5.3. (*b*) ONE-DIMENSIONAL SIMPLE HARMONIC OSCILLATOR IN QUANTUM MECHANICS

Wave Equation for the Oscillator

The time-independent Schrödinger wave equation for linear motion of a particle along the x-axis is :

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

or
$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}(E-V)\,\psi=0 \qquad \text{... (1)}$$

where E is the total energy of the particle, V the potential energy, and ψ the wave-function for the particle, which is a function of x alone.

For a linear oscillator along the x-axis with the angular frequency ω under a restoring force proportional to the displacement x, the potential energy is given by :

$$\boxed{V=\frac{1}{2}m\omega^2x^2} \qquad \text{... (2)}$$

Substituting the value of V in Eq. (1) we get :

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}\left(E-\frac{1}{2}m\omega^2x^2\right)\psi=0 \qquad \text{... (3)}$$

or
$$\frac{d^2\psi}{dx^2}+\left(\frac{2mE}{\hbar^2}-\frac{m^2\omega^2}{\hbar^2}x^2\right)\psi=0 \qquad \text{... (4)}$$

This is the Schrödinger wave equation for the oscillator.

Simplification of the Wave Equation

To simplify Eq. (4), we introduce a dimensionless independent variable y which is related to x by the equation :

$$y=ax \qquad \text{... (5)}$$

so that
$$x=\frac{y}{a},$$

where
$$a=\sqrt{\frac{m\omega}{\hbar}}$$

Now we have,

$$\frac{d\psi}{dx}=\frac{d\psi}{dy}\frac{dy}{dx}=\frac{d\psi}{dy}a$$

and
$$\frac{d^2\psi}{dx^2}=\frac{d^2\psi}{dy^2}\frac{dy}{dx}a=\frac{d^2\psi}{dy^2}a^2$$

$$= a^2 \frac{d^2\psi}{dy^2} \quad \text{... (6)}$$

Substituting the values of $d^2\psi / dx^2$ and x^2 in Eq. (4), we get

$$a^2 \frac{d^2\psi}{dy^2} + \left(\frac{2mE}{\hbar^2} - a^4 \frac{y^2}{a^2} \right) \psi = 0$$

Dividing through by a^2

$$\frac{d^2\psi}{dy^2} + \left(\frac{2mE}{a^2\hbar^2} - y^2 \right) \psi = 0$$

or

$$\frac{d^2\psi}{dy^2} + \left(\frac{2E}{\hbar\omega} - y^2 \right) \psi = 0 \quad \text{... (7)}$$

or

$$\boxed{\frac{d^2\psi}{dy^2} + (\lambda - y^2)\, \psi = 0} \quad \text{where } \lambda = \frac{2E}{\hbar\omega} \quad \text{... (8)}$$

Though Eq. (7) is in a simplified form, it is not easy to solve it. Therefore, its solution in detail is not given here.

In the following paragraphs, we discuss the results of its solution.

Eigen-values of the total energy E_n

The wave equation for the oscillator is satisfied only for discrete values of total energies given by

$$\boxed{\frac{2E}{\hbar\omega} = (2n+1)}$$

or

$$E_n = \frac{1}{2}(2n+1)\,\hbar\omega$$

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega \quad \text{... (9)}$$

Substituting $\hbar = \frac{h}{2\pi}$ and $\omega = 2\pi\nu$, this expression has the form :

$$E_n = \left(n + \frac{1}{2} \right) h\nu \quad \text{... (10)}$$

where, $n = 0, 1, 2, ...$, ω is the angular frequency and ν is the frequency of the classical harmonic oscillator, given by

$$\nu = \frac{\omega}{2\pi} = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$$

From Eq. (9), we get the *following conclusions* :

(1) The lowest energy of the oscillator is obtained by putting $n = 0$ in Eq. (9) and it is :

$$E_0 = \frac{1}{2}\hbar\omega \quad \text{... (11)}$$

This is called the ground state energy or the *zero point* vibrational energy of the harmonic oscillator. The zero-point energy is the characteristic result of quantum mechanics. The values of E_n in terms of E_0 are given by :

$$E_n = (2n+1)\, E_0 \quad \text{... (12)}$$

where $n = 0, 1, 2, 3, ...$

(2) The eigen-values of the total energy depend only on one quantum number n. Therefore all the energy-levels of the oscillator are non-degenerate.

(3) The successive energy-levels are equally spaced; the separation between two adjacent energy-levels being $\hbar\omega$. The energy-level diagram for the harmonic oscillator is shown in Fig. 5.7.

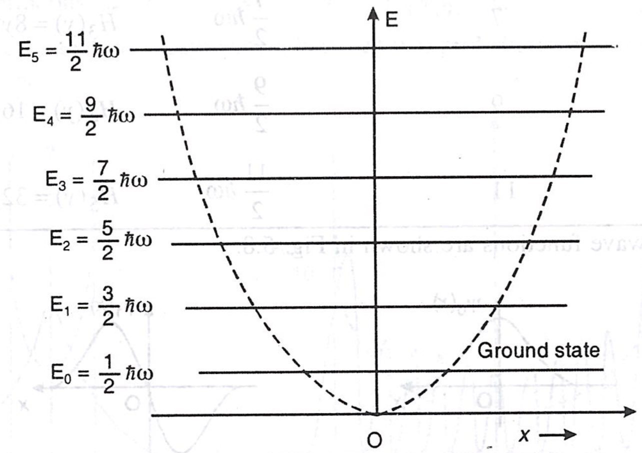

Fig. 5.7

In the figure the horizontal lines show the energy levels and the *dashed curve* is parabola representing the potential energy $V = \frac{1}{2} k x^2$.

(**Ans.** The ground-state energy is $E_1 = \dfrac{\pi^2\hbar^2}{2ma^2}$ the maximum uncertainty in the position of the particle in the box is $\Delta x = a$, where a is the width of the box.

From the uncertainty relation the uncertainty in the momentum is given by :

$$\Delta p_x \gtrsim \frac{h}{\Delta x} \gtrsim \frac{h}{a}$$

$\therefore$ the min. uncertainty in the momentum in + *ive* or − *ive* x-direction is $h/2a$, *i.e.*, the minimum possible momentum in either direction is $h/2a$.

Hence the ground state energy is

$$E_1 = \frac{p_x^2}{2m} = \frac{1}{2m}\left(\frac{h}{2a}\right)^2 = \frac{h^2}{8ma^2} = \frac{(2\pi)^2}{8ma^2}\left(\frac{h}{2\pi}\right)^2$$

$$= \frac{\pi^2\hbar^2}{2ma^2}.$$

10. (*a*) A beam of electrons, each of energy E, is incident on a rectangular potential barrier of width a and height V_0, where $V_0 > E$. Obtain an expression for the transmission-coefficient through the barrier.
(*b*) Explain the phenomenon of α-decay of a radio-active nucleus.

11. A beam of particles each of mass m and energy E, moving in a region of zero potential energy, approaches a rectangular potential barrier of width a and height V_0, where $V_0 > E$. If $\beta a >> 1$, where $\beta = \sqrt{\dfrac{2m(V_0 - E)}{\hbar^2}}$, prove that the transmission : coefficient is given by

$$T = \frac{16E}{V_0}\left(1 - \frac{E}{V_0}\right)e^{-2\beta a}$$

12. Find the reflection and transmission coefficients for a rectangular barrier of width a and height V_0 for the case where $E > V_0$. Show that the transmission coefficient is 1 for certain value of the energy, given by :

$$E = \frac{n^2\pi^2\hbar^2}{2ma^2} + V_0, \text{ where } n = 1, 2, 3, ...$$

13. Explain the problem of the leaking of a particle through a rectangular potential barrier of finite width and explain theory of α-particle decay. (Bangalore, 2005)

14. Show that the reflection coefficient R for a step barrier for the case $E > V_0$ is given by:

$$R = \left[\frac{1 - \sqrt{1 - V_0/E}}{1 + \sqrt{1 - V_0/E}}\right]^2$$

15. Explain why the quantum number n in the energy equation for a particle in one dimensional box cannot take zero value. (N.U., 2006)

CHAPTER 6

THE HYDROGEN ATOM

The hydrogen atom is a system of two particles, a proton and a single electron bound by electrostatic force of attraction. It, being the simplest atom, forms the basis for the theoretical treatment of more complex atomic systems. Bohr's theory of the hydrogen atom marked the beginning of the old quantum theory of atomic structure. Wave mechanics had its beginning when Schrödinger in 1926 gave the solution of the wave equation for the hydrogen atom. Subsequently there was extensive development of quantum mechanical theory of the hydrogen atom by Heisenberg, Max Born, and Jordan, before the treatment was finally given by Pauli.

The quantum mechanical treatment given in this chapter is due to Sommerfeld. It differs in some minor details from that of Schrödinger.

6.1. WAVE EQUATION FOR THE HYDROGEN ATOM

In the hydrogen atom the charge of the proton is + e and that of the electron − e. Therefore, the electrostatic potential energy of the system in the absence of external fields is (in SI units) :

$$V = \frac{e(-e)}{4\pi\varepsilon_0 r} = -\frac{e^2}{4\pi\varepsilon_0 r} \qquad ...(1)$$

where r is the distance between the particles and ε_0 the permittivity of free space.

The proton is 1836 times heavier than the electron. So for convenience the proton can be considered to be stationary with the electron in motion around it. The time-independent Schrödinger's wave equation in three dimensions for the electron is :

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

where m is the mass of the electron,
V is its potential energy,
E is its total energy,
$\psi(x, y, z)$ is the wave function for the electron, and

$\nabla^2 = \dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2}$ is the Laplacian of $\psi(x, y, z)$ in the Cartesian coordinates x, y, z. We write Eq. (2) in a convenient form as :

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\,\psi = 0 \qquad \dots (3)$$

The variables in this equation cannot be separated in the Cartesian coordinates. Therefore, the Cartesian coordinates of the electron relative to the proton are replaced by the spherical polar coordinates (r, θ, ϕ) and the Laplacian operator ∇^2 is transformed into these coordinates by using the equations: (See Fig. 6.1)

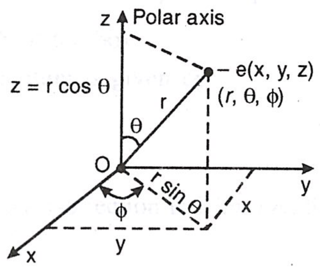

Fig. 6.1

$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$

The Laplacian operator, in spherical polar coordinates, is :

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \qquad \dots (4)$$

Therefore, the Schrödinger equation in spherical polar coordinates becomes :

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} + \frac{2m}{\hbar^2}\left[E + \frac{e^2}{4\pi\varepsilon_0 r}\right]\psi = 0 \qquad \dots (5)$$

In this equation the wave-function ψ is a function of (r, θ, ϕ).

Separation of Variables

The equation in spherical polar coordinates can be easily separated into three equations, each involving a single independent variable. For this purpose, we assume the wave-function $\psi(r, \theta, \phi)$ to be a product of three functions,

$$\psi(r, \theta, \phi) = R(r)\,Q(\theta)\,F(\phi) \qquad \dots (6a)$$

where $R(r)$ is a function of r alone,

$Q(\theta)$ is a function of θ alone and

$F(\phi)$ is a function of ϕ alone.

(**Note** : we use the symbols Q and F for the functions of θ and ϕ respectively and not the symbols θ and Φ to avoid any confusion in writing).

The function $R(r)$ will show the variation of the wave function ψ along a *radius vector* from the nucleus, when θ and ϕ are constant. The function $Q(\theta)$ will show the variation of ψ with *zenith angle* θ along a circle on a sphere with nucleus as the centre, when r and ϕ are constant. The function $F(\phi)$ will show the variation of ψ with *azimuthal angle* ϕ along a circle with centre on OZ, where r and θ are constant.

In a simple form Eq. (6a) is written as :

$$\psi = RQF \qquad \dots (6b)$$

Substituting this equation into Eq. (5), we get

$$\frac{QF}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{RF}{r^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dQ}{d\theta}\right) + \frac{RQ}{r^2\sin^2\theta}\frac{d^2F}{d\phi^2}$$
$$+\frac{2m}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right)RQF = 0 \qquad \dots (7)$$

In this equation we have used ordinary derivatives instead of partial derivatives because each function depends on only one variable.

Now multiplying Eq. (7) by $\dfrac{r^2\sin^2\theta}{RQF}$, we get

$$\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{\sin\theta}{Q}\frac{d}{d\theta}\left(\sin\theta\frac{dQ}{d\theta}\right) + \frac{1}{F}\frac{d^2F}{d\phi^2} + \frac{2m}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right)r^2\sin^2\theta = 0$$

Transposing the third term to the right-hand side, we get

$$\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{\sin\theta}{Q}\frac{d}{d\theta}\left(\sin\theta\frac{dQ}{d\theta}\right) + \frac{2m}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right)r^2\sin^2\theta = -\frac{1}{F}\frac{d^2F}{d\phi^2} \qquad \dots (8)$$

Azimuthal Wave Equation, or the ϕ Equation

The left side of Eq. (8) is a function of r and θ and the right side is a function of ϕ only. Thus each side can be varied independently of the other. Therefore, the equation will be true only if both sides are equal to the same constant. This constant is denoted by m_l^2, where m_l is called the *orbital magnetic quantum number*.

Therefore, the right side of Eq. (8) becomes :

$$-\frac{1}{F}\frac{d^2F}{d\phi^2} = m_l^2$$

or

$$\frac{d^2F}{d\phi^2} + m_l^2 F = 0 \qquad \dots (9)$$

This is the *first* of the *three* differential equations, and is called the *azimuthal wave equation*, or the ϕ equation. In the solution of Eq. (9) we will see that m_l must be a positive or negative integer or zero.

Polar and Radial Wave Equations

Equating the left side of Eq. (8) to m_l^2 and then dividing it by $\sin^2\theta$, we get :

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{1}{Q\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dQ}{d\theta}\right) + \frac{2m\,r^2}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right) = \frac{m_l^2}{\sin^2\theta}$$

Transporing the second term on the left side to the right side, we get :

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2mr^2}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right) = \frac{m_l^2}{\sin^2\theta} - \frac{1}{Q\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dQ}{d\theta}\right) \qquad \dots (10)$$

The left side of this equation is a function of r only, while the right side is a function of θ only, and hence both sides of the equation must be equal to the same constant. We denote this constant by β.

Equating both sides of the equation separately to the same constant β, we get the following equations :

$$\frac{m_l^2}{\sin^2\theta} - \frac{1}{Q\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dQ}{d\theta}\right) = \beta \qquad \text{... (11)}$$

This equation is called the *polar wave equation or the* θ *equation.*

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2m\,r^2}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right) = \beta \qquad \text{... (12)}$$

This equation is called the *radial wave equation*. Thus the Schrödinger wave equation (5) for the hydrogen atom has been separated into three equations (9), (11) and (12). Each of the equations depends on only one variable.