Solution of Hermite's differential equation ⟹ The solution of Hermite's differential equation is a power series in positive powers of y. If the lowest power of y is zero, the solution will be of the form

$$H(y) = A_0 + A_1 y + A_2 y^2 + A_3 y^3 + \ldots..$$

$$= \sum_{n=0}^{n=\infty} A_n y^n \qquad \ldots (14)$$

On differentiating equation (14) w.r.t. y, we get

$$\frac{dH(y)}{dy} = A_1 + 2A_2 y + 3A_3 y^2 + \ldots\ldots. \qquad \ldots (15)$$

Multiplying equation (15) by $-2y$, we get

$$-2y.\frac{dH(y)}{dy} = -2\,(A_1 y + 2A_2 y^2 + 3A_3 y^3 + \ldots.)$$

$$= \sum_{n=0}^{n=\infty} -2n\, A_n y^n \qquad \ldots (16)$$

Differentiating equation (15) w.r.t. y, we get

$$\frac{d^2H(y)}{dy^2} = 2A_2 + 3\times 2\,A_3 y + 4\times 3\,A_4 y^2 + \ldots$$

$$= \sum_{n=0}^{n=\infty} (n+2)(n+1)\,A_{n+2}\cdot y^n \qquad \ldots(17)$$

Multiplying both sides of equation (14) by $(\lambda - 1)$, we get

$$(\lambda - 1)\,H(y) = \sum_{n=0}^{n=\infty} (\lambda - 1)\,A_n y^n \qquad \ldots(18)$$

Substituting equations (16), (17) and (18) in equation (13), we get

$$\sum_{n=0}^{n=\infty} [(n+2)(n+1)\,A_{n+2} - (2n+1-\lambda)\,A_n]\,y^n = 0 \qquad \ldots(19)$$

This equation must be true for all values of y and, therefore, the coefficient of each power of y must vanish separately. Hence, we have

$$(n+2)(n+1)\,A_{n+2} - (2n+1-\lambda)\,A_n = 0$$

$$\text{or,}\quad A_{n+2} = \frac{(2n+1-\lambda)}{(n+1)(n+2)}\cdot A_n \qquad \ldots(20)$$

This is **recursion formula** relating the coefficients A_{n+2} and A_n.

In the solution of any second-order differential equation; there must be two arbitrary constants, So, let us consider A_0 and A_1 as the two arbitrary constants and all other coefficients are determined in terms of A_0 and A_1.

On substituting $n = 0, 2, 4, 6$ ..... in eq^n. (20), we get

$$A_2 = \frac{(1-\lambda)}{2\,!}A_0$$

$$A_4 = \frac{(5-\lambda)}{3\times 4}A_2 = \frac{(5-\lambda)}{3\times 4}\,\frac{(1-\lambda)}{2!}A_0 = \frac{(1-\lambda)(5-\lambda)}{4\,!}A_0$$

$$A_6 = \frac{(9-\lambda)}{5\times 6}A_4 = \frac{(9-\lambda)}{5\times 6}\cdot\frac{(1-\lambda)(5-\lambda)}{4\,!}A_0$$

$$= \frac{(1-\lambda)(5-\lambda)(9-\lambda)}{6\,!}A_0$$

Substituting $n = 1, 3, 5, 7$ .... in eqⁿ. (20), we get

$$A_3 = \frac{(3-\lambda)}{2\times 3}A_1 = \frac{(3-\lambda)}{3\,!}A_1$$

$$A_5 = \frac{(7-\lambda)}{4\times 5}A_3 = \frac{(7-\lambda)}{4\times 5}\cdot\frac{(3-\lambda)}{3\,!}A_1$$

$$= \frac{(3-\lambda)\,(7-\lambda)}{5\,!}A_1$$

$$A_7 = \frac{(3-\lambda)\,(7-\lambda)\,(11-\lambda)}{7\,!}A_1$$

On substituting the values of these coefficients in equation (14), we get

$$H(y) = A_0\left[1 + \frac{(1-\lambda)}{2!}y^2 + \frac{(1-\lambda)(5-\lambda)}{4\,!}y^4 + \frac{(1-\lambda)\,(5-\lambda)\,(9-\lambda)}{6\,!}y^6 + ..\right]$$

$$+A_1\left[y + \frac{(3-\lambda)}{3!}y^3 + \frac{(3-\lambda)(7-\lambda)}{5!}y^5 + \frac{(3-\lambda)\,(7-\lambda)\,(11-\lambda)}{7\,!}y^7 + ...\right] \quad ...(21)$$

This is solution of Hermite's differential equation (13). This equa shows that the polynomial $H(y)$ is the sum of two infinite series. This means that if $H(y)$ does not terminate for some value of n, the wavefunction

$$\psi = e^{-y^2/2}\,H(y)$$

will become infinite as y becomes infinite.

(c) Expression for energy eigen value for simple harmonic oscillator :

The wavefunction, $\psi = e^{-y^2/2}H(y)$, will have a finite value if $H(y)$ terminates at some value on n. For this to happen, A_{n+2} must vanish for some value of n, i.e.,

$$A_{n+2} = 0$$

or, $$\frac{(2n+1-\lambda)}{(n+1)\,(n+2)}A_n = 0$$

or, $$2n+1-\lambda = 0$$

or, $$\lambda = 2n+1 \quad ...(22)$$

Putting $\lambda = \frac{2E}{\hbar\omega}$ from equation (8) in equation (22), we get

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

or, $$E_n = \left(\frac{n+1}{2}\right)\hbar\omega \quad \text{... (23)}$$

Putting $\hbar = \frac{h}{2\pi}$ and $\omega = 2\pi\nu$ in equation (23),

We get $$E_n = \left(n + \frac{1}{2}\right)h\nu \quad \text{... (24)}$$

where $n = 0, 1, 2, 3$ ..... , ω is the angular frequency and ν is the frequency of the classical harmonic oscillator, given by

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

Equation (24) is the quantum mechanical energy of simple harmonic oscillator in its n^{th} vibrational state, n being vibrational quantum number.

(d) **Zero-point energy :** The energy of a simple harmonic oscillator is given by

$$E_n = \left(n + \frac{1}{2}\right)h\nu, \text{ where } n = 0, 1, 2, 3. \ldots$$

For $n = 0$, we have

$$E_0 = \frac{1}{2}h\nu = \frac{1}{2}\hbar\omega$$

This is called ground state vibrational energy or zero-point energy of the harmonic oscillator. The existence of zero-point energy indicates that even in ground state, the oscillator has some energy and still vibrating which is consistent with the Heisenberg's uncertainty principle.