Chapter Four

The Linear Harmonic Oscillator

6.1 The Time-Independent Schrödinger Equation and its Solution

The force acting on a particle executing linear harmonic oscillation can be written as

$$F = -kx \qquad \dots(6.1)$$

where x is the displacement from the equilibrium position and k is called the force constant. The potential energy corresponding to this force is

$$V(x) = \frac{1}{2}kx^2 \qquad \dots(6.2)$$

If ω is the "classical" angular frequency of the oscillator and m is its mass, then

$$\omega = \sqrt{k/m}$$

or

$$k = m\omega^2$$

Therefore

$$V(x) = \frac{1}{2}m\omega^2x^2 \qquad \dots(6.3)$$

The time-independent Schrödinger equation for the harmonic oscillator is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x) \qquad \dots(6.4)$$

or

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

or

$$\frac{d^2\psi(x)}{dx^2} + \frac{m\omega}{\hbar}\left[\frac{2E}{\hbar\omega} - \frac{m\omega}{\hbar}x^2\right]\psi(x) = 0 \qquad \dots(6.5)$$

It is convenient to simplify this equation by introducing the dimensionless eigenvalue

$$\lambda = \frac{2E}{\hbar\omega} \qquad \dots(6.6)$$

and the dimensionless variable

$$y = \alpha x \qquad \dots(6.7)$$

Where $$\alpha = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} \qquad \ldots(6.8)$$

we have $\frac{dy}{dx} = \alpha$

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

$$\frac{d^2\psi}{dx^2} = \frac{d}{dy}\left(\frac{d\psi}{dx}\right)\frac{dy}{dx} = \alpha^2\frac{d^2\psi}{dy^2} = \frac{m\omega}{\hbar}\frac{d^2\psi}{dy^2}$$

Substituting in (6.5),

$$\frac{m\omega}{\hbar}\left[\frac{d^2\psi(y)}{dy^2} + (\lambda - y^2)\psi(y)\right] = 0$$

$$\frac{d^2\psi(y)}{dy^2} + (\lambda - y^2)\psi(y) = 0 \qquad \ldots(6.9)$$

As a first step towards finding acceptable solutions of this equation, we first examine the behavior of ψ in the asymptotic region $|y| \to \infty$ In this limit (6.9) reduces to

$$\frac{d^2\psi(y)}{dy^2} - y^2\psi(y) = 0 \qquad \ldots(6.10)$$

It can be easily verified that for large values of $|y|$ the functions

$$\psi(y) = y^n e^{\pm\frac{y^2}{2}}$$

n being any constant, satisfy Equation (6.10) so far as the leading terms, which are of order $y^2\psi(y)$, are concerned.

Since the wave function must be bounded everywhere, the positive sign in the exponent is not acceptable. This suggests that we should look for exact solution to (6.9) having the form

$$\psi(y) = e^{-\frac{y^2}{2}}H(y) \qquad \ldots(6.11)$$

where $H(y)$ are functions which do not affect the required asymptotic behavior of $\psi(y)$. Substituting (6.11) into (6.9) we find that $H(y)$ satisfy the **Hermite equation:**

…(6.12)

$$\frac{d^2H(y)}{dy^2} - 2y\frac{dH(y)}{dy} + (\lambda - 1)H(y) = 0$$

This equation can be solved by assuming a power series of the form

$$H(y) = \sum_{k=0}^{\infty} a_k y^k = a_0 + a_1 y + a_2 y^2 + \cdots \qquad \ldots(6.13)$$

This gives

$$\frac{dH(y)}{dy} = \sum_{k=1}^{\infty} k a_k y^{k-1} \qquad and \qquad \frac{d^2H(y)}{dy^2} = \sum_{k=2}^{\infty} k(k-1) a_k y^{k-2}$$

Substituting in Equation (6.12),

$$\sum_{k=2}^{\infty} k(k-1) a_k y^{k-2} - 2\sum_{k=1}^{\infty} k a_k y^{k-1} + (\lambda - 1)\sum_{k=0}^{\infty} a_k y^k = 0$$

Or

$$\sum_{k} k(k-1) a_k y^{k-2} - \sum_{k} (2k - \lambda + 1) a_k y^k = 0$$

For this equation to be satisfied identically for all y, the coefficient of each power of y must vanish. Setting the coefficient of y^k equal to zero, we obtain

$$(k+2)(k+1)a_{k+2} - (2k + 1 - \lambda)a_k = 0$$

$$a_{k+2} = \frac{2k + 1 - \lambda}{(k+2)(k+1)} a_k , \qquad k = 0, 1, 2, \ldots \qquad \ldots(6.14)$$

This equation is called the **recurrence relation**. It shows that all the coefficients can be determined from a_0 and a_1.

The general solution of (6.12) has two adjustable parameters. It can be written as the sum of two series, one containing only ***even powers*** and the other only ***odd powers***:

$$H(y) = (a_0 + a_2 y^2 + a_4 y^4 + \cdots) + (a_1 y + a_3 y^3 + a_5 y^5 + \cdots) \qquad \ldots(6.15)$$

Let us now look at the behavior of this series as $y \to \infty$. It is clear that for large y, the higher (large k) terms in the series will dominate. Therefore, we examine the behavior of this series for large k. We have, from (6.14),

$$\frac{a_{k+2}}{a_k} \to \frac{2}{k} \qquad \text{for large k} \qquad \ldots(6.16)$$

Let us now consider the expansion of the function e^{y^2}:

$$e^{y^2} = \sum_{k=0,2,4,\ldots} b_k y^k, \qquad b_k = \frac{1}{(k/2)!}$$

The ratio of two consecutive terms is

$$\frac{b_{k+2}}{b_k} = \frac{(k/2)!}{[(k+2)/2]!} = \frac{2}{k+2} \to \frac{2}{k} \qquad \text{for large k} \qquad \ldots(6.17)$$

Equations (6.16) and (6.17) show that for large k, $H(y)$ behaves as e^{y^2}.

Thus, (6.11) shows that for large k,

$$\psi(y) \approx e^{y^2/2} \qquad \ldots(6.18)$$

which diverges as $y \to \infty$. Therefore, in order to obtain a physically acceptable wave function it is necessary that the series is terminated to a polynomial. The recursion relation (6.14) tells us that this can happen only when λ is an odd integer:

$$\lambda = 2n + 1, \qquad n = 0, 1, 2, \ldots \qquad \ldots(6.19)$$

In that case one of the two series will terminate at $k = n$. The other series is eliminated by setting $a_0 = 0$ if n is odd and $a_1 = 0$ if n is even. In either case, Equations (6.6) and (6.19) yield the **energy eigenvalues**

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, \ldots \qquad \ldots(6.20)$$

We have labelled the energy eigenvalues by the index n which indicates the degree of the polynomial appearing in the solution.

Note that:

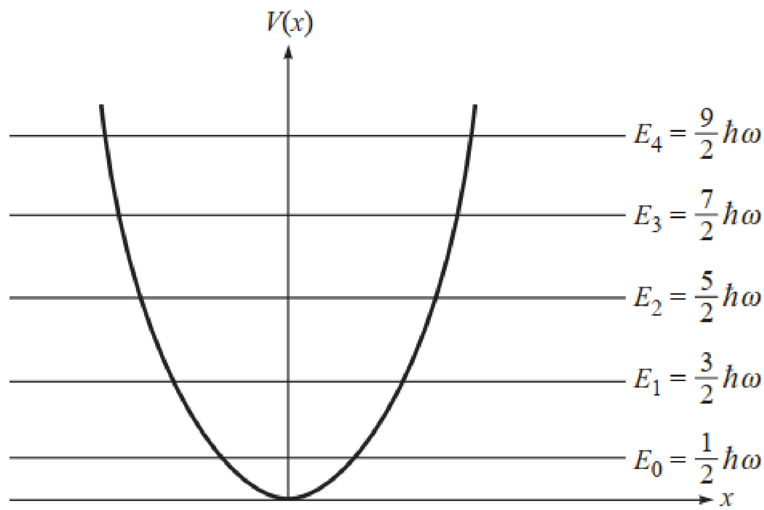
- The infinite sequence of energy levels has the equal spacing $\hbar\omega$ postulated by Planck in 1900.

- It is also in agreement with the quantization rules of the old quantum theory.
- Unlike old quantum theory, ***the ground state energy is not zero***, but is

$$E_0 = \frac{1}{2}\hbar\omega \qquad \ldots(6.21)$$

This is called the ***zero-point energy***.

- The eigenvalues (6.20) are ***nondegenerate***, because for each value of the quantum number *n* there exists only one eigenfunction.



The harmonic oscillator potential and its energy levels.

6.2 The Hermite Polynomials

Substituting $\lambda = 2n + 1$ in Equation (6.12), we get

$$H_n''(y) - 2yH_n'(y) + 2nH_n(y) = 0 \qquad \ldots(6.22)$$

The polynomial $H_n(y)$ of order *n* that is a solution of this equation is called the ***nth Hermite polynomial***.

We record here some important properties Hermite polynomial.

Recurrence Relations

$$H_n' = 2nH_{n-1} \qquad \ldots(6.23a)$$

$$H_{n+1} = 2yH_n - 2nH_{n-1} \qquad \ldots(6.23b)$$

Generating Function

The function

$$G(y,s) = e^{-s^2+2sy}$$

is called *the generating function of Hermite polynomials*. It can be shown that

$$e^{-s^2+2sy} = \sum_{n=0}^{\infty} \frac{H_n(y)}{n!} s^n \qquad \ldots(6.24)$$

Rodrigues' Formula

The Hermite polynomials can be evaluated from the following formula:

$$H_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n}\left(e^{-y^2}\right) \qquad \ldots(6.25)$$

The first few Hermite polynomials are:

$$\left.\begin{aligned} H_0(y) &= 1 \\ H_1(y) &= 2y \\ H_2(y) &= 4y^2 - 2 \\ H_3(y) &= 8y^3 - 12y \\ H_4(y) &= 16y^4 - 48y^2 + 12 \\ H_5(y) &= 32y^5 - 160y^3 + 120y \end{aligned}\right\} \qquad \ldots(6.26)$$

Orthogonality

If $H_n(y)$ and $H_m(y)$ are Hermite polynomials of orders *n* and *m* respectively, then

$$\int_{-\infty}^{\infty} e^{-y^2} H_n(y) H_m(y)\, dy = 0 \qquad n \neq m \qquad \ldots(6.27)$$

For $n = m$, it can be shown that

$$\int_{-\infty}^{\infty} e^{-y^2} H_n^2(y)\, dy = \sqrt{\pi}\, 2^n n! \qquad \ldots(6.28)$$