of one qubit is directly correlated with the state of another, no matter how far apart they are. Entanglement is crucial for many quantum computing algorithms and quantum communication.
3. **Quantum Measurement:**
   - Measuring a qubit collapses its state into one of its basis states ($|0\rangle$ or $|1\rangle$).
   - The outcome is probabilistic, determined by the amplitudes $|\alpha|^2$ and $|\beta|^2$.

4. **Quantum Interference:**
   - Qubits can interfere with each other due to their wave-like properties, enabling complex manipulations and amplifying correct solutions in quantum algorithms.

Qubit vs. Classical Bit

Aspect	Classical Bit	Qubit
States	000 or 111	Superposition
Information	Encodes one state at a time	Encodes multiple states simultaneously (via superposition)
Operations	Classical logic gates (e.g., AND, NOT)	Quantum gates (e.g., Hadamard, CNOT)
Entanglement	Not possible	Possible, enabling correlated states between qubits
Power	Limited by sequential processing	Exploits parallelism and interference

Applications of Qubits

- Quantum Computing: Solve problems like factoring large numbers (Shor's algorithm) and database searches (Grover's algorithm).
- Quantum Communication: Enable secure communication through quantum key distribution (QKD) protocols.
- Quantum Simulation: Model complex quantum systems, such as molecules and materials.
- Quantum Cryptography: Ensure secure data transmission using principles of quantum mechanics.
- Qubits are the heart of quantum computing and quantum information science, offering capabilities far beyond classical systems by harnessing the unique properties of quantum mechanics.

3.8.2 Quantum Logic Gates

Quantum logic gates are the fundamental building blocks of quantum circuits, similar to how classical logic gates (AND, OR, NOT, etc.) are the basis of classical computing. They operate on quantum bits (qubits) and leverage the principles of quantum superposition, entanglement, and unitary transformations to perform operations that classical gates cannot achieve.

Properties of Quantum Logic Gates

1. **Qubit Operations:**
    - Qubits can exist in a superposition of $|0\rangle$ and $|1\rangle$, meaning they can hold more information than a classical bit.
    - Quantum gates manipulate the state of one or more qubits.
2. **Reversible Operations:**
    - Quantum gates are unitary, meaning they preserve the total probability of the system and are always reversible (unlike many classical gates, such as AND or OR).
3. **Linear Algebra Representation:**
    - Quantum gates are represented by unitary matrices.
    - The action of a gate on a qubit or system of qubits is described by matrix multiplication with the state vector.

In quantum computing, ***unitary matrices*** are the mathematical representation of quantum gates, which perform operations on qubits. These matrices govern the evolution of quantum states while preserving the core properties of quantum mechanics, such as normalization and reversibility.

A matrix U is unitary if it satisfies the following condition:

$$U^\dagger U = UU^\dagger = I,$$

where:

- $U^\dagger$ is the **conjugate transpose** (Hermitian conjugate) of U.
- I is the identity matrix.

Properties of Unitary Matrices:

1. **Reversibility:**

- All quantum operations must be reversible, which is ensured by the unitary condition.
- The inverse of a unitary matrix is its conjugate transpose: $U^{-1} = U^\dagger$.

2. **Preservation of Norm:**

   - A unitary matrix ensures that the probability of all possible outcomes (the norm of the state vector) is preserved:

$$\|U|\psi\rangle\| = \||\psi\rangle\| = 1$$

Role of Unitary Matrices in Quantum Gates

Quantum gates are operations applied to qubits and are represented by unitary matrices. These gates transform quantum states in a manner that preserves their quantum mechanical properties.

Common Quantum Logic Gates

1. Single-Qubit Gates:

- **Hadamard Gate (H):**
  - Creates superposition:

$$H|0\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}, \; H|1\rangle = \frac{|0\rangle-|1\rangle}{\sqrt{2}}$$

  - Matrix:

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

- **Pauli Gates:**
  - X (Pauli-X): Quantum analog of the NOT gate, flips $|0\rangle \leftrightarrow |1\rangle$

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

  - Y (Pauli-Y): Rotates qubit around the Y-axis of the Bloch sphere.

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

- Z (Pauli-Z): Flips the phase of |1⟩: Z|0⟩=|0⟩, Z|1⟩=−|1⟩

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

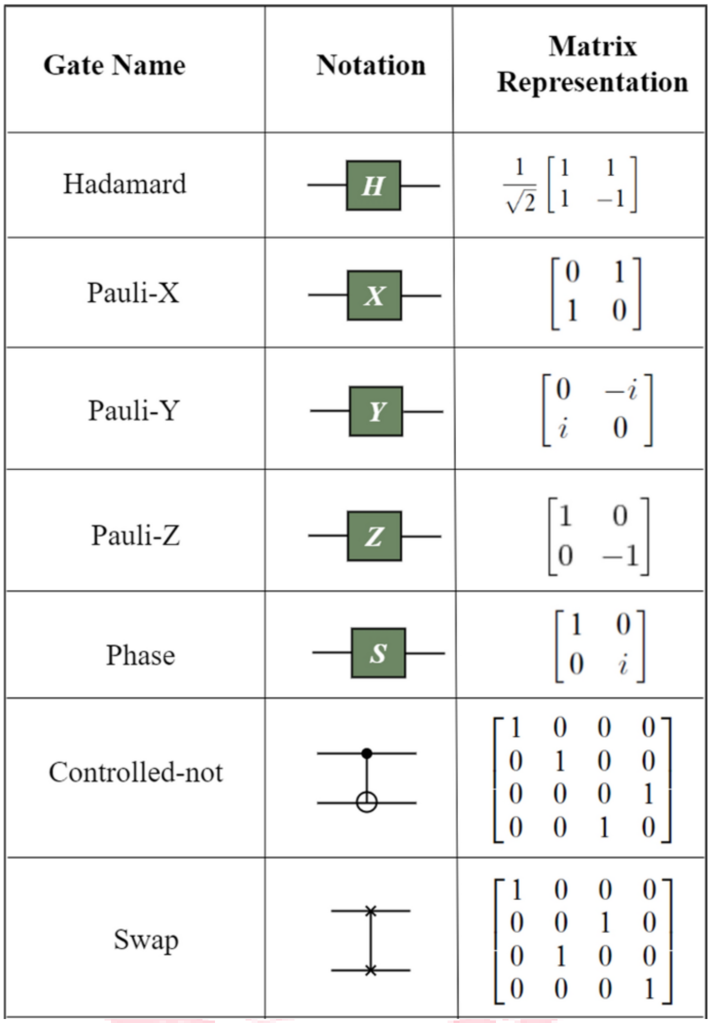
2. Multi-Qubit Gates:

- **CNOT (Controlled NOT):**
  - A 2-qubit gate where the second qubit (target) is flipped if the first qubit (control) is |1⟩.
  - Matrix:

$$\text{CNOT=} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

- **SWAP Gate:**
  - Swaps the states of two qubits, represented by the following 4×44 \times 44×4 unitary matrix:

$$\text{SWAP=} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$



Gate Name	Notation	Matrix Representation
Hadamard	H	$\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}$
Pauli-X	X	$\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}$
Pauli-Y	Y	$\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}$
Pauli-Z	Z	$\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$
Phase	S	$\begin{bmatrix}1 & 0\\ 0 & i\end{bmatrix}$
Controlled-not		$\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{bmatrix}$
Swap		$\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}$

Figure 3.3. Commonly used quantum gates.[1]

Applications of Quantum Logic Gates

1. **Quantum Algorithms:**
    - Used in algorithms like Shor’s (for factoring large numbers) and Grover’s (for database search).
2. **Quantum Communication:**
    - Facilitate secure communication using principles like entanglement.
3. **Quantum Cryptography:**
    - Basis for protocols like quantum key distribution.

4. **Simulating Quantum Systems:**
    - Model physical systems that are computationally infeasible for classical computers.

3.9 Comparison between Classical Computing and Quantum Computing

Classical computing and quantum computing are two fundamentally different paradigms for processing information. Each has its own strengths, limitations, and applications. Classical and quantum computing are not direct competitors but complementary technologies. Classical computing will likely remain dominant for everyday tasks, while quantum computing is expected to revolutionize specific domains like cryptography, optimization, and quantum simulation. As quantum technology advances, hybrid systems combining classical and quantum processors may become the standard for tackling complex, large-scale problems.

Below is a detailed comparison based on key aspects.

1. Fundamental Unit of Information

Aspect	Classical Computing	Quantum Computing
Unit of Information	Bit (000 or 111)	Qubit
Representation	Deterministic (definite state)	Probabilistic state
State	Fixed: 000 or 111	Superposed

2. Information Processing

Aspect	Classical Computing	Quantum Computing
Data Manipulation	Logical gates (AND, OR, NOT)	Quantum gates (Hadamard, CNOT, etc.), all unitary

Parallelism	Sequential or limited parallelism	Massive parallelism via superposition and entanglement
Interference	Not applicable	Exploits constructive and destructive interference to amplify correct solutions
Error Correction	Achieved through redundancy	Requires specialized quantum error correction (e.g., surface codes)

3. Computational Power

Aspect	Classical Computing	Quantum Computing
Speed	Efficient for most tasks	Exponentially faster for specific tasks (e.g., factoring with Shor's algorithm)
Problem Types	Best for deterministic, well-defined tasks	Suitable for problems involving large state spaces, optimization, or simulation
Algorithm Examples	Sorting, arithmetic operations, etc.	Quantum Fourier Transform, Grover's Search, Shor's Algorithm

4. Physical Principles

Aspect	Classical Computing	Quantum Computing
Underlying Physics	Follows classical mechanics	Based on quantum mechanics principles
Key Principles	Boolean logic, binary state manipulation	Superposition, entanglement, and quantum interference
Reversibility	Irreversible gates (e.g., NAND, AND)	All quantum gates are reversible (unitary)

6. Applications

Aspect	Classical Computing	Quantum Computing
Everyday Tasks	Suitable for tasks like word processing, browsing, etc.	Not practical for everyday use (yet)
Specialized Uses	Cryptography, simulations, AI, and ML	Cryptography (breaking RSA), quantum simulations, optimization problems
Advantage	General-purpose, robust, and scalable	Exponential speedup in specific areas (e.g., factoring, searching large datasets)

7. Limitations

Aspect	Classical Computing	Quantum Computing
Scalability	Scalable with improved hardware	Limited by qubit coherence and noise
Error Correction	Well-established	Complex and resource-intensive
Development	Fully developed and reliable	Experimental and prone to errors

Questions:

1. State the de Broglie hypothesis and derive the equation of de Broglie wavelength in terms of energy.

2. Show that the wavelength associated with an electron, accelerated by a potential difference of V volts, is given by h/√2meV.

3. Find the expression for de Broglie wavelength?

4. What is wave function Ψ? State the conditions for a "well behaved wave function".

5. Derive an expression for the Schrodinger Time Independent Wave Equation.

6. Derive an expression for the eigen energy of a particle enclosed in an infinite potential well (rigid box).

7. Define Quantum tunneling effect and explain tunneling of electron for particle in finite potential well (non- rigid box)

8. What is the tunneling effect?

9. Explain the working and principle of Scanning Tunneling Microscope with a neat diagram.

10. State De-Broglie's hypothesis. State the expressions for De Broglie wavelength in terms of 1) Velocity 2) Kinetic Energy.

11. Define operators. State the types of operators.

12. Explain qubit and quantum logic gates.

13. Compare classical computing and quantum computing.

Critical Thinking Questions:

<1> Consider two particles: **Particle A** is an electron with a kinetic energy of 150 eV and **Particle B** is a proton with the same kinetic energy (150 eV). Calculate the De Broglie wavelength for each particle. Discuss how the difference in their masses affects their wavelengths. If both particles were used in a double-slit experiment, which one would exhibit more noticeable diffraction patterns and why?

<2> Connect the abstract wave function to practical scenarios, such as the effect of external potentials.

<3> In nanoscale devices, such as transistors, quantum tunneling can lead to current leakage. What design considerations might engineers use to minimize tunneling effects in such devices?

<4> Explore potential real-world applications of hybrid computational models.

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