

UNIT-1

1. Failure of Classical Electromagnetic Theory

At the end of the 19th century, classical physics (Newtonian mechanics, Maxwell's electrodynamics, and classical thermodynamics) failed to account for phenomena occurring at atomic and subatomic scales:

- **Blackbody Radiation Spectrum:** Classical electrodynamics combined with the equipartition theorem (Rayleigh-Jeans Law) predicted that the energy density emitted by a blackbody tends to infinity at high frequencies: $u(\nu) d\nu = (8\pi\nu^2 / c^3) k_B T d\nu$. This catastrophic prediction at short wavelengths is known as the **Ultraviolet Catastrophe**.
- **Photoelectric Effect:** Classical wave theory predicts that energy is distributed continuously across a wavefront. Consequently, electron emission should involve a measurable time lag while absorbing energy, and kinetic energy should depend on light *intensity* rather than *frequency*—both contradicted by experiment.
- **Atomic Stability:** According to Maxwell's theory, an electron in a circular orbit experiences centripetal acceleration and must continuously radiate electromagnetic energy. The electron should lose energy, spiral inward, and collapse into the nucleus within $\sim 10^{-10}$ seconds.

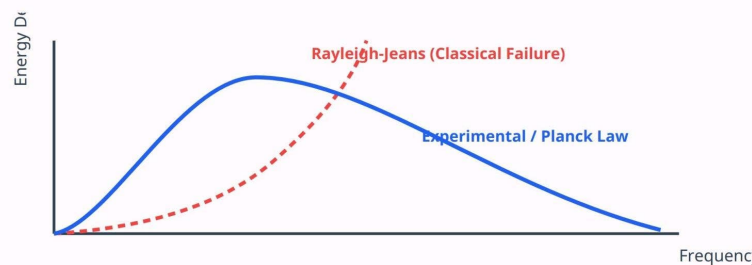


Figure 1.1: Comparison between Rayleigh-Jeans classical prediction and experimental blackbody spectrum.

2. Quantum Theory of Radiation (Old Quantum Theory)

In 1900, **Max Planck** resolved the blackbody spectrum anomaly by introducing the revolutionary hypothesis that atomic oscillators exchange energy with radiation only in discrete units (quanta).

Planck's Quantum Postulate

An oscillator of frequency ν can only possess energies given by integer multiples of a fundamental quantum:

$$E = n h \nu \quad (n = 0, 1, 2, 3, \dots)$$

where $h = 6.626 \times 10^{-34} \text{ J}\cdot\text{s}$ is Planck's constant.

Planck's Radiation Law Derivation Summary:

The average energy $\langle E \rangle$ of an oscillator in thermal equilibrium at temperature T is calculated using Boltzmann statistics:

$$\langle E \rangle = \sum_{n=0}^{\infty} (n h \nu e^{-n h \nu / k_B T}) / \sum_{n=0}^{\infty} (e^{-n h \nu / k_B T}) = (h \nu) / (e^{h \nu / k_B T} - 1)$$

Multiplying by the density of modes per unit volume in frequency range $[v, v+dv]$, $g(v)dv = (8\pi v^2 / c^3) dv$, yields Planck's formula:

$$u(v) dv = (8\pi h v^3 / c^3) \cdot [1 / (e^{h v / k_B T} - 1)] dv$$

3. Photon Concept

In 1905, **Albert Einstein** extended Planck's concept, proposing that light propagates as localized packets of energy called **photons**.

Property	Mathematical Expression / Value
Energy	$E = h\nu = \hbar\omega$ (where $\hbar = h / 2\pi$, $\omega = 2\pi\nu$)
Rest Mass	$m_0 = 0$
Momentum	$p = E / c = h\nu / c = h / \lambda$
Relativistic Energy	$E = \sqrt{(p^2 c^2 + m_0^2 c^4)} = pc$
Charge & Spin	Neutral (Charge = 0), Intrinsic Spin = $1 \hbar$ (Boson)

4. Photoelectric Effect & Einstein's Photoelectric Equation

The photoelectric effect is the emission of electrons from a metallic surface when irradiated by light of suitable frequency.

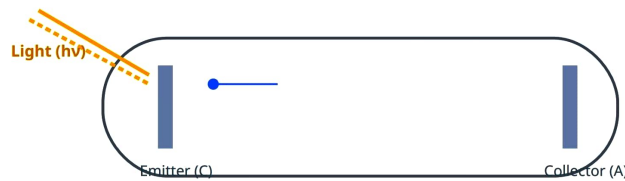


Figure 4.1: Schematic diagram of Photoelectric Effect experimental setup.

Derivation of Einstein's Photoelectric Equation

When a photon of energy $h\nu$ strikes an electron in the metal, the photon transfers its entire energy to the single electron in a 1-to-1 process:

1. Part of the energy is used to liberate the electron from the surface against binding forces: **Work Function (W_0 or ϕ)**.
2. The remaining energy imparts maximum kinetic energy (K_{max}) to the photoelectron.

By Conservation of Energy:

$$h\nu = W_0 + K_{max}$$

At the threshold frequency ν_0 , the incident photon has just enough energy to eject an electron with zero kinetic energy ($K_{max} = 0$):

$$W_0 = h\nu_0$$

Substituting Eq. (4.2) into Eq. (4.1):

$$K_{max} = \frac{1}{2} m v_{max}^2 = h(\nu - \nu_0)$$

If V_0 is the stopping potential (retarding voltage required to reduce photocurrent to zero), then $K_{max} = e V_0$:

$$e V_0 = h\nu - h\nu_0 \implies V_0 = (h/e) \nu - (W_0/e)$$

5. Compton Effect (Theory and Complete Derivation)

The **Compton Effect** is the phenomenon in which high-frequency X-rays or γ -ray photons scattered by stationary free electrons suffer an increase in wavelength (decrease in energy).

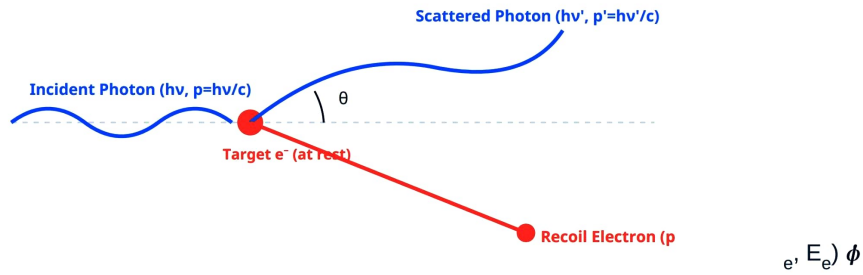


Figure 5.1: Geometry of Compton Scattering collision between photon and electron.

Step-by-Step Derivation of Compton Shift

Initial State (Before Collision):

- Incident Photon: Energy $E = h\nu$, Momentum $p = h\nu/c$
- Electron (at rest): Energy $E_e = m_0c^2$, Momentum $p_e = 0$

Final State (After Collision):

- Scattered Photon: Energy $E' = h\nu'$, Momentum $p' = h\nu'/c$ at angle θ
- Recoil Electron: Total Energy $E_e' = \sqrt{p_e'^2c^2 + m_0^2c^4}$, Momentum p_e at angle ϕ

1. Conservation of Total Relativistic Energy:

$$h\nu + m_0c^2 = h\nu' + E_e' \implies E_e' = h(\nu - \nu') + m_0c^2$$

Squaring both sides:

$$(E_e')^2 = h^2(\nu - \nu')^2 + m_0^2c^4 + 2h(\nu - \nu')m_0c^2$$

2. Conservation of Momentum:

- Along X-axis (incident direction):

$$(h\nu/c) = (h\nu'/c) \cos \theta + p_e \cos \phi \implies p_e c \cos \phi = h(\nu - \nu' \cos \theta)$$

- Along Y-axis (perpendicular):

$$0 = (h\nu'/c) \sin \theta - p_e \sin \phi \implies p_e c \sin \phi = h\nu' \sin \theta$$

Squaring and adding both momentum components:

$$p_e^2 c^2 (\cos^2 \phi + \sin^2 \phi) = h^2 [(v - v' \cos \theta)^2 + (v' \sin \theta)^2]$$

$$p_e^2 c^2 = h^2 [v^2 - 2vv' \cos \theta + v'^2 (\cos^2 \theta + \sin^2 \theta)] = h^2 [v^2 + v'^2 - 2vv' \cos \theta]$$

3. Relativistic Invariant Relation:

From relativistic energy-momentum relation: $(E_e')^2 - p_e^2 c^2 = m_0^2 c^4$. Substituting Eqs. (5.1) and (5.2):

$$h^2(v - v')^2 + m_0^2 c^4 + 2h(v - v')m_0 c^2 - h^2[v^2 + v'^2 - 2vv' \cos \theta] = m_0^2 c^4$$

Expanding $h^2(v - v')^2 = h^2(v^2 + v'^2 - 2vv')$ and cancelling $m_0^2 c^4$, $h^2 v^2$, $h^2 v'^2$:

$$-2h^2 vv' + 2h(v - v')m_0 c^2 = -2h^2 vv' \cos \theta$$

$$2h(v - v')m_0 c^2 = 2h^2 vv' (1 - \cos \theta)$$

Dividing both sides by $2 h m_0 c^2 v v'$:

$$(v - v') / (v v') = (h / m_0 c^2) (1 - \cos \theta) \implies (1 / v') - (1 / v) = (h / m_0 c^2) (1 - \cos \theta)$$

Since $\lambda = c / v$ and $\lambda' = c / v'$, multiplying by c gives the final **Compton Shift Formula**:

$$\Delta \lambda = \lambda' - \lambda = (h / m_0 c) (1 - \cos \theta)$$

Key Physical Results of Compton Effect

- **Compton Wavelength:** $\lambda_C = h / (m_0 c) = 0.02426 \text{ \AA} = 2.426 \times 10^{-12} \text{ m}$.
- **Maximum Shift ($\theta = 180^\circ$):** $\Delta \lambda_{\max} = 2 \lambda_C = 0.0485 \text{ \AA}$.
- **Unmodified Line ($\theta = 0^\circ$):** $\Delta \lambda = 0$ (No wavelength change in forward scattering).

6. Franck-Hertz Experiment

Performed by James Franck and Gustav Hertz in 1914, this experiment provided direct proof of discrete energy states in free atoms, validating Bohr's atomic model.

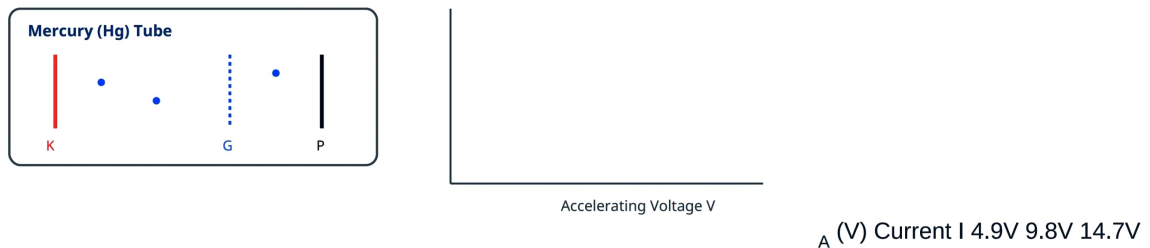


Figure 6.1: Franck-Hertz tube schematic and characteristic periodic current drop curve.

Experimental Mechanism:

- Electrons emitted from cathode K are accelerated toward grid G by voltage V_A . A small retarding voltage $V_R \approx 1.5 \text{ V}$ exists between grid G and collector P .

- When $E_k < 4.9 \text{ eV}$, collisions between electrons and Mercury atoms are **elastic**; electrons retain kinetic energy and reach plate P .
- When $V_A = 4.9 \text{ V}$, electron kinetic energy equals the first excitation energy of Mercury ($6^1S_0 \rightarrow 6^3P_1$). Collisions become **inelastic**, transferring energy to excite Hg atoms. The electrons lose energy and cannot overcome retarding potential V_R , causing a sharp drop in current.
- Periodic drops occur at integer multiples of 4.9 V (e.g., 9.8 V , 14.7 V), proving atomic excitation states are quantized.

7. Inadequacy of Old Quantum Theory

Although Old Quantum Theory (Planck, Einstein, Bohr, Sommerfeld) successfully explained specific isolated phenomena, it was ad-hoc and incomplete:

1. It combined classical mechanics equations with arbitrary quantization conditions (e.g., $\oint p dq = n h$) without an underlying foundational wave equation.
2. It failed to predict transition probabilities, spectral line intensities, or selection rules.
3. It could not be extended to multi-electron systems (even two-electron Helium atoms).
4. It could not explain fine structure features or the anomalous Zeeman effect.

8. de-Broglie Hypothesis (Wave-Particle Duality)

In 1924, **Louis de Broglie** proposed that matter exhibits dual wave-particle properties. Since radiation possesses wave-particle duality, symmetry in nature implies material particles must also possess associated "matter waves".

Derivation of de-Broglie Wavelength

For a photon: $E = h\nu$ and $E = mc^2 \Rightarrow mc^2 = h\nu \Rightarrow p = mc = h\nu / c = h / \lambda$.

Extending this momentum-wavelength relation to a material particle of mass m moving with velocity v :

$$\lambda = h / p = h / (m v)$$

de-Broglie Wavelength of an Electron Accelerated through Potential V :

Kinetic energy acquired $K = e V = p^2 / (2m) \Rightarrow p = \sqrt{2 m e V}$.

$$\lambda = h / \sqrt{2 m e V}$$

Substituting numerical values ($h = 6.626 \times 10^{-34} \text{ J}\cdot\text{s}$, $m = 9.1 \times 10^{-31} \text{ kg}$, $e = 1.6 \times 10^{-19} \text{ C}$):

$$\lambda = 12.27 / \sqrt{V} \text{ \AA} = \sqrt{(150 / V)} \text{ \AA}$$

9. Davisson and Germer Experiment

In 1927, C.J. Davisson and L.H. Germer provided direct experimental confirmation of de-Broglie matter waves by demonstrating electron diffraction from a Nickel crystal.

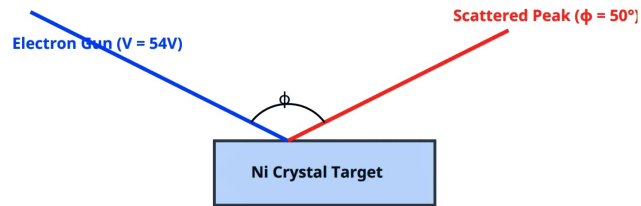


Figure 9.1: Davisson-Germer electron scattering experiment setup.

Quantitative Comparison:

A maximum in scattered electron intensity was observed at accelerating potential $V = 54 \text{ V}$ and scattering angle $\phi = 50^\circ$.

- **Bragg Angle (θ):** $\theta = 90^\circ - (\phi / 2) = 90^\circ - 25^\circ = 65^\circ$.
- **Experimental Wavelength (Bragg's Law for Nickel lattice spacing $d = 0.91 \text{ \AA}$, $n = 1$):**

$$\lambda = 2 d \sin \theta = 2 \times (0.91 \text{ \AA}) \times \sin 65^\circ = 1.65 \text{ \AA}$$

- **Theoretical Wavelength (de-Broglie Formula):**

$$\lambda = 12.27 / \sqrt{54} = 12.27 / 7.348 = 1.66 \text{ \AA}$$

The remarkable agreement ($1.65 \text{ \AA} \approx 1.66 \text{ \AA}$) unequivocally established the wave nature of electrons.

10. Phase Velocity and Group Velocity

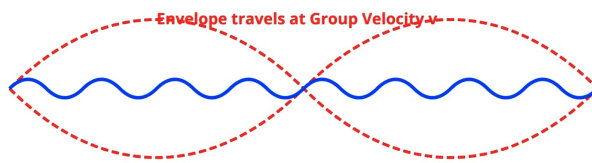
1. Definitions

- **Phase Velocity (v_p):** Velocity of propagation of individual monochromatic wave phases:

$$v_p = \omega / k$$

- **Group Velocity (v_g):** Velocity of the envelope of a wave packet formed by superposition of waves, representing energy/particle velocity:

$$v_g = d\omega / dk$$



_g Phase travels at v_p

Figure 10.1: Representation of a Wave Packet showing envelope and carrier phase wave.

Derivation of Rayleigh's Relation between v_g and v_p

Since $\omega = k v_p$:

$$v_g = d / dk (k v_p) = v_p + k (dv_p / dk)$$

Since $k = 2\pi / \lambda \Rightarrow dk = - (2\pi / \lambda^2) d\lambda \Rightarrow k / dk = - \lambda / d\lambda$:

$$v_g = v_p - \lambda (dv_p / d\lambda)$$

Proof that Particle Velocity Equals Group Velocity ($v_{particle} = v_g$)

For a relativistic particle of rest mass m_0 :

- $\omega = E / \hbar = \gamma m_0 c^2 / \hbar$
- $k = p / \hbar = \gamma m_0 v / \hbar$

Group velocity $v_g = d\omega / dk = dE / dp$.

Differentiating relativistic relation $E^2 = p^2 c^2 + m_0^2 c^4$ with respect to p :

$$2 E (dE / dp) = 2 p c^2 \implies v_g = dE / dp = p c^2 / E$$

Substituting $p = \gamma m_0 v$ and $E = \gamma m_0 c^2$:

$$v_g = (\gamma m_0 v c^2) / (\gamma m_0 c^2) = v$$

Conclusion: The group velocity of the de-Broglie wave packet exactly equals the particle velocity ($v_g = v$).

11. Heisenberg's Uncertainty Principle

Formulated by Werner Heisenberg in 1927: *It is fundamentally impossible to simultaneously measure both the exact position and exact momentum of a quantum mechanical particle.*

$$\Delta x \cdot \Delta p_x \geq \hbar / 2 \quad (\text{where } \hbar = h / 2\pi = 1.054 \times 10^{-34} \text{ J}\cdot\text{s})$$

Canonical Conjugate Relations:

1. **Position – Momentum:** $\Delta x \cdot \Delta p_x \geq \hbar / 2$
2. **Time – Energy:** $\Delta E \cdot \Delta t \geq \hbar / 2$
3. **Angular Position – Angular Momentum:** $\Delta L_z \cdot \Delta \theta \geq \hbar / 2$

12. Uncertainty Principle from de-Broglie Wave Packet

A quantum particle is represented by a wave packet formed by superposing plane waves over a range of wave vectors Δk :

$$\psi(x, t) = \int_{k_0 - \Delta k}^{k_0 + \Delta k} A(k) e^{i(kx - \omega t)} dk$$

From standard Fourier transform analysis of wave packets, spatial extension Δx and wavenumber spread Δk satisfy:

$$\Delta x \cdot \Delta k \approx 2\pi \quad (\text{or } \geq 1)$$

Using de-Broglie relation $p = \hbar k \implies \Delta p_x = \hbar \Delta k$:

$$\Delta x \cdot (\Delta p_x / \hbar) \geq 1 \implies \Delta x \cdot \Delta p_x \geq \hbar$$

Rigorous definition in terms of standard deviation yields $\Delta x \cdot \Delta p_x \geq \hbar / 2$.

13. Gamma-Ray Microscope Thought Experiment

Heisenberg proposed a thought experiment involving the measurement of an electron position using a hypothetical high-energy γ -ray microscope to illustrate the physical origin of uncertainty.

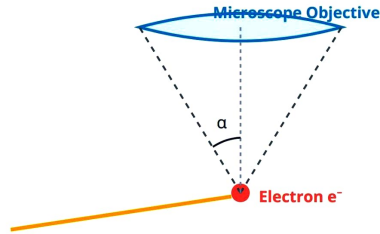


Figure 13.1: Heisenberg's Gamma-Ray Microscope thought experiment.

Mathematical Derivation:

Position Uncertainty (Δx):

By wave optics, the resolving limit of a microscope with semi-vertical angle α using light of wavelength λ is:

$$\Delta x = \lambda / (2 \sin \alpha)$$

Momentum Uncertainty (Δp_x):

To observe the electron, at least one scattered photon of initial momentum $p = h / \lambda$ must enter the microscope lens within the angle cone $-\alpha$ to $+\alpha$.

- Maximum X-momentum transferred to electron: $+(h / \lambda) \sin \alpha$
- Minimum X-momentum transferred to electron: $-(h / \lambda) \sin \alpha$

The uncertainty in electron recoil momentum along X-axis is:

$$\Delta p_x = (h / \lambda) \sin \alpha - [- (h / \lambda) \sin \alpha] = (2 h / \lambda) \sin \alpha$$

Product of Uncertainties:

$$\Delta x \cdot \Delta p_x = [\lambda / (2 \sin \alpha)] \cdot [(2 h / \lambda) \sin \alpha] = h$$

This demonstrates that the very act of measurement introduces a unavoidable quantum disturbance, confirming Heisenberg's principle.

Unit-2

1 Fundamental Postulates of Quantum Mechanics

Quantum mechanics replaces classical deterministic mechanics with a linear statistical state space built on complex Hilbert spaces. The physical framework is established through five fundamental postulates:

Postulate 1: System State Vector / Wave Function

The state of a quantum mechanical system at any time t is completely specified by a continuous, complex state function $\Psi(\mathbf{r}, t)$ residing in Hilbert space $\mathcal{H}$.

Postulate 2: Physical Observables and Linear Operators

Every physically measurable quantity A (e.g., position, momentum, energy) corresponds to a linear Hermitian operator $\hat{A}$ operating on the state space:

$$\text{Position Operator: } \hat{\mathbf{r}} = \mathbf{r}$$

$$\text{Linear Momentum Operator: } \hat{\mathbf{p}} = -i\hbar\nabla = -i\hbar\left(\hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}\right)$$

$$\text{Hamiltonian (Total Energy): } \hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}, t)$$

Postulate 3: Measurement Outcomes & Eigenvalues

The only possible outcomes of a measurement of an observable A are the real eigenvalues a_n obtained from the eigenvalue equation:

$$\hat{A}\psi_n(\mathbf{r}) = a_n\psi_n(\mathbf{r})$$

Postulate 4: Expectation Values (Ensemble Averages)

When a system is in a normalized state $\Psi(\mathbf{r}, t)$, the expectation value (average value over an ensemble of identical measurements) of observable A is:

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi^*(\mathbf{r}, t) \hat{A} \Psi(\mathbf{r}, t) d^3r$$

Postulate 5: Time Evolution of State

The time evolution of an undisturbed quantum state $\Psi(\mathbf{r}, t)$ is deterministically dictated by the

Time-Dependent Schrödinger Equation:

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

2 Properties and Physical Acceptability of Wave Functions

2.1 Born Interpretation of the Wave Function

In quantum mechanics, the wave function $\Psi(\mathbf{r}, t)$ is generally a complex-valued quantity and cannot be directly measured. Max Born (1926) proposed that the square of its absolute magnitude represents a **probability density**:

$$\rho(\mathbf{r}, t) = |\Psi(\mathbf{r}, t)|^2 = \Psi^*(\mathbf{r}, t) \Psi(\mathbf{r}, t)$$

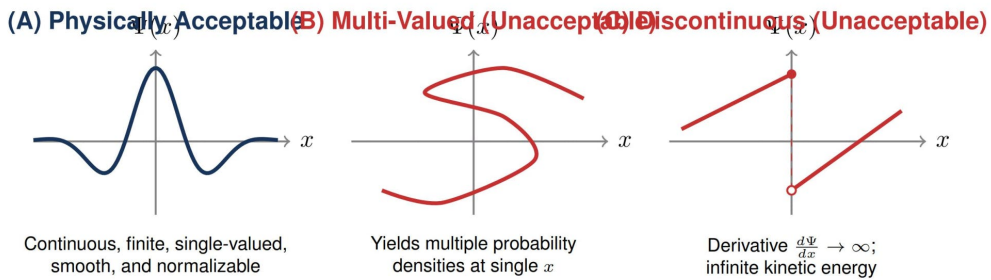
The quantity $dP = |\Psi(\mathbf{r}, t)|^2 d^3r$ represents the probability of locating the particle inside an infinitesimal volume element $d^3r = dx dy dz$ centered at position $\mathbf{r}$ at time t .

2.2 Conditions for Physical Acceptability

For $\Psi(\mathbf{r}, t)$ to yield meaningful physical probabilities, it must satisfy four strict mathematical criteria across its entire domain:

1. **Single-Valuedness:** At every spatial coordinate $\mathbf{r}$, $\Psi(\mathbf{r})$ must have exactly one value. Multi-valued wave functions would imply multiple distinct probability values at the exact same location, which is physically impossible.
2. **Continuity of Ψ and its Spatial Derivative $\nabla\Psi$:** Both $\Psi(\mathbf{r})$ and its first partial derivatives $\left(\frac{\partial\Psi}{\partial x}, \frac{\partial\Psi}{\partial y}, \frac{\partial\Psi}{\partial z}\right)$ must be continuous everywhere. Discontinuities in spatial derivatives would lead to infinite kinetic energy ($\hat{T} \propto \nabla^2$). *Exception:* $\frac{\partial\Psi}{\partial x}$ can have a kink only where potential $V(x)$ becomes infinite (e.g., infinite square well boundary or delta-function potential).
3. **Finiteness Everywhere:** $\Psi(\mathbf{r})$ must remain finite throughout space. If $\Psi \rightarrow \infty$ at any point, the probability density would be undefined at that point.
4. **Square Integrability (Normalizability):** The particle must exist somewhere in the universe. Hence, the integral over all space must equal unity:

$$\int_{-\infty}^{\infty} |\Psi(\mathbf{r}, t)|^2 d^3r = 1$$



3 Eigenvalues and Eigenfunctions

When a quantum operator $\hat{A}$ acts on a state function $\psi_n(x)$ yielding the function multiplied by a constant scalar a_n :

$$\hat{A}\psi_n(x) = a_n\psi_n(x)$$

$\psi_n(x)$ is defined as the **eigenfunction** of $\hat{A}$, and a_n is the corresponding **eigenvalue**.

3.1 Properties of Hermitian Operators

Physical observables are represented by Hermitian operators ($\hat{A} = \hat{A}^\dagger$). Hermitian operators possess two critical mathematical properties:

1. **Real Eigenvalues:** Every eigenvalue of a Hermitian operator is strictly real ($a_n \in \mathbb{R}$).
2. **Orthogonality of Eigenfunctions:** Eigenfunctions corresponding to distinct eigenvalues ($a_m \neq a_n$) are orthogonal:

$$\int_{-\infty}^{\infty} \psi_m^*(x) \psi_n(x) dx = \delta_{mn} = \begin{cases} 1 & \text{if } m = n \\ 0 & \text{if } m \neq n \end{cases}$$

4 Derivation of Time-Dependent and Time-Independent Schrödinger Equations

4.1 Derivation of Time-Dependent Schrödinger Equation (TDSE)

Consider a free particle of mass m moving in 1D with momentum p and total energy E . According to de Broglie's hypothesis, the matter wave is described by a plane wave function:

$$\Psi(x, t) = Ae^{i(kx - \omega t)} = Ae^{\frac{i}{\hbar}(px - Et)} \quad (1)$$

where $k = \frac{p}{\hbar}$ and $\omega = \frac{E}{\hbar}$.

Differentiating Equation (1) with respect to space x :

$$\frac{\partial \Psi}{\partial x} = \frac{\partial}{\partial x} \left[Ae^{\frac{i}{\hbar}(px - Et)} \right] = \frac{ip}{\hbar} \Psi(x, t)$$

Multiplying both sides by $-i\hbar$:

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

Differentiating twice with respect to x :

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{\partial}{\partial x} \left(\frac{ip}{\hbar} \Psi \right) = \left(\frac{ip}{\hbar} \right)^2 \Psi = -\frac{p^2}{\hbar^2} \Psi(x, t)$$

Multiplying by $-\frac{\hbar^2}{2m}$:

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

Next, differentiating Equation (1) with respect to time t :

$$\frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial t} \left[Ae^{\frac{i}{\hbar}(px - Et)} \right] = -\frac{iE}{\hbar} \Psi(x, t)$$

Multiplying both sides by $i\hbar$:

$$i\hbar \frac{\partial \Psi}{\partial t} = E\Psi(x, t) \implies \hat{E} = i\hbar \frac{\partial}{\partial t}$$

For a non-relativistic particle in a potential field $V(x, t)$, total energy is the sum of kinetic and potential energies:

$$E = \frac{p^2}{2m} + V(x, t)$$

Operating this total energy relation on the wave function $\Psi(x, t)$:

$$E\Psi(x, t) = \frac{p^2}{2m} \Psi(x, t) + V(x, t)\Psi(x, t)$$

Substituting the operator expressions derived above yields the **1D Time-Dependent Schrödinger Equation**:

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

In three dimensions ($\mathbf{r} = (x, y, z)$), replacing $\frac{\partial^2}{\partial x^2}$ with the Laplacian operator $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$:

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

4.2 Derivation of Time-Independent Schrödinger Equation (TISE)

If the potential energy function $V(\mathbf{r})$ is stationary (independent of time t), we apply the **method of separation of variables**:

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) \phi(t)$$

Substituting this product ansatz into the 3D Time-Dependent Schrödinger Equation:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} [\psi(\mathbf{r}) \phi(t)] &= -\frac{\hbar^2}{2m} \nabla^2 [\psi(\mathbf{r}) \phi(t)] + V(\mathbf{r}) \psi(\mathbf{r}) \phi(t) \\ i\hbar \psi(\mathbf{r}) \frac{d\phi(t)}{dt} &= -\frac{\hbar^2}{2m} \phi(t) \nabla^2 \psi(\mathbf{r}) + V(\mathbf{r}) \psi(\mathbf{r}) \phi(t) \end{aligned}$$

Dividing both sides by $\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) \phi(t)$:

$$\frac{i\hbar}{\phi(t)} \frac{d\phi(t)}{dt} = \frac{1}{\psi(\mathbf{r})} \left[-\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + V(\mathbf{r}) \psi(\mathbf{r}) \right]$$

The left side depends solely on t , while the right side depends solely on spatial coordinates $\mathbf{r}$. For this equation to hold universally, both sides must equal a common separation constant E (the energy eigenvalue):

1. Temporal Equation:

$$\frac{i\hbar}{\phi(t)} \frac{d\phi(t)}{dt} = E \implies \frac{d\phi(t)}{dt} = -\frac{iE}{\hbar} \phi(t)$$

Integrating gives the time-dependent phase factor:

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

2. Spatial Equation:

$$\frac{1}{\psi(\mathbf{r})} \left[-\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + V(\mathbf{r}) \psi(\mathbf{r}) \right] = E$$

Multiplying by $\psi(\mathbf{r})$ yields the **Time-Independent Schrödinger Equation (TISE)**:

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

The full time-dependent state for a stationary energy eigenstate is thus:

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) e^{-iEt/\hbar}$$

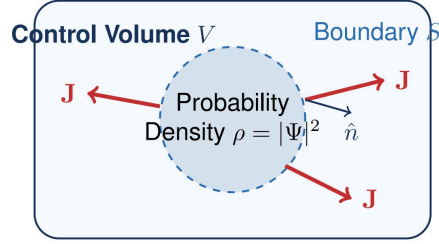
Notice that for stationary states, the probability density is time-invariant:

$$|\Psi(\mathbf{r}, t)|^2 = \left(\psi^*(\mathbf{r}) e^{iEt/\hbar} \right) \left(\psi(\mathbf{r}) e^{-iEt/\hbar} \right) = |\psi(\mathbf{r})|^2$$

5 Derivation of Probability Current Density (J)

Conservation of probability requires that any local change in probability density $\rho(\mathbf{r}, t) = |\Psi(\mathbf{r}, t)|^2$ within a volume element must equal the net flux of probability flowing through its bounding surface. This is governed by the **Continuity Equation**:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0$$



5.1 Step-by-Step Complete Derivation

Start by taking the partial time derivative of the probability density $\rho = \Psi^* \Psi$:

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial t}(\Psi^* \Psi) = \Psi^* \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t} \Psi \quad (2)$$

From the 3D Time-Dependent Schrödinger Equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi \implies \frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m} \nabla^2 \Psi - \frac{i}{\hbar} V\Psi$$

Taking the complex conjugate of TDSE (assuming real potential $V^* = V$):

$$-i\hbar \frac{\partial \Psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi^* + V\Psi^* \implies \frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m} \nabla^2 \Psi^* + \frac{i}{\hbar} V\Psi^*$$

Substitute $\frac{\partial \Psi}{\partial t}$ and $\frac{\partial \Psi^*}{\partial t}$ back into Equation (2):

$$\frac{\partial \rho}{\partial t} = \Psi^* \left(\frac{i\hbar}{2m} \nabla^2 \Psi - \frac{i}{\hbar} V\Psi \right) + \left(-\frac{i\hbar}{2m} \nabla^2 \Psi^* + \frac{i}{\hbar} V\Psi^* \right) \Psi$$

Expand terms:

$$\frac{\partial \rho}{\partial t} = \frac{i\hbar}{2m} \Psi^* \nabla^2 \Psi - \frac{i}{\hbar} V\Psi^* \Psi - \frac{i\hbar}{2m} \Psi \nabla^2 \Psi^* + \frac{i}{\hbar} V\Psi^* \Psi$$

Notice that the potential energy terms cancel exactly ($-\frac{i}{\hbar} V\Psi^* \Psi + \frac{i}{\hbar} V\Psi^* \Psi = 0$):

$$\frac{\partial \rho}{\partial t} = \frac{i\hbar}{2m} (\Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^*)$$

Using vector differential calculus identity: $\nabla \cdot (f \nabla g - g \nabla f) = f \nabla^2 g - g \nabla^2 f$, we rewrite the bracketed expression:

$$\frac{\partial \rho}{\partial t} = \frac{i\hbar}{2m} \nabla \cdot (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*)$$

Rearranging to match standard continuity equation $\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0$:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left[-\frac{i\hbar}{2m} (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) \right] = 0$$

Multiplying numerator and denominator inside bracket by i (since $-i = \frac{1}{i}$):

$$\mathbf{J} = \frac{\hbar}{2mi} (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) = \frac{\hbar}{m} \text{Im}(\Psi^* \nabla \Psi)$$

1D Form:

$$J_x = \frac{\hbar}{2mi} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right)$$

6 Expectation Values of Position and Linear Momentum

6.1 Expectation Value of Position $\langle x \rangle$

The expectation value of position for a normalized particle state in 1D is defined as:

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) x \Psi(x, t) dx$$

6.2 Expectation Value of Linear Momentum $\langle p_x \rangle$

To derive the momentum operator form, we compute the time derivative of $\langle x \rangle$:

$$\frac{d\langle x \rangle}{dt} = \frac{d}{dt} \int_{-\infty}^{\infty} \Psi^* x \Psi dx = \int_{-\infty}^{\infty} \left(\frac{\partial \Psi^*}{\partial t} x \Psi + \Psi^* x \frac{\partial \Psi}{\partial t} \right) dx$$

Substitute $\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V \Psi$ and $\frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V \Psi^*$:

$$\frac{d\langle x \rangle}{dt} = \int_{-\infty}^{\infty} \left[\left(-\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V \Psi^* \right) x \Psi + \Psi^* x \left(\frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V \Psi \right) \right] dx$$

The potential terms cancel ($V x \Psi^* \Psi - V x \Psi^* \Psi = 0$):

$$\frac{d\langle x \rangle}{dt} = \frac{i\hbar}{2m} \int_{-\infty}^{\infty} x \left(\Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \frac{\partial^2 \Psi^*}{\partial x^2} \Psi \right) dx$$

Integrating the second integral term $\int_{-\infty}^{\infty} x \frac{\partial^2 \Psi^*}{\partial x^2} \Psi dx$ by parts twice (using surface boundary conditions $\Psi, \frac{\partial \Psi}{\partial x} \rightarrow 0$ as $x \rightarrow \pm\infty$):

$$\int_{-\infty}^{\infty} x \frac{\partial^2 \Psi^*}{\partial x^2} \Psi dx = \int_{-\infty}^{\infty} \Psi^* \frac{\partial^2}{\partial x^2} (x \Psi) dx$$

Expanding $\frac{\partial^2}{\partial x^2} (x \Psi) = \frac{\partial}{\partial x} (\Psi + x \frac{\partial \Psi}{\partial x}) = 2 \frac{\partial \Psi}{\partial x} + x \frac{\partial^2 \Psi}{\partial x^2}$:

$$\frac{d\langle x \rangle}{dt} = \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \left(\Psi^* x \frac{\partial^2 \Psi}{\partial x^2} - \Psi^* \left[2 \frac{\partial \Psi}{\partial x} + x \frac{\partial^2 \Psi}{\partial x^2} \right] \right) dx$$

The $x \frac{\partial^2 \Psi}{\partial x^2}$ terms cancel:

$$\frac{d\langle x \rangle}{dt} = \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \left(-2 \Psi^* \frac{\partial \Psi}{\partial x} \right) dx = \frac{1}{m} \int_{-\infty}^{\infty} \Psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi dx$$

According to Ehrenfest's theorem, classical velocity relates to quantum expectation value by $\frac{d\langle x \rangle}{dt} = \frac{\langle p_x \rangle}{m}$. Multiplying by m :

$$\langle p_x \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi(x, t) dx$$

This rigorously establishes that the quantum mechanical position-space momentum operator is:

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

7 Summary of Key Operators and Formulas

Observable	Operator	Expectation Value Formula
Position (x)	$\hat{x} = x$	$\langle x \rangle = \int \Psi^* x \Psi dx$
Momentum (p_x)	$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$	$\langle p_x \rangle = \int \Psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi dx$
Kinetic Energy (T)	$\hat{T} = -\frac{\hbar^2}{2m} \nabla^2$	$\langle T \rangle = \int \Psi^* \left(-\frac{\hbar^2}{2m} \nabla^2 \right) \Psi d^3r$
Potential Energy (V)	$\hat{V} = V(\mathbf{r})$	$\langle V \rangle = \int \Psi^* V(\mathbf{r}) \Psi d^3r$
Total Energy (H)	$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V$	$\langle H \rangle = \int \Psi^* \hat{H} \Psi d^3r = E$

1. Core Postulates & Mathematical Properties

Normalization

The wave function $\Psi(x, t)$ completely specifies the quantum state of a particle. According to the Born statistical interpretation, $|\Psi(x, t)|^2 dx$ represents the probability of finding the particle in the infinitesimal interval between x and $x + dx$. Since the particle must exist somewhere in continuous space ($-\infty$ to $+\infty$), total probability is normalized to unity:

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

If an unnormalized state function $\phi(x)$ is given, a normalization constant A is determined via:

$$A = \left(\int_{-\infty}^{+\infty} |\phi(x)|^2 dx \right)^{-1/2}$$

Orthogonality

Two stationary quantum states $\psi_m(x)$ and $\psi_n(x)$ corresponding to non-degenerate energy eigenvalues ($E_m \neq E_n$) are mathematically **orthogonal** if their inner product vanishes:

$$\int_{-\infty}^{+\infty} \psi_m^*(x) \psi_n(x) dx = 0 \quad (m \neq n)$$

Combining normalization and orthogonality yields the **orthonormality relation**, expressed using the Kronecker delta δ_{mn} :

$$\int_{-\infty}^{+\infty} \psi_m^*(x) \psi_n(x) dx = \delta_{mn} = \{ 1 \text{ if } m = n; 0 \text{ if } m \neq n \}$$

Observables & Operators

Every physically measurable quantity (observable) corresponds to a linear **Hermitian operator** acting on the Hilbert space.

Observable	Operator Symbol	Mathematical Form (1D)
Position	$\hat{x}$	x
Linear Momentum	$\hat{p}_x$	$-i\hbar \partial/\partial x$
Total Energy (Hamiltonian)	H	$-(\hbar^2 / 2m) \partial^2/\partial x^2 + V(x)$

An operator $\hat{A}$ is defined as **Hermitian** if it obeys:

$$\int \psi_m^* (A \psi_n) dx = \int (A \psi_m)^* \psi_n dx$$

Hermitian operators guarantee two fundamental properties: (1) all physical measurement eigenvalues are strictly real numbers, and (2) eigenvectors belonging to distinct eigenvalues are mutually orthogonal.

2. Application: Free Particle in a 1D Infinite Potential Well

Consider a quantum particle of mass m trapped inside an infinitely deep 1D box of length L bounded between $x = 0$ and $x = L$.

POTENTIAL PROFILE $V(x)$

$$\begin{array}{ccccc}
 V(x) = \infty; & | & V(x) = 0 \text{ (Free Region)} & | & V(x) = \infty; \\
 \text{-----+-----+-----} & & & & \\
 x \leq 0 & | & 0 < x < L & | & x \geq L
 \end{array}$$

Because $V(x) = \infty$ outside the interval $(0, L)$, the probability density vanishes identically everywhere outside: $\psi(x) = 0$ for $x \leq 0$ and $x \geq L$.

Step 1: Solving the Time-Independent Schrödinger Equation (TISE)

Inside the box where $V(x) = 0$, the TISE reduces to:

$$-(\hbar^2 / 2m) (d^2 \psi / dx^2) = E \psi \implies (d^2 \psi / dx^2) + k^2 \psi = 0$$

where the wavenumber k is defined as $k = \sqrt{2mE} / \hbar$.

The general mathematical solution to this second-order ordinary differential equation is:

$$\psi(x) = A \sin(kx) + B \cos(kx)$$

Step 2: Applying Boundary Conditions

- **Boundary at $x = 0$:** Continuity requires $\psi(0) = 0$.

$$\psi(0) = A \sin(0) + B \cos(0) = 0 \implies B = 0.$$

Thus, $\psi(x) = A \sin(kx)$.

- **Boundary at $x = L$:** Continuity requires $\psi(L) = 0$.

$$\psi(L) = A \sin(kL) = 0.$$

To avoid the trivial solution ($A = 0$), we enforce:

$$kL = n\pi \implies k = n\pi / L \quad (n = 1, 2, 3, \dots)$$

Step 3: Quantization of Energy & Momentum

Equating the expressions for k yields the quantized energy eigenvalues E_n :

$$E_n = \hbar^2 k^2 / 2m = n^2 \pi^2 \hbar^2 / (2mL^2) = n^2 h^2 / (8mL^2) \quad (n = 1, 2, 3, \dots)$$

Similarly, the magnitude of the linear momentum inside the box is quantized as:

$$p_n = \hbar k = n \pi \hbar / L = n h / (2L)$$

Step 4: Eigenfunctions & Normalization

To evaluate constant A , integrate $|\psi_n(x)|^2$ across the box domain:

$$\int_0^L A^2 \sin^2(n\pi x / L) dx = A^2 (L / 2) = 1 \text{ \&implies; } A = \sqrt{2 / L}$$

Thus, the complete normalized **eigenfunctions** are:

$$\psi_n(x) = \sqrt{2 / L} \sin(n\pi x / L) \quad \text{for } 0 \leq x \leq L$$

3. Key Physical Features of the 1D Box Solution

1. Nodes & Anti-Nodes

Nodes: Points within the interior box region ($0 < x < L$) where wave amplitude and probability density vanish ($\psi_n(x) = 0$).

$$\sin(n\pi x / L) = 0 \text{ \&implies; } x = m L / n \quad (m = 1, 2, \dots, n - 1)$$

The n -th energy state has exactly $(n - 1)$ interior nodes.

- **Anti-Nodes:** Positions where wave magnitude reaches maximum value ($|\psi_n(x)| = \sqrt{2/L}$).

$$x = (2m - 1) L / (2n) \quad (m = 1, 2, \dots, n)$$

The n -th energy state has exactly n anti-nodes.

2. Zero-Point Energy (Ground State E_1)

The ground state corresponds to quantum number $n = 1$:

$$E_1 = h^2 / (8mL^2) > 0$$

Physical Consequence: The minimum kinetic energy cannot be zero ($E_1 \neq 0$). If $E = 0$, momentum uncertainty $\Delta p = 0$, which by Heisenberg's Uncertainty Principle ($\Delta x \cdot \Delta p \geq \hbar / 2$) would imply spatial extent $\Delta x = \infty$. This contradicts physical confinement inside box length L . Hence, quantum particles can never be completely at rest.

unit-3

1. NUCLEAR MASS, BINDING ENERGY, AND SYSTEMATICS

1.1 Nuclear Mass and Mass Defect

A nucleus consisting of Z protons and $N = A - Z$ neutrons has a total rest mass $M(Z,A)$. Experimentally, the mass of a bound nucleus is always less than the total mass of its free constituent nucleons. This mass difference is defined as the **mass defect** (Δm):

$$\Delta m = [Z m_p + (A - Z) m_n] - M(Z,A)$$

where $m_p = 1.007276 \text{ u}$ is the proton mass, $m_n = 1.008665 \text{ u}$ is the neutron mass, and u is the atomic mass unit ($1 \text{ u} = 931.5 \text{ MeV}/c^2$).

1.2 Binding Energy (BE) and Proof of Formula

By Einstein's mass-energy equivalence principle, the binding energy B is the energy liberated when free nucleons coalesce into a nucleus, or equivalently, the work required to completely disassemble a nucleus into constituent free nucleons:

$$B(Z,A) = \Delta m \cdot c^2 = [Z m_p + (A - Z) m_n - M(Z,A)] c^2$$

The **Binding Energy per Nucleon** (B/A) measures the relative stability of a nucleus:

$$B/A = \frac{1}{A} [Z m_p + (A - Z) m_n - M(Z,A)] c^2$$

1.3 Systematics of Binding Energy Curve

A plot of average binding energy per nucleon (B/A) against mass number (A) reveals critical characteristics of nuclear forces:

- **Saturation Property:** For mass numbers $40 < A < 120$, B/A remains remarkably constant at approximately **8.5 MeV/nucleon**. This indicates that a nucleon only interacts with its nearest neighbors (short-range saturated nuclear force).
- **Peak Stability:** The curve reaches a global maximum of **8.8 MeV/nucleon** around $A = 56$ (specifically ^{56}Fe and ^{62}Ni), making these the most stable isotopes.
- **Light Nuclei Behavior:** Light nuclei ($A < 20$) have lower B/A values due to a large fraction of nucleons occupying the surface, where they have fewer neighbors. Local peaks appear at $A = 4, 8, 12, 16$ (^4He , ^8Be , ^{12}C , ^{16}O), signifying exceptional stability of tight α -like cluster structures.
- **Heavy Nuclei Drop-off:** Beyond $A = 120$, B/A gradually decreases to $\sim 7.6 \text{ MeV}$ for Uranium ($A = 238$). This reduction is driven by increasing long-range Coulomb repulsion among protons ($\propto Z^2$).

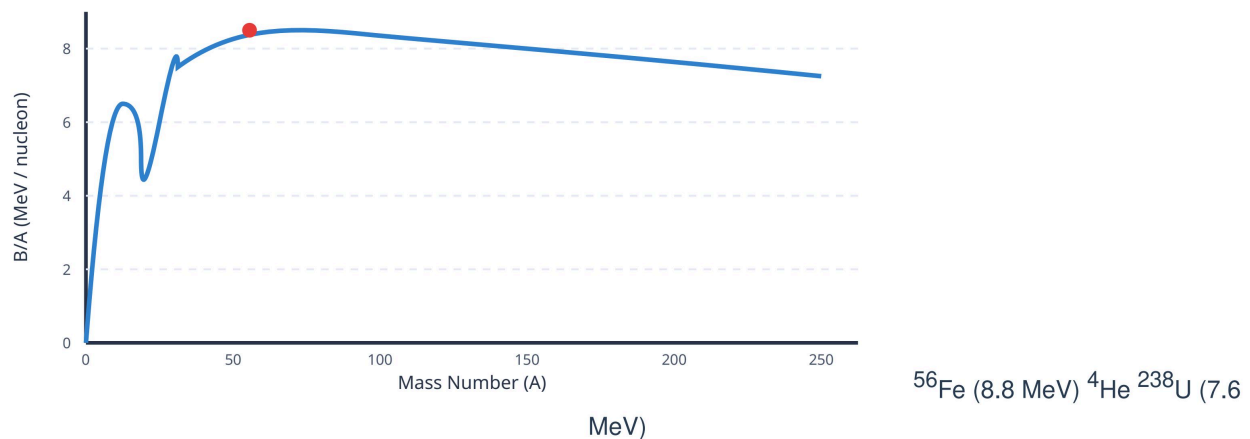


Figure 1.1: Binding Energy per Nucleon (B/A) vs Mass Number (A).

2. NUCLEAR STABILITY AND NUCLEAR SIZE

2.1 Nuclear Stability & The N-Z Valley of Stability

The stability of a nucleus depends on the balance between attractive strong nuclear forces among nucleons and repulsive electrostatic forces between protons.

- **Light Nuclei ($Z \leq 20$):** Stable nuclei lie along the line $N = Z$ (or $N/Z = 1$).
- **Heavy Nuclei ($Z > 20$):** As Z increases, electrostatic repulsion grows as $Z(Z-1)$. To remain bound, nuclei require additional neutrons to add attractive strong forces without adding charge. Thus, the ratio increases up to $N/Z \approx 1.5$ for Uranium.
- **Unstable Regions:** Nuclei above the stability band are neutron-rich and undergo β^- decay. Nuclei below are proton-rich and undergo β^+ decay or electron capture. Very heavy nuclei ($A > 210$) undergo α emission.

2.2 Nuclear Radius & Proof of Nuclear Density

DERIVATION: NUCLEAR RADIUS & DENSITY INDEPENDENCE

Scattering experiments demonstrate that nuclear matter volume V is directly proportional to the total mass number A :

$$V \propto A \implies \frac{4}{3}\pi R^3 = k A$$

Taking the cube root yields the fundamental nuclear radius formula:

$$R = R_0 A^{1/3}$$

where $R_0 \approx 1.2 \times 10^{-15} \text{ m} = 1.2 \text{ fm}$ is the empirical nuclear radius parameter.

To prove that nuclear matter density ρ is constant across all nuclei:

$$\rho = \frac{\text{Mass}}{\text{Volume}} \approx \frac{A \cdot m_u}{\frac{4}{3}\pi R^3} = \frac{A \cdot m_u}{\frac{4}{3}\pi (R_0 A^{1/3})^3} = \frac{m_u}{\frac{4}{3}\pi R_0^3}$$

Substituting $m_u = 1.66 \times 10^{-27} \text{ kg}$ and $R_0 = 1.2 \times 10^{-15} \text{ m}$:

$$\rho \approx \frac{1.66 \times 10^{-27} \text{ kg}}{\frac{4}{3}\pi (1.2 \times 10^{-15} \text{ m})^3} \approx 2.3 \times 10^{17} \text{ kg/m}^3$$

Conclusion: Nuclear matter density ρ is independent of mass number A and is extremely dense ($\sim 10^{14}$ times denser than normal matter).

3. SPIN, PARITY, STATISTICS & ELECTROMAGNETIC MOMENTS

3.1 Nuclear Spin (I) & Parity (π)

The total angular momentum of a nucleus, called **nuclear spin (I)**, is the vector combination of orbital angular momentum L and intrinsic spin angular momentum S of all constituent nucleons: $\mathbf{I} = \sum (\mathbf{L}_i + \mathbf{S}_i)$.

- **Even-Even Nuclei (Even Z , Even N):** Ground state spin is always $I = 0$ due to anti-parallel nucleon pairing.
- **Odd- A Nuclei:** Half-integer spin ($I = 1/2, 3/2, 5/2, \dots$).
- **Odd-Odd Nuclei:** Integer spin ($I = 1, 2, 3, \dots$).

Parity (π) describes the behavior of the nuclear wave function under spatial coordinate inversion ($\mathbf{r} \rightarrow -\mathbf{r}$). It is defined as $\pi = (-1)^I$, where I is the orbital quantum number.

3.2 Quantum Statistics

Nucleus Type	Total Spin (I)	Quantum Statistics	Wavefunction Exchange Symmetry
Even Mass Number (Even A)	Integer ($0, 1, 2, \dots$)	Bose-Einstein (BE)	Symmetric under exchange
Odd Mass Number (Odd A)	Half-Integer ($1/2, 3/2, \dots$)	Fermi-Dirac (FD)	Antisymmetric under exchange

3.3 Magnetic Dipole Moment (μ)

The magnetic dipole moment arises from intrinsic spins and orbital motion of charged nucleons. It is measured in **nuclear magnetons (μ_N)**:

$$\mu_N = \frac{e \hbar}{2 m_p} = 5.05078 \times 10^{-27} \text{ J/T}$$

3.4 Electric Quadrupole Moment (Q) and Shape Concept

The electric quadrupole moment measures the departure of the nuclear charge distribution from pure spherical symmetry:

$$Q = \frac{1}{2} e \int \rho(r) (3z^2 - r^2) dV$$

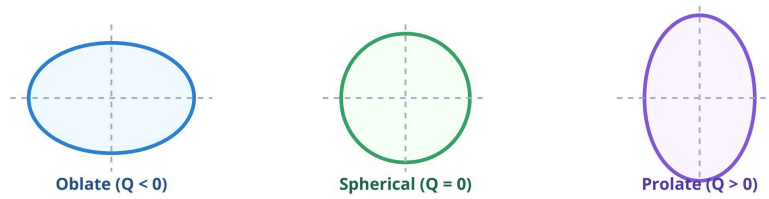


Figure 3.1: Nuclear shapes corresponding to Electric Quadrupole Moment (Q).

4. DETERMINATION OF NUCLEAR CHARGE & SIZE

4.1 Determination of Nuclear Charge by Moseley's Law

Henry Moseley systematically studied characteristic X-ray emission spectra (K_α lines) across various elements. He observed that the frequency ν of the emitted X-ray is directly linked to the atomic number Z :

$$\sqrt{\nu} = a(Z - b)$$

where a is a proportionality constant and $b \approx 1$ is the screening constant for K -shell transitions. This experiment proved that nuclear charge $Q = +Ze$ is the fundamental defining property of elements.

4.2 Determination of Nuclear Size by Rutherford Backscattering

PROOF: DISTANCE OF CLOSEST APPROACH (RUTHERFORD SCATTERING)

Consider an energetic α -particle (charge $q = +2e$, mass m) fired directly head-on (impact parameter $b = 0$) toward a heavy target nucleus (charge $Q = +Ze$).

As the α -particle approaches, it experiences repulsive Coulomb force and decelerates, momentarily coming to complete rest at a distance d (distance of closest approach) before rebounding at 180° .

By conservation of mechanical energy:

$$E_k \text{ (Initial Kinetic Energy)} = U \text{ (Electrostatic Potential Energy at } d\text{)}$$

$$\frac{1}{2} m v^2 = \frac{1}{4\pi\epsilon_0} \cdot \frac{(2e)(Ze)}{d}$$

Solving for the distance of closest approach d :

$$d = \frac{1}{4\pi\epsilon_0} \cdot \frac{2Ze^2}{E_k}$$

Because the α -particle does not penetrate the nuclear surface at standard decay energies, d provides an upper limit for the nuclear radius ($R < d$).

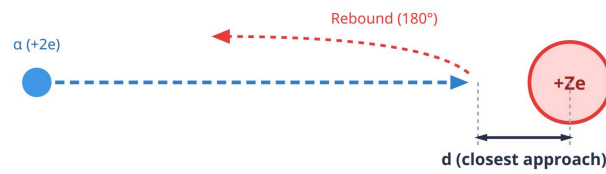


Figure 4.1: Rutherford backscattering head-on collision trajectory.

5. INTERACTION OF HEAVY CHARGED PARTICLES

5.1 Energy Loss Mechanics

When heavy charged particles (α -particles, protons) pass through matter, they lose energy primarily via **inelastic Coulomb collisions** with atomic electrons, causing ionization and atomic excitation.

5.2 Bethe-Bloch Formula (Qualitative Idea)

The linear stopping power $-dE/dx$ (energy loss per unit path length) for a heavy charged particle of charge ze and velocity v moving through a medium with atomic number Z and electron density n is given by:

$$-\frac{dE}{dx} = \frac{4\pi z^2 e^4 n}{m_e v^2} \left[\ln \left(\frac{2 m_e v^2}{I} \right) - \ln(1 - \beta^2) - \beta^2 \right]$$

where $\beta = v/c$ and I is the mean excitation potential of medium atoms.

KEY PHYSICAL INSIGHTS FROM BETHE FORMULA

- $-dE/dx \propto z^2$: Particles with higher charge lose energy dramatically faster.
- $-dE/dx \propto 1/v^2$: As the particle slows down, its rate of energy loss *increases*, culminating in a sharp ionization peak called the **Bragg Peak** near the end of its trajectory.

5.3 Range and Straggling

Range (R): The total mean thickness of matter traversed by a charged particle before coming to rest:

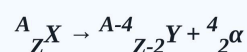
$$R = \int_0^{E_0} \left(-\frac{dE}{dx} \right)^{-1} dE$$

Straggling: Because energy loss occurs through stochastic discrete collisions, identical particles with identical initial energies exhibit small statistical fluctuations in total path length (**Range Straggling**) and final energy (**Energy Straggling**).

6. ALPHA DECAY ENERGISTICS & QUANTUM TUNNELING THEORY

6.1 Alpha Decay Energetics & Q-Value Proof

A parent nucleus undergoes spontaneous alpha disintegration via:



DERIVATION: KINETIC ENERGY OF ALPHA PARTICLE

The total decay energy (Q -value) is given by:

$$Q = [M_X - M_Y - M_\alpha] c^2$$

Assuming parent nucleus X is initially at rest, linear momentum conservation gives:

$$p_Y + p_\alpha = 0 \text{ \&implies; } |p_Y| = |p_\alpha| = p$$

The total energy released Q is split as kinetic energy between daughter Y and α -particle:

$$Q = K_Y + K_\alpha = \frac{p^2}{2 M_Y} + \frac{p^2}{2 M_\alpha} = K_\alpha \left(1 + \frac{M_\alpha}{M_Y} \right)$$

Approximating masses by mass numbers ($M_\alpha \approx 4$, $M_Y \approx A - 4$):

$$Q = K_\alpha \left(1 + \frac{4}{A - 4} \right) = K_\alpha \left(\frac{A}{A - 4} \right)$$

$$K_\alpha = \left(\frac{A - 4}{A} \right) Q$$

Conclusion: The alpha particle carries away most of the decay energy (~98% for heavy nuclei).

6.2 Gamow's Quantum Tunneling Theory of Alpha Decay

Classically, an α -particle inside a nucleus ($E \approx 4\text{--}9 \text{ MeV}$) cannot escape because it faces a potential barrier height of $V_C \approx 25\text{--}30 \text{ MeV}$. Gamow (and independently Gurney & Condon) solved this paradox using **quantum mechanical barrier tunneling**.

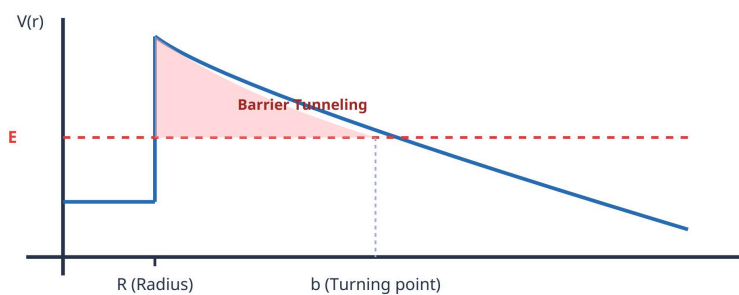


Figure 6.1: Gamow potential barrier and quantum tunneling of alpha particle.

The barrier transmission coefficient T evaluated using WKB approximation is:

$$T = \exp\left(-2 \int_R^b \gamma(r) dr\right) = \exp\left(-2 \int_R^b \frac{\sqrt{2m(V(r) - E)}}{\hbar} dr\right)$$

6.3 Geiger-Nuttall Law Proof

The **Geiger-Nuttall Law** is an empirical relationship connecting the decay constant λ of an α -emitter to the range R_α or energy E of the emitted α -particle:

$$\log_{10} \lambda = A \log_{10} R_\alpha + B \quad \text{or} \quad \log_{10} \lambda = C - \frac{D}{\sqrt{E}}$$

MATHEMATICAL DERIVATION FROM GAMOW THEORY

Decay constant is product of collision frequency ν and barrier transmission probability P :

$$\lambda = \nu \cdot P \approx \left(\frac{\nu}{2R} \right) \exp(-2G)$$

where Gamow factor G is obtained by integrating the barrier:

$$2G = \frac{2}{\hbar} \int_R^b \sqrt{2m \left(\frac{2Ze^2}{4\pi\epsilon_0 r} - E \right)} dr$$

Evaluating this integral yields:

$$2G \approx C_1 Z E^{-1/2} - C_2 Z^{1/2} R^{1/2}$$

Taking natural logarithm on both sides:

$$\ln \lambda = \ln \nu - C_1 Z E^{-1/2} + C_2 Z^{1/2} R^{1/2}$$

Converting to base-10 logarithm for a given isotope series (constant Z):

$$\log_{10} \lambda = C - \frac{D}{\sqrt{E}}$$

Since alpha range in air scales as $R_\alpha \propto E^{3/2}$ ($\log R_\alpha \propto \log E$), this directly proves the empirical relation:

$$\log_{10} \lambda = A \log_{10} R_\alpha + B$$

Unit-4

1. Beta Decay (β -Decay) & Energetics

1.1 Introduction to Beta Particles

Beta particles (β) are high-speed electrons (β^-) or positrons (β^+) emitted spontaneously by unstable atomic nuclei undergoing weak interaction decay to achieve optimal stability.

- **Rest Mass:** $m_e \approx 9.1 \times 10^{-31} \text{ kg}$ ($\approx 0.511 \text{ MeV}/c^2$)
- **Charge:** $-e$ for β^- , $+e$ for β^+
- **Ionization Power:** Significantly lower than α -particles ($\approx 1/100\text{th}$), resulting in greater penetration range in matter.

1.2 Origin of Continuous Beta Spectrum & Neutrino Hypothesis

Unlike α -decay where emitted particles possess discrete energy levels, measurements show that β -particles are emitted with a *continuous energy spectrum* ranging from zero up to a characteristic maximum endpoint kinetic energy (E_{max}).

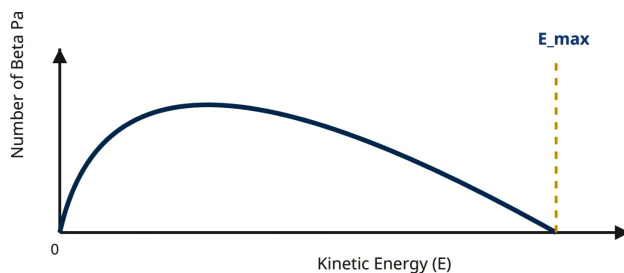


Figure 1.1: Continuous Kinetic Energy Spectrum of Beta Particles

PAULI'S NEUTRINO HYPOTHESIS (1930)

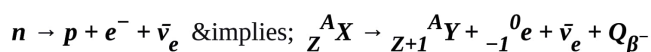
To resolve the apparent violation of energy, momentum, and angular momentum conservation in β -decay, Wolfgang Pauli postulated the simultaneous emission of a third neutral particle—the **neutrino** (ν) or **antineutrino** ($\bar{\nu}$).

- **Spin:** $1/2$ (Fermion) | **Charge:** 0 | **Rest Mass:** Extremely small (≈ 0)
- Total decay energy Q is shared continuously between the β -particle and the neutrino: $Q = E_\beta + E_\nu$. When $E_\nu \approx 0$, $E_\beta = E_{\text{max}}$.

1.3 Types of Beta Decay and Q -Value Derivations

1. Beta-Minus Decay (β^-)

A nuclear neutron converts into a proton, emitting an electron and an electron antineutrino:



Proof of Q -Value Formula (using neutral atomic masses):

Let $m_{\text{Nuc}}(Z, A)$ represent nuclear mass, and $M(Z, A)$ represent neutral atomic mass.

$$Q_{\beta^-} = [m_{Nuc}(Z, A) - (m_{Nuc}(Z+1, A) + m_e)] c^2$$

Expressing nuclear masses in terms of atomic masses (neglecting small electron binding energies):

$$m_{Nuc}(Z, A) = M(Z, A) - Z m_e$$

$$m_{Nuc}(Z+1, A) = M(Z+1, A) - (Z+1) m_e$$

Substituting into the energy balance equation:

$$Q_{\beta^-} = [(M(Z, A) - Z m_e) - (M(Z+1, A) - (Z+1)m_e + m_e)] c^2$$

$$Q_{\beta^-} = [M(Z, A) - M(Z+1, A)] c^2$$

2. Beta-Plus Decay (β^+)

A proton converts into a neutron, emitting a positron and an electron neutrino:

$$p \rightarrow n + e^+ + \nu_e \text{ \&imples; } {}^A_ZX \rightarrow {}^A_{Z-1}Y + {}^0_{+1}e + \nu_e + Q_{\beta^+}$$

Proof of Q-Value Formula:

$$Q_{\beta^+} = [m_{Nuc}(Z, A) - (m_{Nuc}(Z-1, A) + m_e)] c^2$$

Substituting atomic masses:

$$Q_{\beta^+} = [(M(Z, A) - Z m_e) - (M(Z-1, A) - (Z-1)m_e + m_e)] c^2$$

$$Q_{\beta^+} = [M(Z, A) - Z m_e - M(Z-1, A) + Z m_e - m_e] c^2$$

$$Q_{\beta^+} = [M(Z, A) - M(Z-1, A) - 2 m_e] c^2$$

3. Electron Capture (EC)

An inner orbital electron (K-shell) is captured by the nucleus:

$${}^A_ZX + {}^0_{-1}e \rightarrow {}^A_{Z-1}Y + \nu_e + Q_{EC}$$

$$Q_{EC} = [M(Z, A) - M(Z-1, A)] c^2 - B_e$$

(where B_e is the binding energy of the captured atomic electron)

2. Energy Loss & Absorption of Beta Particles

2.1 Mechanisms of Energy Loss

1. **Collisional Loss (Ionization & Excitation):** Inelastic Coulomb interactions with atomic electrons, governed by the Bethe-

Bloch relation: $(-dE/dx)_{coll} \propto n_e / v^2$.

2. **Radiative Loss (Bremsstrahlung):** Deceleration of energetic electrons in the strong electric field of target nuclei producing continuous X-radiation: $(-dE/dx)_{rad} \propto E \cdot Z^2$.

$$\text{Ratio: } -(dE/dx)_{rad} / -(dE/dx)_{coll} \approx (E \cdot Z) / 800 \text{ MeV}$$

2.2 Range and Absorption Law

Due to severe multiple scattering, electron trajectories are zigzag. The total penetration depth is defined as range **R**. For continuous β -spectrum, attenuation obeys an exponential empirical absorption law:

$$I = I_0 e^{-\mu x}$$

Feather's Empirical Relation for maximum range R_{max} (in g/cm²) for $E_{max} > 0.6 \text{ MeV}$:

$$R_{max} = 0.542 E_{max} - 0.133$$

3. Interaction of Gamma Rays with Matter

3.1 Nature and Primary Interaction Mechanisms

Gamma rays (γ) are high-energy photons ($E = h\nu$) emitted during nuclear transitions. They interact with matter via three main primary mechanisms depending on photon energy $h\nu$ and atomic number **Z**:

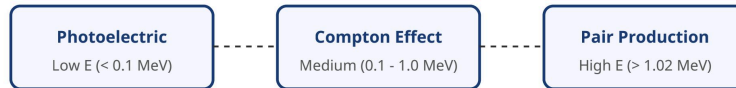


Figure 3.1: Dominant Regions of Gamma-Ray Interaction Mechanisms

3.2 Rigorous Proof of Compton Scattering Formula

Consider a photon of frequency ν colliding elastically with a stationary electron of rest mass m_0 . The scattered photon has frequency ν' at angle θ , and the recoil electron moves at angle ϕ .

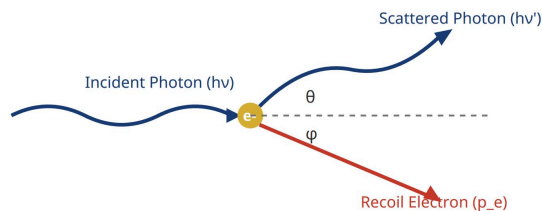


Figure 3.2: Geometry of Compton Scattering Interaction

Step 1: Conservation of Relativistic Energy

$$h\nu + m_0 c^2 = h\nu' + m c^2 \quad \&implies; \quad m c^2 = h(\nu - \nu') + m_0 c^2 \quad \text{--- (1)}$$

Step 2: Conservation of Momentum

- Along x-axis: $h\nu/c = (h\nu'/c) \cos\theta + p_e \cos\phi \quad \&implies; \quad p_e c \cos\phi = h\nu - h\nu' \cos\theta \quad \text{--- (2)}$

- Along y-axis: $0 = (hv'/c) \sin\theta - p_e \sin\phi$ & implies; $p_e c \sin\phi = hv' \sin\theta$ — (3)

Step 3: Eliminating Recoil Angle (ϕ)

Squaring and adding equations (2) and (3):

$$(p_e c)^2 (\cos^2\phi + \sin^2\phi) = (hv - hv' \cos\theta)^2 + (hv' \sin\theta)^2$$

$$p_e^2 c^2 = h^2 v^2 - 2h^2 v v' \cos\theta + h^2 v'^2 \cos^2\theta + h^2 v'^2 \sin^2\theta$$

$$p_e^2 c^2 = h^2 v^2 + h^2 v'^2 - 2h^2 v v' \cos\theta \quad \text{— (4)}$$

Step 4: Using Relativistic Energy-Momentum Relation

From relativistic dynamics: $E^2 = p^2 c^2 + m_0^2 c^4$ & implies; $m^2 c^4 = p_e^2 c^2 + m_0^2 c^4$ — (5)

Squaring Equation (1):

$$m^2 c^4 = [h(v - v') + m_0 c^2]^2 = h^2 (v - v')^2 + 2h(v - v') m_0 c^2 + m_0^2 c^4$$

$$m^2 c^4 = h^2 v^2 + h^2 v'^2 - 2h^2 v v' + 2h m_0 c^2 (v - v') + m_0^2 c^4 \quad \text{— (6)}$$

Equating (5) and (6) and substituting $p_e^2 c^2$ from (4):

$$h^2 v^2 + h^2 v'^2 - 2h^2 v v' \cos\theta + m_0^2 c^4 = h^2 v^2 + h^2 v'^2 - 2h^2 v v' + 2h m_0 c^2 (v - v') + m_0^2 c^4$$

Canceling common terms on both sides:

$$-2h^2 v v' \cos\theta = -2h^2 v v' + 2h m_0 c^2 (v - v')$$

$$2h^2 v v' (1 - \cos\theta) = 2h m_0 c^2 (v - v')$$

Dividing both sides by $2 h^2 c^2 v v'$:

$$(v - v') / (v v') = (h / m_0 c^2) (1 - \cos\theta) \quad \& \text{ implies; } 1/v' - 1/v = (h / m_0 c^2) (1 - \cos\theta)$$

Multiplying by velocity of light c (since $\lambda = c/v$):

$$\Delta\lambda = \lambda' - \lambda = (h / m_0 c) (1 - \cos\theta)$$

Where $\lambda_C = h / (m_0 c) \approx 0.02426 \text{ \AA}$ (or $2.426 \times 10^{-12} \text{ m}$) is the **Compton Wavelength**.

3.3 Pair Production and Electron-Positron Annihilation

- **Pair Production:** Photon energy converts directly into electron-positron pair in nuclear Coulomb field: $\gamma \rightarrow e^- + e^+$.

Threshold energy: $h\nu_{\min} = 2 m_0 c^2 = 1.02 \text{ MeV}$.

- **Positron Annihilation:** Thermalized positron meets electron, annihilating into two photons emitted back-to-back (180°) for momentum conservation: $e^- + e^+ \rightarrow \gamma_1 + \gamma_2$ ($E_\gamma = 0.511 \text{ MeV}$ each).

3.4 Attenuation Proof (Beer-Lambert Exponential Law)

Consider a narrow beam of photons with intensity I passing through an absorber layer of thickness dx . Reduction in intensity dI is proportional to I and dx :

$$dI = -\mu I dx \quad \& \text{ implies; } dI / I = -\mu dx$$

Integrating from $x = 0$ ($I = I_0$) to thickness x (I):

$\int_{I_0}^I \frac{dI}{I} = -\mu \int_0^x dx$ & implies; $\ln(I/I_0) = -\mu x$

$$I(x) = I_0 e^{-\mu x}$$

Mass Attenuation Coefficient: $\mu_m = \mu / \rho$ (expressed in cm^2/g), which is independent of the physical density ρ of the absorbing medium.

4. Nuclear Reactors

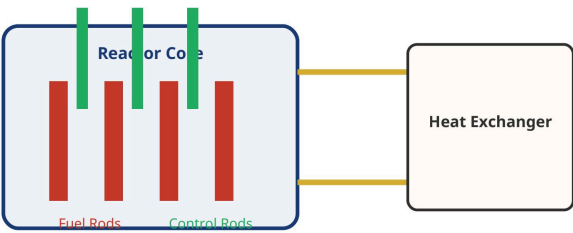


Figure 4.1: Schematic Core Layout of Nuclear Fission Power Reactor

4.1 Fission vs. Fusion Comparison

Parameter	Nuclear Fission Reactor	Nuclear Fusion Reactor (Tokamak)
Core Principle	Splitting heavy nucleus: $^{235}\text{U} + n \rightarrow F_1 + F_2 + 2.5n + 200\text{ MeV}$	Fusing light nuclei: $^2\text{H} + ^3\text{H} \rightarrow ^4\text{He} + n + 17.6\text{ MeV}$
Operating Condition	Thermal neutrons ($E \approx 0.025\text{ eV}$)	Ultra-high temperature plasma ($T \sim 10^8\text{ K}$)
Primary Fuel	Enriched Uranium (^{235}U), Plutonium (^{239}Pu)	Deuterium (^2H) and Tritium (^3H)
Multiplication Factor	Controlled via neutron absorption ($k = 1$)	Lawson criterion ($n \cdot \tau \cdot T$ Lawson limit)

4.2 Components of Fission Reactor

- **Fuel:** Fissile material (^{235}U).
- **Moderator:** Slows fast fission neutrons ($\sim 2\text{ MeV}$) to thermal energies ($\sim 0.025\text{ eV}$) via elastic collisions (e.g., Heavy Water D_2O , Graphite).
- **Control Rods:** Strong neutron absorbers (Cd, B) to maintain criticality factor $k = 1$.
- **Coolant:** Transfers thermal energy to heat exchanger (e.g., Liquid Sodium, Pressurized Water).

5. Gas-Filled Radiation Detectors

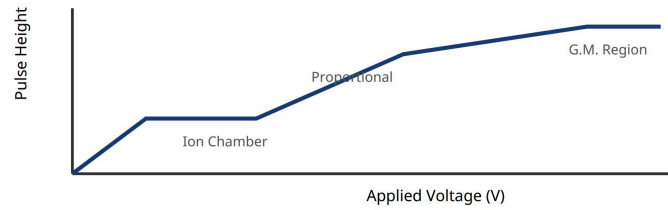


Figure 5.1: Collected Pulse Height vs Applied Voltage Operating Regions

5.1 Comparison of Detector Types

Feature	Ionization Chamber	Proportional Counter	Geiger-Müller (G.M.) Counter
Voltage Range	Low (100 – 300 V)	Medium (300 – 1000 V)	High (1000 – 1500 V)
Gas Amplification (M)	$M = 1$ (No multiplication)	$10^2 \leq M \leq 10^5$	$10^6 \leq M \leq 10^8$ (Avalanche discharge)
Output Pulse	Proportional to primary E	Proportional to primary E	Constant height (Independent of E)
Discrimination	Distinguishes α, β	Particle discrimination possible	Cannot distinguish particle type or energy

5.2 Detailed Study of Geiger-Müller (G.M.) Counter

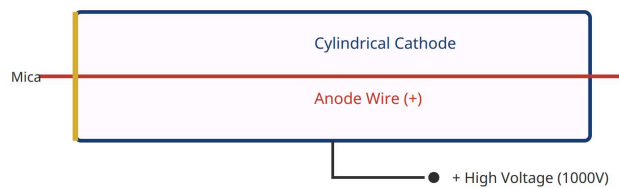


Figure 5.2: Structural Schematic of Geiger-Müller Counter Tube

Working Mechanism & Quenching

- Townsend Avalanche & Geiger Discharge:** Incident particle produces primary ion pairs in Argon gas ($\sim 90\%$). Extremely high electric field near central anode wire triggers massive secondary ionization cascade (Townsend avalanche) spreading along entire wire length via UV photon emission.
- Dead Time ($t_d \approx 100 \mu s$):** Slow-moving positive ion sheath (Ar^+) surrounds central wire, shielding electric field below threshold and rendering detector insensitive to subsequent incoming radiation.
- Quenching Mechanism:** To prevent continuous false discharge caused by secondary electron emission when Ar^+ strikes cathode wall, quenching gas (e.g., 10% Ethyl Alcohol or Halogen Br_2) is added. Alcohol molecules ($IP \approx 11.3 eV$) transfer charge from Argon ($IP \approx 15.8 eV$):

$$Ar^+ + Alcohol \rightarrow Ar + Alcohol^+$$

Neutralized alcohol ions dissociate safely upon reaching cathode without releasing secondary electrons.