Linear Harmonic oscillator

A point mass undergoing simple harmonic oscillations in one dimension, due to attraction by a force proportional to the displacement x from the equilibrium position, constitutes a linear harmonic oscillator. The restoring force $F = -kx$ — ① is derivable ($F = -\frac{\partial V}{\partial x}$) from the Potential energy $V = \frac{1}{2}kx^2$.

The classical equation of motion is

$$m\frac{d^2x}{dt^2} = -kx$$ where m is the mass of the oscillating Particle.

or $$\frac{d^2x}{dt^2} + \frac{k}{m}x = 0 \qquad \text{—— ②}$$

Here $\frac{k}{m} = \omega_c^2$

The general solution of this equation is

$$x = A\sin(\omega_c t + C) \qquad \text{—— ③}$$

where $\omega_c = \sqrt{\frac{k}{m}}$ is the angular frequency of the classical oscillator.

In quantum mechanics, the wave equation for the harmonic oscillator is given by (Directly from S-equation)

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}kx^2\right)\psi = 0 \qquad \text{—— ④}$$

For Convenience, we rewrite the above equation in a dimensionless form by introducing a new independent variable $\eta = \alpha x$, so that

$$\frac{d\psi}{dx} = \frac{d\psi}{d\eta}\cdot\frac{d\eta}{dx} = \alpha\frac{d\psi}{d\eta}$$

or $$\frac{d^2\psi}{dx^2} = \alpha^2\frac{d^2\psi}{d\eta^2} \qquad \text{—— ⑤}$$

Then eqn ④ becomes

$$\frac{d^2\psi}{d\eta^2} + (\lambda - \eta^2)\psi = 0 \qquad \text{—— ⑥}$$

where $\alpha^4 = \frac{mK}{\hbar^2}$ and $\lambda = \frac{2mE}{\hbar^2\alpha^2} = \frac{2E}{\hbar}\left(\frac{m}{K}\right)^{\frac{1}{2}}$

$$= \frac{2E}{\hbar \omega_c} \quad \text{—— (7)}$$

$$\left[\alpha^2 \frac{d^2\psi}{d\eta^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}Kx^2\right)\psi = 0 \right]$$

To solve the eqn. (6), let us first make an attempt to obtain an assymptotic solution for the case when $\eta \geq \lambda$ and $\eta \to \pm\infty$, eqn. (6) reduces to

$$\frac{d^2\psi}{d\eta^2} - \eta^2\psi = 0 \quad \text{—— (8)}$$

which has the solution of the form

$$\psi = e^{\pm\eta^2/2}, \text{ for this gives}$$

$$\frac{d^2\psi}{d\eta^2} = (\eta^2 \pm 1)\psi \to \eta^2\psi$$

when $\eta \to \infty$

As $\eta \to \pm\infty$, $\eta^2 \to +\infty$ and $\psi = e^{\eta^2/2}$ becomes arbitrarily large therefore boundary condition allow us only to retain the $-$ exponent term.

In view of above discussion it might be possible to find an exact solution of eqn (5) of the form

$$\psi = e^{-\eta^2/2}\phi(\eta) \quad \text{—— (9)}$$

Now, differentiating it twice w.r.t η, one get the values of $\frac{d^2\psi}{d\eta^2} = e^{-\eta^2/2}\left[\frac{d^2\phi}{d\eta^2} - 2\eta\frac{d\phi}{d\eta} + (\eta^2-1)\phi\right]$

Thus putting the value of $\frac{d^2\psi}{d\eta^2}$ and ψ in eqn. (5), we get

$$\frac{d^2\phi}{d\eta^2} - 2\eta\frac{d\phi}{d\eta} + (\lambda-1)\phi = 0 \quad \text{—— (10)}$$

This differential equation is solved by the method of Series. We then wish to express the function $\phi(\eta)$ by a

Power Series

$$\phi(\eta) = \sum_{n=0}^{\infty} a_n \eta^{n+s} \quad \text{--- (11)}$$

Differentiating eqn. (11) term by term and substituting in eqn (10), we obtain

$$\sum_{n=0}^{\infty} \left\{ (n+s)(n+s-1) a_n \eta^{n+s-2} - 2(n+s) a_n \eta^{n+s} + (\lambda-1) a_n \eta^{n+s} \right\} = 0. \quad \text{--- (12)}$$

For this equation to be satisfied identically in η, co-eff of each power of η must vanish. Hence we require

$$\left.\begin{aligned} s(s-1)\, a_0 &= 0 \\ \text{and } s(s+1)\, a_1 &= 0 \end{aligned}\right\} \quad \text{--- (13)}$$

therefore, we find that $s=0$ or 1. If $s=0$ is chosen, we obtain

$$(n+1)(n+2) a_{n+2} - (2n+1-\lambda) a_n = 0$$

or

$$\frac{a_{n+2}}{a_n} = \frac{(2n+1-\lambda)}{(n+1)(n+2)} \quad \text{(14)} \rightarrow \frac{2}{n} \text{ when } n \rightarrow \infty$$

This expression is called recursion formula from which the remaining co-efficients are calculated with known values of a_0 and a_1.

On examination it is demonstrated that the ratio of eqn. (14) is same as that of the co-efficients of η^{n+2} and η^n in the expansion of $e^{\eta^2/2}$ is allowed to recur to unlimited no. of terms, the wave fn. given by eqn (9) will behave as $e^{\eta^2/2}$ for large η and ~~would~~ therefore would diverge for $\eta \rightarrow \pm\infty$ thus making the wave fn physically unacceptable.

Therefore, to find the admissible wave fn we must put certain restrictions so that the series break off after a finite no. of terms. This is so if and only if we put in eqn (14), $2n+1-\lambda=0$ —— (15)

or $\lambda = 2n+1$

Thus well behaved wave fns are obtained if

$$\lambda = \frac{2E}{\hbar w_c} = 2n+1 \quad (\text{where } n = 0,1,2 \cdots)$$

which gives $E_n = (n+\frac{1}{2})\hbar w_c$ —— (16)

This gives an infinite set of discrete energy level and known as Eigen values of the harmonic oscillator. Also the above equation indicates that the energy levels of harmonic oscillator are equally spaced. The ground state ($n=0$) of the oscillator has the energy $E_0 = \frac{1}{2}\hbar w_c$ which is called zero-point energy and its existence is related to the uncertainty principle. Classically this energy would be zero. This is regarded as an important difference between classical and quantal calculations.

Eigen fn of Harmonic oscillator:

It has been seen clearly from the examination of series $\phi(\eta)$, that it should be a polynomial rather than a power series. Thus the wave fn can be given by

$$\psi_n(x) = N_n e^{-\eta^2/2} H_n(\eta) \; ; \; [\eta = \alpha x] \quad \text{—— (17)}$$

where N_n is a normalisation factor and $H_n(\eta)$ represents the Hermite polynomial of nth degree and is defined by

$$H_n(\eta) = (-1)^n e^{\eta^2} \frac{d^n}{d\eta^n}(e^{-\eta^2}) \quad \text{—— (18)}$$

The normalising condition is given by

$$\int_{-\infty}^{\infty} \psi_n(x)^* \psi_m(x)\, dx = \delta_{mn}$$

$$= \int_{-\infty}^{+\infty} \psi_n^*(x)\,\psi_n(x)\,dx = 1$$

which gives $N_n = \left[\frac{\alpha}{\sqrt{\pi}\, 2^n\, n!}\right]^{1/2}$

Thus the normalised wave fns of harmonic oscillator are

$$\psi_n(x) = \left[\frac{\alpha}{\sqrt{\pi}\, 2^n\, n!}\right]^{\frac{1}{2}} e^{-\frac{1}{2}\alpha^2 x^2} H_n(\alpha x), \quad \text{—19.}$$

where $\alpha^2 = \sqrt{\frac{mk}{\hbar^2}} = \frac{m\omega_c}{\hbar} = \frac{k}{\hbar\omega_c}$ — (20)

Few Hermite Polynomials are given

for $n=0$, $H_0(\eta) = 1$, for $n=1$ $H_1(\eta) = 2\eta$, $H_2(\eta) = 4\eta^2 - 2$

$H_3(\eta) = 8\eta^3 - 12\eta$

The above eqn (19) for wave fn gives the eigen functions of the harmonic oscillator.