6.2.4. The Harmonic Oscillator:

6.2.4.1. The Anisotropic Oscillator,

Consider a particle of mass "m" executing harmonic motion in x-direction. The force acting on the particle is.

$$F = -Kx \quad \text{(Hook's Law)}$$

where "x" is the displacement of the particle from mean position. The equation of motion is

$$m\frac{d^2x}{dt^2} = -Kx, \quad F = ma = m\frac{d^2x}{dt^2}$$

or. $$\frac{d^2x}{dt^2} + \frac{K}{m}x = 0, \quad \sqrt{\frac{K}{m}} = \omega$$

ω → angular frequency

or. $$\boxed{\frac{d^2x}{dt^2} + \omega^2 x = 0.}$$

The general solution of the above equation is.

$$\boxed{x = A\cos\omega t}$$

where A is the amplitude of oscillation and ω is the angular frequency. The Potential energy can be calculated as

$\hat{F} = -Kx$

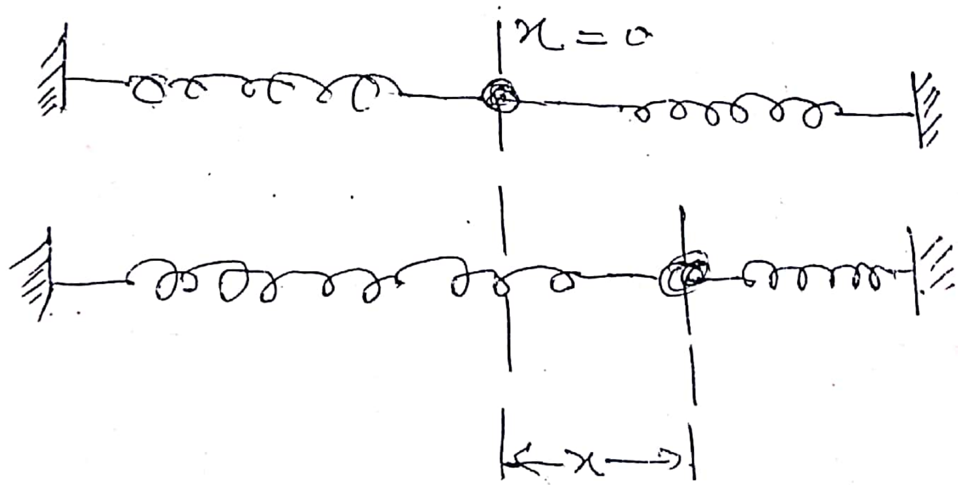
$K = m\omega^2$

$$\boxed{\hat{F} = -m\omega^2 x}$$

$$F = -\frac{\partial V}{\partial x},$$

$$-m\omega^2 x = -\frac{\partial V}{\partial x}$$

$$\boxed{V(x) = \frac{1}{2} m\omega^2 x^2 + C}$$



At $x = 0$, $V(x) = 0$, therefore $C = 0$

then

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

$\llcorner$ 1D.

In 3D. -

$$\boxed{\bar{V}(x,y,z) = \frac{1}{2} m \left[\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right]}$$

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The Schrodinger wave equ. will become

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + \frac{1}{2}m\omega_x^2 x^2 \psi(x) = E_x \psi(x)$$

with similar equations for y and z - components.

The eigenenergies corresponding to the potential

$$V(x,y,z) = \frac{1}{2}m\omega_x^2 x^2$$

is of the form.

$$E_{n_x} = \left(n_x + \frac{1}{2}\right)\hbar\omega_x \quad - 1D.$$

$$E_{n_x n_y n_z} = E_{n_x} + E_{n_y} + E_{n_z}.$$

$$\boxed{E_{n_x n_y n_z} = \left(n_x + \frac{1}{2}\right)\hbar\omega_x + \left(n_y + \frac{1}{2}\right)\hbar\omega_y + \left(n_z + \frac{1}{2}\right)\hbar\omega_z}$$

6.2.4.2. The Isotropic Harmonic Oscillator:

For an isotropic Harmonic oscillator potential:

$$\omega_x = \omega_y = \omega_z = \omega.$$

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Hence, its energy eigenvalues can be written as

$$E_{n_x n_y n_z} = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega.$$

The ground state energy, when

$n_x = n_y = n_z = 0$ → non-degenerate

$$\boxed{E_{000} = \frac{3}{2}\hbar\omega}.$$

The first excited state is 3-fold degenerate, since there are three different states $\psi_{100}, \psi_{010}, \psi_{001}$; which correspond to same energy $\frac{5}{2}\hbar\omega$.

The 2nd excited state is 6-fold degenerate with energy eigen value $\frac{7}{2}\hbar\omega$.

The degeneracy of nth excited state is given by

$$\boxed{g_n = \frac{1}{2}(n+1)(n+2)}$$

which is equal to the number of ways the non-negative integers n_x, n_y, n_z which may be chosen to total to "n". $\boxed{n = n_x + n_y + n_z}$

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Quantum Theory of Harmonic Oscillator:

Since the Potential is constant in time, the time-independent Schroedinger equation determines the solutions ψ_n and Corresponding eigenvalues (energies) E_n. The time-independent Schroedinger equation of the Problem is

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

where $V(x) = \frac{1}{2} kx^2$

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

or we may write it as

$$\frac{d^2\psi}{dx^2} + \left(k_1^2 - \lambda^2 x^2\right)\psi = 0. \quad \text{—(1)}$$

where $K_1 = \frac{\sqrt{2mE}}{\hbar}$

$$\lambda = \frac{\sqrt{mk}}{\hbar}$$

Equation ① is known as Weber's differential equation. For more simplification we introduce a reparameterization.

$$z^2 = \lambda x^2$$

or $$z = \sqrt{\lambda}\, x$$

This gives

$$\sqrt{\lambda} = \frac{dz}{dx}$$

with

$$\frac{d\psi}{dx} = \frac{d\psi}{dz} \cdot \frac{dz}{dx} = \sqrt{\lambda}\, \frac{d\psi}{dz}$$

$$\frac{d^2\psi}{dx} = \sqrt{\lambda}\, \frac{d^2\psi}{dz^2} \frac{dz}{dx} = \lambda \frac{d^2\psi}{dz^2}$$

The equ ① can be re-expressed as

$$\frac{d^2\psi}{dz^2} + \left[\frac{K_1^2}{\lambda} - z^2\right]\psi = 0.$$

If we set $\mu = \frac{K_1^2}{\lambda}$, we get

$$\frac{d^2\psi}{dz^2} + (\mu - z^2)\,\psi = 0 \quad ②$$

Let us look for the asymptotic solution of equ. (2) i.e. when

$$|z| >> \mu$$

and $|z| \to \infty$ (The asymptotic region.)

⇒ Asymptotic analysis is a method of describing limiting behaviour. The method has applications across science. ~~It~~ used to get the ~~approximation~~ approximated solutions.

In the asymptotic form, equ (2) can be written as

$$\frac{d^2\psi}{dz^2} - z^2\psi = 0 \quad \text{--- (3)}$$

$$|z| >> \mu$$
$$\text{and } |z| \to \infty$$

Suppose that the above equ. has a solution of the form

$$\psi = A e^{-z^2/2} + B e^{z^2/2}$$

This solution must satisfy the equation ③. ꞓ'

Check!

$$\frac{d\psi}{dz} = -Az\cdot e^{-z^2/2} + Bz\,e^{z^2/2}$$

$$\frac{d^2\psi}{dz^2} = (z^2-1)A\,e^{-z^2/2} + (z^2+1)B\,e^{z^2/2}$$

for asymptotic values of z, we take

$$(z^2 \pm 1) \simeq z^2$$

So that, we have

$$\frac{d^2\psi}{dz^2} = z^2\left(A e^{-z^2/2} + B e^{z^2/2}\right)$$

$$= z^2\psi$$

Hence, the equ. ③ is satisfied with this solution.

$$\psi = A e^{-z^2/2} + B e^{z^2/2}$$

Since $e^{z^2/2} \longrightarrow \infty$, as $|z| \longrightarrow \infty$

Therefore, we set $B = 0$.

The asymptotic solution of the Weber's differential equation is. therefore,

$$\psi(z) = A\, e^{-z^2/2}, \quad |z| \to \infty$$

The general solution of equation (2) is obtained by multiplying the asymptotic solution with a function say $F(z)$. Hence, the general solution has the form.

$$\psi(z) = \left(A\, e^{-z^2/2}\right) F(z).$$

The function $F(z)$ can be determined as follows:

Let us first differentiate $\psi(z)$ with respect to z

$$\frac{d\psi}{dz} = -z A e^{-z^2/2} F(z) + A e^{-z^2/2} F'(z)$$

$$\frac{d^2\psi}{dz^2} = A e^{-z^2/2}\left[(z^2-1)F(z) - 2zF'(z) + F''(z)\right]$$

The Weber's differential equ.(2) no

takes the form

$$A e^{-z^2/2}\left[(z^2-1)F(z) - 2zF'(z) + F''(z)\right]$$
$$+ (\mu - z^2)\left[A e^{-z^2/2} F(z)\right] = 0$$

or.

$$A e^{-z^2/2}\left[F''(z) - 2zF'(z) + (\mu-1)F(z)\right] = 0$$

Since $A e^{-z^2/2} \neq 0$, therefore

$$F''(z) - 2zF'(z) + (\mu-1)F(z) = 0 \quad \text{— (4)}$$

The standard way to solve this differential equ.(4) is to assume the power series as:

$$F(z) = \sum_{n=0}^{\infty} a_n z^n$$
$$= a_0 + a_1 z + a_2 z^2 + \cdots$$

and then, to determine the value of the co-efficients a_n.

Differentiating $F(z)$ yields.

$$F'(z) = \sum_{n=0}^{\infty} n a_n z^{n-1}$$

$$F''(z) = \sum_{n=0}^{\infty} n(n-1) a_n z^{n-2}$$

Put in equ. (ii), we get.

$$\sum_{n=0}^{\infty} n(n-1) a_n z^{n-2} - 2z \sum_{n=0}^{\infty} n a_n z^{n-1}$$

$$+ (\mu-1) \sum_{n=0}^{\infty} a_n z^{n} = 0$$

or.

$$\sum_{n=0}^{\infty} a_n \left[n(n-1) z^{n-2} + (\mu-1-2n) z^{n} \right] = 0$$

Comparing the co-efficients of $z^0, z^1, z^2, \dots$

$O(z^0)$: $2a_2 + (\mu-1) a_0 = 0$

$O(z^1)$: $3.2\, a_3 + (\mu-3) a_1 = 0$

$O(z^2)$: $4.3\, a_4 + (\mu-5) a_2 = 0$

⋮

$O(z^p)$: $(p+2)(p+1) a_{p+2} + [\mu - (2p+1)] a_p = 0$

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The last equation gives the recursion relation

$$a_{p+2} = \frac{-[l - (2p+1)]}{(p+2)(p+1)} a_p$$

for

$p=0$ $\quad a_2 = \frac{-l+1}{2 \cdot 1} a_0$

$p=1$ $\quad a_3 = \frac{-l+3}{3 \cdot 2} a_1$

$p=2$ $\quad a_4 = \frac{-l+5}{4 \cdot 3} a_2$

$p=3$ $\quad a_5 = \frac{-l+7}{5 \cdot 4} a_3$

These relations allows us to calculate successive co-efficients $a_2, a_4, a_6, \ldots$ in terms of a_0 and the co-efficients $a_3, a_5, a_7, \ldots$ in terms of a_1. So a_0 and a_1 are the two arbitrary constants of the second order differential equations.

Let us write

$$f(z) = a_0 + a_2 z^2 + a_4 z^4 + \cdots$$

$$g(z) = a_1 z + a_3 z^3 + a_5 z^5 + \cdots$$

So that

$$F(z) = f(z) + g(z) = H(z)$$

Then the solution is of the form.

$$\psi(z) = A e^{-z^2/2} \left[f(z) + g(z) \right]$$

The function $f(z)$ can be compared with.

$$e^{z^2} = \sum_{n=0}^{\infty} \frac{(z^2)^n}{n!} = \sum_{n=0}^{\infty} Q_n$$

$$= 1 + z^2 + \frac{z^4}{2!} + \frac{z^6}{3!} + \cdots + \frac{z^{2p}}{p!} + \frac{z^{2(p+1)}}{(p+1)!}$$

For this series the ratio of the two successive terms is.

$$\frac{Q_{p+1}}{Q_p} = \frac{\left(\frac{z^{2(p+1)}}{(p+1)!}\right)}{\left(\frac{z^{2p}}{p!}\right)} = \frac{z^2}{p+1} \simeq \frac{z^2}{p}$$

for $p \gg 1$

which is same for $f(z)$, so that one can write.

$$\boxed{f(z) = C e^{z^2}}$$

Similarly

$$g(z) = a_1 z + a_3 z^3 + a_5 z^5 + \dots$$

$$= z\,(a_1 + a_3 z^2 + a_5 z^4 + \dots)$$

$$\boxed{g(z) = z D e^{z^2}}$$

Now the solution will become.

$$\psi(z) = AC\, e^{z^2/2} + z AD\, e^{z^2/2}$$

However, the function $\psi(z)$ is not finite at $z = \pm\infty$ and therefore not physically acceptable. In order to have finite wavefunction, the series

$$H(z) = \sum_{n=0}^{\infty} a_n z^n$$

must terminate after a finite number of terms. The series can be terminated at z^n by making $\mu = 2n+1$.