PREFACE

In a bid to standardize higher education in the country, the University Grants Commission (UGC) has introduced Choice Based Credit System (CBCS) based on five types of courses viz. *core, discipline specific, generic elective, ability and skill enhancement* for graduate students of all programmes at Honours level. This brings in the semester pattern, which finds efficacy in sync with credit system, credit tranafer, comprehensive continuous assessments and a graded pattern of evaluation. The objective is to offer learners ample flexibility to choose from a wide gamut of courses, as also to provide them lateral mobility between various educational institutions in the country where they can carry their acquired credits. I am happy to note that the University has been recently accredited by National Assessment and Accreditation Council of India (NAAC) with grade "A".

UGC (Open and Distance Learning Programmes and Online Programmes) Regulations, 2020 have mandated compliance with CBCS for U. G. programmes for all the HEIs in this mode. Welcoming this paradigm shift in higher education, Netaji Subhas Open University (NSOU) has resolved to adopt CBCS from the academic session 2021-22 at the Under Graduate Degree Programme level. The present syllabus, framed in the spirit of syllabi recommended by UGC, lays due stress on all aspects envisaged in the curricular framework of the apex body on higher education. It will be imparted to learners over the six semesters of the Programme.

Self Learning Materials (SLMs) are the mainstay of Student Support Services (SSS) of an Open University. From a logistic point of view, NSOU has embarked upon CBCS presently with SLMs in English/Bengali. Eventually, the English version SLMs will be translated into Bengali too, for the benefit of learners. As always, all of our teaching faculties contributed in this process. In addition to this we have also requisitioned the services of best academics in each domain in preparation of the new SLMs. I am sure they will be of commendable academic support. We look forward to proactive feedback from all stakeholders who will participate in the teaching-learning based on these study materials. It has been a very challenging task well executed by the teachers, officers & staff of the University and I heartily congratulate all concerned in the preparation of these SLMs.

I wish you all a grand success.

Professor (Dr.) Ranjan Chakrabarti

Vice-Chancellor

Netaji Subhas Open University

Under Graduate Degree Programme

Choice Based Credit System (CBCS)

Subject : Honours in Physics (HPH)

Course Code : GE-PH-41

Course : Elements of Modern Physics

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: Course Writer :

Unit 1–4 Dr. Baibaswata Bhattacherjee

Unit 5–7 Dr. Gahul Amin
Associate Professor of Physics, NSOU

: Course Editor :

Dr. Gahul Amin
Associate Professor of Physics, NSOU

Dr. Malay Kumar Ghosh

: Format Editor :

Dr. Gahul Amin

Notification

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Unit - 1 ❑ Quantum N ature of Light

Structure

1.1 Objective

This chapter intends to impart knowledge to the students regarding the following topics :

- Planck's concept of quantum, Planck's constant and light as a collection of photons
- Black body radiation, Photoelectric effect and Compton scattering
- De Broglie wavelength and matter waves, Davisson-Germer experiment.

1.2 Introduction

By the end of the 19th centruy, the battle over the nature of light as a wave or a collection of particles seemed over. James Clerk Maxwell's synthesis of electric, magnetic and optical phenomena and the discover by Heinrich Hertz of electromagnetic waves were theoretical and experimental triumphs of the first order. Along with Newtonian mechanics and thermodynamics, Maxwell's electromagnetism took its place as a foundational element of physics. However, just when everthing seemed to be settled, a period of revolutionary change was ushered in at the beginning of the 20th century. A new interpretation of the emission of light by heated objects and new experimental methods that opened the atomic world for study led to a radical departure from the classical theories of Newton and Maxwell—quantum mechanics was born. Once again the question of the nature of light was reopened. The first two decades of the 20th century left the status of the nature of light confused. That light is a wave phenomenon was indisputable : there were countless examples of interference effects—the signature of waves—and a well-developed electromagnetic wave theory. However, there was also undeniable evidence that light consists of a collection of particles with well-defined energies and momenta. In 1923 the French physcist Louis de Broglie suggested that wave-particle duality is a feature common to light and all matter.

1.3 Planck's constant

Classical physics is dominated by two fundamental concepts. The first is the concept of a particle, a discrete entity with difinite position and momentum which moves in accordance with Newton's laws of motion. The second is the concept of an electromagnetic wave, an extended physical entity with a presence at every point in space that is provided by electric and magnetic fields which change in accordance with Maxwell's laws of electromagnetism. The classical world picture is neat and tidy : the laws of particle motion account for the material world around us and the laws of electromagnetic fields account for the light waves which illuminate this world. This classical picture began to crumble in 1900 when Max Planck published a theory of black-body radiation; i.e. a theory of thermal radiation in equilibrium with a perfectly absorbing body. Planck provided an explanation of the observed properties of black-body radiation by assuming that atoms emit and absorb discrete quanta of radiation with energy $\mathbf{E = h\nu}$, where ν is the frequency of the radiation and h is a fundamental constant of nature with value $\mathbf{h = 6.626 \times 10^{-34}\ Js}$. This constant is called Planck's constant.

Planck's constant has a strange role of linking wave-like and particle-like properties. In so doing it reveals that physics cannot be based on two distinct, unrelated concepts, the concept of a particle and the concept of a wave. These classical concepts, it seems, are at best approximate descriptions of reality.

1. Photons

Photons are particle-like quanta of electromagnetic radiation. They travel at the speed of light c with momentum p and energy E give by

$$p = \frac{h}{\lambda} \text{ and } E = \frac{hc}{\lambda} \qquad \dots (1)$$

where λ is the wavelength of the electromagnetic radiation. In comparison with macroscopic standards, the momentum and energy of a photon are tiny. For example, the momentum and energy of a visible photon with wave length $\lambda = 663$ mm are $p = 10^{-27}$ Js and $E = 3 \times 10^{-19}$ J. We note that an electronvolt, **1 eV = 1.602 × 10^{-19} J,** is a useful unit for the energy of a photon. Visible photons have energies of the order of an eV and X-ray photons have energies of the order of 10 keV.

The evidence for the existence of photons emerged during the early years of the twentieth century. In 1923 the evidence became compelling when A. H. Compton showed that the wavelength of an X-ray increases when it is scattered by an atomic electron. This effect, which is now called the Compton effect, can be understood by assuming that the scattering process is a photon-electron collision in which energy and momentum are conserved. Blackbody radiation and Photoelectric effect are the other experiments whose experimental results needed the concept of photon to be explained properly.

2. Black Body Radiation

A hot body emits thermal radiations which depend on composition and the temperature of the body. The ability of the body to radiate is closely related to its ability to absorb radiation. A Body which is capable of absorbing almost all the radiations incident on it is called a black body. A perfectly blackbody can absorb the entire radiations incident on it. Platinum black and Lamp black and absorb almost all the radiations incident on them.

Emissive power of a black body is defined as the total energy radiated per second from the unit surface area of a black body maintained at certain temperature.

Absorptive power of a black body is defined as the ratio of the total energy absorbed by the black body to the amount of radiant energy incident on it in a given time interval. The sbsorptive power of a perfectly black body is 1.

Spectral Distribution of energy in thermal radiation (Black Body radiation spectrum)

A good absorber of radiation is also a good emitter. Hence when a black-body is heated it emits radiations. In practice a black body can be realized with the emission of Ultraviolet. Visible and infrared wavelength on heating a body. German physicists Lammer and Pringsheim studied the energy density (U_λ) as a function of wavelength (λ) for different temperatures (T) of a black body using a spectrograph and a plot is made. This is called Black Body radiation spectrum.

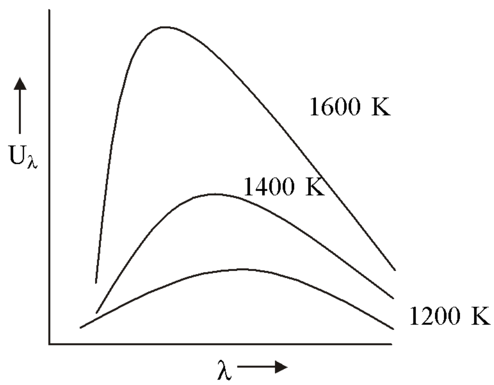


Figure 1.1 : Typical blackbody radiation spectra

The Salient features of black body radiation spectrum are as mentioned below :

1. Theoretically a black-body emits all wavelengths ranging from zero to infinity.
2. The energy density of blackbody radiation increases with wavelength then takes a msximum value U_m for a particular wavelength λ_m and then decrease to a value zero for longer wavelengths. Hence the Energy distribution in the spectrum is not uniform.
3. As the Temperature increases the wavelength (l_m) corresponding to the maximum emission energy (U_m) shifts towards shorter wavelength side. Thus the λ_m is inversely proportional to temperature (T) and is called

Wein's Displacement Law. Mathematically λ_m = **b/T**, Here b is Wein's Constant having value of 2.898 × 20^{-3} mk.

4. The total energy emitted by the black body at a given temperature is given by the area under the curve and is proportional to the fourth power of temperature. This is called Stefan's law of radiation. Mathematically **E = σ T⁴**, here σ is the Stefan's constant of value 5.67 × 10^{-8} Wm^2K^{-4}.

Explanation of Black Body Radiation Spectrum

Classical Theories

(1) Wein's Distribution Law : In the year 1893 Wein using thermodynamics showed that the energy emitted per unit volume in the wavelength range λ and λ + dλ can be expressed using the formula

$$U_\lambda d\lambda = \frac{C_1}{\lambda^5} e^{\frac{-C_2}{\lambda T}} d\lambda \qquad \ldots (2)$$

where C_1 and C_2 are empirical constants. A suitable selection for these constants helps to explain the experimental curve in the shorter wavelength region. The drawback of this law is if fails to explain the curve in the longer wavelength region. Also according to this equation the energy density at high temperatures tends to zero which contradicts experimental observations.

(2) Rayleigh-Jeand Law : British Physicists Lord Rayleigh and James made an attempt to explain the Black Body radiation spectrum Based on the concepts formation of standing electromagnetic waves and the law of equipartition of energy. According to this law the energy density of radiation is given by

$$U_\lambda d = \frac{8\pi kT}{\lambda^4} d \qquad \ldots (3)$$

where 'k' is Boltzmann constant with value 1.38 × 10^{-23} JK^{-1}. This law successfully explains the energy distribution of the black body radiation in the longer wavelength region. According to this law black body is expected to radiate large amount of energy in the shorter wavelength region thus leading to no energy available for emission in the longer wavelength region. Experimental observations show that the most of the emissions of the black body radiation occur in the visible and infrared regions. This discrepancy is called **Ultraviolet Catastrophe**.

Quantum theory of radiation

Planck's law of radiation : German physicist Max Plank successfully explained the energy distribution in the black body radiation based on the following assumptions :

(a) The surface of the black body contains oscillators

(b) These oscillators absorb or emit energy in terms of integral multiples of discrete packets called quanta or photons. The energy E of photons is proportional to the frequency v of the radiation. Mathematically **E = nhv**, where h is a constant called Planck's constant and its value is 6.625×10^{-34} Js, and n can take integral values.

(c) At thermal equilibrium the rate of absorption and emission of radiation are equal.

According to Planck's law of radiation the expression for energy density of radiation is given by

$$U_\lambda d = \frac{8\pi hc}{\lambda^5}\left(\frac{1}{e^{\frac{hc}{\lambda kT-1}}}\right)d \qquad \ldots (4)$$

where c is the velocity of light, k is Boltzmann constant and h is Planck's constant. This law explains the distribution of energy in the black body radiation spectrum completely for all wavelengths and at all temperatures. Also this law can be reduced to Wein's distribution law in the shorter wavelength region and to Rayleigh-Jeans law in the longer wavelength region.

Photo-Electric effect : The emission of electrons from the surface of certain materials when radiation of suitable frequency is incident on it is called the phenomenon of Photo-Electric effect. The electrons emitted are called photo electrons and the material is said to be photo sensitive. This was discovered in the 1887 by Henrich Hertz. This phenomenon cannot be explained using the existing theory of classical physics, Photoelectric effect signifies the particle nature of radiation.

The main characteristics of photo-electric effect are obtained experimentally and mentioned as below :

1. Photo electrons are emitted instantaneously as soon as the radiation is incident.
2. Photo electric emission occurs only if the frequency of the incident radiation is greater than a certain value called Threshold frequency.
3. The kinetic energy acquired by photo electrons is directly proportional to the frequency of the incident radiation and is imjdependent of the intensity.
4. The number of photoelectrons emitted depends on the intensity of the incident radiation and is independent of the frequency.

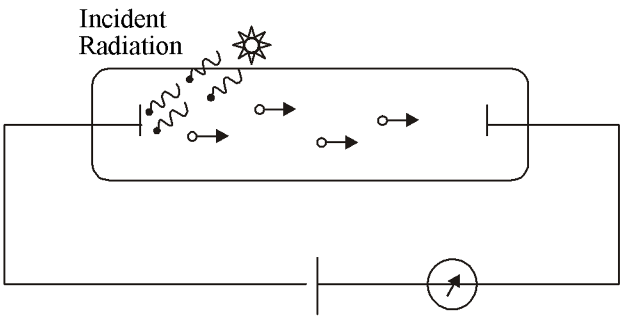


Figure 1.2 : Schematic diagram showing photo electric effect

Einstein's explanation of the photo electric effect

When metal is illuminated with radiation of suitable frequency, the photons of the radiation interact with electrons in the metal. When a photon interacts with an electron, the electron absorbs it and the photon vanishes. The energy acquired by the electron from the photon is made use in two statges. A part of the energy is used by the electron to free itself from the metal since it is bound within metal. Thus some minimum amount of energy is required for the electron just to escape from the metal is called Work Function (φ). The rest of the energy is carried by the clectron as Kinetic Energy (KE). Since the energy of the photon is hv the photoelectric satisfies the following equation

$$hv = \varphi = KE \qquad \text{... (5)}$$

This is called Photoelectric Equation. Here v is the frequency of the incident radition. Equation (5) can also be written in the form

$$hv = hv_0 + \frac{1}{2}mv^2 \qquad \text{... (6)}$$

where v_0 is the threshold frequency and v is the velocity of electron and m the mass. Thus from the photoelectric equation, if the frequency of the radiation $v < v_0$ no photoelectrons and emitted.

1.4 Millikan's Experiment for Verification of Einstein's Photo-electric Equation

The apparatus consists of an evacuated chamber C (Fig. 1.3). At the centre of the chamber drum D is kept which can rotate freely about a vertical axis. Four cylindrical blocks of different materials (sodium, potassium, lithium etc.) are fixed on the surface of the drum. K is a sharp knife edge which can scrap the surface of the metal. W is a quartz window through which monochromatic light of known frequency is allowed fo pass, F is a Faraday cylinder connected to a quadrant etc. trometer. With the help of a sensitive potential divider arrangement, suitable positive or negative potential can be applied to the drum with respect to the cylinder F.

Initially the surface of any one of the metal blocks is scraped with the knife edge K and then by rotating the drum D, the block is turned towards the window W.

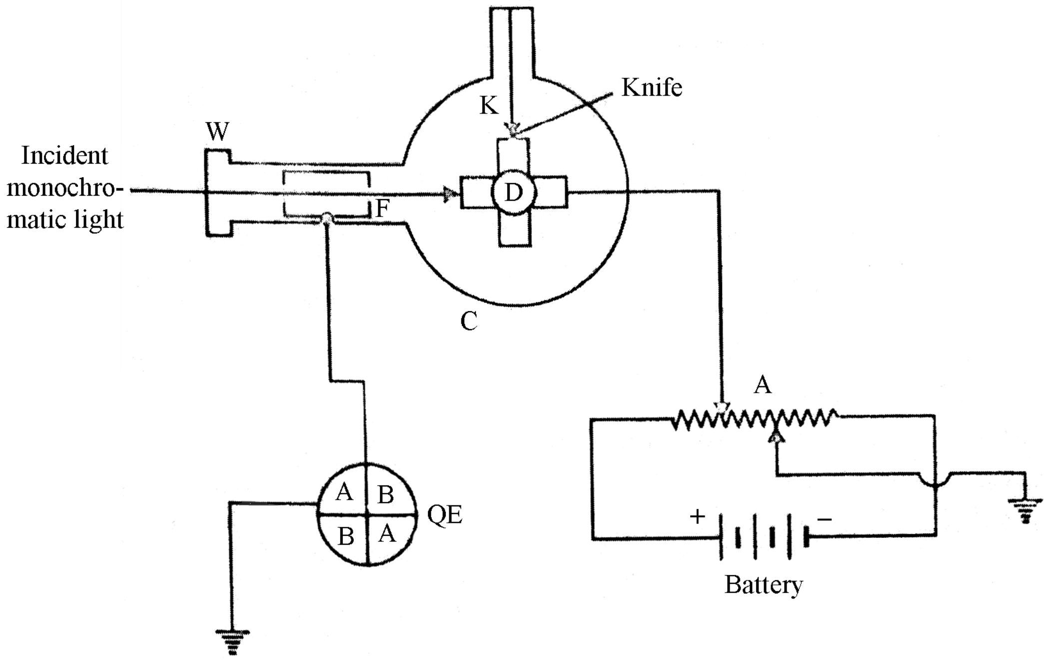


Figure 1.3

Allow monochromatic radiation of known frequency υ to be incident on the surface of the metal block. When the drum is kept at a negative potential with respect to the cylinder F, the photo-electrons ejected from the surface are accelerated towards the cylinder and the quadrant electrometer records the deflection. When a small positive potential is applied to the drum, only the fast moving electrons reach

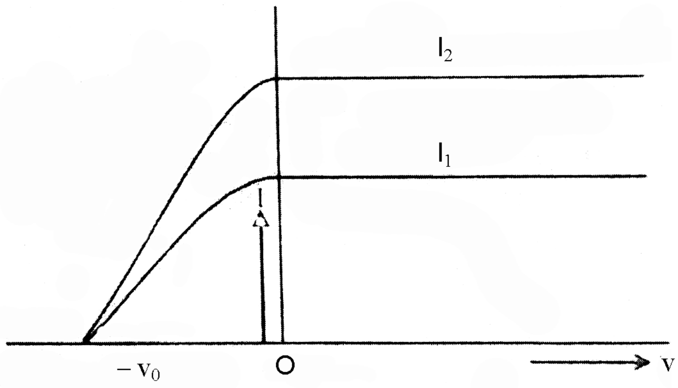


Figure 1.4

the cylinder F, the deflection in the electrometer decreases. Now, the positive potential of the drum is gradually increased till the deflection in the quadrant electrometer is zero. At this stage no photoelectron reaches the cylinder. This particular potential V_0 is called the stopping potential. Even when the intensity of light is increased for the same frequency, the deflection remains zero for the same stopping potential V_0. **It means that the stopping potential V_0 is the same and is independent of the intensity of incident light**. The experiment is repeated for different frequencies for the same metal. It is found that the stopping potential V_0 increases with increase in frequency for a given metal. According to Einstein's photo-electric equations

$$hv - \phi = \frac{1}{2}m\upsilon^2$$

Here $$\phi = hv_0$$

$\therefore$ $$hv = hv_0 = \frac{1}{2}m\upsilon^2$$

Also $$ev_0 = \frac{1}{2}m\upsilon^2$$

$$hv - hv_0 = eV_0$$

$$V_0 = \frac{h}{v}[v - v_0]$$

The experiment is repeated for different metals and graphs are drawn between frequency υ along the X-axis and the stopping potential V_0 along y-axis. The graph is a straight line (Fig 1.5). A straight line graph is obtained in all cases and this is agreement with Einstein's theory.

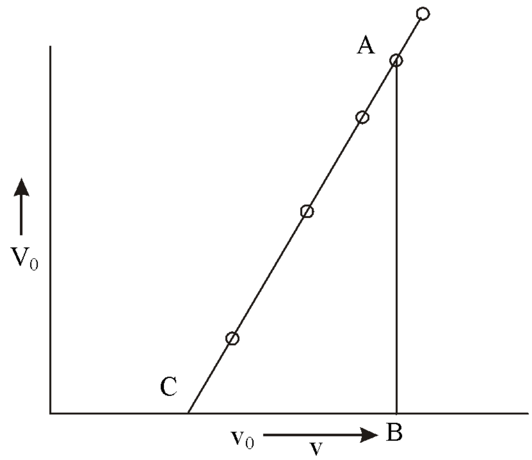


Figure 1.5

Determination of Planck's Constant

As discussed earlier, the stopping potentials of a particular metal are determined for different frequencies. A graph plotted between frequency υ along the X-axis and stopping potential υ_0 along the X-axis. Take a point A on the graph and measure υ_0. Draw AB parallel of Y-axis. The point B gives the value of υ. The graph meets the X-axis and X-axis at the point C corresponding to the threshold frequency υ_0. The slope of the graph

$$= \frac{AB}{BC} = \left(\frac{V_0}{\upsilon - \upsilon_0}\right)$$

But $$V_0 = \frac{h}{e}[\upsilon - \upsilon_0]$$

$$h = e\left[\frac{V_0}{\upsilon - \upsilon_0}\right]$$

$$h = e \text{ [slope of the graph]}$$

Here e is the charge of the electron and it is equal to 1.6×10^{-19} C. Hence the value of Plan constant h can be determined. The value of h was found to be $[6.624 \pm 0.01] \times 10^{-34}$ J–s. This is in agreement with the value determined by other methods.

Problem 1. What is the threshold wavelength for a tungsten surface whose work function 4.5 eV. [Delhi (Hons.)]

Solution. Here $\phi = 4.5$ eV

$= 4.5 \times 1.6 \times 10^{-19}$ Joule

Bur $\phi = h\nu_0$

$$\phi = \frac{hc}{\lambda_0}$$

$$\lambda_0 = \frac{hc}{\phi}$$

Here $h = 6.6 \times 10^{-34}$ Joule-second

$c = 3 \times 10^8$ m/s

$$\therefore \quad \lambda_0 = \frac{6.6 \times 10^{-34} \times 3 \times 10^8}{4.5 \times 1.6 \times 10^{-19}}$$

$$\lambda_0 = 9.640 \times 10^{-7} \text{ m}$$

$\lambda_0 =$ **9640 Å**

Problem 2. A photoelectric surface has a work function of 4 eV. What is the maximum velocity of the photoelectrons emitted by light of frequency 10^{15} hertz incident on the surface

$h = 6.6 \times 10^{-34}$ Joule-second

$e = 1.6 \times 10^{-19}$ Coulomb

$m = 9 \times 10^{-31}$ g

Solution. Here $\phi = 4$ ev

$= 4 \times 1.6 \times 10^{-16}$ Joule

$= 6.4 \times 10^{-19}$ Joule

$$\frac{1}{2}m\upsilon^2 = h\upsilon - \phi = 6.6 \times 10^{-34} \times 10^{-15} - 6.5 \times 10^{-19}$$

$$\frac{1}{2}m\upsilon^2 = 0.2 \times 10^{-19}$$

$$\upsilon = \sqrt{\frac{0.4\times10^{-19}}{m}} = \sqrt{\frac{0.4\times10^{-19}}{9\times10^{-31}}}$$

$$\upsilon = \mathbf{2.107 \times 10^5\ m/s.}$$

Problem 3. Calculate the energy in electron-volts of the photoelectrons from the surface of a tungsten emitter when it is iradiated with light of wavelength 1800 Å, given that the threshold wavelength for photoelectric emission in this case is 2300 Å. [Delhi (Hons.) 1981]

Solution. $E = h(\upsilon - \upsilon_0)$

$$E = hc\left[\frac{1}{\lambda} - \frac{1}{\lambda_0}\right] = hc\left[\frac{\lambda_0 - \lambda}{\lambda\lambda_0}\right]$$

Here $h = 6.6 \times 10^{-34}$ J-s

$c = 3 \times 10^8$ m/s

$\lambda = 1800$ Å $= 18 \times 10^{-18}$ m

$\lambda = 2300$ Å $= 23 \times 10^{-8}$ m

$$E = 6.6 \times 10^{-34} \times 2 \times 10^8 \left[\frac{5\times10^{-8}}{18\times10^{-8}\times23\times10^{-8}}\right]$$

$$E = \frac{6.6\times10^{-34}\times3\times10^8\times5}{18\times23\times10^{-18}}$$

$$E = 2.4 \times 10^{-19} \text{ Joule}$$

But $1\text{eV} = 1.6 \times 10^{-19}$ Joule

or $$1 \text{ Joule} = \frac{1}{1.6\times10^{-19}}\text{eV}$$

$\therefore$ $$E = \frac{2.4\times10^{-19}}{1.6\times10^{-19}} = 1.5 \text{ eV}$$

Hence the energy of each photoelectron emitted from the sufrace is 1.5 eV.

Problem 4. Calculate the longest wavelength of the incident radiation which well eject electrons from a metal work function of 6 electron volts. Planck's constaht $h = 6.624 \times 10^{-34}$ joule second. [Delhi 1982]

Solution. Here, work function $\phi = h\upsilon_0$ electron volts

$$= 6 \times 1.6 \times 10^{-19} \text{ joule}$$

$$u_0 = \frac{6\times1.6\times10^{-19}}{h} = \frac{6\times1.6\times10^{-19}}{6.624\times10^{-34}} \text{ hertz}$$

$$\lambda_0 = \frac{c}{\upsilon_0} = \frac{3\times10^{8}\times6.624\times10^{-34}}{6\times1.6\times10^{-19}}$$

$$\lambda = 2.07 \times 10^{-7} \text{ m} = \mathbf{2070\ Å.}$$

Problem 5. Calculate the threshold frequency and the corresponding wavelength of radiation incident on a certain metal whose work function is 3×10^{-19} J. Given, Planck's constant $= 6.62 \times 10^{-34}$ J-s. [Delhi (Sub) 1985]

Solution. Here, work function

$$\phi = h\upsilon_0 = 3.31 \times 10^{-19} \text{ J}$$

$$h = 6.62 \times 10^{-34} \text{ J-s}$$

$$\upsilon_0 = \frac{\phi}{h} = \frac{3.31\times10^{-19}}{6.62\times10^{-34}}$$

$$= 5 \times 10^{14} \text{ hertz}$$

$$\lambda_0 = \frac{c}{v_0} = \frac{3\times10^{8}}{5\times10^{14}} = 6\times10^{-7} \text{ m}$$

$$= \mathbf{6000\ Å}$$

Problem 6. Light of wavelength 4300 Å is incident on (a) nickel surface of work function 5 electron volts and (b) a potassium surface of work function 2.3 electron volts. Find out, if electrons will be emitted, and if so, the maximum velocity of the emitted electrons in each case. [Delhi 1985]

Solution. (a) For the nickel surface

$$\phi = h\upsilon_0 \text{ electron volts}$$

$$= 5 \times 1.6 \times 10^{-19} \text{ Joule}$$

$$\upsilon_0 = \frac{\phi}{h} = \frac{5 \times 1.6 \times 10^{-19}}{6.624 \times 10^{-34}} \text{ hertz}$$

$$\lambda_0 = \frac{c}{v_0} = \frac{3 \times 10^8 \times 6.624 \times 10^{-34}}{8 \times 10^{-19}}$$

$$= 2484 \times 10^{10} \text{ m}$$

$$= \mathbf{2484 \ Å}$$

As λ_0 is less than the wavelength of the incident radiation, (λ = 4300 Å), electrons will not be emitted.

(b) For the potassium surface,

$$\phi = 2.3 \text{ electrons volts}$$

$$= 2.3 \times 1.6 \times 10^{-19} \text{ joule}$$

$$l_0 = \frac{ch}{\phi}$$

$$= \frac{3 \times 10^8 \times 6.624 \times 10^{-34}}{2.3 \times 1.6 \times 10^{-19}}$$

$$= 4389 \times 10^{-10} \text{ m}$$

$$= \mathbf{4389 \ Å.}$$

As λ_0 is greater than l electrons will be emitted. Let the maximum velocity of the ejected electrons be υ_0

$$\frac{1}{2}m\upsilon^2 = h\upsilon - h\upsilon_0$$

$$= hc\left[\frac{1}{\lambda} - \frac{1}{\lambda_0}\right]$$

$$\frac{1}{2}m\upsilon^2 = \frac{hc(\lambda_0 - \lambda)}{\lambda\lambda_0}$$

$$\upsilon = \left[\frac{2hc(\lambda_0 - \lambda)}{m\lambda\lambda_0}\right]^{\frac{1}{2}}$$

$$\upsilon = \left[\frac{2\times6.624\times10^{-34}\times3\times10^{8}\times89\times10^{-10}}{9.1\times10^{-31}\times4300\times10^{-10}\times4389\times10^{-10}}\right]$$

$$\upsilon = \mathbf{1.423 \times 10^{5}\ m/s.}$$

Problem 7. The wavelength of the photoelectric threshold for silver is 3250 Å. Determine the maximum energy if the ejected electrons from a silver surface by light of wavelength 2537 Å. [I.A.S. 1983]

Solution. $U = h(u - u_0)$

$$U = hc\left[\frac{1}{\lambda}-\frac{1}{\lambda_0}\right]=\left[\frac{\lambda_0-\lambda}{\lambda\times\lambda_0}\right]$$

Here $h = 6.6 \times 10^{-34}$ J-s and $c = 3 \times 10^{-8}$ m/s

$\lambda = 2537$ Å $= 2537 \times 10^{-10}$ m

$\lambda_0 = 3250$ Å $= 3250 \times 10^{-10}$ m

$$U = 6.6 \times 10^{-34}\times3 \times 10^{8}\left[\frac{3250\times10^{-10}-2537\times10^{-10}}{3250\times10^{-10}\times2537\times10^{-10}}\right]$$

$$U = \mathbf{1.625 \times 10^{-19}\ J}$$

Problem 8. A surface having work function 1.51 eV is illuminated by light of wavelength 4000 Å. Calculate (i) the maximum kinetic energy of the ejected electrons and (ii) the stopping potential. [I.A.S.]

Solution. Here $\phi_0 = 1.51$ ev

$= 1.51 \times 1.6 \times 10^{-19}$ J

$= 2.416 \times 10^{-19}$ J

$\lambda = 4000$ Å $= 4 \times 10^{-7}$ m

$$v = \frac{c}{\lambda}=\frac{3\times10^{8}}{4\times10^{-7}}=7.5\times10^{14}\ \text{Hz}$$

(i) $$h\upsilon - \phi_0 = \frac{1}{2}m\upsilon^2 = U$$

$U = 6.624 \times 10^{-34} \times 7.5 \times 10^{14} - 2.416 \times 10^{-19}$

$U = 4.968 \times 10^{-19} - 2.416 \times 10^{-19}$

$U = 2.552 \times 10^{-19}$ J

$$U = \frac{2.552\times10^{-19}}{1.6\times10^{-19}}\ \text{eV}$$

$$U = 1.595\ \text{eV}$$

(ii) Also $h\upsilon - \phi_0 = e\upsilon = U$

stopping potential $V = \dfrac{U}{e}$

$$V = \frac{2.552\times10^{-19}}{1.6\times10^{-19}}$$

$$V = \mathbf{1.595\ volts.}$$

Problem 9. The stopping potential for the electrons emitted from a metal due to photoelectric effect is found to be 1 V for light of 2500 Å. Calculate the work function of the metal in eV.

Solution. Here $V = 1$ Volt

$\lambda = 25000$ Å $= 2.5 \times 10^{-7}$ m

$$\upsilon = \frac{c}{\lambda} = \frac{3\times10^{8}}{2.5\times10^{-7}}$$

or $\upsilon = 1.2 \times 10^{15}$ Hz

$\phi = ?$

$e = 1.6 \times 10^{-19}$ C

$h\upsilon = \phi = eV$

$$\phi = h\upsilon - eV$$

$$= 6.624 \times 10^{-34} \times 1.2 \times 10^{15} - 1.6 \times 10^{-19} \times 1$$

$$= 7.9488 \times 10^{-19} - 1.6 \times 10^{-19}$$

$$= 6.3488 \times 10^{-19}\ \text{J}$$

$$= \frac{6.3488\times10^{-19}}{1.6\times10^{-19}}\ \text{eV}$$

$$= \mathbf{3.968\ eV.}$$

Problem 10. The photoelectric threshold wavelength for Tungsten is 2300 Å. Find the energy in eV of the emitted electrons from the surface by ultraviolet light of wavelength 1800 Å. [Delhi, 1990]

Solution. $E = h(\upsilon - \upsilon_0)$

$$E = hc\left[\frac{1}{\lambda} - \frac{1}{\lambda_0}\right]$$

$$E = hc\left[\frac{\lambda_0 - \lambda}{\lambda\lambda_0}\right]$$

Here $h = 6.6 \times 10^{-34}$ J-s

$c = 3 \times 10^8$ ms/

$\lambda = 1800$ Å $= 1800 \times 10^{-10}$ m $= 18 \times 10^{-8}$ m

$\lambda_0 = 2300$ Å $= 2300 \times 10^{-10}$ m $= 23 \times 10^{-8}$ m

$$E = 6.6 \times 10^{-34} \times 3 \times 10^8 \left[\frac{23\times10^{-8} - 18\times10^{-8}}{18\times10^{-8}\times23\times10^{-8}}\right]$$

$$E = \frac{6.6\times10^{-34}\times3\times10^{8}\times5}{18\times23\times10^{8}}$$

$$E = 2.4 \times 10^{-19} \text{ J}$$

But $1 \text{ eV} = 1.6 \times 10^{-19}$ J

or $$1 \text{ J} = \left(\frac{1}{1.6\times10^{-19}}\right)\text{eV}$$

$$E = \frac{2.4\times10^{-19}}{1.6\times10^{-19}}$$

$E =$ **1.5 eV**

Hence, the energy of each photoelectron emitted from the surface is **1.5 eV**.

Problem 11. Calculate the energy of a photon having the same momentum as that of 10 MeV proton. [Osmania, 1992]

Solution. Mass of proton, $m = 1.67 \times 10^{-27}$ kg

Energy of proton, $U = \frac{1}{2}m\upsilon^2 = 10^7 \times 1.6\times10^{-19}$ J

$$U = 1.6 \times 10^{-12} \text{ J}$$

$$\upsilon = \left[\frac{2U}{m}\right]^{\frac{1}{2}}$$

$$\text{Momentum, } p = m\upsilon = m\left[\frac{2U}{m}\right]^{\frac{1}{2}}$$

$$p = [2mU]^{\frac{1}{2}}$$

$$\text{Energy of photon, } E = pc = [2mU]^{\frac{1}{2}}$$

$$E = \left[2\times1.67\times10^{-27}\times1.6\times10^{-12}\right]^{\frac{1}{2}}\times3\times10^{8}\text{ J}$$

$$E = \mathbf{21.9 \times 10^{-12}\ J}$$

$$E = \frac{21.9\times10^{-12}}{1.6\times10^{-19}} = \mathbf{13.69 \times 10^{7}\ eV.}$$

Problem 12. The wavelength of light falling on the surface of a metal of work function 2.3 eV is 4300Å. With what velocity will the electron be emitte.

[Delhi (Hons.) 1992]

Solution. Here

$$m = 9.1 \times 10^{-31}\text{ kg}$$

$$\phi = 2.3\text{ eV}$$

$$= 2.3 \times 1.6 \times 10^{-19}\text{ J}$$

$$= \mathbf{3.68 \times 10^{-19}\ J}$$

$$\lambda = 4300\text{ Å} = 4.3 \times 10^{-17}\text{ m}$$

$$\frac{1}{2}m\upsilon^2 = h\upsilon - \phi = \left(\frac{hc}{\lambda}\right) - \phi$$

$$= \left(\frac{6.624\times10^{-34}\times3\times10^{8}}{4.3\times10^{-7}}\right) - 3.86\times10^{-19}$$

$$= 4.62 \times 10^{-19} - 3.68 \times 10^{-19}$$

$$= 0.94 \times 10^{-19}\text{ J}$$

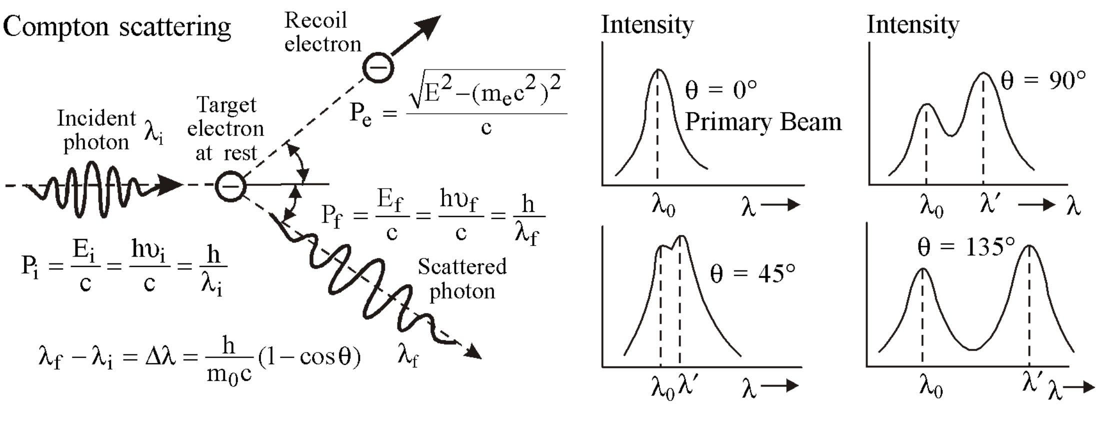
$$\upsilon = \left[\frac{2\times0.94\times10^{-19}}{m}\right]^{\frac{1}{2}} = \left[\frac{2\times0.94\times10^{-19}}{9.1\times10^{-31}}\right]^{\frac{1}{2}}$$

$$\upsilon = \mathbf{4.55 \times 10^{5}\ m/s.}$$

1.5 Compton Effect

The phenomenon of scattering of X-rays from suitable material and hence increase in its wavelength is called Compton Effect. When X-rays are incident on certain materials they are scattered and the scattered X-rays contain two components. One component has the same wavelength as the incident x-ray and the other with wavelength greater than the incident X-rays. This is due to the scattering X-ray photons from the electrons present in the material. Due to the transfer of energy from X-ray photon to electron the wavelength of X-ray increases and the electron recoils. This can be treated as collision between two particles. Thus Compton Effect signifies particle nature of radiation. The change in wavelength which is also called Compton Shift is given by

$$\Delta\lambda = \lambda_1 - \lambda = \frac{h}{m_0 c}(1-\cos\theta) \qquad \dots (7)$$



(a) (b)

Figure 1.6 : (a) Schematic representation of Compton scattering (b) Compton shift

Considering the elastic collide between a photon and an electron, the following is the derivation :

$h\nu_0$: energy of photon

$p_i = \frac{h\nu_0}{c}$

momentum of the photon

$p_i = pf\cos\Theta + p_e\cos\phi$ (1)

(conservation of momentum in x direction)

$0 = p_f\sin\Theta + p_e\sin\phi$ (2)

(conservation of momentum in x direction)

$$p_e^2 = p_e^2(\cos^2\phi + \sin^2\phi)$$

$$= (p_i - p_f\cos\Theta)^2 + p_f^2\sin^2\Theta$$

$$= p_i^2 + p_f^2 - 2p_i p_f\cos\Theta$$

$$hv_0 + m_0c^2 = hv + \sqrt{\left(m_0^2c^4 + p_e^2c^2\right)}$$

$$m_0^2c^4 + p_e^2c^2 = (hv_0 - hv + m_0c^2)^2$$

$$= (hv_0 - hv)^2 + m_0^2c^4 + 2m_0c^2(hv_0 - hv)$$

$$p_e^2c^2 = (hv_0 - hv)^2 + 2m_0c^2(hv_0 - hv)$$

$$p_i^2c^2 + p_f^2c^2 - 2p_ip_f\cos\Theta c^2 = (hv_0 - hv)^2 + 2m_0c^2(hv_0 - hv)$$

$$hvv_0(1-\cos\Theta) = m_0c^2(v_0 - v)$$

$$\therefore\ \lambda_s - \lambda_0 = \frac{h}{m_0c}(1-\cos\Theta)$$

Therefore, above is the Compton effect equation and $\frac{h}{m_0c} \equiv \lambda_c$ is Compton wavelength of an electron.

Difference between Compton Effect and Photoelectric Effect

Compton effect	Photoelectric effect
This is the effect caused by the inelastic scattering of high-energy photons that are bound to free electrons.	This is the effect caused by the weakly bound electrons that are ejected from the surface of the material when electromagnetic radiation interacts with the electrons.

Compton effect	Photoelectric effect
The energy associated with the recoil electrons falls in the mid-energy range.	The energy associated with the emitted electrons fall in the low-energy range.
The wavelength of the scattered photon is higher than that of the incident photon.	The wavelength is not observed as the photon disappears after interacting with the electrons.
Arthur Compton explained the effect.	Albert Einstein explained the effect.

1.6 Energy of recoil electron

Direction of Recoil electron. Dividing Eq. (5) by Eq. (4), we get

$$\tan\phi = \frac{h\nu'\sin\theta}{h(\nu - \nu'\cos\theta)} = \frac{\nu'\sin\theta}{(\nu - \nu'\cos\theta)} \quad \text{... (12)}$$

Using Eq. (10), we get

$$\frac{1}{\nu'} = \frac{1}{\nu} + \frac{h}{m_0c^2}(1-\cos\theta) = \frac{1}{\nu} + \frac{h}{m_0c^2}.2\sin^2\frac{\theta}{2}$$

or, $$\nu' = \frac{\nu}{1+\left(\frac{h\nu}{m_0c^2}\right)2\sin^2\frac{\theta}{2}} = \frac{\nu}{1+2\beta\sin^2\left(\frac{\theta}{2}\right)} \text{ where } \beta = \frac{h\nu}{m_0c^2} \quad \text{... (13)}$$

Substituting this value of ν' in Eq. (12), we get

$$\tan\phi = \frac{\nu\sin\theta/\left[1+2\beta\sin^2\left(\frac{\theta}{2}\right)\right]}{\left[\nu - \left\{\nu\cos\theta/\left(1+2\beta\sin^2\frac{\theta}{2}\right)\right\}\right]} = \frac{\cot\left(\frac{\theta}{2}\right)}{(1+\beta)}$$

$$\therefore \quad \tan\phi = \frac{\cot\left(\frac{\theta}{2}\right)}{1+\left(\frac{h\nu}{m_0c^2}\right)} \quad \text{... (14)}$$

Kinetic Energy of Recoil electron. The K. E. of recoil electron is the difference between the nergies of incident and scattered photons, i.e.

$$K.E. = hv - hv'$$

$$K.E. = hv - h\left[\frac{v}{1+2\beta\sin^2(\theta/2)}\right] = hv\left[\frac{2\beta\sin^2(\theta/2)}{1+2\beta\sin^2(\theta/2)}\right] \quad \text{... (15)}$$

where $\beta = hv/\ m_0c^2$

Problem 1. X-rays of wavelength 0.7080 Å are scattered from a carbon block through a angle of 90° and are analysed with a calcite crystal, the interplanar distance of whose reflecting planers is 3.13 Å. Determine the angular separation, in the first order, between the modified and the unmodified rays.

Sol. Wavelength of the modified rays = $\lambda' = \lambda + \frac{h}{m_0c}(1-\cos\theta)$

$$= 0.7080 \times 10^{-10}\ m + \left(\frac{6.63\times10^{-34}}{9.11\times10^{-31}\times3\times10^{8}}\right) m = 0.7323\ Å$$

Let θ and θ' be the angles of Bragg reflections corresponding to the wavelengths λ and λ'. Then, for n = 1 (first order),

$$2d\sin\theta = n\lambda = 0.7080 \times 10^{-10}\ m$$

and $$2d\sin\theta' = n\lambda' = 0.7323 \times 10^{-10}\ m.$$

Here, $d = 3.13 \times 10^{-10}$ m; $\therefore\ \theta = 6°30'$ and $\theta' = 6°\ 43'$.

$\therefore$ $\left.\begin{array}{l}\text{The angular separation, in the first order,}\\ \text{between the modified and un modified rays}\end{array}\right\} = \theta' - \theta = 13'$

Problem 2. A photon of ene]rgy E is Compton scattered by an angle θ. Show the kinetic energy of the recoiled electron is

$$E' = \frac{E^2(1-\cos\phi)}{E(1-\cos\phi)+m_ec^2}$$

Calculate the value of E′ for E = 40 KeV and ϕ = 60°.

Solution : From $\lambda = \frac{h}{p}$ and (2.5.9) we get

$$\frac{h}{p'} - \frac{h}{p_0} = \frac{h}{m_e c}(1 - \cos\phi)$$

$$\therefore \qquad p' = \frac{p_0 m_e c}{m_e c + p_0(1 - \cos\phi)}$$

From (2.5.5) the kinetic energy of the recoiled electron is

$$E' = (p_0 - p')\, c$$

$$= \frac{p_0^2 (1 - \cos\phi)\, c}{m_e c + p_0(1 - \cos\phi)}$$

Finally $\qquad p_0 = E/c$

$$E' = \frac{E^2(1 - \cos\phi)}{E(1 - \cos\phi) + m_e c^2}$$

Taking E = 40 keV, ϕ = 60° and $m_e c^2$ = .511 MeV we get

$$E' = \frac{16 \times 10^8 \left(1 - \frac{1}{2}\right)}{4 \times 10^4 \left(1 - \frac{1}{2}\right) + .511 \times 10^6} \approx 1.5 \text{ keV}.$$

Dual Nature of Radiation and de Broglie's hypothesis :

The phenomenon like Interference. Diffraction and Polarization are attributed to the wave properties of radiation. The Quantum theory of radiation and experiments like Photoelectric effect and Compton Effect describe the particle nature of radiation. Thus radiation behaves like waves and like particles under different suitable circumstances. Hence radiation exhibits dual nature. In the year 1924 French physicist Louis de Broglie made a daring suggestion "If radiant energy could behave like waves in some experiments and particles or photons in others and since nature loves symmetry, then one can except the particles like protons and electrons to exhibit wave nature under suitable circumstances." This is well known as de

Broglie's hypothesis. Therefore waves can be even associated with moving material particles called Matter waves and the wavelengths associated with matter waves is called de Broglie wavelength. The de Broglie wavelength is given by

$$\lambda = \frac{h}{mv} \qquad \ldots (8)$$

where m is the mass of the particle and v is its velocity.

Expression of de Broglie wavelength :

According to the Einstein's photon theory the energy of the photon is given by

$$E = hv$$

Here 'v' is the frequency of the incident radiation and 'h' is Planck's constant. If 'm' is the mass equivalent of the energy of the photon then

$$mc^2 = hv$$

Since the frequency of the incident radiation could be expressed in terms of wavelength 'λ' as $v = \frac{c}{\lambda}$ we get

$$mc^2 = \frac{hc}{\lambda} \Rightarrow mc = \frac{h}{\lambda} = p \qquad \ldots (9)$$

Here 'p' is the momentum of photon

$$\text{Therefore } \lambda = \frac{h}{mc} = \frac{h}{p} \qquad \ldots (10)$$

Thus, according to de Broglie's hypothesis, for a particle moving with velocity 'v' the above equation can be modified by replacing the momentum of photon with the momentum of the moving particle 'mv'. Therefore the de Broglie wavelength associated with a moving particle is given by

$$\lambda = \frac{h}{p} = \frac{h}{mv} \qquad \ldots (11)$$

Here 'm' is the mass of the moving particle.

de Broglie wavelength of an electron accelerated with a potential difference of 'V' volt.

Consider an electron accelerated by a potential difference 'V' volts. The kinetic energy acquired by the electron is given by

$$E = \frac{1}{2}mv^2 \qquad \Rightarrow v = \sqrt{\frac{2E}{m}}$$

Here 'm' is the mass of the electron and is given by 9.1×10^{-31} kg

Substituting the value of 'v' in equation (1) we get

$$\lambda = \frac{h}{m\sqrt{\frac{2E}{m}}} = \frac{h}{\sqrt{2mE}} \qquad \text{... (12)}$$

Since the electron acquires kinetic energy from the applied potential differenve 'V'

The kinetic energy of the electron is also given by E = eV where 'e' is the charge on electron with value 1.6×10^{-19}C

Hence the expression for the de Broglie wavelength $\lambda = \frac{h}{\sqrt{2meV}}$ ... (13)

Substituting the values for the constants h, ma and e we get

$$\lambda = \frac{12.26}{\sqrt{V}} \text{ Å} \qquad \text{... (14)}$$

Problem 1. Calculate the De-Broglie wavelength of a beam of electrons whose energy is 100 eV. Take h = 6.6×10^{-34} Joule-second and

Solution. $m = 9.1 \times 10^{-31}$ kg.

Energy $E = \frac{1}{2}m\upsilon^2 = 100 \text{ eV} = 100 \times 1.6 \times 10^{-19}$ Joule

$$\upsilon^2 = \frac{2E}{m} \text{ or } \upsilon = \sqrt{\frac{2E}{m}}$$

Momentum, $m\upsilon = m\sqrt{\frac{2E}{m}} = \sqrt{2mE}$

$$\lambda = \frac{h}{m\upsilon} = \frac{h}{\sqrt{2mE}} \text{ metres}$$

Hence, $h = 6.6 \times 10^{-34}$ kg

$$\lambda = \frac{6.6\times10^{-34}}{(2\times9.1\times10^{-31}\times100\times1.6\times10^{-19})^{1/2}}$$

$= 1.23 \times 10^{-19}$ metre

= **1.23 Å**

Problem 2. What is the momentum of a photon of wavelength 6×10^{-7} m?

Solution. Momentum of photon = $\frac{hv}{c} = \frac{h}{c/v}$

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

$$= \frac{6.624\times10^{-34}}{6\times10^{-7}}$$

= $\mathbf{1.104 \times 10^{-27}}$ **kg-m/s.**

Problem 3. Deduce the momentum of an electron having kinetic energy 1 BeV.

Solution. $E = \frac{p^2}{2m}$

or $p = \sqrt{2mE}$

Here $m = 9.1 \times 10^{-31}$ kg

$E = 1 \text{ Bev} = 10^9 \text{ ev} = 10^9 \times 1.6 \times 10^{-19}]$

$E = 1.6 \times 10^{-10}$ J

$p = [2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{10}]^{1/2}$

= $\mathbf{1.7 \times 10^{-20}}$ **kg-m/s**

Problem 4. A particle of mass 0.51 MeV/c^2 has kinetic energy 100 eV. Final its De-Broglie wavelength.

Solution. U = 100 eV

$$= 100 \times 1.6 \times 10^{-19} \text{ J}$$
$$= 1.6 \times 10^{-17} \text{ J}$$

$$\text{mass, m} = \frac{0.51 \text{ MeV}}{c^2} = \frac{0.51 \times 10^6 \times 1.6 \times 10^{19}}{(3 \times 10^8)^2}$$

$$= 9 \times 10^{-31} \text{ kg}$$

$$U = \frac{1}{2} m\upsilon^2$$

$$\upsilon = \sqrt{\frac{2U}{m}}$$

$$\lambda = \frac{h}{m\upsilon} - \frac{h}{m\sqrt{2U/m}}$$

$$\lambda = \frac{h}{\sqrt{2mU}}$$

$$\lambda = \frac{6.624 \times 10^{-34}}{[2.9 \times 19^{-31} \times 1,6 \times 10^{-17}]^{1/2}}$$

$$= \mathbf{1.234 \times 10^{-10} \text{ m} = 1.234 \text{ Å}.}$$

Problem 5. Compare the energy of a photon with that of a neutron when both are associated with wavelength 1 Å. Mass of neutron = 1.67×10^{-27} kg.

$1\text{Å} = 10^{-10}$ m

Solution. (i) Energy of Photon

$$U_1 = h\nu = \frac{hc}{\lambda}$$

$$U_1 = \frac{6.624 \times 10^{-34} \times 3 \times 10^8}{10^{-10}}$$

$$U_1 = \mathbf{19.872 \times 10^{-16} \text{ J}}$$

(i) Energy of neutron,

$$\lambda = \frac{h}{m\upsilon} \text{ or } v = \frac{h}{m\lambda}$$

$$U_2 = \frac{1}{2}m\upsilon^2$$

$$U_2 = \frac{h^2}{2m\lambda^2}$$

$$U_2 = \frac{(6.624\times10^{-34})^2}{2\times1.67\times10^{-27}\times(10^{-10})^2}$$

$$U_2 = 13.14 \times 10^{-21} \text{ J}$$

$$\frac{U_1}{U_2} = \frac{19.872\times10^{-16}}{13.14\times10^{-21}}$$

$$= \mathbf{1.51 \times 10^5}$$

Problem 6. Photoelectrons are liberated by ultraviolet light of wavelength 3000 Å from metallic surface for which the photoelectric threshold is 4000 Å. Calculate the De-Broglie was length of electrons emitted with maximum kinetic energy.

Solution. Here, $\lambda = 3000 \text{ Å} = 3 \times 10^{-7}$ m

$\lambda = 4000 \text{ Å} = 4 \times 10^{-7}$ m

$$h\nu - h\nu_0 = U$$

$$\frac{hc}{\lambda} - \frac{hc}{\lambda_0} = U$$

$$U = hc\left[\frac{1}{\lambda} - \frac{1}{\lambda_0}\right]$$

$$U = 6.624 \times 10^{-34} \times 3 \times 10^8 \left[\frac{1}{3\times10^{-7}} - \frac{1}{4\times10^{-7}}\right]$$

$$U = \mathbf{1.656 \times 10^{-19} \text{ J}}$$

De-Broglie wavelength

$$\lambda = \frac{h}{m\upsilon}$$

$$U = \frac{1}{2}m\upsilon^2$$

$$\lambda = \frac{h}{\sqrt{2mU}} = \left[\frac{h^2}{2mU}\right]^{\frac{1}{2}}$$

$$\lambda = \left[\frac{(6.624\times10^{-34})^2}{2\times9.1\times10^{-31}\times1.656\times10^{-19}}\right]$$

$$= \mathbf{1.2 \times 10^{-9}\ m = 12Å}$$

Problem 7. Show that the De-Broglie wavelength of electrons accelerated through V volts is very nearly given by

$$\lambda\ (\text{in Å}) = \left[\frac{150}{v(\text{volts})}\right]^{\frac{1}{2}}$$ [Kanpur, 1991]

Solution. Here, $eV = \frac{1}{2}m\upsilon^2$

$$\upsilon = \left[\frac{2eV}{m}\right]^{\frac{1}{2}}$$

$$\lambda = \frac{h}{m\upsilon}$$

$$= \frac{h}{m\left[\frac{2eV}{m}\right]^{1/2}}$$

$$= \left[\frac{h^2}{2meV}\right]^{\frac{1}{2}}$$

$h = 6.624 \times 10^{-34}$

$m = 9.1 \times 10^{-31}$ kg

$e = 1.6 \times 10^{-19}$ C

$$\lambda = \left[\frac{(6.624\times10^{-34})^2}{2\times9.1\times10^{-31}\times1.6\times10^{-19}\times V}\right]^{\frac{1}{2}}$$

$$\lambda = \left[\frac{150}{V}\right]^{\frac{1}{2}}\times10^{-10}\,\text{m}$$

$$= \left[\frac{150}{V}\right]^{\frac{1}{2}}\,\text{Å}$$

Example 8. Calculate the wavelength of matter-waves associated with an electron which has been accelerated from rest, through a potential difference of 1.25 kV.

Solution. Here $E = eV = 1.6 \times 10^{-19} \times 1.25 \times 10^{3}$ J

$$E = 2 \times 10^{-16}\text{ J}$$

Also $E = \frac{1}{2}m\upsilon^2$

$$u = \sqrt{\frac{2E}{m}}$$

$$\lambda = \frac{h}{m\upsilon}$$

$$\lambda = \frac{h}{n\sqrt{\frac{2E}{m}}}$$

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$E = 2 \times 10^{-16}\text{ J}$$

$$h = 6.624 \times 10^{-34}\text{ J-s}$$

$$m = 9.1 \times 10^{-31}\text{ kg}$$

$$\lambda = \frac{6.624\times10^{-34}}{(2\times9.1\times10^{-31}\times2\times10^{-16})^{1/2}}$$

$$\lambda = \mathbf{0.348 \times 10^{-10}\ m}$$

$$= \mathbf{0.348\ Å}$$

Problem 9. What is the momentum of a proton having kinetic energy 1 B e v? [G.N.D.U. 1991]

Solution. Here $U = 1\ B\ e\ V = 10^9\ eV = 10^9 \times 1.6 \times 10^{-19}\ J$

$$U = 1.6 \times 10^{-10}\ J$$

$$m = 1.67 \times 10^{-27}\ kg$$

$$U = \frac{1}{2}m\upsilon^2$$

$$p = mv = m\left[\frac{2U}{m}\right]^{\frac{1}{2}}$$

$$p = [2mU]^{1/2}$$

$$p = [2 \times 1.67 \times 10^{-27} \times 1.6 \times 10^{-10}]^{1/2}$$

$$p = 7.31 \times 10^{-19}\ kgm/s$$

Problem 10. Calculate the wavelength of an electron of I MeV (non-relativistic) [Kanpur, 1991]

Solution. $U = 10^6\ eV = 10^6 \times 1.6 \times 10^{-19}\ J$

$$U = 1.6 \times 10^{-13}\ J$$

$$m = 9.1 \times 10^{-31}\ kg$$

$$U = \frac{1}{2}m\upsilon^2$$

$$\upsilon = \left[\frac{2U}{m}\right]^{\frac{1}{2}}$$

$$\lambda = \frac{h}{m\left[\frac{2U}{m}\right]^{1/2}} = \frac{h}{[2mU]^{1/2}}$$

$$= \frac{6.624\times10^{-34}}{[2\times9.1\times10^{-31}\times1.6\times10^{-13}]^{1/2}}$$

$$= 1.227 \times 10^{-12} \text{ m}$$

$$= 1.227 \times 10^{-2} \text{ Å}$$

Problem 11. Calculate the most probable De-Broglie wavelength associated with thermal neutrons. Given, temperature = 27°C, k = 1.38×10^{-21} J/K, mass of neutron = 1.6749×10^{-27} kg [Kolkata, 1992]

Solution. For neutron,

$$U = \frac{3}{2}kT$$

or $$\frac{1}{2}m\upsilon^2 = \frac{3}{2}kT$$

or $$\upsilon = \left[\frac{3kT}{m}\right]^{\frac{1}{2}}$$

$$\lambda = \frac{h}{mv} = \frac{h}{m\times\left[\frac{3kT}{m}\right]^{\frac{1}{2}}}$$

$$\lambda = \frac{h}{[3kTm]^{1/2}}$$

Here $h = 6.624 \times 10^{-34}$ J.S, $m = 1.6749 \times 10^{-27}$ kg

$k = 1.38 \times 10^{-21}$ J/kg, $T = 27 + 273 = 300$ K

$$l = \frac{6.624\times10^{-34}}{[3\times1.38\times10^{-21}]\times300\times1.6749\times10^{-27}]^{1/2}}$$

$$l = 1.45 \times 10^{-27} \text{ m} = \mathbf{0.145\ Å.}$$

Problem 12. The De-Broglie wavelength of a proton is 1 Å. Find its kinetic energy in eV. [Delhi, 1992]

Solution. Mass of proton

$$m = 1.67 \times 10^{-27} \text{ kg}$$

$$l = 1 \text{ Å} = 10^{-10} \text{ m}$$

$$l = \frac{h}{mv} \text{ or } m = \frac{h}{m\lambda}$$

$$\upsilon_k = \frac{1}{2}m\upsilon^2$$

$$= \frac{1}{2}m\left[\frac{h}{m\lambda}\right]^2$$

$$= \frac{h^2}{2\lambda^2 m}$$

$$= \frac{(6.624\times10^{-34})^2}{2\times(10^{-10})^2\times1.67\times10^{-27}}$$

$$= 1.34 \times 10^{-20} \text{ J}$$

$$= \frac{1.314\times10^{-20}}{1.6\times10^{-19}} = \mathbf{8.2 \times 10^{-2}\ eV.}$$

1.7 Davisson and Germer Experiment (Experimental evidence of de Broglie's hypothesis)

The experimental set up is as shown in figure 1.7. It consists of an arrangement to study Bragg diffraction of electrons generated from an electron gun E. The electrons can be accelerated to a desire velocity. Then the electrons are made to incident on the nickel crystal C mounted on the turntable which can be rotated. The electrons are scattered in all direction by the atomic planes of the cyrstal. The No. of electrons scattered (Intensity) in a direction can be measured by a detector (Ionization Chamber) to which a galvanometer G is connected. The deflection in the galvanometer is proportional to the intensity of the electron beam entering the detector. The angle φ can be measured using a circular scale S. The whole instrument is placed in an evacuated chamber. During the investigation, The Electrons accelerated by a potential difference of 54 V are made to incident on the nickel crystal. The first order electron beam reflection intensity is found to be maximum for a value of φ = 50° (Fig 1.8 and 1.9) with the glancing angle of incidence 65°. The spacing of family of Bragg's planes involved in the reflection is determined using X-rays and is found to be 0.091 nm.

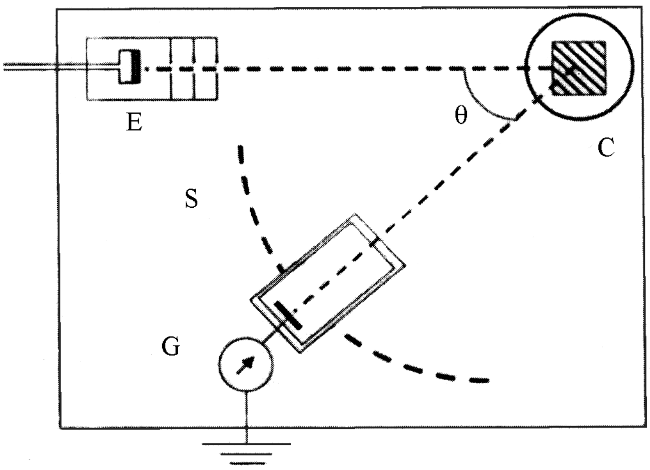
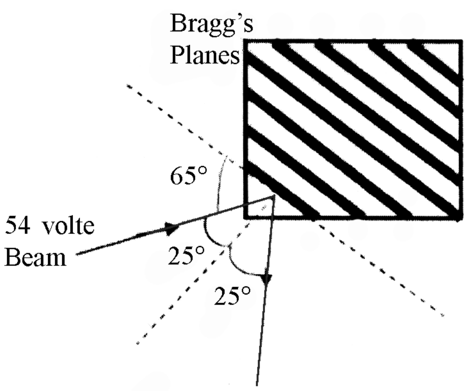


Figure 1.7 : Schematic diagram of Davison and Germer experiment



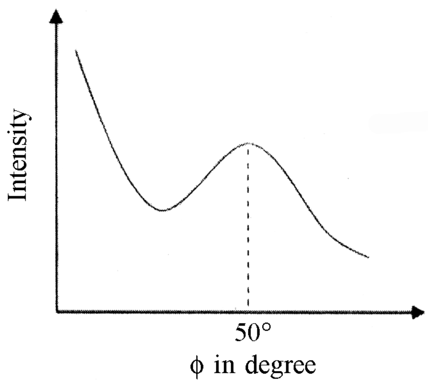


Figure 1.8 : Electron scattering from Ni crystal **Figure 1.9 :** Variation of intensity with φ

According to Bragg's law for the first order reflection maxima (n = 1)

$$2d \text{ Sin } \theta = n\lambda$$

$$\Rightarrow \lambda = 2d \text{ Sin } \theta = 2 \times 0.091 \times 10^{-9} \times \text{Sin } (65°)$$

$$= 0.165 \times 10^{-9} \text{ m}$$

According to de Broglie's hypothesis for an electron accelerated by potential differeen of 54 V the de Broglie wavelength is given by

$$1 = \text{Å} = = 0.166 \times 10^{-9} \text{ m}$$

The experimentally determined value is in good agreement with the value calculated according to de Broglie's hypothesis. Thus Divisson and Germer experiment not only confirms the wave associated with moving particle it also verifies the de Broglie's hypothesis.

1.8 Summary

In this chapter, The Planck's concept of light as a collection of photons is introduced to the students. The experimental evidence of quantum nature of light such as Black body radiation, Photoelectric effects and Compton scattering are discussed and the problems related to these topics are introduced to the students. The de Boglie's concept of wave-particle duality is introduced and the experimental evidence of the existence of matter wave (Davisson-Germer experiment) is discussed.

1.9 Questions

1. What is the significance of Planck's constant in Physics? What are photons ?
2. What is a black body ? Discuss the distribution of energy in the spectrum of a black body.
3. What do you mean by ultraviolet catastrophe ? How Planck successfuly explained the energy distribution in black body radiation ?
4. What is the photoelectric effect ? What are the characteristics of photoelectric effect ? How Einstein's photoelectric equation explains these characte ?

5. How was Millikan able to verify Einsteins photoelectric equation exerimentally ?

6. How will you determine experimentally Planck's constant by cut off potential method ?

7. What is the Compton effect ? Why Compton scattering is known as an incoherent scattering ?

8. Obtain the equation for calculating the Compton shift. What is the Compton wavelength ?

9. Discuss briefly the wave nature of matter. Obtain an expression of de Broglie wavelength for matter waves.

10. Describe the Davisson and Germer experiments for the study of electron diffraction. What are the results of the experiment`?

Unit - 2 ❑ Structure of Atom

Structure

2.1 Objective

This chapter intends to impart knowledge to the students regarding the following topics :

- Problems with Rutherford model : instability of atoms ad observation of discrete atomic spectra
- Bohr's quantization rule and atomic stability
- Calculation of energy levels for hydrogen like atoms and their spectra

2.2 Introduction

The Bohr model of the atom was proposed by Neil Bohr in 1915. It came into existence with the modification of Rutherford's model of an atom. Rutherford's model introduced the nuclear model of an atom, in which he explained that a nucleus (positively charged) is surrounded by negatively charged electrons. Bohr theory modified the atomic structure model by explaining that electrons more in fixed orbitals (shells) and not anywhere in between and he also explained that each orbit (shell) has a fixed energy. Rutherford explained the nucleus of an atom and Bohr modified that model into electrons and their energy levels. Bohr's model consists of a small nucleus (positively charged) surrounded by negative electrons moving around the nucleus in orbits. Bohr found that an electron located away from the nucleus has more energy, and the electron which is closer to nucleus has less energy.

2.3 Rutherford's Experiment

Rutherford atomic model was the firs step in the evolution of the modern atomic model. Ernest Rutherford was a keen scientist who worked to understand the distribution of electrons in an atom. He performed an experiment using alpha particles and gold foil and made the following observations :

1. Most of the alpha particles passed straight through the gold foil (A).
2. There was a deflection of the alpha particles by a small angle (B).
3. Very small amount of alpha particles rebounded (C).

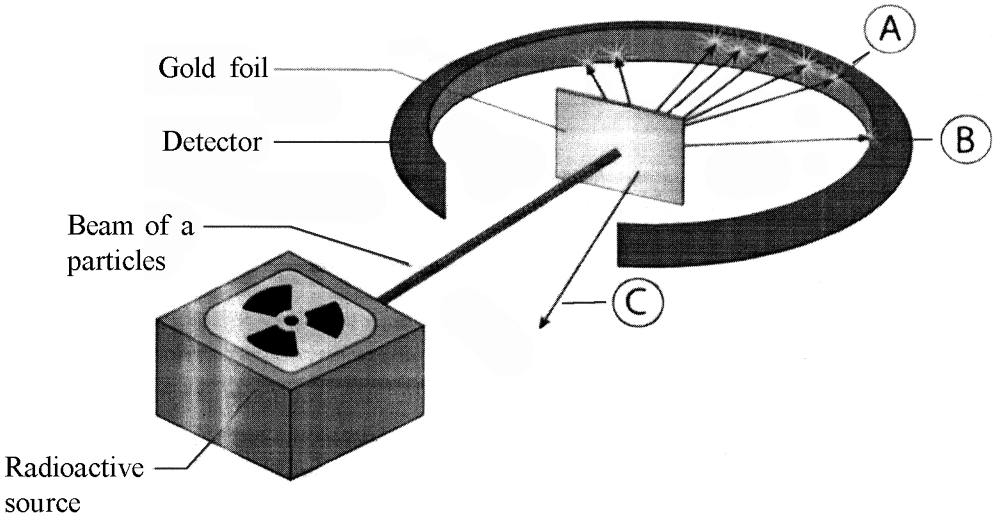


Figure 2.1 : Schematic diagram of Rutherford's experiment

From his experiment, Rutherford came to the following conclusions :

1. Most of the space in an atom is empty.
2. The space occupied by the positive charges is very small.
3. The positive charges mass of the atom were concentrated in a very small volume within an atom.

Rutherford atomic model

Rutherford developed a nuclear model of the atom on the basis of his experiment and observations. The Rutherford atomic model has the following features :

1. The centre of an atom is called the nucleus. It is positively charged and almost all mass of the atom resides in it.
2. Electrons spin around the nucleus in a circular path.
3. Comparatively, the size of the nucleus is smaller than the size of the atom.

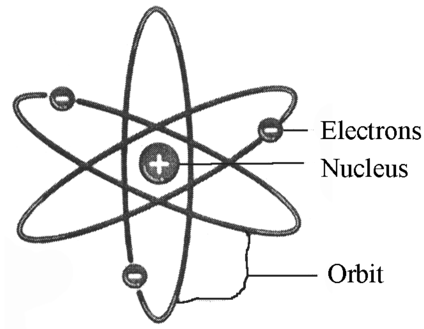


Figure 2.2 : Rutherford atomic model

Drawbacks of Rutherford's atomic model :

Rutherford's atomic model suffers from the following drawbacks :

1. This atomic model failed to explain the stability of atoms. According to the model, electrons revolve around the positively charged nucleus.

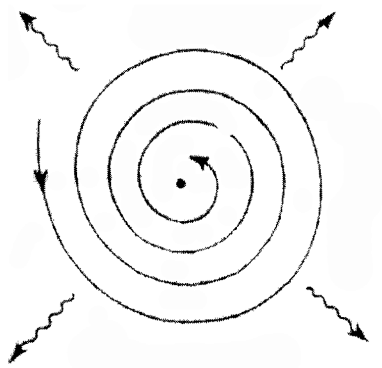


Figure 2.3 : Spiral path of accelarating electrons

It's not possible for the long run as we know atoms are stable while any particle in a circular orbit would undergo acceleration. During acceleration charged particles would radiate energy. Thus the revolving electrons will lose energy and finally fall into the nucleus following spiral paths.

2. This model of the atom also failed to explain the existence of definite lines in the hydrogen spectrum.

Bohr Atomic Model :

In 1913 Bohr proposed his quantized shell model of the atom to explain how electrons can have stable orbits around the nucleus. To get a remedy of the stability problem. Bohr modified the Rutherford model by requiring that the electrons move in orbits of fixed size and energy. The energy of an electron depends on the size of the orbit and is lower for smaller orbits. Radiation can occur only when the electron jumps from one orbit to another. The atom will be completely stable in the state with the smallest orbit, since there is no orbit of lower energy into which the electron can jump. The model was based on the quantum theory of radiation and the classical law of physics. It gave new idea of atomic structure in order to explain the stability of the atom and emission of sharp spectral lines.

Postulates of Bohr atomic model :

(i) The atom has a central massive core nucleus where all the protons and neutrons are present. The size of the nucleus is very small.

(ii) The electron in an atom revolves around the nucleus in certain discrete orbits. Such orbits are known as stable orbits or non-radiating or stationary orbits.

(iii) The force of attraction between the nucleus and the electron is equal to centrifugal force of the moving electron. Force of attraction towards nucleus = centrifugal force.

(iv) An electron can move only in those premissive orbits in which the angular momentum (mvr) of the electron is an integral multiple of $h/2\pi$. Thus, mvr = n $2\pi/h$ Where, m = mass of the electron, r = radius of the electron orbit, v = velocity of the electron in its orbit. This principal is know as quantization of angular momentum. In the above equation 'n' is any integer which has been called as principal quantum number. It can have the values n = 1, 2, 3, ...(from the nucleus). Various energy levels are designed as K (n = 1), L (n = 2), M (n = 3)...... etc. Since the electron present in these orbits is associated with some energy, these orbits are called energy levels.

(v) The emission or absorption of radiation by the atom takes place when an electron jumps from one stationary orbit to another.

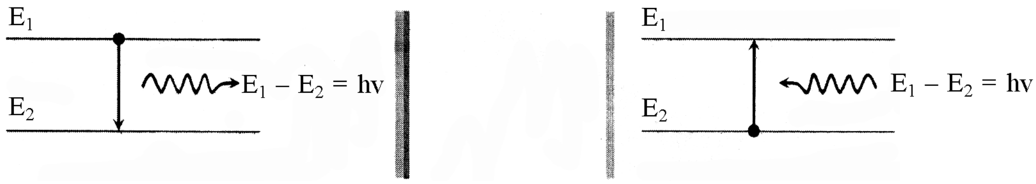


Figure 2.4 : Schematic representation of emission and absorption in Bohr atom

(vi) The radiation is emitted or absorbed as a single quantum (photon) whose energy hv is equal to the difference in energy ΔE of the electron in the two orbits involved. Thus, hv = ΔE Where 'h' = Planck's constant, v = frequency of the radiant energy. Hence the spectrum of the atom will have certain fixed frequency.

(vii) The lowest energy state (n = 1) is called the ground state. When an electron absorbs energy, it gets excited and jumps to an outer orbit. It has to fall back to a lower orbit with the release of energy.

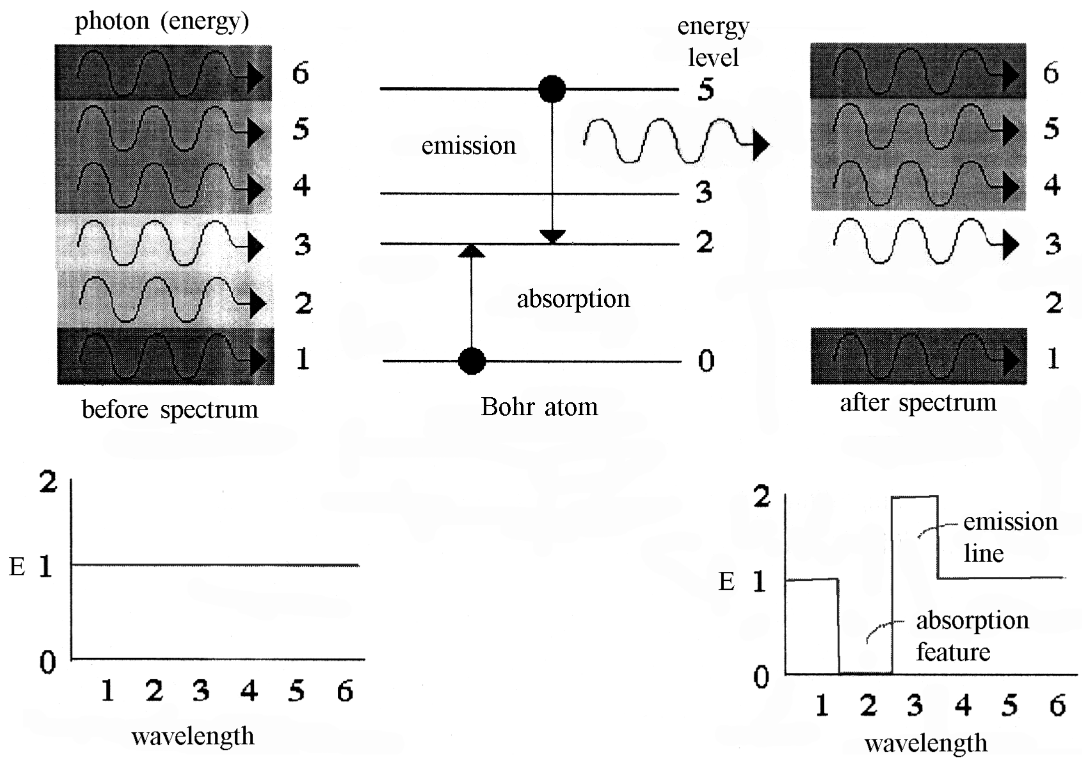
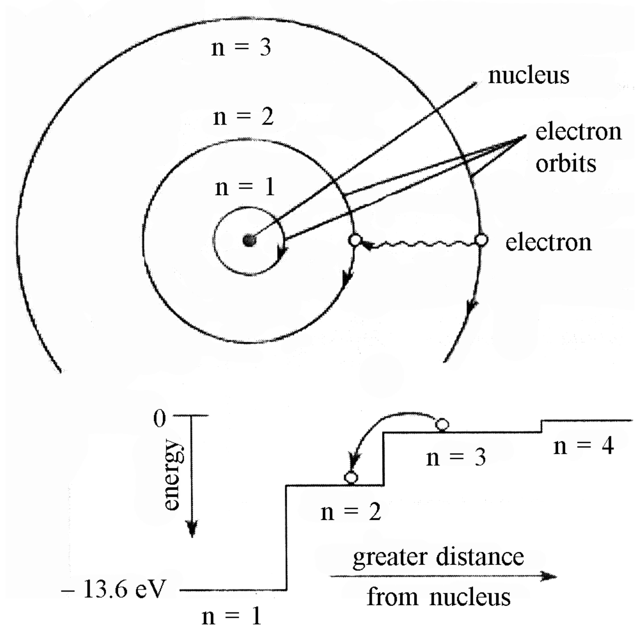


Figure 2.5 : Energy level diagram, asborption and emission spectra in a Bhor atom



The electron travel in circular orbits around the nucleus. The orbits have quantized sizes and energies. Energy is emitted from the atom when the electron jumps from one orbit to another close to the nucleus. Show here is the first Balmer transition, in which an electron jumps from orbit n = 3 to orbit n = 2, producing a photon of red light with an energy of 1.89 eV and a wavelength of 656×10^{-9} m.

Figure 2.6 : Schematic representation of Bohr's atomic model

Calculation of energy levels for hydrogen like atoms and their spectra :

Let us suppose that the hydrogen-like atom has a nucleus of charge +Ze and mass M and the electron has charge –e and mass m, and that the distance between them is a. The distance of the nucleus from the centre of mass is ma/(M + m) and the distance of the electron from the centre of mass is Ma/(M + m). We'll suppose that the speed of the electron in its orbit around the centre of mass is v. The angular momentum of the sytem is mva, then using Bohr's first assumption we can write

$$mua = n\hbar,$$

where n is an integer.

The Coulomb force on the electron is equal to its mass times its centripetal acceleration :

$$\frac{Ze^2}{4\pi \in_0 a^2} = \frac{m\upsilon^2}{Ma/(M+m)}$$

It you eliminate u from these, you obtain an expression for the radius of the nth orbit :

$$a = \frac{4\pi \epsilon_0 \hbar^2 n^2}{Ze^2 \mu},$$

Where

$$\mu = \frac{mM}{m+M}$$

The quantity represented by the symbol μ is called the reduced mass of the electron. It is slightly less than the actual mass of the electron. In the hydrogen atom, in which the nucleus is just a proton, the ratio M/m is about. 1836, so that μ = 0.9946m. For heavier hydrogen-like atoms it is closer to m. From equation (2) we can get the explicit expression of v as

$$\upsilon = \frac{MZe^2}{4\pi \epsilon_0 (M+m)\hbar n}$$

The energy of the atom is the sum of the natural potencial energy between nucleus and electron and the orbital kinetic energies of the particles. That is :

$$E = -\frac{Ze^2}{4\pi \epsilon_0 a} + \frac{1}{2}m\upsilon^2 + \frac{1}{2}M\left(\frac{m\upsilon}{M}\right)^2$$

If we make use of equation 7.4.2 this becomes

$$E = -\frac{m(M+m)\upsilon^2}{M} = \frac{1}{2}m\upsilon^2 + \frac{1}{2}\frac{m^2}{M}\upsilon^2$$

$$= -\frac{1}{2}m\left(\frac{M+m}{M}\right)\upsilon^2$$

Then, making use of equation 7.4.5 we obtain for the energy

$$E = -\frac{\mu Z^2 e^4}{2(4\pi \epsilon_0)^2 \hbar^2} \cdot \frac{1}{n^2}$$

In deriving this expression for the energy, we had taken the potential energy to be zero at infinite separation of proton and nucleus, which is a frequent convention in electrostatics. This is, the energy level we have calculated for a bound orbit is expressed relative to the energy of ionized hydrogen. Hence the energy of all bound orbits is negative. In tables of atomic energy levels, however, it is more usual to take the energy of the ground state (n = 1) to be zero. In that case the energy levels are given by

$$E = \frac{\mu Z^2 e^4}{2(4\pi \in_0)^2 \hbar^2} . \left(1 - \frac{1}{n^2}\right)$$

It is customary to tabulate term values T rather than energy levels, and this is achieved by dividing by hc. Thus

$$T = \frac{\mu Z^2 e^4}{2(4\pi \in_o)^2 \hbar^2 hc} . \left(1 - \frac{1}{n^2}\right)$$

The expression before the large parentheses is called the Rydberg constant for the atom is question. ($^1H : Z = 1$), it has the value $1.09679 \times 10^7\ m^{-1}$

If we put Z = 1 and $\mu = m$ resulting expression is called the Rydberg constant for a hydrogen nucleus of infinite mass; it is the expression one would arrive at if one neglected the motion of the nucleus. It is one of the physical constants whose value is known with greatest precision, its value being

$$R_\infty = 1.097373153 \times 10^7 m^{-1}$$

The term value equal to $1.097373 \times 10^7\ m^{-1}$ or the corresponding energy, which is 2.1799×10^{-18} J or 13.61 eV is called a rydberg.

Hydrogen Emission Spectrum

We all know that electrons in an atom or a molecule absorb energy and get excited, they jump from a lower energy level to a higher energy level, and they emit radiation when they come back to their original states. This phenomenon accounts for the emission spectrum through hydrogen too, better known as the hydrogen emission spectrum.

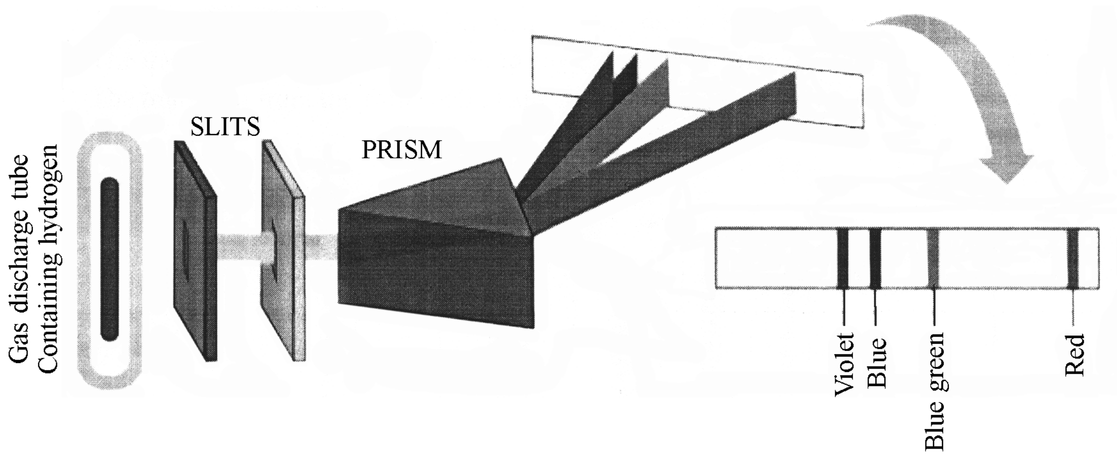


Figure 2.7 : Schematic arrangement of observing Hydrogen emission spectra

The hydrogen spectrum is an important evidence to show the quantized electronic structure of an atom. The hydrogen atoms of the molecule dissociate as soon as an electric discharge is passed through a gaseous hydrogen molecule. It results in the emission of electromagnetic radiation initiated by the energetically excited hydrogen atoms. The hydrogen emission spectrum comprises radiation of dicrete frequencies. These series of radiation are named after the scientists who discovered them.

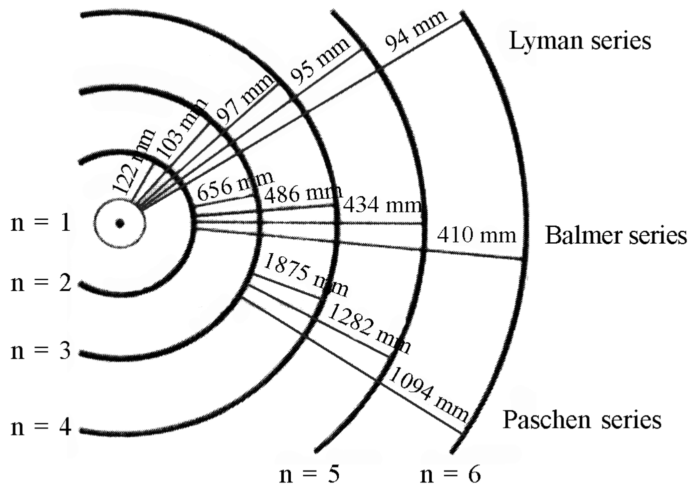


Figure 2.8 : Schematic representation Hydrogen emission spectra

In the year 1885, on the basis of experimental observations, Balmer proposed the formula for correlating the wave number of the spectral lines emitted and the energy shells involved. This formula is given as :

$$\bar{v} = 109677\left(\frac{1}{2^2} - \frac{1}{n^2}\right)$$

This series of the hydrogen emission spectrum is known as the Balmer series. This is the only series of lines in the electomagnetic spectrum that lies in the visible region. The value, 109,677 cm^{-1}, is called the Rydberg constant for hydrogen. The Balmer series is basically the part of the hydrogen emission spectrum responsible for the excitation of an electron from the second shell to any other shell. Similarly, other transitions also have their own series names. Some of them are listed below :

1. The transition from the first shell to any other shell—Lyman series
2. The transition from the second shell to any other shell—Balmer series
3. The transition from the third shell to any other shell—Paschen series
4. The transition from the fourth shell to any other shell—Brackett series
5. The transition from the fifth shell to any other shell—Pfund series

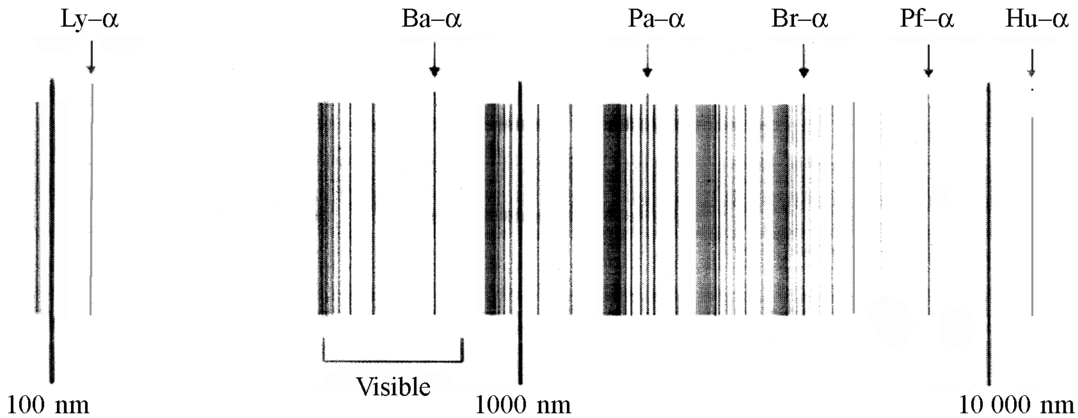


Figure 2.9 : Soectral lines of Hydrogen emission spectra

Johannes Rydberg, a Swedish spectroscopist, derived a general formula for the calculation of wave number of hydrogen spectral line emissions due to the transition of an electron from one orbit to another. The general formula for the hydrogen emission spectrum is given by :

$$\bar{v} = 109677\left(\frac{1}{n_1^2} = \frac{1}{n_2^2}\right)$$

Where, n_1 = 1, 2, 3, 4, ...

$n_2 = n_1 + 1$

v = wave number of electromagnetic radiation. The value 109,677 cm^{-1} is known as Rydberg constant for hydrogen.

Problem 1. The Rydberg constant for hydrogen is 1.09678×10^7/m and ionized helium 1.09722 × 107/m. Calculate the ratio of the mass of the proton to that of the electron, assuaning the helium nucleus to be four times the mass of proton.

[I.A.S. 1976]

Solution. The nucleus of the atom has motion though it is too heavy as compared to the electron. Due to this reason the reduced mass of the electron is

$$m = \left[\frac{M}{M+m}\right] = \frac{1}{1+\frac{m}{M}}$$

Here m is the mass of the electron and M is the mass of the nucleus. For hydrogen, Rudberg constant,

$$R_H = \frac{R}{\left[1+\frac{m}{M_H}\right]}$$

For ionized helium, Rydberg constant

$$R_H = \frac{R}{\left[1+\frac{m}{M_{He}}\right]}$$

Here $$R = \frac{me^4}{8\in_0^2 ch^3} \text{ per metre}$$

Dividying (ii) by (i)

$$\frac{R_{He}}{R_H} = \frac{\left[1+\frac{m}{M_H}\right]}{\left[1+\frac{m}{M_{He}}\right]}$$

Taking $M_{He} = 4M_H$ and simplifying

$$\frac{M_H}{m} = \frac{R_H - \frac{1}{4}R_{He}}{R_{He} - R_H}$$

Here $R_H = 1.09678 \times 10^7$/m and $R_{He} = 1.09722 \times 10^7$/m

$$\frac{M_H}{m} = \frac{10^7}{10^7}\left[\frac{1.09678 - \frac{1}{4}\times 1.09722}{1.09733 - 1.09722 - 1.09678}\right] = 1869$$

Problem 2. Calculate the radius of the hydrogen atom. Show that the velocity of the electron in the first Bohr orbit in hydrogen atom is (1/37) c, where c is velocity of light. [Delhi (Hons.) 1922], [Delhi 1992]

Solution. (i) Radius $r = \frac{\epsilon_o n^2 h^2}{\pi m Z e^2}$

Here $n = 1$

$h = 6.624 \times 10^{-34}$ J-s

$\epsilon_0 = 8.85 \times 10^{-12}$ C^2/N–m^2

$m = 9.1 \times 10^{-31}$ kg

$e = 1.6 \times 10^{-19}$ C

$$r = \frac{8.85 \times (6.624 \times 10^{-34})^2}{\pi \times 9.1 \times 10^{-31} \times (1.6 \times 10^{-19})^2}$$

$r =$ **5.29×10^{-11} m**

$=$ **0.529 Å**

Velocity, $\upsilon = \frac{Ze^2}{2\epsilon_0 hn}$

Here $Z = 1$, $n = 1$

$$\therefore \qquad \upsilon = \frac{(1.6\times10^{-19})^2}{2\times8.85\times10^{-12}\times6.624\times10^{-34}}$$

$$\frac{\upsilon}{c} = \frac{(1.6\times10^{-19})^2}{2\times8.85\times10^{-12}\times6.624\times10^{-34}\times3\times10^{8}}$$

$$\frac{\upsilon}{c} = \frac{1}{137}$$

$$\upsilon = \left(\frac{1}{137}\right)c$$

2.4 Resonance, excitation and Ionization Potentials

Resonance Potential. The minimum potential required to provide energy to the electron in the ground state of the first excited state i.e., from n = 1 to n = 2 is called resonance potential.

The energy of electron in the gound state of hydrogen atom is – 13.6 eV and first excited state (n = 2) is – 3.4 eV. Therefore, the energy required to move and the electron from the ground state to the first excited state is (– 3.4) eV – (– 13.6) eV = 10.2 eV.

Therefore the resonance potential for hydrogen is 10.2 V.

Excitation Potential. The state n > 1 are called excited states. The energy required to move the electron to the first, second, third excited states is given by

$$E_1 = 10.2 \text{ eV}$$

$$E_2 = -\left(\frac{13.6}{3^2}\right)-(-13.6)$$

$$= -1.51 + 13.60 = 12.09 \text{ eV}$$

$$E_3 = -\left[\frac{13.6}{3^2}\right]-(-13.6)$$

$$= -0.85 + 13.60 = 12.75 \text{ eV}$$

Therefore the successive exciation potentials are 10.2 V, 12.09 V, 12.75 V and so on.

The excitation potential is the potential required to provide energy to raise the electron from the ground state to the state n > 1 i.e., n = 2, 3, 4....

Ionization Potential. It is the minimum potential required that provides energy to bring the electron from the ground state out of the atom.

For hydrogen atom, ionization potential = 13.6 V

The energy to the electron in the atom can be provided by electron emitted from a hot filament and accelerated though a creation potential V.

The electron will move with a velocity υ where $\upsilon = \left[\frac{2eV}{m}\right]^{\frac{1}{2}}$.

(1) If the energy of the striking electron is just equal to or more than the energy required by the electron to come of the atom, the electron in the atom absorbs energy and comes out of the atom.

Problem 1. Wavelength of Balmer H_α line is 6563 Å. Calculate the wavelength of H_β line.

Solution. For H_α line of Balmer series i.e., the first number,

$$\bar{v}_1 = R\left[\frac{1}{2^2} - \frac{1}{3^2}\right]$$

$$\frac{1}{\lambda_1} = \frac{5}{36}R \qquad \text{... (i)}$$

For H_β line of Balmer series i.e., the second number,

$$\bar{v}_2 = R\left[\frac{1}{2^2} - \frac{1}{4^2}\right]$$

$$\frac{1}{\lambda_2} = \frac{3}{16}R \qquad \text{... (ii)}$$

Dividing (i) by (ii)

$$\frac{\lambda_2}{\lambda_1} = \frac{20}{27}$$

$$\lambda_2 = \left(\frac{20}{27}\right)\lambda_1$$

But $\lambda_1 = 6563$ Å

$$\lambda_2 = \left(\frac{20}{27}\right)6563$$

$\therefore$ $\lambda_2 =$ **4861 Å**

Problem 2. Calculate the energy required to excite the hydrogen atom from the ground state (n = 1) to the first excited state (n = 2). [Delhi (Hons.)]

Solution. Energy required

$$U = \frac{me^4}{8 \in_0^2 h^2}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

$$U = \frac{me^4}{8 \in_0^2 h^2}\left[\frac{1}{1^2} - \frac{1}{2^2}\right]$$

$$U = \frac{3me^4}{32 \in_0^2 h^2}$$

Here $m = 9.1 \times 10^{-31}$ Kg, $e = 1.6 \times 10^{-19}$ C

$\in_0 = 8.85 \times 10^{-12}$ $C^2/N\text{-}m^2$

$h = 6.624 \times 10^{-34}$ J-s

$$U = \frac{3 \times 9.1 \times 10^{-31} \times (1.6 \times 10^{=19})^4}{32 \times (8.85 \times 10^{-12})^2 \times (6.624 \times 10^{-34})^2} \text{Joules}$$

$$U = \frac{3 \times 9.1 \times 10^{-31} \times (1.6 \times 10^{=19})^4}{32 \times (8.85 \times 10^{-12})^2 \times (6.624 \times 10^{-34})^2 \times 1.6 \times 10^{-15}} \text{eV}$$

$U = 10.13$ eV.

Problem 3. The wavelength of sodium D_1 line is 590 nm. Calculate the difference in energy levels involved in the emission or absorption of this line.

Solution. Here $E_{(n_2-n_1)} = h\upsilon = \frac{hc}{\lambda}$

Here,

$$h = 6.624 \times 10^{-34} \text{ J-s}$$

$$c = 3 \times 10^{8} \text{ m/s}$$

$$h = 590 \text{ nm} = 590 \times 10^{-9} \text{ m}$$

$$\therefore \quad E_{(n_2-n_1)} = \frac{(6.624 \times 10^{-34}) \times 3 \times 10^{8}}{590 \times 10^{-9}}$$

$$= \mathbf{3.37 \times 10^{-19}\ J}$$

Problem 4. The wavelength of the second line of the Balmer series in the hydrogen spectram is 4861 Å. Calcutta the wavelength of the first line. [Rajasthan]

Solution. For the second line,

$$\bar{v} = R\left[\frac{1}{2^2} - \frac{1}{4^2}\right]$$

$$\bar{v}_2 = \frac{3}{16}R$$

$$\frac{1}{\lambda_2} = \frac{3}{16}R$$

For the first line,

$$\bar{v} = R\left[\frac{1}{2^2} - \frac{1}{3^2}\right]$$

$$\bar{v}_1 = \frac{5}{36}R$$

or

$$\frac{1}{\lambda_1} = \frac{5}{36}R$$

Dividing (i) by (ii)

$$\frac{\lambda_1}{\lambda_2} = \frac{27}{20}$$

$\therefore$ $$\lambda_1 = \frac{27\lambda_2}{20}$$

But $$\lambda_2 = 4861 \text{ Å}$$

$$\lambda_1 = \frac{27 \times 4861}{10}$$

or $$\lambda_1 = \mathbf{6563 \text{ Å}.}$$

Problem 5. A beam of electrons is used to bombard gaseous hydrogen. What is the minimum energy in electron-volts the electrons must have if the first number of the Balmer series corresponding to a transition from $n_2 = 3$ state to $n_1 = 2$ state is to be emitted?

$$h = 6.6 \times 10^{-34} \text{ Joule second.}$$

[Mumbai, 1981, Kolkata,1992]

Solution. Energy required

$$= \frac{me^4}{8 \epsilon_0^2 h^2}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

Here $$n_1 = 2,\ n_2 = 3$$

$\therefore$ $$\text{Energy requird} = \left(\frac{me^4}{8 \epsilon_0^2 h^2}\right) \times \left(\frac{5}{36}\right) \text{ Joule}$$

But $$1 \text{ eV} = 1.6 \times 10^{-19} \text{ Joule}$$

$\therefore$ $$\text{Energy required} = \frac{5me^4}{8 \times 36 \times \epsilon_0^2 h^2 \times (1.6 \times 10^{-19})} \text{ electron volts}$$

$$= \frac{5 \times 9 \times 10^{-31} \times (1.6 \times 10^{-19})^4}{8 \times 36 (8.85 \times 10^{-12})^2 \times (6.6 \times 10^{-34})^2 \times (1.6 \times 10^{-19})}$$

$$= \mathbf{1.88 \text{ eV}.}$$

Problem 6. Calculate the ionization potential in electron volts for hydrogen atom. Given that

$$e = 1.6 \times 10^{-19} \text{ coulomb}$$
$$m = 9 \times 10^{-31} \text{ kg}$$
$$h = 6.6 \times 10^{-34} \text{ Joule-second}$$
$$\epsilon_0 = 8.85 - 10^{-19} \text{ coulomb}^2/\text{Newton-m}^2$$

Solution. Work function,

$$\phi = \frac{me^4}{8\epsilon_0^2 h^2} \text{ Joules}$$

$$\phi = \frac{9\times10^{-31}\times(1.6\times10^{-19})^4}{8\times(8.85\times10^{-12})^2\times(6.6\times19^{-34})^2} \text{ Joule}$$

But $1\text{eV} = 1.6 \times 10^{-19}$ Joule

$$\phi = \frac{9\times10^{-31}\times(1.6\times10^{-19})^4}{8\times(8.85\times10^{-19})^2\times(6.6\times10^{-34})^2\times1.6\times10^{-19}}$$

$$\phi = \mathbf{13.51\ eV.}$$

Problem 7. The wavelength of the first number of Balmer series of hydrogen is 6563×10^{-10} m. Calculate the wavelength of its second number. [Delhi, 1982]

Solution. For the first number

$$\bar{v}_1 = R\left[\frac{1}{2^2}-\frac{1}{3^2}\right]$$

$$\bar{v}_1 = \frac{5}{36}R$$

or $$\frac{1}{\lambda_1} = \frac{5}{36}R$$

For the second number,

$$\bar{v}_2 = R\left[\frac{1}{2^2}-\frac{1}{4^2}\right]$$

or $$\frac{1}{\lambda_2} = \frac{3}{16}R$$

Dividing (i) by (ii)

$$\frac{\lambda_2}{\lambda_1} = \frac{20}{27}$$

$$\lambda_2 = \frac{20}{27}\lambda_1$$

But $$\lambda_1 = 6563 \times 10^{-19} \text{ m}$$

$$\lambda_2 = \frac{20 \times 6563 \times 10^{-10}}{27}$$

$$= \mathbf{4861 \times 10^{-10} \text{ m}}$$

Problem 8. The ionization potential of atomic hydrogen is 13.6 V. Calculate the wavelength of light emitted in a transition starting at the first excited state of hydrogen atom. [I.A.S. 1985]

Solution. Ionization potential = 13.6

Energy of electron in the first orbit

$$U_1 = -13.6 \text{ eV}$$

Energy of electron in the second orbit

$$U_2 = \frac{-13.6}{n^2} = \frac{-13.6}{4} = -3.4 \text{ eV}$$

$$U_1 - U_2 = -3.4 + 13.6$$

$$h\nu = 10.2 \text{ eV}$$

$$\frac{hc}{\lambda} = 10.2 \times 1.6 \times 10^{-19} \text{ J} = 1.632 \times 10^{-18} \text{ J}$$

$$\lambda = \frac{hc}{1.632 \times 10^{-18}}$$

$$= \frac{6.624 \times 10^{-34} \times 3 \times 10^{8}}{1.632 \times 10^{-18}}$$

$$= 1.271 \times 10^{-7} \text{ m}$$

$$= \mathbf{1217 \text{ Å}.}$$

Problem 9. Find the radius and speed of the electron in the first Bohr orbit of the hydrogen atom. How will the radius and speed of electron change with the increase in atomic number of the atom? [I.A.S.]

Solution. (i) The radius of the Bohr orbit is given by

$$r = \frac{\epsilon_0 n^2 h^2}{\pi m Z e^2}$$

For hydrogen, $Z = 1, n = 1$

$$r_H = \frac{\epsilon_0 h^2}{\pi m e^2}$$

Here $\epsilon_0 = 8.85 \times 10^{-12} C^2/N\text{-}m^2$

$m = 1.6 \times 10^{-19}$ C

$h = 6.624 \times 10^{-34}$ J-s

$$\therefore \quad r_H = \frac{8.85 \times 10^{-12} \times (6.624 \times 10^{-34})^2}{\pi \times 9.1 \times 10^{-31} \times (1.6 \times 10^{-19})^2}$$

$$r_H = 5.30 \times 10^{-11} \text{ m}$$

Also $r = \frac{r_H}{Z}$

Therefore radius of the orbit will decrease with increase in atomic number Z.

(ii) Velocity of the electron

$$\upsilon = \frac{Ze^2}{2\epsilon_0 nh}$$

In hydrogen $Z = 1, n = 1$

$$\upsilon_H = \frac{Ze^2}{2\epsilon_0 h} = \frac{(1.6 \times 10^{-19})^2}{2 \times 8.85 \times 10^{-12} \times 6.624 \times 10^{-34}}$$

$$= 2.2 \times 10^6 \text{ m/s}$$

Also $\upsilon = Z\upsilon_H$

Therefore velocity of the electron in the orbit will increase with increase at atomic number Z.

Problem 10. Calculate the radius of the first Bohr orbit for (i) H and (ii) He atoms and also the velocity of the electron in these orbits as compared to the velocity of light. [I.A.S.]

Solution. For hydrogen atom, the radius of the orbit is

$$r_H = \frac{\epsilon_0 n^2 h^2}{\pi m Z e^2}$$

Here $n = 1, Z = 1$

$\hat{I}_0 = 8.85 \times 10^{-12}\ C^2/N\text{-}m^2$

$m = 9.1 \times 10^{-31}$ kg

$e = 1.6 \times 10^{-19}$ C

$h = 6.624 \times 10^{-34}$ J-s

$$\therefore \quad r_H = \frac{8.85\times10^{-12}\times1\times(6.624\times10^{-34})^2}{3.142\times9.1\times10^{-31}\times(1.6\times10^{-19})^2}$$

$$r_H = \mathbf{5.3 \times 10^{-11}\ m}$$

For helium, atom, $n = 1$, $Z = 2$

$$r_H = \frac{r_H}{Z} = \frac{5.30\times10^{-11}}{2}$$

$$= \mathbf{2.65 \times 10^{-11}\ m}$$

(ii) Velocity of the electron,

$$\upsilon = \frac{Ze^2}{2\epsilon_0 nh}$$

For hydrogen $Z = 1$ and $n = 1$

$$\upsilon_H = \frac{e^2}{2\epsilon_0 h}$$

$$= \frac{(1.6\times10^{-19})^2}{2\times8.85\times10^{-12}\times6.624\times10^{-34}}$$

$$= \mathbf{2.2 \times 10^6\ m/s}$$

Also $$\frac{\upsilon_H}{c} = \frac{2.2\times10^6}{3\times10^8} = \mathbf{7.33 \times 10^{-3}}$$

For helium $$\upsilon_{He} = \frac{Ze^2}{2\in_0 nh}$$

Here n = 1, Z = 2

$$\upsilon_{He} = \frac{Ze^2}{2\in_0 h} = 2\upsilon_H$$

$$\upsilon_{He} = 2 \times 2.2 \times 10^6$$
$$= \mathbf{4.4 \times 10^6\ m/s}$$

$$\frac{\upsilon_{He}}{c} = \frac{4.4\times10^6}{3\times10^8}$$
$$= \mathbf{1.466 \times 10^{-2}}$$

Problem 11. Calculate the difference in wavelength in the spectra of hydrogen and heavy hydrogen corresponding to the first line on the long wave side of Balmer series.

$$\begin{bmatrix} R_H = 1.097\times10^7 / m \\ m = 0.000549 M_H \end{bmatrix}$$ [I.A.S.]

Solution. $$R_H = \frac{R}{1+\frac{m}{M_H}}$$

$$R_D = \frac{R}{1+\frac{m}{M_D}}$$

$$\frac{m}{M_H} = 0.000549$$

$$\frac{m}{M_D} = \frac{m}{2M_H} = 0.000274$$

$$\frac{R_D}{R_H} = \frac{1+\frac{M}{M_H}}{1+\frac{m}{M_D}} = \frac{1+0.000549}{1+0.000274}$$

$$\frac{R_D}{R_H} = 1.00027$$

$$R_D = (R_H)\ 1.00027$$

$$R_D = 1.097 \times 10^7 \times 1.00027$$

$$R_D = 1.0973 \times 10^7/\text{m}$$

In the case of Balmer series, for the first member

$$n_1 = 2,\ n_2 = 3$$

$$\frac{1}{\lambda_H} = R_H\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] = \left(\frac{5}{36}\right)R_H$$

$$\lambda_H = \frac{36}{4R_H} = \frac{1}{5\times1.097\times10^7}$$

$$\lambda_H = 6.5633 \times 10^7\ \text{m}$$

Similarly $$\frac{1}{\lambda_D} = R_D\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] = \left(\frac{5}{36}\right)R_D$$

$$\lambda_D = \frac{36}{5R_D}$$

$$\lambda_D = \frac{36}{5\times1.0973\times10^7}$$

$$\lambda_D = 6.5615 \times 10^{-7}\ \text{m}$$

$$\lambda_D = \lambda_H - \lambda_D$$

$$= 6.5633 \times 10^{-7} - 6.5615 \times 10^{-7}$$

$$= 0.0018 \times 10^{-7}\ \text{m}$$

$$= \mathbf{1.8\ \text{Å}}$$

Problem 12. In hydrogen atom the electron is replaced by a muon whose mass is 200 times that of an electron and charge is same as that of electron, calculate the oinization on the basis of Bohr's theory. [I.A.S.]

Solution. In the case of hydrogen atom, having an electron, the ionization potential

$$\phi = \frac{me^4}{8 \in_0^2 h^2} \quad \text{.... (i)}$$

when electron is replaced by muon.

$$m_1 = 200 \text{ m}$$

$$\phi_1 = \frac{m_1 e^4}{8 \in_0^2 h^2} = \frac{(200m)e^4}{8 \in_0^2 h^2}$$

Dividing (ii) by (i)

$$\frac{\phi_1}{\phi} = 200$$

But $\phi = 13.6 \text{ eV}$

$\therefore$ $\phi_1 = 200 \times 13.6$

$= 2.72 \times 10^3 \text{ eV}$

Problem 13. What is the energy, momentum and wavelength of the photon emitted by a hydrogen atom when an electron makes a transition from n = 2 to n = 1 state? Given inoization potential = 13.6 eV.

Solution. Energy of electron in the first orbit of hydrogen atom,

$$E_1 = -13.6 \text{ eV}$$

Energy of electron is second orbit

$$E_2 = \frac{E_1}{n^2} = \frac{E_1}{4} = \frac{-13.6}{4}$$

$$E_2 = -3.4 \text{ eV}$$

(1) Energy of photon emitted $= E_2 - E_1$

$$E = -3.4 + (13.6)$$

$$= \mathbf{10.2\ eV}$$

$$= 10.2 \times 1.6 \times 10^{-19} \text{ J}$$

$$= 16.32 \times 10^{-19} \text{ J}$$

(2) Momentum, $P = \frac{E}{c} = \frac{16.32 \times 10^{-19}}{3 \times 10^{8}}$

$$P = 5.44 \times 10^{-27} \text{ kg-m/s}$$

(3) Wavelength, $\lambda = \frac{h}{p} = \frac{6.624 \times 10^{-34}}{5.44 \times 10^{-27}}$

$$= 1.218 \times 10^{-7} \text{ m}$$

$$= 1218 \text{ Å}.$$

Limitations of the Bohr's Theory

In spite of the extraordinary success of the Bohr's theory there were some serious limitations

1. It could not account for the spectra of complex atoms.
2. Even simple atoms as neutral helium having more than one electron could not be dealt with by the Bohr's theory.
3. Intensities of lines could not be calculated.
4. It failed to give correct results in the complicated conditions of the splitting of lines in the presence of a magnetic field, known as the anomalous Zeeman effect.
5. It did not account for the fine structure of the hydrogen lines and it did not account for the doublet structure of all alkali metal spectra.

2.5 Summary

In this chapter the Rutherford model of atoms and its limitations are discussed. The Bohr quantization rules and Bohr atomic model are introduced to the students. Atomic stability is discussed in the view of Bohr atomic model. Calculation of energy levels of hydrogen like atoms, their spectra and related problems are discussed in this chapter.

2.6 Questions

1. Describe Rutherford's model of the atom and the evidence that led to it. What are the drawbacks of this model ?
2. State the postulates of Bohr atomic model. Obtain the expressions for the radius and electron energy of the nth orbit.
3. Explain how Bohr's atomic model successfully accounts for the hydrogen emission spectrum.
4. Define the terms (i) Critical potential, (ii) Excitation potencial and (iii) lonisation potential.
5. The energy of the electron in the nth orbit in hydrogen atom is negative, explain the fact.
6. Find the wavelength of the photon emitted when the hydrogen atom goes from n = 10 state to the ground state. Why couldn't Bohr allow the quantum number n to take on the value n = 0 ?

Unit - 3 ❑ Introduction to quantum mechanics

Structure

3.1 Objective

This chapter intends to impart knowledge to the students regarding the following topics :

- Wave-particle duality and Heisenberg uncertanity principle. Application of this principle for estimating minimum energy of a confined particle. Energy-time uncertainty principle.
- Two slit interference experiment; linear superposition principle as a consequence; Matter waves and wave amplitude
- Schrodinger equation for non-relativistic particles; Momentum and Energy operators; stationary states; physical interpretation of wavefunction; probabilities and normalization; Probability and probability current densities in one dimension.

3.2 Introduction

Bohr's theory of the hydrogen atom led de Broglie to the conception of matter waves. According to the Bohr's theory, the stable states of electrons in the atoms are governed by "integer rules". The only phenomena involving integers in physics are those of interference and modes of vibration of stretched strings, both of which imply wave motion. Hence de Broglie thought that the electrons may also be characterized by a periodicity. So he proposed that matter, like radiation has dual nature.

3.3 Heisenberg's Uncertainty Principle

Statement. It is impossible to determine precisely and simultaneously the values of both the members of a pair physical variables which describe the motion of an atomic system. Such pairs of variables are called cononically conjugate variables.

Example. According to this principle, the position and momentum of a particle (say electron) cannot be determined simultaneously to any desired degree of accuracy.

Taking Δx as the error in determining its position and Δp the error in determining its momentum at the same instant, these quantities are related as follows :

$$\Delta x \, \Delta p = h/2\pi$$

The product of the two error is approximately of the order of Planck's constant. If Δx is small, Δp will be large and vice versa. It means that if one quantity is measured accurately, the other quantity becomes less accurate. Thus any instrument cannot measure the quantities more accurately than predicted by Heisenberg's principle of uncertainty of indeterminacy. The same relation holds for the energy and time related to any given event.

i.e.,
$$\Delta E \, \Delta t = h/2\pi$$

According to classical ideas, it is possible for a particle to occupy a fixed position and have a definite momentum and we can predict exactly its position and momentum at any time later. But according to the uncertainty principle, it is not possible to determine accurately the simultaneous values of position and momentum of a particle at any time. Heisenberg's principle implies that in physical measurements probability takes the place of exactness and as such phenomena which are impossible according to classical may find a small but finite probability of occurrence.

Illustration (i) : Determination of position with g-ray-microscope. Suppose we try to measure the position and linear momentum of an electron using an imaginary microscope with a very high resolving power (Fig. 3.1). The electron can be observed if atleast one photon is scattered by it into the microscope leans. The resolving power of the microscope is given by the relation

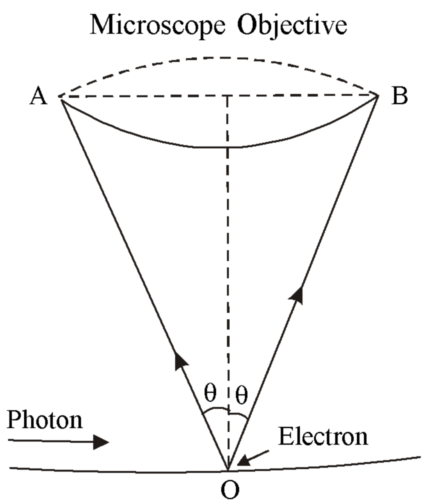


Figure 3.1

$$\Delta x = \frac{\lambda}{2\sin\theta}$$

where Δx is the distance between two points which can be just resolved by microscope. This is the range in which the electron would be visible when disturbed by the photon. Hence Δx is the uncertainty involved in the position measurement of the electron.

However, the incoming photon will interact with the electron through the Compton effect. To be able to see this electron, the scattered photon should enter the microscope within the angle 2θ. The momentum imparted by the photon to the electron during the impact is of the order of h/λ. The component of this momentum along OA is $-\frac{h}{\lambda}\sin\theta$ and that along OB is $\frac{h}{\lambda}\sin\theta$.

Hence the uncertainty in the momentum measurement in the x-direction is

$$\Delta p_X - \frac{h}{\lambda}\sin\theta - \left(-\frac{h}{\lambda}\sin\theta\right) = \frac{2h}{\lambda}\sin\theta.$$

$$\therefore \quad \Delta x \times \Delta p_X = \frac{\lambda}{2\sin\theta} \times \frac{2h}{\lambda}\sin\theta = h$$

A more sophisicated approach will show that $\Delta x\ \Delta p_X \geq h/2\pi$.

It is clear that the process of measurement itself perturbs the particle whose properties are being measured.

Illustration (ii) : Diffraction of a beam of electrons by a slit. A beam of electrons is transmitted through a slit and received on a photographic plate P kept at some distance from the slit (Fig 3.2). We can only say that the electron must have passed through the slit and cannot specify its exact location it the slit as the electron crosses it. Hence the position of any electron recorded on the plate is uncertain by an amount equal to the width of the slit (Δ y). Let λ be the wavelength of the electrons and θ be the angle of deviation corresponding to first minimum. From the theory of diffraction in optics. This is the uncertainty in determining the position of electron along y-axis.

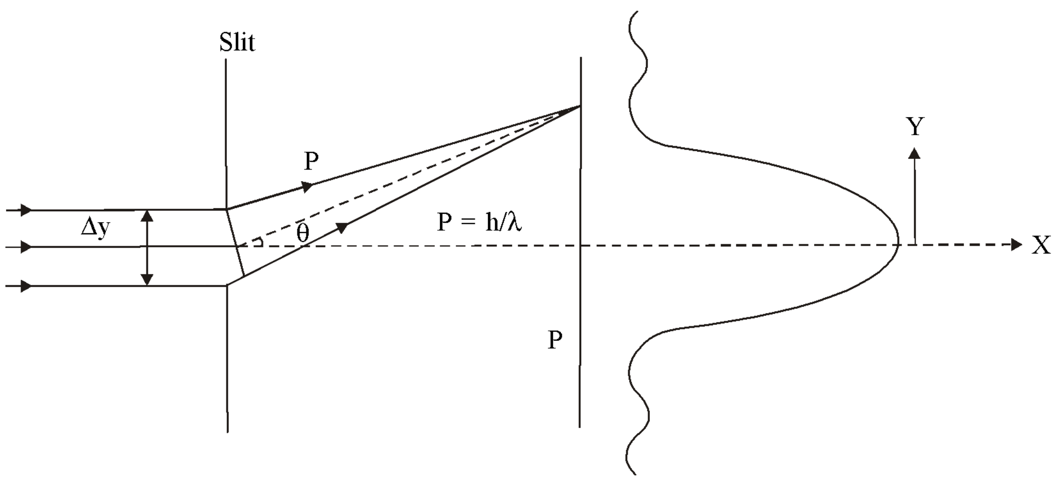


Figure 3.2

Initially the electrons are moving along X-axis and so they have no component of momentum along y-axis. As the electrons are deviated at the slit from their initial

Figure 1.3 : Typical blackbody radiation spectra

path to form the pattern, they acquire an additional component of momentum along y-axis. If p is the momentum of the electron on emerging from the slit, the component of momentum of electron along y-axis is p sin θ. As the electron may be where within the pattern from angle – θ to + θ, the y-component of momentum of the electron may be anywhere between –p sin θ and + p sin θ.

Therefore, the uncertainty in the y-component of momentum of the electron

$$\Delta p_y = 2p \sin\theta = \sin\theta \qquad \left(\text{since } \lambda = \frac{h}{p}\right)$$

$$\therefore \quad \Delta y\, \Delta p_y = \frac{\lambda}{\sin\theta} \times \frac{2h}{\lambda} \sin\theta = 2h$$

i.e., $\Delta y\, \Delta p_y \geq h/2\pi$, which is Heisenberg's uncertainty principle.

Problem 1. A microscope, using photons, is employed to locate an electron in an atom to within a distance of 0.2 Å. What is the uncertainty in the momentum of the electron located in this way?

Sol. Here, $\Delta x = 0.2$ Å $= 0.2 \times 10^{-10}$ m. Δp?

We have, $\Delta x\, \Delta p \approx \frac{h}{2\pi}$ or $\Delta p = \frac{h}{2\pi \Delta x}$

$$\therefore \quad \Delta p = \frac{6.626 \times 10^{-34}}{2\pi(0.2 \times 10^{-10})} = 5.274 \times 10^{-24}\, \text{kg ms}^{-1}$$

Problem 2. An electron has a speed of 600 ms^{-1} with an accuracy of 0.005%. Calculate the certainty with which we can locate the position of the electron. $h = 6.6 \times 10^{-34}$ J and $m = 9.1 \times 10^{-31}$ kg.

Sol. Momentum of the electron = $mv = 9.1 \times 10^{-31} \times 600$ kg ms^{-1}

$$\Delta p = \left(\frac{0.005}{100}\right) mv = (5 \times 10^{-5})(9.1 \times 10^{-31} \times 600)\ \text{kg ms}^{-1}$$

From uncertainty principle, $\Delta x\, \Delta p = h/2\pi$

$$\therefore \qquad \Delta x \approx \frac{h}{2\pi\Delta p} = \frac{6.6\times10^{-34}}{2\pi(5\times10^{-5}\times9.1\times10^{-31}\times600)}$$

$$= 0.003846 \text{ m.}$$

Problem 3. The lifetime of an excited state of an atom is about 10^{-8} sec. Calculate the minimum uncertainty in the determination of the energy of the excited state.

Sol. We have, $\Delta E\ \Delta t \geq h/2\pi$

$$\therefore \qquad \Delta E \geq \frac{h}{2\pi\Delta t} = \frac{6.6\times10^{-34}}{2\pi(10^{-8})}$$

$$\therefore \qquad \Delta E \geq 1.0 \times 10^{-26}\ \text{J} = 6.5 \times 10^{-8}\ \text{eV.}$$

This is known as the energy width of an excited state.

Problem 4. Consider an electron of momentum p in the Coulomb field of a proton. The field energy is

$$E = \frac{p^2}{2m} - \frac{e^2}{(4\pi\varepsilon_0)r},$$

where r is the distance of the electron from the proton. Assuming that the uncertainty Dr of the radial coordinate is $\Delta r \approx r$ and tha $\Delta p \approx p$, use Heisenberg's uncertainty principle to obtain at estimate of the size and the energy of the hydrogen atom in the ground state.

Sol. From the uncertainty principle, $\Delta p \geq \dfrac{(h/2\pi)}{\Delta r}$

Making the assumption $\Delta p \geq \dfrac{(h/2\pi)}{\Delta r} = \dfrac{(h/2\pi)}{r}$, we obtain

$$E = \frac{(h/2\pi)^2}{2m}\frac{1}{r^2} - \left(\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}\right)$$

The radius at which E is a minimum is given by the condition dE/dr = 0, from which we find

$$r = \frac{(4\pi\varepsilon_0)(h/2\pi)^2}{me^2} = a_0$$

The corresponding lowest value of E is

$$E_0 = \frac{e^4 m}{(4\pi\varepsilon_0)^2 2(h/2\pi)^2} = -13.6 \text{ eV}.$$

Problem 5. Compare the kinetic energies of an electron and a proton to localize them within an atomic radius which may be taken to be 10^{-8} cm, assuming the momenta of the particles to be equal to the uncertainties in their momentum.

From the uncertainty relation we have

$$\Delta p = \frac{\hbar}{\Delta x} = \frac{1.05\times10^{-27}}{10^{-8}} = 1.05 \times 10^{-19} \text{ gm cm/sec}$$

So the kinetic energy is

$$E_k = \frac{p^2}{2m} = \frac{\Delta p^2}{2m} = \frac{(1.05\times10^{-19})^2}{2\times1.6\times10^{-12} m} \text{eV} = \frac{3.445\times10^{-27}}{m} \text{eV}$$

For the electron, $m = 9.11 \times 10^{-28}$ gm

$$\therefore \; E_k = \frac{3.445\times10^{-27}}{9.11\times10^{-28}} = 3.78 \text{ eV}$$

For the proton, $m = 1.67 \times 10^{-24}$ gm

$$\therefore \; E_k = \frac{3.445\times10^{-27}}{1.67\times10^{-24}} = 0.0021 \text{ eV}$$

Problem 6. An atomic nucleus is made up of protons and neutrons, collectively known as nucleons. Calculate the uncertainty in the momentum of a nucleon inside a nucleus of mass number A = 64 and radius R = 48 × 10^{-13} cm and hence estimate its kinetic energy.

Volume of the nucleus is

$$V = \frac{4}{3}\pi R^3 = \frac{4}{3}\pi \times (4.8 \times 10^{-13})^3 = 463.2 \times 10^{-39}\,\text{cm}^3$$

Hence the volume available for each nucleon is

$$v = \frac{V}{A} = \frac{463.2 \times 10^{-39}}{64} = 7.24 \times 10^{-39}\,\text{cm}^3$$

Since the nucleons are strongly attracted by the neighbouring necleons, we assume that they are more or less confined within the volume *v*. So the uncertanity in the position of a nucleon is equal to the radius r or a sphere of volume $v = \frac{4}{3}\pi r^3$.

Hence

$$r = \left(\frac{3v}{4\pi}\right)^{1/3} = \left(\frac{3 \times 7.24 \times 10^{-39}}{4\pi}\right)^{1/3} = 1.2 \times 10^{-13}\,\text{cm}$$

So the uncertanity in the momentum of the nucleon is

$$\Delta p = \frac{\hbar}{r} = \frac{1.05 \times 19^{-27}}{1.2 \times 10^{-13}} = 8.75 \times 10^{-15}\,\text{gm cm / sec}$$

Assuming the momentum of the nucleon to be of the order of Δp, we get the kinetic energy of the nucleon

$$E_k = \frac{\Delta p^2}{2M} = \frac{(8.75 \times 10^{-15})^2}{2 \times 1.67 \times 10^{-24} \times 1.6 \times 10^{-6}} - 14.3\text{ MeV}$$

Problem 7. An atomic nucleus in an excited state makes transition to the ground state by the emission of γ-ray. If it remains in the excited state for about 10^{-13} sec, what is the uncertainty in the energy of the excited state? Compare it with the uncertainty in the energy of an atomic energy level which has a life time of about 10^{-8} sec.

Since $\Delta t = 10^{-3}$ sec

$$\Delta E = \frac{\hbar}{\Delta t} = \frac{1.05 \times 10^{-27}}{10^{-13} \times 1.6 \times 10^{-6}} = 6.56 \times 10^{-9} \text{ MeV} = 0.00656 \text{ eV}$$

Note that this is also the broadening of the γ-ray line during the transition since the ground state for which $\Delta t = \infty$ has zero energy broadening, i.e., $\Delta E = 0$.

For the atomic energy level, since $\Delta t = 10^{-8}$ sec, we have

$$\Delta E = \frac{\hbar}{\Delta t} = \frac{1.05 \times 10^{-27}}{10^{-8} \times 1.6 \times 10^{-12}} = 6.56 \times 10^{-8} \text{ eV}$$

Problem 8. An electron is observed by scattering a beam of protons from it in a so-called proton microscope. If the electron is initially at rest, show that the smallest distance within which it can be localized is equal to $(M_p/m_e)\ \bar{\lambda}_p$ where $\bar{\lambda}_p = \lambda_p/2p$; λ_p is the de Broglie wavelength of the proton.

Consider are incident proton of kinetic energy E_p to be scattered by the electron at an angle θ while the electron recoils at the angle ϕ. Then applying the laws of conservation of energy and momentum we can write (p' is the scattered proton).

$$E_p = E_{p'} + E_e$$

$$\text{or,} \quad \frac{p_p^2}{2M_p} = \frac{p_{p'}^2}{2M_p} + \frac{p_e^2}{2m_e}$$

where p's are the momenta, we also have

$$p_p = p_{p'} \cos\theta + p_e \cos\phi$$

$$0 = p_{p'} \sin\theta - p_e \sin\phi$$

Squaring and adding we get

$$p_{p'}^2 = (p_p - p_e \cos\phi)^2 + p_e^2 \sin^2\phi = p_p^2 + p_e^2 - 2p_p p_e \cos\phi$$

From the energy conservation equation, we also have

$$p_{p'}^2 = p_p^2 - \frac{M_p}{m_e} . p_e^2$$

Subtracting we have

$$0 = p_e^2(1 + m_p / m_e) - 2p_p p_e \cos\phi$$

or,

$$p_e = \frac{2p_p \cos\phi}{1 + M_p / m_e} \approx \frac{2m_e}{M_p} . p_p \cos\phi$$

Thus, the limits of p_e are $- 2m_e\, p_p/M_p$ and $+ 2m_e p_p/M_p$.

Hence

$$\Delta p_e = \frac{4me}{M_p} p_p$$

So from the uncertainty relation

$$(\Delta\, x)_{min} = \frac{\hbar}{\Delta p_e} = \frac{\hbar}{p_p} . \frac{M_p}{4m_e} = \frac{M_p}{4m_e} . \bar{\lambda}_p$$

3.4 The particle in a box

Let us discuss the possible energy states of a particle in a box on the basis of de Broglie's hypothesis. Consider a particle of mass m enclosed in a box of length L with impenetrable walls (Fig. 3.3). Suppose the (bound) particle is moving back and forth in the x-direction with constant speed v, making perfectly elastic collisions with the walls of the box. Since the walls of box are impenetrable, the particle cannot move beyond the walls and so the amplitude of the associated wave must drop to zero at the walls. In other words, the particle moving back and forth between opposite walls will form a stationary-wave pattern with nodes at the walls. Wave functions of the particle trapped in the box are shown in Fig 3.4. The general formula for the permitted by Broglie wavelength of the particle is

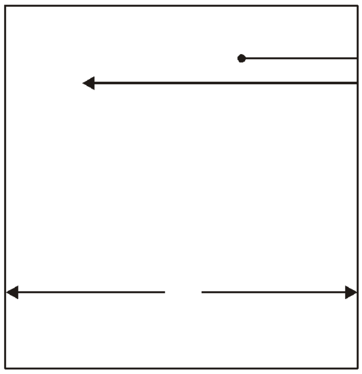


Figure 3.3

$$\lambda_n = \frac{2L}{n},\ n = 1, 2, 3 \qquad \text{.... (1)}$$

The possible values of the momentum of the particle are therefore,

$$p = \frac{h}{\lambda_n} = n\frac{h}{2L}$$

Consequently, the possible values of the kinetic energy of the particle are

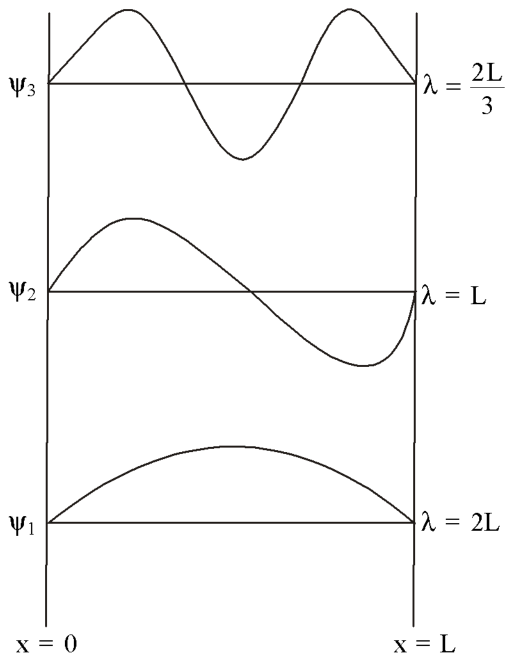


Figure 3.4

$$E_n = \frac{p^2}{2m} = n^2 \frac{h^2}{8mL^2} \quad .... (2)$$

Thus only certain discrete energy states are possible for the particle bound in a box. Each permitted energy is called an energy level. The integer n that specifies an energy level E_n is called is quantum number.

3.5 Mathematical Proof of Uncertanity Principle for one Dimensional Wave-packet

We shall derive the position-momentum uncertainty relation by using the theory of Fourier analysis. A moving particle corresponds to a single wave group. An isolated wave group is the result of superposing an infinite number of waves with different angular frequencies ω, continuous range of wave numbers k and amplitudes (Fig. 3.5). The composition produces oscillations confined to a single region of space and thus provides and idealized picture of a localized matter wave.

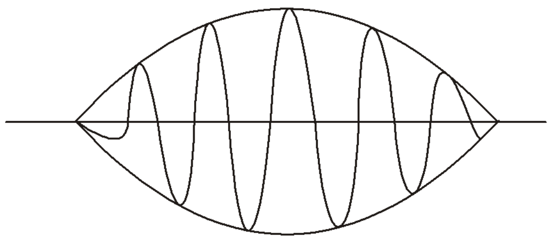


Figure 3.5

At a certain time t, the wave group ψ (x) can be represented by the Fourier intergal.

$$\psi(x) = \int_0^\infty g\,(k) \cos\, kx\, dk.$$

Here the amplitude function g (k) describes how the amplitudes of the waves that contributed to ψ (x) vary with wave number k. ψ (x) and g (k) are just Fourier transforms of each other. Fig. 3.6 shows Gaussian distribution for the amplitude function g (k) and the wave packet ψ (x). The relationship between distance Δx and the wave number Δk depends upo the shape of the wave group and upon how Δx and

Δk are defined. The widths Δx and Δk obey a reciprocal relation in which the product $\Delta s\ \Delta k$ is equal to pure number. The minimum value of the product $\Delta x\ \Delta k$ occurs when the envelope of the group has the bell shape of a Gaussian function (Fig. 3.6). Thus, the Gaussian wave packets happedn to be minimum uncertanity wave packets. If Δx and Δk are taken as the standard deviations of the respective functions ψ (x) and g (k), then this minimum value is 1/2. Wave groups in general do not have Gaussian forms. So we can write

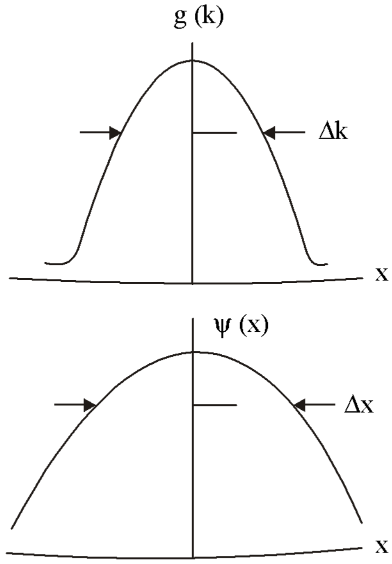


Figure 3.6

$$\Delta x\ \Delta k \geq \frac{1}{2} \qquad \text{... (1)}$$

Let λ be the de Broglie wavelength of the particle. We see from

$$k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h}$$

that the momentum of the particle is determined by the wave number k.

$$\therefore \qquad p = \frac{hk}{2\pi}$$

$$\Delta p = \frac{h\Delta k}{2\pi} = \hbar\Delta k$$

Hence an uncertanity Δk in the wave number of the de Brogile waves associated with the article results in an uncertainity Δp in the particle's momentum.

From Eq. (1) $\Delta x \, \Delta k \geq 1/2$ or $\Delta k \geq 1/2 \, \Delta x$

$$\Delta x \, \Delta p \geq \hbar/2 \qquad \text{... (2)}$$

This is Heisenberg uncertainty relation for position and momentum, according to which is uncertanity Δx is measuring the x coordinate of a particle is related to the uncertanity Δp_x in easurning the x component of the momentum, the product of the uncertainities being equal to or eater than $\hbar/2$.

The three-dimensional from of the Heisenberg uncertainty relations for position and momentum now

$$\Delta x \, \Delta p_x \geq \frac{\hbar}{2}, \; \Delta y \, \Delta p_y \geq \frac{\hbar}{2}, \; \Delta z \, \Delta p_z \geq \frac{\hbar}{2} \qquad \text{... (3)}$$

The theory of Fourier analysis may also be invoked to obtain a time-energy uncertanity relation Indeed, according to Fourier analysis, a wave packet of duration Δt must be composed of plane have components whose angular frequencies extend over a range Δw such that $\Delta t \, \Delta \omega \geq 1/2$. Since $\Delta t = \hbar\omega$ we therefore, have

$$\Delta t \, \Delta E \geq \hbar/2 \qquad \text{... (4)}$$

which is the Heisenberg uncertanity relation for time and energy. It connects the uncertainty DE in the determination of the energy of a system with the time interval Δt available for this energy determination. Thus, if a system does not stay longer than a time Δt in a given state or motion, its energy in that state will be uncertain by an amount $\Delta E \geq \hbar/2 \, \Delta t$.

3.6 Basic postulates of Wave Mechanics

In the development of Wave Mechanics, there are certain basic postulates, which are of fundamental importance. The fundamental postulates are three in number. Other wave properties follow from them.

(1) Each dynamical variable relating to the motion of a particle can be represented by a linear operator.

Explanation. In classical Physics certain definite functions of suitable variables are associated with each observable quantity. Thus (x, y, z) are associated with position, mv is associated with momentum $\frac{1}{2}mv^2$ associated with K.E. and so on.

Similarly, in wave mechanics and quantum mechanics, certain operators are associated with observable quantities. For the x-component of the linear momentum of a particle which has a classical expression $p_x = m\left(\frac{dx}{dt}\right)$ we have a quantum mechanical operator $-i\left(\frac{h}{2\pi}\right)\frac{\partial}{\partial x}$. In the vector from, this operator is $-i\left(\frac{h}{2\pi}\right)\nabla$. For angular momentum we can write the operator as $(r \times p) = -i\left(\frac{h}{2\pi}\right)(r\times\nabla)$. Similarly, for the observable total energy, the classical representation is $\frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + V(x, y, z)$

and the quantum mechanical operator is $-\frac{(h/2\pi)^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(x, y, z)$.

An operator tells us what operation to carry out on the quantity that follows it. The operator $t\left(\frac{h}{2\pi}\right)\frac{\partial}{\partial t}$ instructs us to take the partial derivative of what comes after it with respect to t and multiply the result by $i\left(\frac{h}{2\pi}\right)$.

Table 11.1 summarises the quantum operators for several physical quantities.

Table 11.1. Quantum operators

Quantity	Classical definition	Quantum operator
Position	r	r
Momentum	p	$-i\frac{h}{2\pi}\nabla$
Angular momentum	r × p	$-i\frac{h}{2\pi}r\times\nabla$
Kinetic energy	$p^2/2m$	$-\left(h^2/8\pi^2 m\right)\nabla^2$
Total energy	$p^2/2m + E_p(r)$	$-(h^2/8\pi^2 m)\nabla^2 + E_p(r)$

(2) A linear eigenvalue equation can be always linked with each operator.

Example. The total energy operator is $i\left(\frac{h}{2\pi}\right)\frac{\partial}{\partial t}$. Consider the eigen value equation $i\left(\frac{h}{2\pi}\right)\frac{\partial\psi}{\partial t} = E\psi$. Here ψ is said to be an eigenfunction of the operator $i\left(\frac{h}{2\pi}\right)\frac{\partial}{\partial t}$ and E is called the corresponding energy eigenvalue.

(3) In general, when a measurement of a dynamical quantity a is made on a particle for which the wave function ψ, we get different values of a during different trials. This is in conformity with the uncertanity principle. The most probable value of a is given by

$$< a > = \int_0^{\infty} \psi^* \hat{A}\psi \, dV$$

where $\hat{A}$ is the operator associated with the quantity a and ψ^* is the complex conjugate of ψ. The quantity < a > is called the expectation value of $\hat{A}$ (that is the value of a obtained in the majority of the trials). The expectation value of momentum and energy may be found by using the corresponding differential operator. Thus

$$< \vec{p} > = \int_{-\infty}^{\infty} \psi^*\left(-\frac{ih}{2\pi}\nabla\right)\psi \, dx\, dy\, dz$$

$$< E > = \int_{-\infty}^{\infty} \psi^*\left(i\frac{ih}{2\pi}\frac{\partial}{\partial t}\right)\psi \, dx\, dy\, dz$$

3.7 Derivation of Time-dependent form of Schrodinger Equation

The quantity that characterises the de Broglie waves is called the wave function. It is denoted by ψ. It may be a complex function. Let us assume that ψ is specified in the x direction by

$$\psi = Ae^{-i\omega(t - x/v)} \quad \dots (1)$$

If v is the frequency, then $\omega = 2\pi v$ and $v = v\lambda$.

$$\therefore \qquad \psi = Ae^{-2\pi(vt - x/\lambda)} \qquad \text{... (2)}$$

Let E be the total energy and p the momentum of the particle. Then E = hv and $\lambda = h/p$. Making these substitutions in Eq. (2).

$$\psi = Ae^{-(2\pi i/h)(Et - px)} \qquad \text{... (3)}$$

Eq. (3) is a mathematical description of the wave equivalent of an unrestricted particle of total energy E and momentum p moving in the +x directrion.

Differentiating Eq. (3) twice with respect to x, we get

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{4\pi^2 p^2}{h^2}\psi \qquad \text{... (4)}$$

Differentiating Eq. (3) twice with respect to t, we get

$$\frac{\partial\psi}{\partial t} = -\frac{2\pi i E}{h}\psi \qquad \text{... (5)}$$

At speeds small compared with that of light, the total energy E of a particle is the sum of its kinetic energy $p^2/2m$ and its potential energy V. V is in general a function of position x and time t.

$$\therefore \qquad E = \frac{p^2}{2m} + V \qquad \text{... (6)}$$

Multiplying both sides of Eq. (6) by ψ we get

$$E\psi = \frac{p^2\psi}{2m} + V\psi \qquad \text{... (7)}$$

From Eqs. (5) and (4) we see that

$$E\psi = -\frac{h}{2\pi i}\frac{\partial\psi}{\partial t} \qquad \text{... (8)}$$

and

$$p^2\psi = -\frac{h^2}{4\pi^2}\frac{\partial^2\psi}{\partial x^2} \qquad \text{... (9)}$$

Substituting these expressions for $E\psi$ and $p^2\psi$ into Eq. (7) we obtain

$$-\frac{h}{2\pi i}\frac{\partial\psi}{\partial t}=-\frac{h^2}{8\pi^2 m}\frac{\partial^2\psi}{\partial x^2}+V\psi$$

or
$$\frac{ih}{2\pi}\frac{\partial\psi}{\partial t}=-\frac{h^2}{8\pi^2 m}\frac{\partial^2\psi}{\partial x^2}+V\psi \qquad \text{... (10)}$$

Eq. (10) is the time-dependent form of Schrodinger's equation.

In three dimensions the time-dependent form of Schrodinger's equation is

$$\frac{ih}{2\pi}\frac{\partial\psi}{\partial t}=-\frac{h^2}{8\pi^2 m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+V\psi$$

Schrodinger's equation : Steady-state form

In a great many situations the potential energy of a particle does not depend upon time explicility. The forces that act upon it, and hence V, vary with the position of the particle only. When this is true. Schrodinger's equation may be simplified by removing all reference to t. The one-dimesional wave function ψ of an unrestricted particle may be written in the form

$$\psi = Ae^{-(2\pi i/h)(Et - px)}$$

$$= Ae^{-(2\pi i/E/h)t}.e^{+(2\pi ip/h)x}$$

$$\therefore \qquad \psi = \psi_0 e^{-(2\pi iE/h)t}$$

Here, $\psi_0 = Ae^{+(2\pi ip/h)x}$. That is, y is the product of a position dependent function ψ_0 and a time dependent function $e^{-(2\pi iE/h)t}$.

Differentiating Eq. (1) with respect to t, we get

$$\frac{\partial\psi}{\partial t}=-\frac{2\pi iE}{h}\psi_0 e^{-(2\pi iE/h)t} \qquad \text{... (2)}$$

Differentiating Eq. (1) twice with respect to x, we get

$$\frac{\partial^2\psi}{\partial x^2}=\frac{\partial^2\psi_0}{\partial x^2}e^{-(2\pi iE/h)t} \qquad \text{... (3)}$$

We can substitute these values in the time-dependent from of Schrodinger's equation

$$\frac{ih}{2\pi}\frac{\partial\psi}{\partial t} = -\frac{h^2}{8\pi^2 m}\frac{\partial^2\psi}{\partial x^2} + V\psi$$

$$\therefore \quad E\psi_0 e^{-(2piE/h)t} = -\frac{h^2}{8\pi^2 m}\frac{\partial^2\psi_0 e}{\partial x^2} e^{-(2\pi iE/h)t} + V\psi_0 e^{-(2\pi iE/h)t}$$

Dividing through by the common exponential factor, we get

$$\frac{\partial^2\psi_0}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi_0 = 0 \qquad \text{... (4)}$$

Eq. (5) is the steady-state form of Schrodinger's equation.

In three dimensions it is

$$\nabla^2\psi_0 + \frac{8\pi^2 m}{h^2}(E - V)\psi_0 = 0 \qquad \text{... (5)}$$

Usually it is written in the form

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

3.8 Properties of the Wave Function

Physical significance of ψ. The probability that a particle will be found at a given place in space at a given instant of time is characterised by the function ψ (x, y, z, t). It is called the wave function. This function can be either real or complex. The only quantity having a physical meaning is the square of its magnitude $P = \psi\psi^*$ where ψ^* is the complex conjugate of ψ. The quantity Pis the probability density. The probability of finding a particle in a volume dx, dy, dz, is $|\psi|^2$ dx dy dz. Further, since the particle is certanily to be found somewhere in space.

$$\iiint |\psi|^2 \; dx.\, dy.\, dz = 1$$

the triple integral extending over all possible values of x, y, z.

A wave function (ψ) satisfying this relation is called a normalised wave function.

Orthogonal and normalised wave functions. If the product of function $\psi_1(x)$ and the complex conjugate $\psi_2^*(x)$ of a function ψ_2 (x) vanishes when integrated with respect to x over the interval $a \le x \le b$, thatis, if

$$\int \psi_2{}^*(x)\psi_1(x)\,dx = 0$$

then ψ_1 and ψ_2 are said to be orthogonal in the interval (a, b).

We know that the probability of finding a particle in the volume element dV is given by $\psi\psi^*$ dV. The total probability of finding the particle in the entire space, is of course, unity, i.e.,

$$\int |\psi|^2\,dV = 1.$$

where the integration extends over all space. The above equation can also be written as

$$\int \psi\psi^*\,dV = 1.$$

Any wave function satisfying the above equation is said to be normalised to unity or simply normalised.

Very often ψ is not a normalized wave function. We know that it is possible to multiply ψ by a constant A, to give a new wave function. Aψ, which is also a solution of the wave equation. Now the problem is to choose the proper value of A such that the new wave function is a normalized function. In order that it is a normalized function, it must meet the requirement.

$$\int (A\psi)^* A\psi\,dx\,dy\,dz = 1$$

or, $$\left|A^2\right| \int \psi\psi^* dx\,dy\,dz = 1$$

or, $$\left|A^2\right| = \frac{1}{\int \psi\psi^*\,dx\,dy\,dz}$$

|A| is known as normalizing constant.

1. It must be well behaved, that is, single-valued and continuous everywhere.
2. If ψ_1 (x), ...ψ_n (x) are solutions of Schrodinger equation, then the linear combination y (x) = $a_1 \psi_1$ (x) + $a_2 \psi_2$ + ...$a_n \psi_n$ (x) must be a solution.
3. The wave function ψ (x) must approach zero as $x \to \pm \infty$

Eigenfunctions and Eigenvalues. Schrodinger's time-independent equation is an example of a type of differential equation called an eigenvalue equation. In general, we can write an eigenvalue equation as

$$F_{op} \psi = f\psi$$

The differential operator F_{op} operates on a function ψ, and this yields a constant f times the function. The function ψ is them called an eigenfunction of the operator F_{op}, and the corresponding value for f is called the eigenvalue.

Physical interpretation of ψ in Schrödinger representation ;

We have seen that the wave function ψ (x, t) which describes the complete space-time behaviour of a particle in one dimensional motion has appreciable amplitudes in those regions where the particle is likely to be found with greater probability. As discussed in § 3.3, quantities which are quadratic in the amplitude of the wave function are to be interpreted as the probability of finding a particle in a given region of space.

We shall assume that the quantity

$$|\Psi (x,t)|^2 dx = \Psi^* (x, t) \Psi (x, t) dx$$

is proportional to the probability of finding the particle in the interval x to x + dx at the time t where Ψ^* is the complex conjugate of Ψ. The total probability of finding the particle anywhere in space is

$$P \propto \int_{-\infty}^{\infty} |\Psi (x,t)|^2 dx$$

We define the position probability density as

$$\rho\ (x,\ t) = |\Psi\ (x,\ t)\ |^2 \,/ \int_{-\infty}^{\infty} |\Psi\ (x,t)|^2\ dx \tag{3.8.1}$$

Hence, the total probability will be

$$P = \int_{-\infty}^{\infty} P(x,t)dx = \int_{-\infty}^{\infty} |\Psi(x,t)|^2\, dx \,/ \int_{-\infty}^{\infty} |\Psi(x,t)|^2\, dx = 1 \tag{3.8.2}$$

This is as it should be, since the total probability must be unit.

Since $|Y\ (x,\ t)|^2$ is necessarily positive. Eq. (4.6-1) shows that the probability density ρ (x, t) is always positive which is consistent with the expected behaviour of probability.

If Ψ (x, t) is multiplied by a complex constant N such that Ψ_N (x, t) = Ψ_N (x, t) where Ψ_N (x, t) satisfies the relation

$$\int_{-\infty}^{\infty} |\psi_N(x,t)|^2\, dx = |N|^2 \int_{-\infty}^{\infty} |\Psi(x,t)|^2\, dx = 1 \tag{3.8.3}$$

then Ψ_N (x, t) is said to be the mormalized wave function. From Eq. (38) we have

$$|N|^2 = 1 / \int_{-\infty}^{\infty} |\Psi(x,t)|^2\, dx \tag{3.8.4}$$

N is called the normalization constant. Obviously a wave function is normalizable

if $\int_{-\infty}^{\infty} |\Psi(x,t)|^2\, dx$ or more generally $\int_{\tau} |\Psi(r,t)|^2\, d\tau$ over all space remains finite.

This is known as the square-integrability of the wave function. It should be noted that since the modulus squared $|N|^2$ is determined by Eq (38), the normalization constant N remains undefined to the extent of a phase factor.

Using Eqs. (4.6-1), (4.6-3) and (4.6-4), we get

$$\rho\ (x, t) = |\Psi_N\ (x, t)|^2 = \Psi_N^*(x, t)\ \Psi_N\ (x, t) \qquad (3.8.5)$$

Obviously the probability of finding the particle in an interval x to x + dx will be

$$\rho\ (x, t)\ dx = |\Psi_N\ (x, t)|^2\ dx \qquad (3.8.6)$$

The above relations can be generalised for the case of three dimensinal motion to give

$$\rho\ (r, t) = |\Psi\ (r, t)|^2 = \Psi^*\ (r, t)\ \Psi\ (r, t) \qquad (3.8.7)$$

$$P = \int_\tau |\Psi(r,t)|^2\, d\tau = 1 \qquad (3.8.8)$$

where Ψ (r, t) is here regarded as normalized and the integration is carred out over the entire three dimensional space.

Probability current density : Conservation of probability

Since the total probability

$$\int_\tau \rho(r,t)\, d\tau = \int_\tau |\psi(r,t)|^2\, d\tau = 1 = \text{cons tan t}$$

at every instant of time, any decrease of probability in a given volume element $d\tau$ must be associated with the corresponding increase of probability in some other element. The situation is analogus to the flow of charge from a given volume element. The change in the total quantity of charge contained in the given volume element should be equal to the net flow of charge through the surfaces enclosing the given volume element which is expressed by the equation of continuity :

$$\frac{\partial \rho}{\partial t} + \nabla . j = 0$$

where ρ is the charge density and j is the current density. An analogous relation can be deduced in the case of probability density.

Considering a finite volume τ enclosed by the surface S, we calculate the rate of change of the probability of finding the particle in τ :

$$\frac{\partial}{\partial t}\int_\tau \rho(r,t)d\tau = \frac{\partial}{\partial t}\int_\tau \Psi^*\Psi d\tau = \int_\tau \left(\frac{\partial \Psi^*}{\partial t}\Psi + \Psi^*\frac{\partial \Psi}{\partial t}\right)d\tau \tag{3.8.9}$$

Now Ψ satisfies the Schrödinger equation

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

Writing $\hat{H}$ explicity, we have

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

Assuming V to be real, we get the complex conjugate of the above equation as

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

So we have

$$\frac{\partial \Psi}{\partial t} = \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi$$

$$\frac{\partial \Psi}{\partial t} = -\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi^*$$

Then $$\frac{\partial \Psi}{\partial t}\Psi + \Psi^*\frac{\partial \Psi}{\partial t}$$

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

$$= -i\frac{\hbar}{2m}(\Psi\nabla^2\,\Psi^* - \Psi^*\nabla^2\,\Psi) \tag{3.8.10}$$

Now we know from vector analysis, that if u and v are two scalars, we can write

$$\nabla.(u\nabla v) = u\nabla^2 v + \nabla u.\nabla v$$

$$\nabla.(v\nabla u) = v\nabla^2 u + \nabla v.\nabla u = v\nabla^2 u + \nabla u.\nabla$$

Hence $$\nabla.(u\nabla v - v\nabla u) = u\nabla^2 v - v\nabla^2 u$$

So we can write

$$\Psi\nabla^2\Psi^* - \Psi^*\nabla^2\Psi = \nabla.(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi)$$

Then we have from Eqs. 3.8.9 & 3.8.10

$$\frac{\partial}{\partial t}\int_\tau \rho dr = -\frac{i\hbar}{2m}\int_\tau \nabla.(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi)\, d\tau \qquad (3.8.11)$$

We define probability current density as

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

Then from Eq. (3.8.11) we get by the application of vector divergence theorem

$$\frac{\partial}{\partial t}\int_\tau \rho d\tau = -\int_\tau \nabla.j\, d\tau = -\oint_S j.dS = -\oint_S j_n\, dS$$

Where n denotes the outward drawn unit vector normal to the surface element dS and j_n denotes the normal component of j.

Since Eq. (4.7-9) must hold for any arbitrary volume element, we have

$$\frac{\partial \rho}{\partial t} + \nabla.j = 0$$

This expresses the conservation of probability density. As stated above it is analogous to the classical conservation law of charge (or matter) in the absence of any source or sink.

Eq. (4.7-8) can also be written as

$$j = -\frac{\hbar}{m}\,\text{Im}\,(\Psi\nabla\Psi^*) = \frac{\hbar}{m}\,\text{Re}\,(i\,\Psi\nabla\Psi^*)$$

For one dimentional motion, the probability current density is given by

$$J_x = \frac{i\hbar}{2m}\left(\Psi\frac{d\Psi^*}{dy} - \Psi^*\frac{d\Psi}{dx}\right)$$

3.9 Summary

In this chapter the students got introduced to the fundamentals of quantum mechanics. They have come to know the Heisenberg's uncertainty principle and its simple applications. They are introduced to the characteristics of matter wave and the concepts of wave function, probability density, normalization, observables, operators and eigenvalues. They have learnt to obtain the time dependent Schrödubger equation and separate it into time dependent and steady state parts.

3.10 Questions

1. State and explain the Heisenberg's uncertainty principle. Why does the principle not reveal itself while working with macroscope object?
2. How and why does the concept of Bohr orbits violate the principle of uncertainty?
3. Discuss how the wave-particle dualism can be reconciled on the basis of the uncertainty principle.
4. Show from Heisenberg uncertainty relation, that electron cannot be a constituent of atomic nucleus.
5. How you would obtain the uncertainty relationship from an analysis for the hypothetical experiment of detection of γ ray photon by microscope?
6. What do you understand by the wave function ψ of a moving particle? Give the physical significance of wave function. What are the conditions and limitations the wave function of a particle must obey?

7. Outline the probability interpretation of the wave function. Obtain and explain the quantum mechanical probability conservation equation. What are stationary states? What are they so called?

8. What is the physical significance of normalization of a wave function? Why can't we represent matter waves associated with a free particle by a wave function ψ (x, t) = a sin (ωt-kx)?

9. Explain the terms "observable" and "operator". What is an eigenfunction and eigenvable?

10. Starting from the wave equation and introducing energy and momentum of the particle, obtain the time dependent Schrödinger equation. Separate the equation into time dependent and time independent parts and obtain the steady state Schrödinger equation.

Unit - 4 ❑ Application of Schrödinger equation to some simple problems

Structure

4.1 Objective

This chapter intends to impart knowledge to the students regarding the following topics :

- To study the application of Schrödinger equation for one dimensional infinitely rigid box and to calculate the energy eigenvalues and eigenfunctions with proper normalization for this problem.
- To study the application of Schrödinger equation in Quantum mechanical scattering and tunnelling in one dimension : across a step potential and across a rectangular potential barrier.

4.2 Introduction

This chapter aims to apply the quantum mechanical method for the study of some simple physical systems. The task would be to set up the Schrödinger's equation for the system concerned and to solve it too obtain the energy eigenvalues and the eigenfunctions and to explain their physical significance. This would provide some insight into the methods of application of quantum mechanics to physical problems.

4.3 Simple Applications of Schrodinger's Equation

The Particle in a Box : Infinite Square Well Potential

Consider a particle moving inside a box along the x-direction. The particle is bouncing back and forth between the walls of the box. The box has insurmountable potential barriers at x = 0 and x = L. i.e., the box is supposed to have walls of infinite height at x = 0 and x = L (Fig. 4.1). The particle has a mass m and its position x at any instant is given by $0 < x < L$.

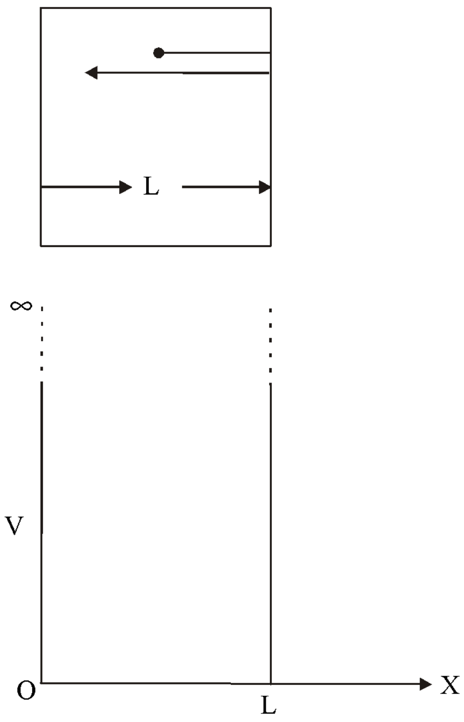


Figure 4.1

The potential energy V of the particle is infinite on both sides of the box. The potential energy V of the particle can be assumed to be zero between x = 0 and x = L.

In terms of the boundary conditions imposed by the probalem, the potential function is

$$V = 0 \text{ for } 0 < x < L$$

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

$$v = \infty \text{ for } x \leq L$$

The particle cannot exist outside the box and so its wave function ψ is 0 for $x \leq 0$ and $x \geq 1$. Our taks is to find what ψ is within the box. viz., between $x = 0$ and $x = L$.

Within the box, the Schrödinger's equation becomes

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi = 0.$$

Putting $\frac{8\pi^2 mE}{h^2} = k^2$, the equation becomes

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0.$$

The general solution of this equation is

$$\psi = A \sin kx + B \cos kx.$$

The boundary conditions can be used to evaluate the constants A and B in equation (1).

$$\psi = 0 \text{ at } x = 0 \text{ and hence } B = 0$$

$$\psi = 0 \text{ at } x = L. \text{ Hence } 0 = A \sin kL$$

Since A ¹ kL = np where n is an integer of $k = \frac{n\pi}{L}$

Thus $\psi_n(x) = A \sin \frac{n\pi x}{L}$

The enerfo of the particle = $E_m = \frac{k^2 h^2}{8\pi^2 m} = \frac{h^2 n^2 \pi^2}{L^2 8\pi^2 m}$

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

For each value of n, there is an energy level and the corresponding wavefunction is given by equation (2). Each value of E_n is called an eigenvalue and the corresponding ψ_n is called eigenfunction. Thus inside the box, the particle can only have the discerete energy values specified by equation t3 Note also that the particle have zero energy.

The particle in a box : Wave functions

It is certain that the particle is somewhere inside the box. Hence for a normalised wave function

$$\int_0^L \psi^* \psi \, dx = 1 \text{ i.e., } A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

i.e.,
$$A^2 \int_0^L \left(\frac{1 - \cos 2n\pi x / L}{2}\right) dx = 1 \text{ or } A^2 \frac{L}{2} = 1$$

or
$$A = \sqrt{\frac{2}{L}}$$

$\therefore$ The normalised wave functions of the partilce $= \psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$

The normalised wave functions ψ_1 ψ_2 and ψ_3 are plotted in Fig. 4.2.

Problem 1. Calculate the permitted energy levels of an electron, in a box 1 Å wide.

Solution. Here, m mass of the electron = 9.1×10^{-31} kg;

$L = 1$ Å $= 10^{-10}$ m.

$E_n = ?$

$\therefore$ The permitted electron energies, $E_n = \dfrac{n^2h^2}{8mL^2}$

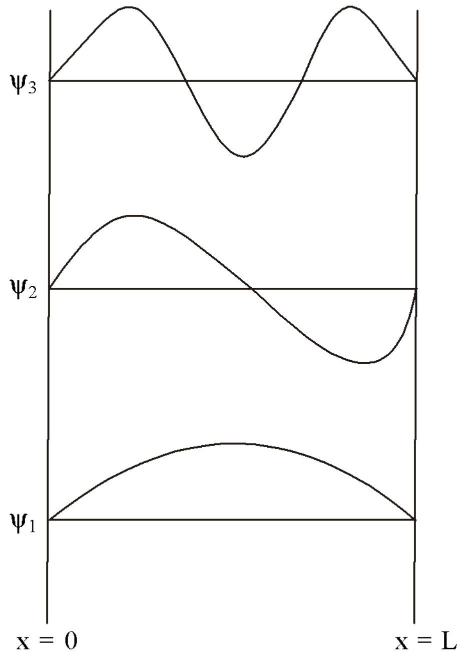


Figure 4.2

$$= \frac{n^2(6.626\times10^{-34})^2}{8(9.1\times10^{-31})(10^{-10})^2}$$

$$= 6 \times 10^{-18}\ n^2\ J = 38n^2\ eV.$$

The minimum energy, the electron can have, is E_1 = 38 eV, corresponding to n = 1.

The other values of energy are $E_2 = 4E_1$ = 152 eV, $E_3 = 9E_1$ = 342 eV and so on.

Problem 2. A particle is moving in a one-dimensional box (of infinite height) of width 10 Å. Calculate the probability of finding the particle within an interval of 1 Å at the centre of the box, when it is in its state of least energy.

Solution. The wave function of the particle in the ground state (n = 1) is

$$\psi_1 = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$$

The probability of finding the particle in unit interval at the centre of the box (x = L/2) is

$$P = \psi_1^2 = \left[\sqrt{\frac{2}{L}} \sin \frac{\pi(L/2)}{L}\right]^2 = \frac{2}{L} \sin^2 \frac{\pi}{2} = \frac{2}{L}.$$

∴ The probability of finding the particle within an interval of Δx at the centre of the box = W = $|\psi|^2 \Delta x = \frac{2}{L} \Delta x$

Here, $L = 10 \times 10^{-10}$ m and $\Delta x = 10^{-10}$ m.

$$\therefore \qquad W = \frac{2}{10 \times 10^{-10}} \times 10^{-10} = -0.2.$$

Problem 3. Calculate the expectation value $< p_x >$ of the momentum of a particle trapped in a one-dimensional box.

Solution. The normalized wave functions of the particle are

$$\psi_n^* = \psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

$$\frac{d\psi}{dx} = \sqrt{\frac{2}{L}} \left(\frac{n\pi}{L}\right) \cos \frac{n\pi x}{L}$$

Now, $$< p_x > = \int_{-\infty}^{\infty} \psi^* \left(-i \frac{h}{2\pi} \frac{d}{dx}\right) \psi \, dx$$

$$= -\frac{ih}{2\pi} \frac{2}{L} \frac{n\pi}{L} \int_0^L \sin \frac{n\pi x}{L} \cos \frac{n\pi x}{L} \, dx$$

$$= 0$$

The expection value $< p_x >$ of the particle's momentum is 0.

Problem 4. Find the expection value $< x >$ of the position of a particle trapped in a box L wide.

Solution. $$< x > = \int_{-\infty}^{\infty} x|\psi|^2 dx = \frac{2}{L}\int_0^L x\sin^2\frac{n\pi x}{L}dx$$

$$= \frac{2}{L}\left[\frac{x^2}{4} - \frac{\sin(2n\pi x/L)}{4n\pi/L} - \frac{\cos(2n\pi x/L)}{8(n\pi/L)^2}\right]_0^L$$

$$\therefore \qquad < x > = \frac{2}{L}\left(\frac{L^2}{4}\right) = \frac{L}{2}$$

This result means that the average position of the particle is the middle of the box in all quantum states.

Problem 5. Consider a one-dimensional of length a. There are two electrons in the box State their quantum numbers and calculate the lowest energy of the system.

Solution. The quantum numbers of the two electrons are

(1) $n = 1, l = 0, m_l = 0, m_s = +\frac{1}{2}$

(2) $n = 1, l = 0, m_l = 0, m_s = -\frac{1}{2}$

For lowest energy the electrons are in the ground state. As both the electrons are in the ground state, the total energy of the system

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

Here n = 1

$$E = \frac{h^2}{4ma^2}$$

Problem 6. Consider that a one-dimensional box of length a has three electrons. State the quantum numbers and the lowest energy of the system.

Solution. Here 2 electrons will be in ground state and 1 electron in the excited state (n = 2) (According to Pauli's exclusion principle) "No two electrons can be in the same quantum state".

(1) $n = 1,\ l = 0,\ m_l = 0,\ m_s = +\frac{1}{2}$

(2) $n = 1,\ l = 0,\ m_l = 0,\ m_s = -\frac{1}{2}$

(3) $n = 1,\ l = 0,\ m_l = 0,\ m_s = +\frac{1}{2}$

The energy of the system

$$E = \left[\frac{h^2}{8ma^2} + \frac{h^2}{8ma^2}\right] + \left(\frac{2^2 h^2}{8ma^2}\right)$$

$$E = \left[\frac{6h^2}{8ma^2}\right]$$

Problem 7. Deduce the zero point energy if the length of the box be 10^{-10} m and there are 10 electrons in it.

(The Coulomb interaction may be disregarded.)

Solution. The eyergy for a particle in a box

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

(i) There will be two electrons in the lowest energy level for n = 1

$$E_1 = 2\times\left(\frac{h^2}{8ma^2}\right)=\frac{h^2}{4ma^2}$$

(ii) There are in all 10 electrons, the next 8 electrons will have n = 2. This is according to the Pauli's exclusio principle. Here n = 2

and $$E_2 = 8x\left[\frac{2^2h^2}{8ma^2}\right]=\frac{4h^2}{ma^2}$$

Therfore total lowest energy of the system.

$$E = E_1 + E_2 = \frac{h^2}{4ma^2}+\frac{4h^2}{ma^2}=\frac{17h^2}{4ma^2}$$

Here $h = 6.624 \times 10^{-34}$ J-s

$m = 9.1 \times 10^{-31}$ kg

$a = 10^{-10}$ m

$$E = \frac{17\times(6.624\times10^{-34})^2}{4\times9.1\times10^{-31}\times(10^{-10})^2}$$

$= \mathbf{2.05 \times 10^{-16}}$ **J**

Problem 8. Calculate the mean energy per electron at 0 K if electrons are enclosed in a long-chain molecule of length 50 Å.

Solution. Here energy per electron

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

$h = 6.624 \times 10^{-34}$ J-s

$m = 9.1 \times 10^{-31}$ kg

$a = 50$ Å $= 50 \times 10^{-10}$ m

$$E = \frac{(6.624\times10^{-34})^2}{8\times9.1\times10^{-31}\times(50\times10^{-10})^2}$$

$E = \mathbf{2.4 \times 10^{-21}\ J}$

$$E = \frac{2.4\times10^{-21}}{1.6\times10^{-19}}$$

$E = \mathbf{1.5 \times 10^{-2}\ eV.}$

Problem 9. Consider that two electrons are confined to a box of length 10^{-10} m. Calculate the lowest energy of the system.

Solution. Here both the electrons are in the ground state for n = 1.

Energy of the system

$$E = 2\left[\frac{n^2h^2}{8ma^2}\right]$$

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

Here $h = 6.624 \times 10^{-34}$ J-s

$m = 9.1 \times 10^{-31}$ kg

$a = 10^{-10}$ m

$$E = \frac{2\times(6.624\times10^{-34})^2}{8\times9.1\times10^{-31}\times10^{-10})^2}$$

$E = \mathbf{1.205 \times 10^{-17}\ J}$

$$E = \frac{1.205\times10^{-17}}{1.6\times10^{-19}}\ \text{eV}$$

$E = \mathbf{75.3\ eV.}$

Problem 10. Consider that there electrons are confined to a one dimensional box of length 1 Å. Calculate the lowest energy of the system.

Solution. According to Pauli's exclusion principle, for first two electrons n = 1 and for the third electron n = 2.

$$a = 1 \text{ Å} = 10^{-10} \text{ m}$$

Total energy of the system

$$E = 2\left(\frac{h^2}{8ma^2}\right)+\left(\frac{2^2 h^2}{8ma^2}\right)$$

$$E = \frac{6h^2}{8ma^2}$$

$$= \frac{6\times(6.624\times10^{-34})^2}{8\times9.1\times10^{-31}\times(10^{-10})^2}$$

$$\mathbf{E = 3.615 \times 10^{-17} \ J}$$

$$E = \frac{3.615\times10^{-17}}{1.6\times10^{-19}} \text{ eV}$$

$$\mathbf{E = 225.93 \ eV.}$$

4.4 Concept of Quantum Confinement (QC)

According to Heisenberg uncertanity principle, if a moving particle with a mass m is confined to a region, say Δx length along the x-axis, then the uncertanity in its momentum (say Δp_x) is given by

$\Delta p_x \approx \hbar/\Delta x$ which can be simply written as, $\Delta p_x \approx \dfrac{\hbar}{\Delta x}$.(cf. $\hbar = h/2\pi$).

The Δp_x may be considered as the measure of momentum of the particle along the x-direction. This confinement along the x-axis, give the particle an additional amount of kinetic energy given by

$$E_{confinement} = \frac{(\Delta p_x)^2}{2m} = \frac{h^2}{2m(\Delta x)^2}$$

This confinement energy is meaningful, if it is comparable to the kinetic energy ($E_{x(T)}$) of the particle due to its thermal motion along the x-direction. Thus the condition is :

$$E_{confinement} = E_{X(T)} \approx \frac{1}{2}k_BT; \text{ or, } \frac{\hbar^2}{2m(\Delta x)^2} \approx \frac{1}{2}k_BT \text{ where } \hbar = \frac{h}{2\pi}$$

or $$\Delta x \approx \sqrt{\frac{\hbar^2}{mk_BT}}; \text{ or } \Delta x \approx \sqrt{\frac{h^2}{mk_BT}} \text{ taking } \Delta p_x\, \Delta x = h$$

The de Broglie wavelength (λ_{DR}) of the particle for its thermal motion along the x-axis given by :

$$\lambda_{DB} \approx \frac{h}{p_{X(T)}} = \frac{h}{\sqrt{2mE_{X(T)}}} = \frac{h}{\sqrt{mk_BT}} = \sqrt{\frac{h^2}{mk_BT}}\Delta x$$

Thus the condition of quantum confinement of a particle along a particular direction is :

The dimension of confinement must to be of the order the de Broglie wavelength (λ_{DB}) for the thermal motion of the particle in the direction.

The above condition tells us how small the dimension must be if we want to observe the size-dependent quantum confinement.

In general, it can be stated that a nanomaterial is in the state of quantum confinement when its size is in the order of de Broglie wavelength (λ_{DB}) of the charge carrier (i.e., electron or hole).

In a semiconducting nanoparticle like quantum dot (QD), its size must be comparable to that of the Bohr radius (r_B) of the exciton (i.e., bound electron-hole pair produced by the absorption of a photon in a semiconductor). This aspect will be discussed later in detail in Sec. 6.1.2.

Conditions of quantum confinement : Size ≈ λ_{DB} of electron of hole ; size ≈ exciton Bohr radius (r_B) in a semiconductor nanoparticle.

2D-Quantum Well : Quantum Confinement along One Direction

Let us consider a 2D-quantum well, where the carrier is allowed to move freely in the xy-plane while its motion is restricted along the z-axis. Then the quantised energy levels of the carrier (say electron) can be obtained by solving the following 1D-form of the time-independent Schrödinger equation.

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

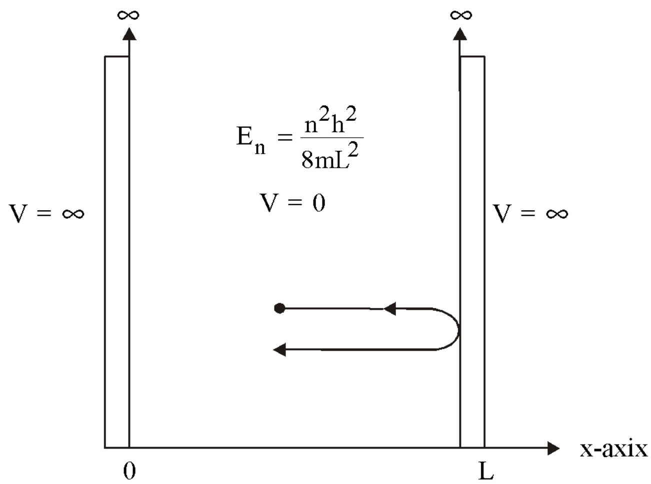


Figure 4.3 : Particle In a box model to describe the fate of electrons in nanoparticles

It is a problem similar to 'particle in a box' (Fig. 4.3) and V(z) is zero within the box which extends z = 0 to z = L_z. Sloving the Schrödinger equation under the boundary conditions and infinite depth approximation, we get :

$$E_{n_z} = \frac{n_z^2h^2}{8mL_z^2}, \quad (n_z, \text{ quantum number} = 1, 2, 3....)$$

$$\Delta E = E_{n_z+1} - E_{n_1} = (2n_z+1)\frac{h^2}{8mL_z^2}$$

It indicates that with the decrease of the dimension (L_z), the energy level spacing increases (of DE μ $1/L_z^2$ and $\Delta E >> k_BT$). In nanomaterials (i.e. L_z in the nanoscale), this effect is prominant and the phenomenon is called quantum size confinement effect.

In the 2D-quantum well, the motion of the carrier is restricted along the direction perpendicular to the plane of the well (i.e, energy levels are quantised in the direction normal to the well plane) but within the plane of the well, the motion of the carrier is unrestricted. Thus the total energy (E_{total}) of the carrier is given by the sum of energy due to the restricted motion along the z-direction (i.e. quantised energy) and unrestricted motion in the xy-plane. The in-plane carrier motion is characterized by a wave vector (k_{II}) which can be express in terms of the wave vectors for motion along the orthogonal in-plane directions (i.e, x- and y-directions) as follows :

$$k_{II} = \sqrt{k_x^2 + k_y^2}$$

The energy due to the unrestricted in-plane motion is given by :

$$E_{k_{II}} = \frac{\hbar^2 k_{II}^2}{2m}, \left(\text{of } E = \frac{p^2}{2m}, k = \frac{2\pi}{\lambda}, p \approx \hbar k = \frac{h}{\lambda}, \hbar = \frac{h}{2\pi} \right)$$

$$\text{i.e., } E_{(k_x, k_y)} = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2\right)$$

Thus the total energy of the carrier is given by :

$$E^{2D}_{n_z,(k_x,k_y)} = \underbrace{\frac{n_z^2 h^2}{8mL_z^2}}_{\substack{\text{(Quantum}\\ \text{cofinement}\\ \text{effect)}}} + \underbrace{\frac{\hbar^2}{2m}(k_x^2 + k_y^2)}_{\substack{\text{(Free carrier}\\ \text{motion in the}\\ \text{xy-plane)}}}$$

$E_{k_{II}}$, i.e. $E_{(k_x,k_y)}$ gives the continuous energy states due to the unrestricted values of k_x and k_y while $E_{n_{II}}$ gives the quantised and discrete energy levels due to the restricted values of n_z.

1D Quantum Wire : Quantum Confinement along Two Directions

In a 1D-quantum wire (having regular square or rectangular cross-sections), the carrier can move freely along the length (say x-direction) while its motion is restricted in the remaining two orthogonal directions (i.e, y- and z-directions). The quantised energies along they y- and z-directions can be calculated independently. The energy due to the free motion along the x-direction can also be calculated. The total energy of the carrier is given by :

$$E_{total}^{1D} = E_{n_y} + E_{n_z} + E_{k_x} = \frac{h^2 n_y^2}{8mL_y^2} + \frac{h^2 n_z^2}{8mL_z^2} + \frac{\hbar^2 k_x^2}{2m}$$

$$\underbrace{\frac{h^2}{8m}\left(\frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)}_{\substack{\text{Quantised energy states}\\ \text{due to confinement}\\ \text{along they y-and z-axes}}} + \underbrace{\frac{\hbar^2 k^2}{2m}}_{\substack{\text{Continuous energy}\\ \text{satesdue to free}\\ \text{movement along}\\ \text{the x-axis}}}$$

Note : For the quantum wires of complex cross-sections, the quantised energy states cannot be calculated by separating them in two terms as E_{n_y} and E_{n_z}. The quantised energy values can be obtained from the numerical solution of the appropriate Schoödinger equation.

0D Quantum Dot or Quantum Box : Quantum Confinement along Three Directions

In a 0D-quantum dot or quantum box, the carrier motion is restricted within the nanoscale in all three orthogonal directions (i.e. x, y and z-axes). For a simple cuboid shape nanocluster of dimensions L_x, L_y and L_z, the quantised energy values in three directions can be obtained separately. The total energy is given by :

$$E_{n_x,n_y,n_z}^{0D} = E_{n_x} + E_{n_y} + E_{n_z} = \underbrace{\frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)}_{\substack{\text{Quantised energy states along}\\ \text{the three orthogonal directions.}}}$$

Note : In all the above energy expressions, the carrier mass m should be replaced by effective mass m*.

Here each energy state is fully quantised and the energy difference between the successive discrete energy states is greater than the thermal energy (i.e. DE > k_BT) as in atoms (cf. continuous energy states in a 3D-bulk material). In reality, the quantum dot (QD), a 0D-particle, may not be necessarily cuboid-shaped and in such cases, a more complicated relationship showing the quantum confinement may be developed.

4.5 Potential step

The potential functional of a potential step is defined by

$$v(x) = 0 \qquad x < 0$$
$$= V_0 \qquad x > 0$$

Let electrons of energy E move from left to right, i.e., along the positive direction of x-axis (Fig. 4.4). It is desired to find the eigenfunction solutions of the time-independent Schrödinger equation.

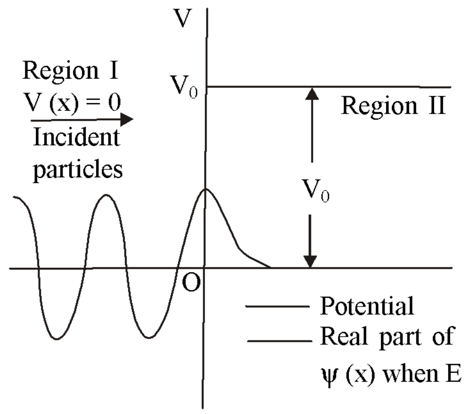


Figure 4.4

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \qquad \text{..... (2)}$$

For I region V(x) = 0. Therefore, the Schrödinger equation takes the form

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \qquad \text{... (3)}$$

The solution of Eq. (3) is

$$\psi_1 Ae^{ip_1x/\hbar} + Be^{-ip_1x/\hbar} \qquad \text{... (4)}$$

where A and B are constants.

$$p_1 = \sqrt{(2mE)}$$

Some particles may be reflected by the potential barrier and some transmitted. The first and second terms respectively represent the incident and reflected particles.

The Schrödinger wave equation for II region is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0 \qquad \text{... (5)}$$

The solution of Eq. (5) is

$$\psi_2 = Ce^{ip_2x/\hbar} + De^{-ip_2x/\hbar} \qquad \text{... (6)}$$

where $p_2 = \sqrt{\left[2m(E - V_0)\right]}$; C and D are constants.

In Eq. (6), the first term represents the transmitted wave. The second term represents a wave coming from + in the negative direction. Clearly for $x > 0$ no particles can flow to the left and D must be zero. Therefore, Eq. (6) becomes

$$\psi_2 = Ce^{ip_2x/\hbar} \qquad \text{... (7)}$$

The continuity of ψ implies that $\psi_1 = \psi_2$ at $x = 0$

$\therefore$ $A + B = C$. ... (8)

The continuity of $\frac{d\psi}{dx}$ implies that $\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$ at $x = 0$.

$\therefore$ $p_1 (A - B) = p_2C$ ... (9)

Solving (8) and (9) we get

$$B = \frac{p_1 - p_2}{p_1 + p_2} A \qquad \text{... (10}$$

and
$$C = \frac{2p_1}{p_1 + p_2} A \qquad \text{... (11)}$$

B and C represents the amplitudes of reflected and transmitted beams respectively in terms of the amplitude of the incident wave.

The reflectance and the transmittance at the potential discontinuity may be defined as follows :

Reflectance $R = \dfrac{\text{magnitude of reflected current}}{\text{magnitude of incident current}}$

Transmittance $T = \dfrac{\text{magnitude of transmitted current}}{\text{magnitude of incident current}}$

Two cases may rise : (i) $E > V_0$ and (ii) $E < V_0$

Case (i) : $E > V_0$. When $E > V_0$, $p_2 = \sqrt{[2m(E - V_0)]}$ is real.

We will now derive expressions for the current density in the I and II regions.

The probability current is defined as

$$J = \frac{\hbar}{2im}[\psi^* \nabla\psi - \psi\nabla\psi^*] \qquad \text{... (12)}$$

$$\therefore \ (J_x)_1 = \frac{\hbar}{2im}\left[\psi^*{}_1 \frac{d\psi_1}{dx} - \psi_1 \frac{d\psi_1^*}{dx}\right]$$

$$= \frac{\hbar}{2im}\left[\left\{\left(A^* e^{-p_1 x/\hbar} + B^* e^{ip_1 x/\hbar}\right) \times \left(\frac{ip_1}{\hbar}\right)\left(Ae^{-p_1 x/\hbar} + Be^{ip_1 x/\hbar}\right)\right\}\right]$$

$$-\left[\left\{\left(Ae^{-p_1 x/\hbar} + Be^{-ip_1 x/\hbar}\right) \times \left(\frac{ip_1}{\hbar}\right)\left(A^* e^{-p_1 x/\hbar} + B^* e^{ip_1 x/\hbar}\right)\right\}\right]$$

$$= \frac{p_1(AA^* - B^*B)}{m} = \frac{p_1}{m}\left[|A|^2 - |B|^2\right] \quad \text{... (13)}$$

From the above relation it is evident that the current in the I region is equal to the difference between two terms. The first term which is proportional to $p_1\ |A|^2$ represents the incident wave. The second term which is proportional to $p_1|B|^2$ represents the reflected wave.

$$\left.\begin{array}{l}\text{The probability current}\\ \text{of the incident beam}\end{array}\right\} = |A|^2 \frac{p_1}{m} \quad \text{... (14)}$$

$$\left.\begin{array}{l}\text{The probability current}\\ \text{of the reflected beam}\end{array}\right\} = |B|^2 \frac{p_1}{m} \quad \text{... (15)}$$

This expression for the probability current in region II is

$$(J_x)_{II} = \frac{\hbar}{2im}\left[\psi_2^* \frac{d\psi_2}{dx} - \psi_2 \frac{d\psi_2^*}{}\right]$$

$$= \frac{\hbar}{2im}\left[\left\{C^* e^{-ip_2x/\hbar}\left(\frac{ip_2}{\hbar}\right)Ce^{ip_2x/\hbar}\right\} - \left\{Ce^{ip_2x/\hbar}\left(\frac{ip_2}{\hbar}\right)C^* e^{-ip_2x/\hbar}\right\}\right]$$

$$= \frac{|C|^2 p_2}{m} \quad \text{... (16)}$$

Eq. (16) represent the transmitted current.

$$R = \frac{\text{magnitude of reflected current}}{\text{magnitude of incident current}}$$

$$= \frac{|B|^2 (p_1/m)}{|A|^2 (p_1/m)}$$

$$R = \frac{(p_1 - p_2)^2}{(p_1 + p_2)^2} \text{ from Eq. (10)} \quad \text{... (17)}$$

$$T = \frac{\text{magnitude of transmitted current}}{\text{magnitude of incident current}}$$

$$= \frac{|C|^2 (p_2/m)}{|A|^2 (p_1/m)}$$

$$= \left(\frac{2p_1}{p_1+p_2}\right)^2 \times \frac{p_2}{p_1} \text{ from Eq. (11)}$$

$$\therefore \quad T = \frac{4p_1p_2}{(p_1+p_2)^2} \qquad \text{... (18)}$$

Case (ii). $E < V_0$. When $E < V_0$, $p_2 = \sqrt{[2m(E-V_0)]}$ is imaginary.

Hence $p_2 = \sqrt{[2m(E-V_0)]}$ and $p_2^* = -i\sqrt{[2m(V_0-E)]} = -p_2$

The probability current in this case is given by

$$J_x = \frac{\hbar}{2im}\left[\psi_2^* \frac{d\psi_2}{dx} - \psi_2 \frac{d\psi_2^*}{dx}\right]$$

$$= \frac{\hbar}{2im}\left[C^* e^{-ip_2x/\hbar}\left(\frac{ip_2}{\hbar}\right)Ce^{ip_2x/\hbar} - Ce^{ip_2x/\hbar}\left(-\frac{ip_2^*}{\hbar}\right)C^* e^{-ip_2^*x/\hbar}\right]$$

Substituting $p_2^* = -p_2$ we get,

$$J_x = \frac{\hbar}{2im}\left[C^* e^{ip_2x/\hbar}\left(\frac{ip_2}{\hbar}\right)Ce^{ip_2x/\hbar} - CC^*\left(\frac{ip_2}{\hbar}\right)e^{ip_2x/\hbar}e^{ip_2x/\hbar}\right]$$

$$= 0$$

Thus the transmitted current is zero.

$$T = \frac{\text{magnitude of transmitted current}}{\text{magnitude of incident current}} = 0$$

$\therefore \quad T = 0$

By definition, $R + T = 1$

$\therefore \quad R = 1$ ... (20)

4.6 The Barrier Penetration Problem

Consider a beam of particles of kinetic energy E incident from the left of a potential barrier of height V and width OA = L (Fig. 4.5). V > E and on both sides of the barrier, V = 0, which means that no forces act upon the particles there. This potential is described by

$V = 0$ for $x < 0$ (region I)

$V = V$ for $0 < x < L$ (region II)

$V = 0$ for $x > L$ (region III) ... (1)

Let ψ_1, ψ_2 and ψ_3 be the respective wave function in regions, I, II and III as indicated in the figure.

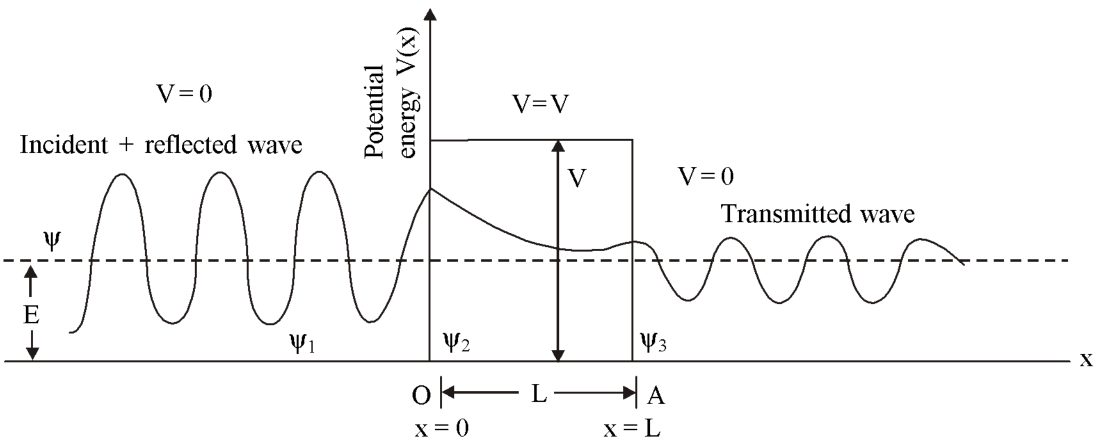


Figure 4.5

The corresponding Schrödinger equations are

region I $\quad \dfrac{d^2\psi_1}{dx^2} + \dfrac{8\pi^2 mE}{h^2}\psi_1 = 0$ since V = 0 region II $$\frac{d^2\psi_2}{dx^2}+\frac{8\pi^2 m}{h^2}(E-V)\psi_2=0 \quad (\because V = V)$$

region III $$\frac{d^2\psi_3}{dx^2}+\frac{8\pi^2 mE}{h^2}\psi_2=0 \quad (\because V = 0) \qquad \text{... (2)}$$

Put $\frac{8\pi^2 mE}{h^2}=\alpha^2$ and $\frac{8\pi^2 m(V-E)}{h^2}=\beta^2$

Then the equations become

region I $$\frac{d^2\psi_1}{dx^2}+\alpha^2\psi_1=0$$

region II $$\frac{d^2\psi_2}{dx^2}+\beta^2\psi_2=0 \qquad \text{... (3)}$$

region III $$\frac{d^2\psi_3}{dx^2}+\alpha^2\psi_3=0$$

The solutions to these equations are

region I $\psi_1 = Ae^{i\alpha x}+Be^{-i\alpha x}$

region II $\psi_2 = Fe^{-\beta x}+Ge^{\beta x}$ ... (4)

region III $\psi_3 = Ce^{i\alpha x}+De^{-i\alpha x}$

Where the constants A, B and so on are the amplitudes of the corresponding components of each wave. They may be recognized as follows :

A is the amplitude of the wave, incident on the barrier from the left,

B is the amplitude of the reflected wave in region I,

F is the amplitude of the wave, penetrating the barrier in region II,

G is the amplitude of the reflected wave (from the surface at A) in region II, C is the amplitude of the transmitted wave, in region III, and

D is the amplitude of a (nonexistent) reflected wave, in region III.

It should be noted that we have drawn the wave function through the three regions in Fig 4.5 so that it is continuous and singly valued everywhere along the x-axis.

Since the probability density associated with a wave function is proportional to the square of the amplitude of that function, we can define the barrier transmission coefficient as

$$T = \frac{|C|^2}{|A|^2}$$

and a reflection coefficient for the barrier surface at x = 0 as

$$R = \frac{|B|^2}{|A|^2}$$

If the barrier is high, compared to the total energy of the particle, or is thick compared to the wavelength of the wave function, then the transmission coefficient becomes

$$T \approx 16\frac{E}{V}\left(1-\frac{E}{V}\right)\exp\left[-\frac{2L}{(h/2\pi)}\sqrt{2m(V-E)}\right]$$

where L is the physical thickness of the barrier. The ratio $\frac{|C|^2}{|A|^2}$ is also called the 'penetrabilny' of the barrier. It represents the probability that a particle incident on the barrier from the side will appear on the other side. Such a probability is zero classically. But a finite quantity in quantum mechanics. We thus conclude that if a particle with energy E is incident on a thin energy barier of height greater than E, there is a finite probability of the particle penetrating the barrier. This phenomenon is called the tunnel effect. This effect was used by George Gamow in 1928 to explain in process of α-decay by radioactive nuclei.

Problem 1. The potential barrier problem is a good approximation to the problem of an electron trapped inside but near the surface of a metal. Calculate the probability of transmission there 1.0 eV electron will penetrate a potential barrier of 4.0 eV when the barrier width is 2.0 Å.

Solution. From equation (7) the transmission coefficient is

$$T = 16\left(\frac{1.0\,eV}{4.0\,eV}\right)\left(1-\frac{1.0\,eV}{4.0\,eV}\right)$$

$$X\exp\left[-\frac{2\times2\times10^{-10}\,m}{1.05\times19^{-34}\,Js}\sqrt{2(9.1\times10^{-31}\,kg)(4-1)(1.6\times10^{-19}\,J)}\right]$$

$$\approx 0.084$$

Thus, only about eight 1.0 eV electrons, out of every hundred, penetrate the barrier.

Problem 2. Calculate the width of the potential barrier of an α particle emitted with kinetic energy 4 MeV from a radioactive atom of atomic weight A = 222 and atomic number Z = 86.

Solution. Here $r_0 = (1.5 \times 10^{-15})\, A^{1/3},$ But A = 222

$$r_0 = (1.5 \times 10^{-15})\,(222)^{1/3}$$

$$r = 9 \times 10^{-15}\ m$$

Let r_1 be the distance from the centre of the nucleus where potential energy of the a particle is equal to the kinetic energy.

$$E = \frac{2(Z-2)e^2}{4\pi\varepsilon_0 r_i}$$

$$r_1 = \frac{2(Z-2)e^2}{4\pi\varepsilon_0 E}$$

Here $Z = 86$

$$\frac{1}{4\pi\varepsilon_0} = 9 \times 10^9$$

$$e = 1.6 \times 10^{-19}\ \text{C}$$

$$E = 4\ \text{MeV} = 4 \times 10^{-6} \times 1.6 \times 10^{-19}\ \text{J}$$

or $$E = 6.4 \times 10^{-13}\ \text{J}$$

$$\therefore \quad r_1 = \frac{2 \times 84 \times (1.6 \times 10^{-19})^2 \times 9 \times 10^9}{6.4 \times 10^{-13}}$$

$$r_1 = 60.48 \times 10^{-15}\ \text{m}$$

Width of the potential barrier

$$a = r_1 - r_0$$

or $$a = 60.48 \times 10^{-15} - 9 \times 10^{-15}$$

$$= \mathbf{51.48 \times 10^{-15}\ m}$$

Problem 3. A beam of electrons is incident on a potential barrier 5 eV high, 0.5 nm wide. What energy should they have if half of them are to get through the barrier ? [G.N.D.U., 1992]

$$h = 1.054 \times 10^{-34}\ \text{J-s}$$

Solution. Here $V_0 = 5\ \text{eV} = 5 \times 1.6 \times 10^{-19}\ \text{J}$

$$V_0 = 8 \times 10^{-19}\ \text{J}$$

$$m = 9.1 \times 10^{-31}\ \text{kg}$$

$$a = 0.5\ \text{nm} = 0.5 \times 10^{-9}\ \text{m}$$

$$a = 5 \times 10^{-10}\ \text{m}$$

$$T = \frac{1}{2}$$

$$E = ?$$

$$T = \frac{1}{1 + \dfrac{mV_0^2 a^2}{2E\hbar^2}}$$

$$1 + \left(\frac{mV_0^2 a^2}{2E\hbar^2}\right) = \frac{1}{T}$$

$$\frac{mV_0^2 a^2}{2E\hbar^2} = \frac{1}{T} = \left(\frac{1}{1/2}\right) - 1 = 1$$

$$\therefore \qquad E = \frac{mV_0^2 a^2}{2E\hbar^2}$$

$$E = \frac{(9.1\times10^{-31})(8\times10^{-19})^2\times(5\times10^{-10})^2}{2\times(1.054\times10^{-34})^2}$$

$$E = 65.53 \times 10^{-19}\ J$$

$$= \frac{65.53\times10^{-19}}{1.6\times10^{-19}} eV$$

$$= \mathbf{40.95\ eV}$$

Problem 4. Calculate the zero point energy of a system, constrained to move only in one direction, consisting of mass 1 gram connected to fixed point by a spring which is stretched 1 cm by a force of 1,000 dynes. [Delhi]

Solution. Displacement

$$x = A \sin 2\pi\ vt$$

$$\text{Restoring Force} = 4\pi^2 r^2\ mx$$

Here

$$m = 10^{-3}\ kg$$

$$x = 10^{-2}\ m$$

$$F = 10^{-2}\ N$$

$$F = 4\pi^2 v^2\ (10^{-3}) \times (10^{-2})$$

$$10^{-2} = 4\pi^2 v^2\ (10^{-5})$$

$$4\pi^2 v^2 = 1000$$

or

$$V = \frac{(1000)^{\frac{1}{2}}}{2\pi}$$

Zero point energy

$$U = \frac{1}{2} hv$$

$$U = \frac{6.6\times10^{-34}\times(1000)^{\frac{1}{2}}}{2\times2\times3.14}$$

$$U = 1.66 \times 10^{-33}\ J$$

4.7 Summary

The students have gathered knowledge about how to apply Schrödinger's equation for the study of some simple systems. They have studied the application of Schrödinger equation for one dimensional infinitely rigid box and calculated the corresponding energy eigenvalues and eigenfunctions with proper normalization. They also have applied the Schrödinger equation to study the Quantum mechanical scattering and tunnelling in one dimension, across a step potential and across a rectangular potential barrier respectively.

4.8 Questions

1. Set Schrödinger equation for a particle confined in a one dimensional infinite square well potential. Solve the equation to obtain the normalized wave function for the particle. Calculate the eigenfunctions and corresponding eigenvalues of momentum and energy.
2. How do the energy levels for a particle inside a box depend upon the box width a? What are the ground state and excited states? Draw the energy level diagram. Explain the term "degeneracy".
3. A particle of mass m is confined to a one-dimensional box of width 1. Derive expression for (i) the wave function and the (ii) probability density of the particle. Show these on separate graphs.
4. A particle of energy $E < V_0$ is approaching a potential barrier of hight V_0. Use quantum mechanical ideas to find the probability that the particle will leak through.
5. A particle of energy $E > V_0$ is incident on a finite potencial barrier of height V_0. Write the Schrödinger equation and the form of the wave function in different regions.

Unit - 5 ❑ Atomic Nucleus and its Structure

Structure

5.1 Objective

In this chapter you will learn about atomic nucleus and its properties.

5.2 Introduction

All nuclei are composed of two types of particles : protons and neutrons. The only exception is the ordinary hydrogen nucleus, which is a single proton. There are strong force which hold the particle together by overcoming the opposing coulomb force. The are certain kind of particle exchange which generates such a strong holding force.

5.3 Atomic Nucleus and its structure

Size and structure of atomic nucleus and its relationship with atomic weight

All nuclei are composed of two types of particles : protons and neutrons. The nuclei of all atoms of a particular element must contain the same number of protons, but they may contain different numbers of neutrons. Nuclei that are related in this way are called isotopes. The isotopes of an element have the same Z value, but different N and A values. The natural abundances of isotopes can differ substantially. For example,

$$^{11}_{6}C,\ ^{12}_{6}C,\ ^{13}_{6}C \text{ and } ^{14}_{6}C$$

are four isotopes of carbon. The natural abundance of the $^{12}_{6}C$ isotope is about

98.9%, whereas that of the $^{13}_{6}C$ isotope is only about 1.1%. Some isotopes don't occur naturally, but can be produced in the laboratory through nuclear reactions.

Mass

Particle	**kg**	**u**	**MeV/c²**
Proton	1.6726×10^{-27}	1.007276	938.28
Neutron	1.6750×10^{-27}	1.008665	939.57

Size of Nuclei

The size and structure of nuclei were first investigated in the scattering experiments of Rutherford. Using the principle of conservation of energy, Rutherford found and expression for how close an alpha particle moving directly towards the nucleus can come to the nucleus before being turned around by Coulomb repulsion.

Rutherford found that alpha particles approached to within 3.2×10^{-14} m of a nucleus when the foil was made of gold, implying that the radius of the gold nucleus must be less than this value. For silver atoms, the distance of closet approach was 2.3×10^{-14} m. From these results, Rutherford concluded that the positive charge in an atom is concentrated in a small sphere, which he called the nucleus, with radius no greater than about 10^{-14} m. Because such small lengths are common in nuclear physics, a convenient unit of length is the femotometer (fm), sometimes called the fermi and defined as 1 fm = 10^{-15} meter.

Nuclei are approximately spherical and have an average radius given by

$$r = r_0 A^{1/3}$$

where r_0 is a constant equal tp 1.2×10^{-15} m and A is the total number of nucleons. This relationship then suggests all nuclei have nearly the same density. Nucleons combine to form a nucleus as though they were tightly packed sphers.

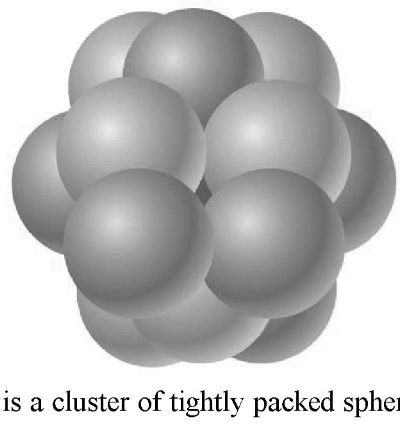


Figure 5.1 : A nucleus is a cluster of tightly packed sphere, each of which is nucleon

Impossibility of an electron being in nucleus as a consequence of the uncertanity principle :

The size of nucleus is 10^{-15} m. If electron exists within nucleus then uncertainty in position is 10^{-15} m. If the uncertainty in momentum is Δp then we can write as per Heisenberg uncertainty principle

$$\Delta x \Delta p \sim \hbar$$

$$\Delta p = \frac{h}{2\pi \Delta x}$$

$$\Delta p = \frac{6.63 \times 10^{-34}}{2\pi \times 10^{-15}}$$

$$\Delta p = 1.05 \times 10^{-19} \text{ kg.m/s}$$

Now we know $E = \sqrt{p^2c^2 + m_0^2 c^4} = T + m_0c^2$

Where T is the kinetic energy of the electron. Putting the value of electron we get

$$T = 19.3 \text{ MeV}$$

If the electron stays within the nucleus, then its kinetic energy at least 19.3 MeV. However, the kinetic energy of electron emitted in β-decay is around 4 MeV. So, we can conclude that the electron cannot stays within nucleus.

Nature of nuclear force :

Given that the nucleus consists of a closely packed collection of protons and neutrons, you might be surprised that it can even exist. The very large repulsive electrostatic forces between protons should cause the nucleus to fly apart. Nuclei, however, are stable because of the presence of another, short-range (about 2-fm) force : the nuclear force, an attractive force that acts between all nuclear particles.

The protons attract each other via the nuclear force, and at the same time they repel each other through the Coulomb force. The attractive nuclear force also acts between pairs of neutrons and between neutrons and protons. The nuclear attractive force is stronger than the Coulomb repulsive force within the nucleus (at short ranges). If it were not, stable nuclei would not exist. Moreover, the strong nuclear force is nearly independent of charge. In other words, the nuclear forces associated

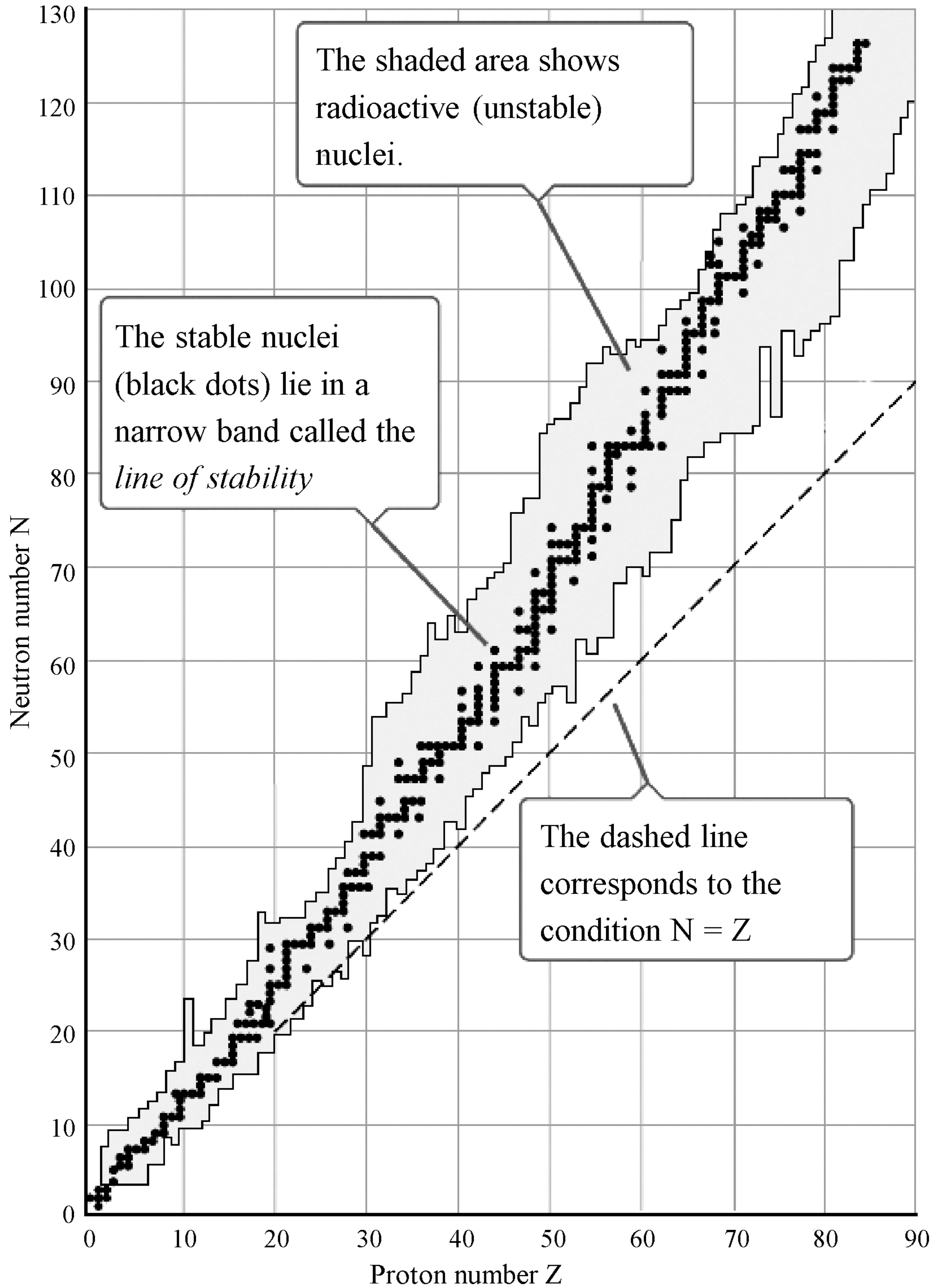


Figure 5.2 : A plot of the neutron number N versus the proton number Z for the stable nuclei (black dots).

with proton–proton, proton–neutron, and neutron– neutron interactions are approximately the same, apart from the additional repulsive Coulomb force for the proton–proton interaction.

There are about 260 stable nuclei; hundreds of others have been observed, but are unstable. A plot of N versus Z for a number of stable nuclei is given in Figure 2. Note that light nuclei are most stable if they contain equal numbers of protons and neutrons so that $N = Z$, but heavy nuclei are more stable if $N > Z$. This difference can be partially understood by recognizing that as the number of protons increases, the strength of the Coulomb force increases, which tends to break the nucleus apart. As a result, more neutrons are needed to keep the nucleus stable because neutrons are affected only by the attractive nuclear forces.

In effect, the additional neutrons "dilute" the nuclear charge density. Eventually, when $Z = 83$, the repulsive forces between protons cannot be compensated for by the addition of neutrons. Elements that contain more than 83 protons don't have stable nuclei, but, rather, decay or disintegrate into other particles in various amounts of time

Binding energy:

The total mass of a nucleus is always less than the sum of the masses of its nucleons. Also, because mass is another manifestation of energy, the total energy of the bound system (the nucleus) is less than the combined energy of the separated nucleons. This difference in energy is called the binding energy of the nucleus and can be thought of as the energy that must be added to a nucleus to break it apart into its separated neutrons and protons.

It's interesting to examine a plot of binding energy per nucleon, BE/A, as a function of mass number for various stable nuclei (Fig. 5.3). Except for the lighter nuclei, the average binding energy per nucleon is about 8 MeV. Note that the curve peaks in the vicinity of $A = 60$, which means that nuclei with mass numbers greater or less than 60 are not as strongly bound as those near the middle of the periodic table. As we'll see later, this fact allows energy to be released in fission and fusion reactions. The curve is slowly varying for $A > 40$, which suggests the nuclear force saturates. In other words, a particular nucleon can interact with only a limited number of other nucleons, which can be viewed as the "nearest neighbours" in the close-packed structure of a nucleus.

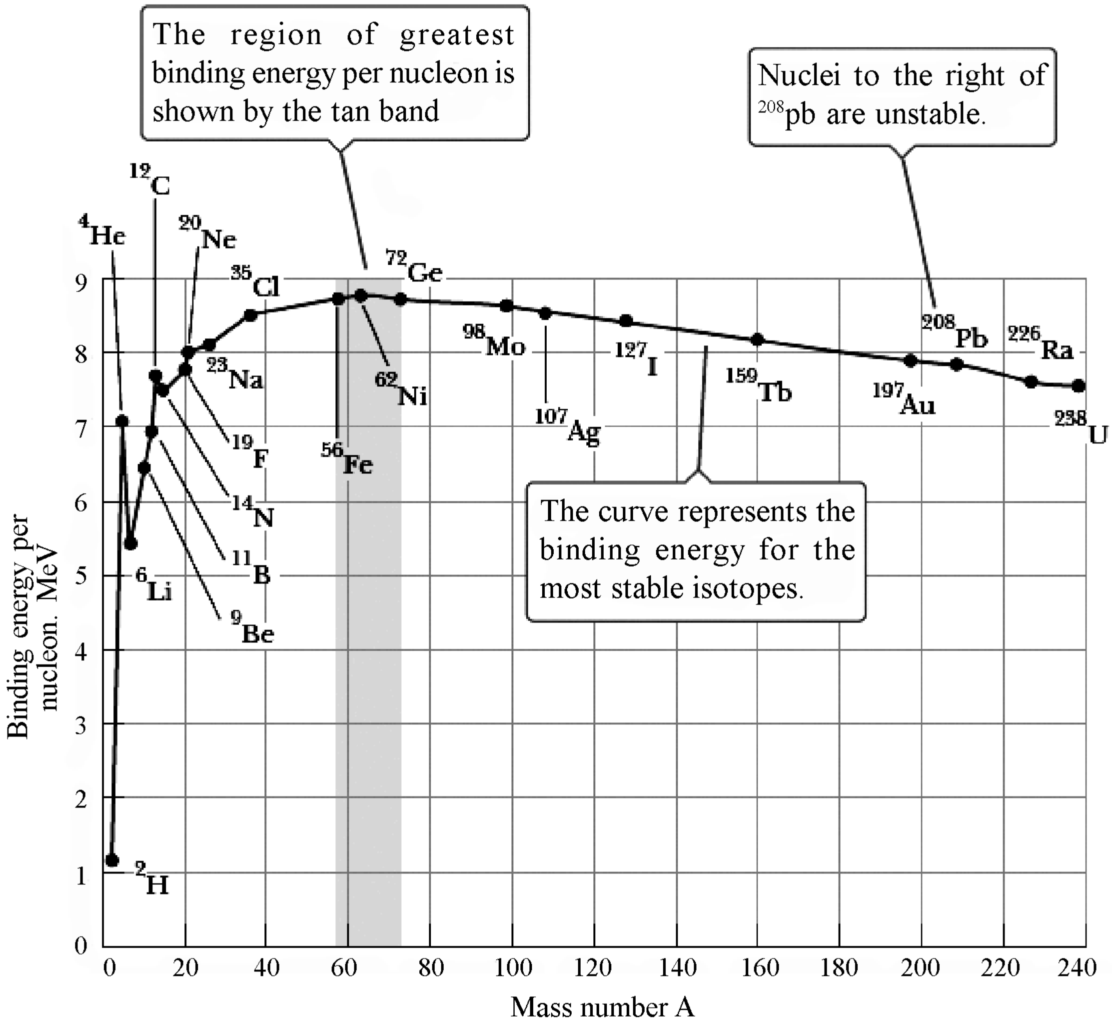


Figure 5.3 : Binding energy per nucleon versus the mass number A for nuclei

Semi-empirical mass formula:

The binding energy can be expressed as

where a_v (the volume term constant) and as (the surface term constant) are parameters to be determined from data.

$$B_E = a_\upsilon A - a_s A^{2/3}$$

The above expression for the binding energy is a reasonable approximation but does not reproduce a lot of the effects we have already seen. It predicts that the ground state binding energy only depends on A but is independent of Z or N, which we have already seen is not correct. It ignores quantum effects such as the Pauli exclusion principle (and others) completely. To get a better agreement we need to add three more terms which explicitly depend on Z and N.

The first term we will now add is easy to understand. We know there is an EM repulsive force between protons due to their charge and so this will reduce the binding energy for nucleons with several protons. As we believe the nuclear force itself is independent of nucleon type, then the protons will on average be spread evenly throughout the nucleus, which means the charge density is uniform. It is a standard problem in electrostatics to calculate the energy required to assemble a sphere of uniform charge density and the result is

$$\frac{3}{5}\frac{Q^2}{4\pi \in_0 r_0}$$

For a nucleus with Z protons, this self-energy is therefore

$$\Delta B_E = -\frac{3}{5}\frac{e^2}{4\pi \in_0 r_0}\frac{Z^2}{A^{1/3}} = -a_c\frac{Z^2}{A^{1/3}}$$

where ac = 0.72 MeV. Note the dependence on Z^2, not Z; the EM force is long range and so every proton affects every other proton in the nucleus, not just its nearest neighbours. Contrast this to the short range nuclear force where the nucleons only affect their nearest neighbours and the energy depends on A. In fact, although this Z^2 form is often used, strictly speaking it is not quite right. The energy given by the expression above is that needed to spread all the charge out throughout all space to an infinitely small density. However, the binding energy is defined as the energy need to break the nucleus into its constituent nucleons, i.e. break it into neutrons and protons, but not to spread the individual proton charges out. Indeed, the equation says even one proton, i.e. Z = 1, gives a correction to the binding energy, even though there is nothing to repel it. This means the correction to the binding energy should not be quite as big. A better form is

$$a_c Z(Z - 1)/A^{1/3}$$

which is now zero for Z = 1. Clearly, for large Z, as found in large nuclei, these two are very similar. We now have

$$B_E = a_\upsilon A - a_s A^{2/3} - a_c \frac{Z(Z-1)}{A^{1/3}}$$

This by itself breaks the independence on Z but clearly predicts the biggest binding energy for any A will be for Z = 0 or 1. We know this isn't right as we have stable nuclei with all values of charge up to Z > 100 in the atomic periodic table. We need to add two more terms to account for quantum effects.

The next term is called the "asymmetry term". The idea here is identical to the concept of a Fermi level in the physics of materials. The nucleons have energy levels in the nucleus and, being spin 1/2 particles, then each level can take two of each type of nucleon.

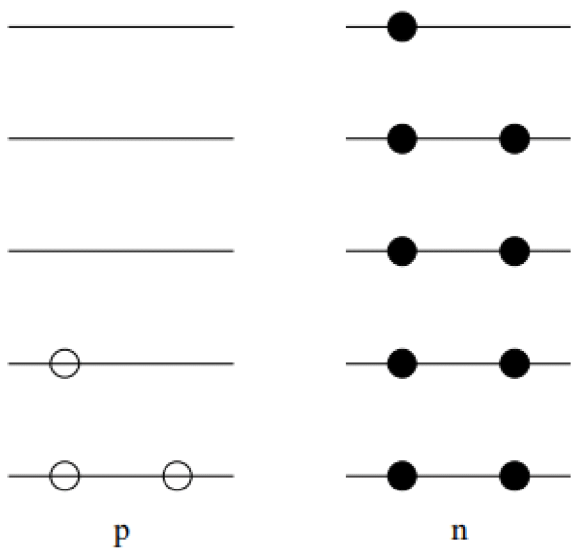


Figure 5.4

If a nucleus purely from neutrons, as implied by the terms it is so far for the binding energy, it would have to be put into higher and higher energy levels and so would be less and less strongly bound, reducing the binding energy. Clearly, putting protons into the nucleus instead would be beneficial for the binding energy as they could go into the deepest empty proton levels. It is clear the best situation is when the two are evenly balanced with N = Z. The details of the exact energy levels and numbers per level will be messy and vary with A, but a reasonable parametrisation turns out to given by ΔBE $\alpha - (N - Z)^2$, i.e. the binding energy is reduced symmetrically for either N > Z or Z >

N. In fact, the spacing between states depends inversely on the size of the nucleus, so that larger nuclei have less of a binding energy loss if $N \neq Z$, hence, the full term used is

$$-a_a (N - Z)^2/A$$

The final term which is needed is called the "pairing term". This occurs because of the different overlap of wavefunctions for pairs of nuclei in various states. For two identical nucleons in the same spatial state, with opposite spins to be antisymmetric as required, then the spatial wavefunctions are effectively identical and have maximal overlap. Because of the short range force, this gives more of a binding energy for this particular pair. This effect occurs for all nucleons except potentially the ones in the highest occupied energy level for each type of nucleon, where there is either one or two nucleons of that type. Hence, the nucleus will be more strongly bound for ones with an even number of nucleons of either type. There are three cases

1. Even-even, meaning an even number of both protons and neutrons, and hence even A. This has both pairs strongly bound.

2. Odd-odd, meaning an odd number of both protons and neutrons, and hence also even A. This is the least strongly bound.

3. Even-odd, meaning an even number of one type and an odd number of the other, and hence odd A. This has one strongly bound pair and so should be half way in between the previous two.

This is therefore simply parametrised by a form $a_p/A^{1/2}$, where a_p is takes its positive value for even-even nuclei, its negative value for odd-odd nuclei and is zero for even-odd nuclei. Note, the 2 pairing term implies even-even nuclei always have the spins of the nucleons in the same spatial state parallel, so all such nuclei would be expected to have ground states with total spin zero; this is observed to be true.

Therefore, the total expression for the binding energy is

$$B_E = a_\upsilon A - a_s A^{2/3} - a_c \frac{Z(Z-1)}{A^{1/3}} - a_a \frac{(N-Z)^2}{A} + a_p \frac{1}{A^{1/2}}$$

and this is the semi-empirical mass formula. The best-fit parameters take values around $a_v = 15.8$ MeV, $a_s = 18.3$ MeV, $a_c = 0.71$ MeV, $a_a = 23.2$ MeV and $a_p \pm 11.2$ MeV.

5.4 Summary

We have seen nuclear force is acting in short range and it is much more stronger than Coulomb repulsion. The nucleus is highly dense, and density of nucleus is almost same for all the elements.

5.5 Question

1. What is nuclear force ?
2. What is the range of nuclear force ?
3. What is binding energy ?
4. Binding energy depends on which factors ?
5. What is semi empirical mass formula ?

Unit - 6 ❑ α-decay; β-decay - Energy Released, Spectrum and Pauli's Prediction of Neutrino; γ-ray Emission

Structure

6.1 Objective

In this unit you will learn about radioactivity, decay of nucleus and energy released due during radioactivity.

6.2 Introduction

In 1896 Becquerel accidentally discovered that uranium salt crystals emit an invisible radiation that can darken a photographic plate even if the plate is covered to exclude light. After several such observations under controlled conditions, he concluded that the radiation emitted by the crystals was of a new type, one requiring no external stimulation. This spontaneous emission of radiation was soon called radioactivity. Subsequent experiments by other scientists showed that other substances were also radioactive.

The most significant investigations of this type were conducted by Marie and Pierre Curie. After several years of careful and laborious chemical separation processes on tons of pitchblende, a radioactive ore, the Curies reported the discovery of two previously unknown elements, both of which were radioactive. These elements were named polonium and radium. Subsequent experiments, including Rutherford's famous work on alpha-particle scattering, suggested that radioactivity was the result of the decay, or disintegration, of unstable nuclei.

6.3 Radioactivity

Three types of radiation can be emitted by a radioactive substance : alpha (a) particles, in which the emitted particles are $_2He^4$ nuclei; beta (b) particles, in which the emitted particles are either electrons or positrons; and gamma (g) rays, in which the emitted "rays" are high-energy photons.

Observation has shown that if a radioactive sample contains N radioactive nuclei at some instant, the number of nuclei, ΔN, that decay in a small time interval dt is proportional to ΔN; mathematically,

$$\frac{\Delta N}{\Delta t} \propto N$$

$$\Delta N = \lambda n \Delta t$$

where l is a constant called the decay constant. The negative sign signifies that N decreases with time; that is, ΔN is negative. The value of l for any isotope determines the rate at which that isotope will decay. The decay rate, or activity R, of a sample is defined as the number of decays per second. The decay rate is

$$R = \left|\frac{\Delta N}{\Delta t}\right| = \lambda N$$

Isotopes with a large l value decay rapidly; those with small l decay slowly.

Integrating the above equation we get

$$N = N_0 e^{-\lambda t}$$

where N is the number of radioactive nuclei present at time t, N_0 is the number present at time t = 0, and e = 2.718 . . . is Euler's constant.

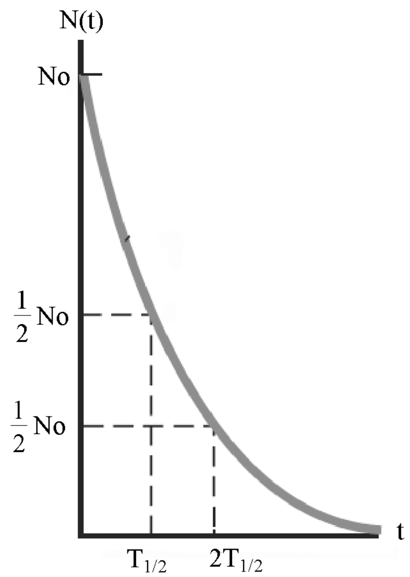


Figure 6.1 : Plot of the exponential decay law for radioactive nuclei

Mean life and half-life :

The half-life of a radioactive substance is the time it takes for half of a given number of radioactive nuclei to decay. From decay equation it can be shown that

$$N = N_0 \left(\frac{1}{2}\right)^n$$

where n is the number of half-lives. The number n can take any nonnegative value and need not be an integer.

Also we can write from the decay equation that

$$\frac{N_0}{2} = N_0 e^{-\lambda T_{1/2}}$$

$$T_{1/2} = \frac{\ell n_2}{\lambda} = \frac{0.693}{\lambda}$$

6.4 α-decay

If a nucleus emits an alpha particle ($_2He^4$), it loses two protons and two neutrons. Therefore, the neutron number N of a single nucleus decreases by 2, Z decreases by 2, and A decreases by 4. The decay can be written symbolically as

$$ {}^{4}_{Z}X \rightarrow {}^{A-4}_{Z-2}Y + {}^{4}_{2}He $$

where X is called the parent nucleus and Y is known as the daughter nucleus. As examples, ^{238}U and ^{226}Ra are both alpha emitters and decay according to the schemes

$$ {}^{238}_{92}U \rightarrow {}^{234}_{90}Th + {}^{4}_{2}He $$

$$ {}^{226}_{88}Ra \rightarrow {}^{222}_{80}Rn + {}^{4}_{2}He $$

The half-life for ^{238}U decay is 4.47×10^9 years, and the half-life for ^{226}Ra decay is 1.60×10^3 years. In both cases, note that the mass number A of the dauther nucleus is four less than of the parent nucleus, and the automic number Z is reduced by two. The differences are accounted for in the emitted alpha particle (the ^4He nucleus).

When one element changes into another, as happens in alpha decay, the process is called spontaneous decay or transmutation. As a general rule, (1) the sum of the mass numbers A must be the same on both sides of the equation, and (2) the sum of the atomic numbers Z must be the same on both sides of the equation.

For alpha emission to occur, the mass of the parent must be greater than the combined mass of the daughter and the alpha particle. In the decay process, this excess mass is converted into energy of other forms and appears in the form of kinetic energy in the daughter nucleus and the alpha particle. Most of the kinetic energy is carried away by the alpha particle because it is much less massive than the daughter nucleus. This can be understood by first noting that a particle's kinetic energy and momentum p are related as follows :

$$ KE = \frac{p^2}{2m} $$

Because momentum is conserved, the two particles emitted in the decay of a nucleus at rest must have equal, but oppositely directed, momenta. As a result, the lighter particle, with the smaller mass in the denominator, has more kinetic energy than the more massive particle.

6.5 β-decay

When a radioactive nucleus undergoes beta decay, the daughter nucleus has the same number of nucleons as the parent nucleus, but the atomic number is changed by 1:

$$^{A}_{Z}X \rightarrow {}^{A}_{Z+1}Y + e^{-}$$

$$^{A}_{Z}X \rightarrow {}^{A}_{Z-1}Y + e^{+}$$

Again, note that the nucleon number and total charge are both conserved in these decays. However, these processes are not described completely by these expressions. A typical beta decay event is

$$^{14}_{6}C \rightarrow {}^{14}_{7}N + e^{-}$$

The emission of electrons from a nucleus is surprising because, the nucleus is composed of protons and neutrons only. This apparent discrepancy can be explained by noting that the emitted electron is created in the nucleus by a process in which a neutron is transformed into a proton. This process can be represented by

$$^{1}_{0}n \rightarrow {}^{1}_{1}p + e^{-}$$

As with alpha decay, we expect the electron to carry away virtually all this energy as kinetic energy because, apparently, it is the lightest particle produced in the decay. As Figure 5 shows, however, only a small number of electrons have this maximum kinetic energy, represented as KE_{max} on the graph; most of the electrons emitted have kinetic energies lower than that predicted value. If the daughter nucleus and the electron aren't carrying away this liberated energy, where has the energy gone? As an additional complication, further analysis of beta decay shows that the principles of conservation of both angular momentum and linear momentum appear to have been violated

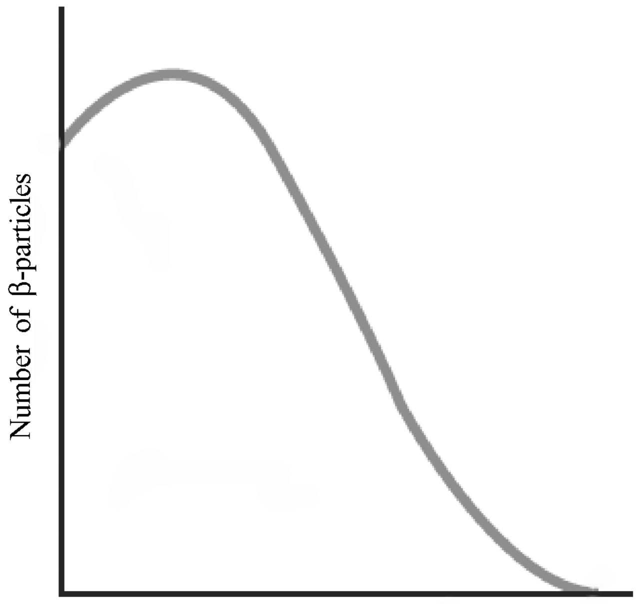


Fig 5.2 : Kinetic Energy of emitted beta particle

In 1930 Pauli proposed that a third particle must be present to carry away the "missing" energy and to conserve momentum. Later, Enrico Fermi developed a complete theory of beta decay and named this particle the neutrino ("little neutral one") because it had to be electrically neutral and have little or no mass. Although it eluded detection for many years, the neutrino (n) was finally detected experimentally in 1956. The neutrino has the following properties :

- Zero electric charge
- A mass much smaller than that of the elctron, but probably not zero. (Recent experiments suggest that the neutrino definitely has mass, but the value is uncertain, perhaps less than 1 eV/c^2).
- A spin of $\frac{1}{2}$
- Very weak interaction with matter, making it difficult to detect

With the introduction of the neutrino, we can now represent the beta decay process

$$^{14}_{6}C \rightarrow {}^{14}_{7}N + e^- + \bar{v}$$

The bar in the symbol $\bar{\nu}$ indicates an antineutrino. To explain what an antineutrino is, we first consider the following decay :

$$^{12}_{7}N \rightarrow \; ^{12}_{6}C + e^{+} + \nu$$

Here, we see that when ^{12}N decays into ^{12}C, a particle is produced that is identical to the electron except that it has a positive charge of 1e. This particle is called a positron. Because it is like the electron in all respects except charge, the positron is said to be the antiparticle of the electron. In beta decay, an electron and an antineutrino are emitted or a positron and a neutrino are emitted.

6.6 γ-ray emission

Very often a nucleus that undergoes radioactive decay is left in an excited energy state. The nucleus can then undergo a second decay to a lower energy state—perhaps even to the ground state—by emitting one or more high-energy photons. The process is similar to the emission of light by an atom. An atom emits radiation to release some extra energy when an electron " jumps" from a state of high energy to a state of lower energy. Likewise, the nucleus uses essentially the same method to release any extra energy it may have following a decay or some other nuclear event. In nuclear de-excitation, the " jumps" that release energy are made by protons or neutrons in the nucleus as they move from a higher energy level to a lower level. The photons emitted in the process are called gamma rays, which have very high energy relative to the energy of visible light.

A nucleus may reach an excited state as the result of a violent collision with another particle. It's more common, however, for a nucleus to be in an excited state as a result of alpha or beta decay. The following sequence of events shows the decay

$$^{12}_{5}B \rightarrow \; ^{12}_{6}C^{*} + e^{-} + \bar{\nu}$$

$$^{12}_{6}C^{*} \rightarrow \; ^{12}_{6}C + \gamma$$

$^{12}C^{*}$, where the asterisk indicates that the carbon nucleus is left in an excited state following the decay. The excited carbon nucleus then decays to the ground state by emitting a gamma ray. Note that gamma emission doesn't result in any change in either Z or A.

6.7 Summary

We have seen that some natural elements and artificial elements shows radioactivity. The decay time is different for different element ranging from few seconds to few thousands' years. Radioactivity is used in carbon dating and in treatment and diagnosis of diseases.

6.8 Questions

1. What is Radioactivity ?
2. What is half life ?
3. What is mean life ?
4. What is alpha and beta decay ?
5. Mention few uses of radioactivity.

Unit - 7 ❑ Fission and Fusion

Structure

7.1 Objective

- To get knowledge about nuclear fission and fusion.
- To know about Nuclear reactor and risk involved to manage a reactor.
- To get knowledge about thermos nuclear reactions.

7.2 Introduction

There are two means by which energy can be derived from nuclear reactions: fission, in which a nucleus of large mass number splits into two smaller nuclei, and fusion, in which two light nuclei fuse to form a heavier nucleus. In either case, there is a release of large amounts of energy that can be used destructively through bombs or constructively through the production of electric power.

7.3 Fission and Fusion

Nuclear Fission :

Nuclear fission occurs when a heavy nucleus, such as ^{235}U, splits, or fissions, into two smaller nuclei. In such a reaction **the total mass of the products is less than the original mass of the heavy nucleus**.

The fission of ^{235}U by slow (low-energy) neutrons can be represented by the sequence of events.

$$ {}^{1}_{0}n + {}^{235}_{92}U \rightarrow {}^{236}_{92}U^{*} \rightarrow X + Y + \text{neutrons} $$

where $^{236}U^{*}$ is an intermediate state that lasts only for about 10^{-12} s before splitting into nuclei X and Y, called fission fragments. Many combinations of X and Y satisfy the requirements of conservation of energy and charge. In the fission of uranium, about 90 different daughter nuclei can be formed. The process also results in the production of several (typically two or three) neutrons per fission event. On the average, 2.47 neutrons are released per event.

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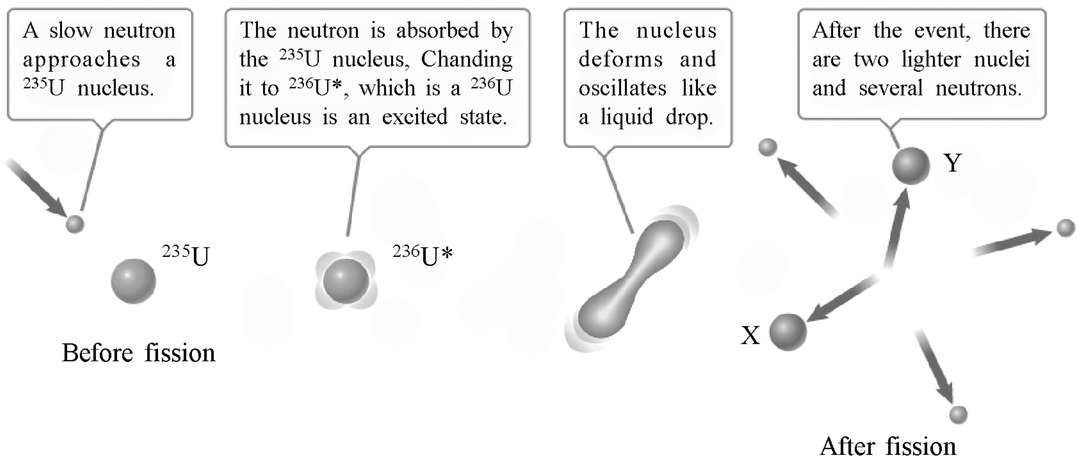

Figure 7.1 A nuclear fission event as described by the liquid drop model of the nucleus.

A typical reaction of this type is

$$ {}^{1}_{0}n + {}^{235}_{92}U \rightarrow {}^{141}_{56}Ba + {}^{92}_{36}Kr + 3\,{}^{1}_{0}n $$

The fission fragments, barium and krypton, and the released neutrons have a great deal of kinetic energy following the fission event. Notice that the sum of the mass numbers, or number of nucleons, on the left is same as the total number of nucleons on the right. The total number of protons (92) is also the same on both sides. The energy Q released through the disintegration 200.422 MeV.

The breakup of the uranium nucleus can be compared to what happens to a drop of water when excess energy is added to it. All the atoms in the drop have energy, but not enough to break up the drop. If enough energy is added to set the drop vibrating, however, it will undergo elongation and compression until the amplitude of vibration becomes large enough to cause the drop to break apart. The sequence of events is as follows :

1. The ^{235}U nucleus captures a thermal (slow-moving) neutron.
2. The capture results in the formation of $^{236}U^*$, and the excess energy of this nucleus causes it to undergo violent oscillations.
3. The $^{236}U^*$ nucleus becomes highly elongated, and the force of repulsion between protons in the two halves of the dumbbell-shaped nucleus tends to increase the distortion.
4. The nucleus splits into two fragments, emitting several neutrons in the process.

Nuclear Fusion :

When two light nuclei combine to form a heavier nucleus, the process is called nuclear fusion. Because the mass of the final nucleus is less than the sum of the masses of the original nuclei, there is a loss of mass, accompanied by a release of energy. Although fusion power plants have not yet been developed, a worldwide effort is under way to harness the energy from fusion reactions in the laboratory.

Fusion in the Sun :

All stars generate their energy through fusion processes. About 90% of stars, including the Sun, fuse hydrogen, whereas some older stars fuse helium or other heavier elements. The energy produced by fusion increases the pressure inside the star and prevents its collapse due to gravity.

Two conditions must be met before fusion reactions in the star can sustain its energy needs. First, the temperature must be high enough (about 10^7 K for hydrogen) to allow the kinetic energy of the positively charged hydrogen nuclei to overcome their mutual Coulomb repulsion as they collide. Second, the density of nuclei must be high enough to ensure a high rate of collision.

It's interesting to note that a quantum effect is key in making sunshine. Temperatures inside stars like the Sun are not high enough to allow colliding protons to overcome the Coulomb repulsion. In a certain percentage of collisions, however, the nuclei pass through the barrier anyway an example of quantum tunneling.

The proton–proton cycle is a series of three nuclear reactions that are believed to be the stages in the liberation of energy in the Sun and other stars rich in hydrogen. An overall view of the proton–proton cycle is that four protons combine to form an alpha particle and two positrons, with the release of 25 MeV of energy in the process.

The specific steps in the proton–proton cycle are

$$ {}^{1}_{1}H + {}^{1}_{1}H \rightarrow {}^{2}_{1}D + e^{-} + v $$

$$ {}^{1}_{1}H + {}^{2}_{1}D \rightarrow {}^{3}_{2}He + \gamma $$

where D stands for deuterium. The second reaction is followed by either hydrogen-helium fusion or helium-helium fusion :

$$ {}^{1}_{1}H + {}^{3}_{2}He \rightarrow {}^{4}_{2}He + e^{+} + v $$

$$ {}^{3}_{2}He + {}^{3}_{2}He \rightarrow {}^{4}_{2}He + 2({}^{1}_{1}H) $$

The energy liberated is carried primarily by gamma rays, positrons, and neutrinos, as can be seen from the reactions. The gamma rays are soon absorbed by the dense gas, raising its temperature. The positrons combine with electrons to produce gamma rays, which in turn are also absorbed by the gas within a few centimeters. The neutrinos, however, almost never interact with matter; hence, they escape from the star, carrying about 2% of the energy generated with them. These energy-liberating fusion reactions are called thermonuclear fusion reactions. The hydrogen (fusion) bomb, first exploded in 1952, is an example of an uncontrolled thermonuclear fusion reaction.

7.4 Nuclear reactor

The neutrons emitted when ^{235}U undergoes fission can in turn trigger other nuclei to undergo fission, with the possibility of a chain reaction. Calculations show that if the chain reaction isn't controlled, it will proceed too rapidly and possibly result in the sudden release of an enormous amount of energy (an explosion), even from only 1 g of ^{235}U.

A nuclear reactor is a system designed to maintain what is called a self-sustained chain reaction, first achieved in 1942 by a team led by Enrico Fermi. Most reactors in operation today also use uranium as fuel. Natural uranium contains only about 0.7% of the ^{235}U isotope, with the remaining 99.3% being the ^{238}U isotope. This fact is important to the operation of a reactor because ^{238}U almost never undergoes fission. Instead, it tends to absorb neutrons, producing neptunium and plutonium.

For this reason, reactor fuels must be artificially enriched so that they contain several percent of the ^{235}U isotope.

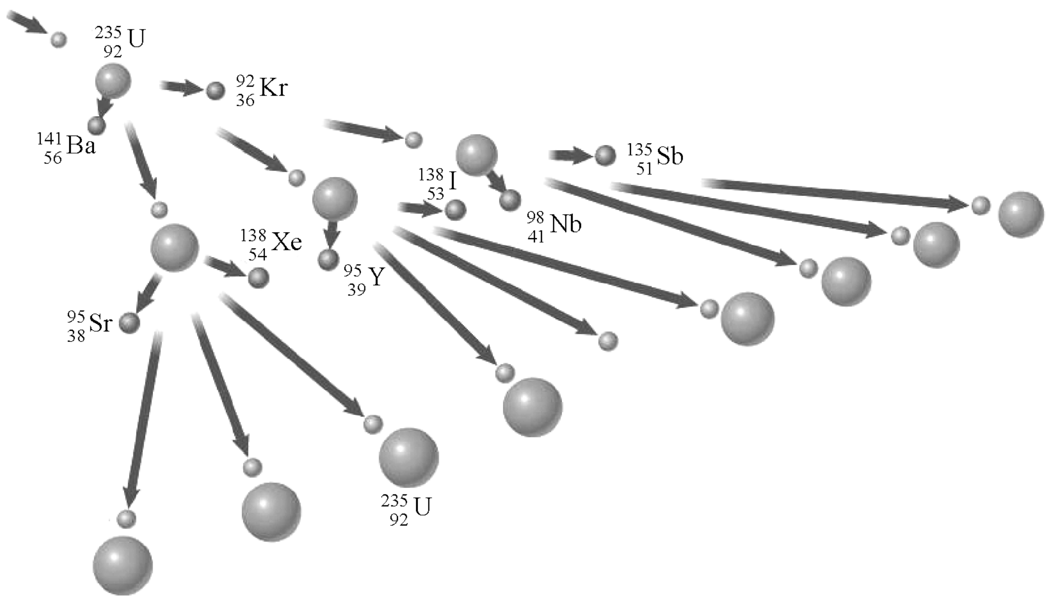

Figure. 7.2

On average, about 2.5 neutrons are emitted in each fission event of ^{235}U. To achieve a self-sustained chain reaction, one of these neutrons must be captured by another ^{235}U nucleus and cause it to undergo fission. A useful parameter for describing the level of reactor operation is the reproduction constant K, defined as the average number of neutrons from each fission event that will cause another event.

A self-sustained chain reaction is achieved when K = 1. Under this condition, the reactor is said to be critical. When K is less than 1, the reactor is subcritical and the reaction dies out. When K is greater than 1, the reactor is said to be supercritical and a runaway reaction occurs. In a nuclear reactor used to furnish power to a utility company, it is necessary to maintain a K value close to 1.

The basic design of a nuclear reactor is shown in Figure 7.3. The fuel elements consist of enriched uranium. The size of the reactor is important in reducing neutron leakage: a large reactor has a smaller surface-to-volume ratio and smaller leakage than a smaller reactor.

It's also important to regulate the neutron energies because slow neutrons are far more likely to cause fissions than fast neutrons in ^{235}U. Further, ^{238}U doesn't absorb slow neutrons. For the chain reaction to continue, the neutrons must, therefore, be slowed down. This slowing is accomplished by surrounding the fuel with a substance called a moderator, such as graphite (carbon) or heavy water (D_2O).

Most modern reactors use heavy water. Collisions in the moderator slow the neutrons and enhance the fissioning of ^{235}U. The power output of a fission reactor is controlled by the control rods depicted in Figure 7.3. These rods are made of materials like cadmium that readily absorb neutrons.

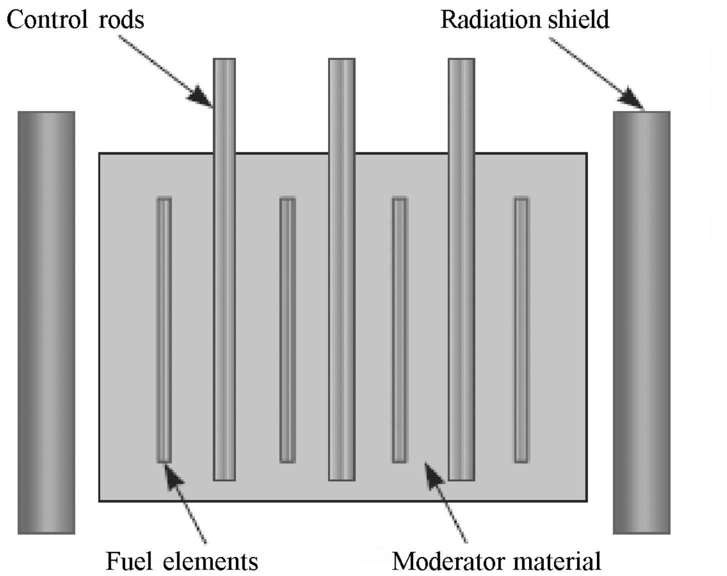

Fig 7.3 Cross section of a reactor core

Fissions in a nuclear reactor heat molten sodium (or water, depending on the system), which is pumped through a heat exchanger. There, the thermal energy is transferred to water in a secondary system. The water is converted to steam, which drives a turbine-generator to create electric power.

7.5 Summary

This nuclear energy may solve our energy crisis for thousands of years. Using safety measure and new technology like breeder reactor may help us to solve the energy crisis. Our ocean has a source of Uranium which may provide us energy security in near future.

7.6 Question

1. What is nuclear fission and fusion ?
2. What is slow neutron and fast neutron ?
3. What is moderator ?
4. Which kind of product used as moderator ?
5. What is the source of energy in Sun ?

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