(D) 1-D Linear Harmonic oscillator (derivation of soln is not required, comparison with classical oscillator) ①

Ex-2 E

Harmonic Oscillator:-

e.g. diatomic molecule, an atom in a crystal lattice.

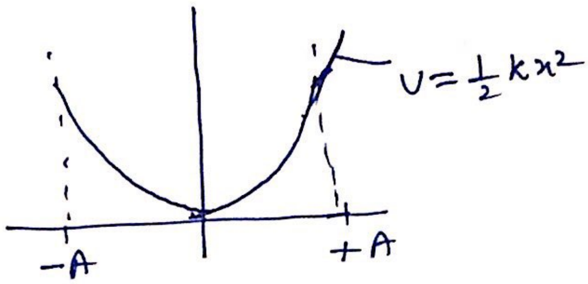


Fig: The potential energy of a harmonic oscillator is proportional to x^2.

There are three quantum-mechanical modifications to this classical picture:

1. The allowed energies will not form a continuous spectrum ~~that~~ but instead a discrete spectrum of certain specific values only.

2. The lowest allowed energy will not be $E=0$, but will be some definite minimum $E=E_0$ (zero-point energy).

3. There will be a certain probability that the particle can penetrate the potential well it may go beyond the limits of $-A$ and $+A$.

$$U(x) = -\int_0^x F(x)\,dx = k\int_0^x x\,dx = \frac{1}{2}kx^2$$

Energy levels:-

Schrödinger eqn for the Harmonic oscillator with $U=\frac{1}{2}kx^2$,

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

It is convenient to simplify eqn ① by introducing the dimensionless quantities.

$$y = \left(\frac{1}{\hbar}\sqrt{km}\right)^{1/2} x = \left(\sqrt{\frac{2\pi m\nu}{\hbar}}\right) x \quad \text{---} ②$$

and
$$\alpha = \frac{2E}{\hbar}\sqrt{\frac{m}{k}} = \frac{2E}{h\nu} \quad \text{---} ③$$

Where ν is the classical frequency.

Here, we change the units in which x and E are expressed from meters and joules, respectively, to dimensionless units.

$F=-kx$

$F=ma$

$$\frac{d^2x}{dt^2} + \frac{k}{m}x = 0$$

$$x = A\cos(2\pi\nu t+\phi)$$

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

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

$$2\pi m\nu = \sqrt{km}$$

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

In terms of y and α Schrödinger eqⁿ becomes

$$\frac{d^2\psi}{dy^2} + [\alpha - y^2]\psi = 0 \quad \text{---} \; (4)$$

[The soln to this eqⁿ that are acceptable here are limited by the condition that $\psi \to 0$ as $y \to \infty$ in order that]

$$\int_{-\infty}^{+\infty} |\psi|^2 dy = 1$$

otherwise the wave function cannot represent an actual particle. The mathematical properties of eqⁿ (4) are such that this condition will be fulfilled only when.

$$\alpha = 2n + 1, \quad \text{where } n = 0, 1, 2, 3, \ldots$$

where $\alpha = \frac{2E}{h\nu}$

$$\boxed{E_n = \left(n + \frac{1}{2}\right) h\nu} \quad \text{where } n = 0, 1, 2, 3, \ldots \quad (5)$$

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

Energy levels of Harmonic oscillator

The energy of a harmonic oscillator is thus quantized in steps of $h\nu$.

When $n = 0$

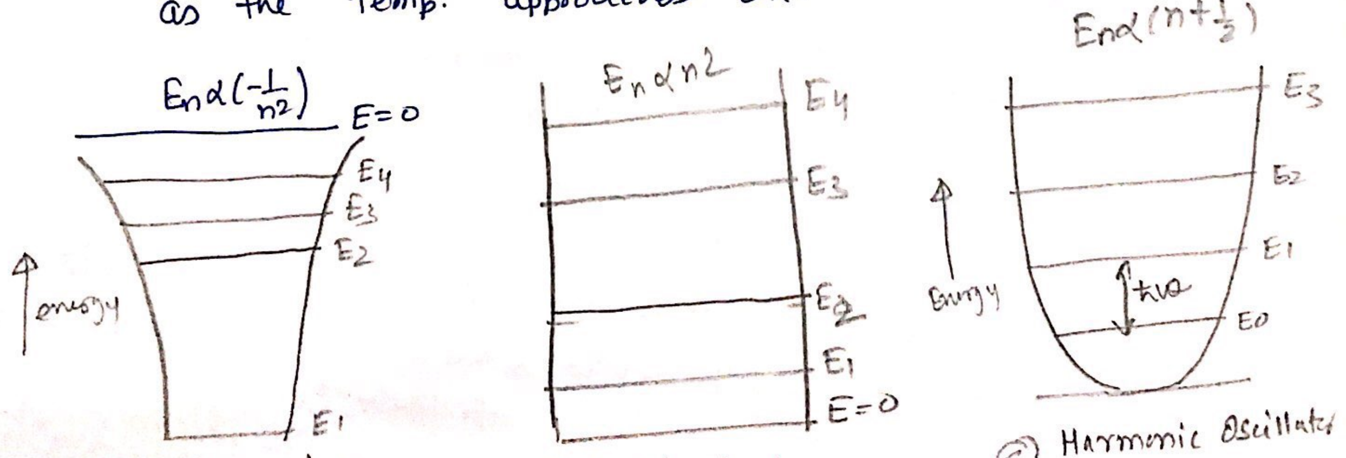
$$\boxed{E_0 = \frac{1}{2} h\nu} \longrightarrow (6)$$

$E = \hbar\omega(2n+1+\frac{3}{2})$

Zero-point energy

This is the lowest value the energy of the oscillator can have.

In case of harmonic oscillator $E = E_0$ and not $E = 0$ as the temp. approaches 0K.



(a) Hydrogen atom (b) Particle in a box (c) Harmonic Oscillator Energy levels

only in case of H.O., the levels are equally spaced.

Wave functions:-

For each choice of the parameter α_n there is a different wave function ψ_n.

Each function consists of a polynomial $H_n(y)$ (called a Hermite polynomial) in either odd or even powers of y, the exponential factor $e^{-\frac{y^2}{2}}$ and a numerical coefficient which is needed for ψ_n to meet the normalization condition

$$\int_{-\infty}^{+\infty} |\psi_n|^2 dy = 1 \qquad n = 0, 1, 2, \ldots$$

The general formula for the nth wave function is

$$\boxed{\psi_n = \left(\frac{2m\nu}{\hbar}\right)^{1/4} \left(2^n n!\right)^{-1/2} H_n(y)\, e^{-\frac{y^2}{2}}} \qquad (7)$$

$H_n(y) \rightarrow$ Hermite polynomial

nth order polynomial called Hermitial polynomial

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

$$H_n(y) = \frac{\lfloor n}{2\pi i} \oint e^{-t^2+2ty}\, t^{-n-1}\, dt$$

Table:- Some Hermite Polynomials

n	$H_n(y)$	$\alpha_n (=2n+1)$	$E_n = (n+\frac{1}{2}) h\nu$
0	1	1	$\frac{1}{2} h\nu$ (or $\frac{1}{2}$ true)
1	$2y$	3	$\frac{3}{2} h\nu$
2	$4y^2 - 2$	5	$\frac{5}{2} h\nu$
3	$8y^3 - 12y$	7	$\frac{7}{2} h\nu$
4	$16y^4 - 48y^2 + 12$	9	$\frac{9}{2} h\nu$
5	$32y^5 - 160y^3 + 120y$	11	$\frac{11}{2} h\nu$

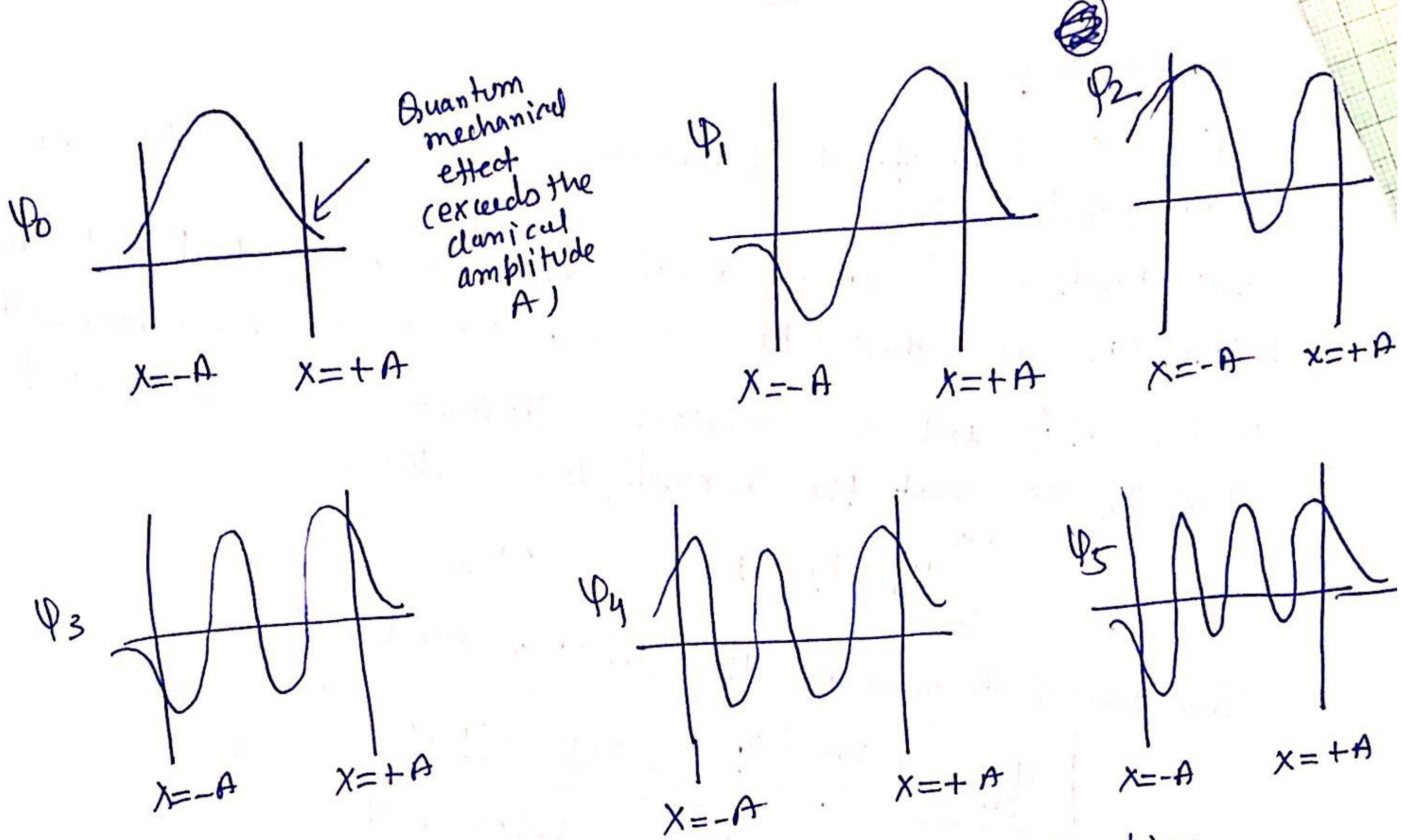
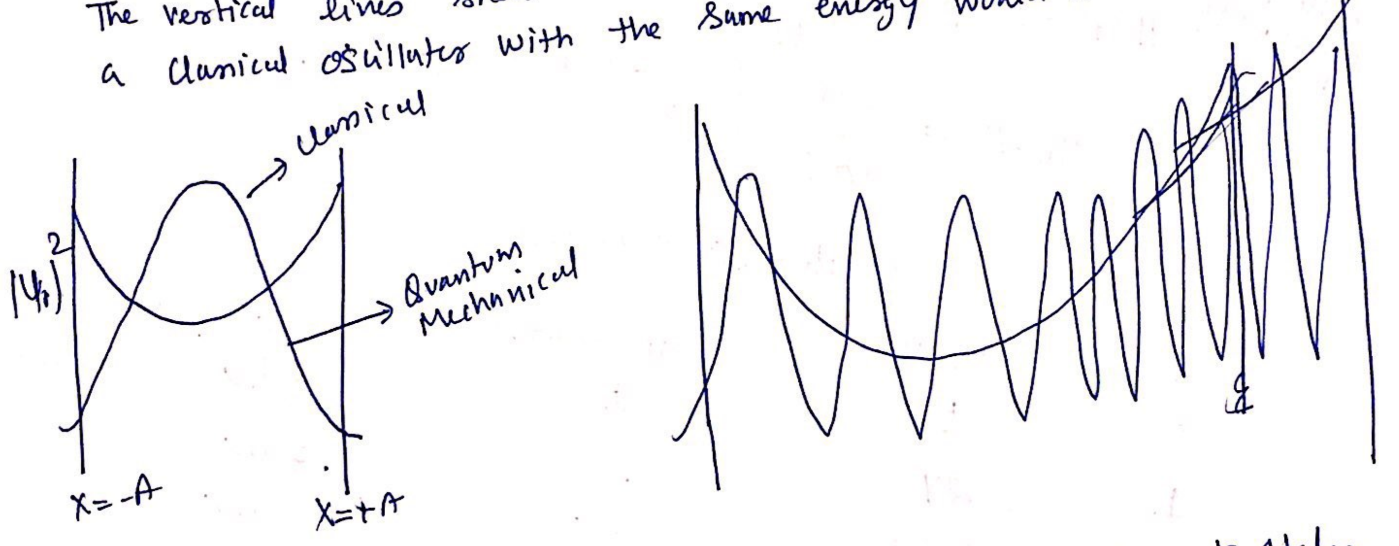


Fig:- The first six harmonic-oscillator wave functions. The vertical lines show the limits -A and +A between which a classical oscillator with the same energy would vibrate.



Fig→ Probabilities densities for the $n=0$ and $n=10$ states.

For $n=0$, opposite behaviour occurs for classical and quantum mechanical oscillator

However, this disagreement becomes less with increasing n.

$$\Downarrow$$

Thus, the classical and quantum picture begin to resemble each other more and more for longer value of n.

First four H.O. normalized wavefunctions

$$\psi_0 = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{y^2}{2}}$$

$$\psi_1 = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2}\, y\, e^{-\frac{y^2}{2}}$$

$$\psi_2 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}} (2y^2-1)\, e^{-\frac{y^2}{2}}$$

$$\psi_3 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{3}} (2y^3-3y)\, e^{-\frac{y^2}{2}}$$

Where $\alpha = \frac{m\omega}{\hbar}$ or $\left(\frac{m(2\pi\nu)}{\hbar}\right)$

$$y = \sqrt{\alpha}\, x$$

Unnormalized

$$\psi_0 = A_0 e^{-\frac{y^2}{2}}$$

$$\psi_1 = A_1\, y\, e^{-\frac{y^2}{2}}$$

$$\psi_2 = A_2 (1-2y^2)\, e^{-\frac{y^2}{2}}$$

$$\psi_3 = A_3 \left(1-\frac{2}{3}y^3\right) e^{-\frac{y^2}{2}}$$

Q: Find the expectation value $\langle x \rangle$ for the first two states of a harmonic oscillator.

Soln: The general formula for $\langle x \rangle$ is

$$\langle x \rangle = \int_{-\infty}^{+\infty} x\,|\psi|^2\,dx$$

$$\psi_n = \left(\frac{2m\nu}{\hbar}\right)^{1/4}\left(2^n n!\right)^{-1/2} H_n(y)\, e^{-\frac{y^2}{2}}$$

Here $H_n(y) = 1$

$$\psi_0 = \left(\frac{2m\nu}{\hbar}\right)^{1/4} e^{-\frac{y^2}{2}}$$

Here $H_n(y) = 2y$

$$\psi_1 = \left(\frac{2m\nu}{\hbar}\right)^{1/4}\left(\frac{1}{2}\right)^{1/2}(2y)\, e^{-\frac{y^2}{2}}$$

The values of $\langle x \rangle$ for $n=0$ and $n=1$ will respectively be proportional to the integrals.

$n=0$

$$\int_{-\infty}^{+\infty} y\,|\psi_0|^2\,dy = \int_{-\infty}^{+\infty} y\,e^{-y^2}\,dy = -\left[\frac{1}{2}e^{-y^2}\right]_{-\infty}^{\infty}$$

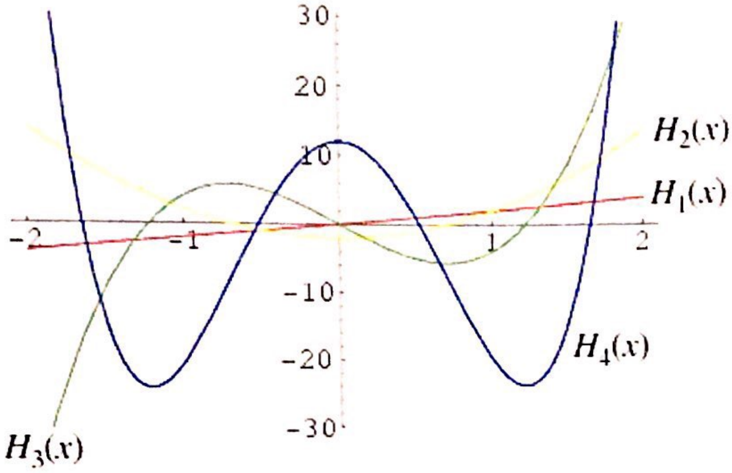
$$= 0$$

$n=1$

$$\int_{-\infty}^{+\infty} y\,|\psi_1|^2\,dy = \int_{-\infty}^{+\infty} y^3\,e^{-y^2}\,dy = -\left[\left(\frac{1}{4}+\frac{y^2}{2}\right)e^{-y^2}\right]_{-\infty}^{+\infty}$$

$$= 0$$

The expectation value $\langle x \rangle$ is therefore 0 in both cases. In fact $\langle x \rangle = 0$ for all states of a harmonic oscillator, which could be predicted since $x=0$ is the equilibrium position of the oscillator where its potential energy is a minimum.



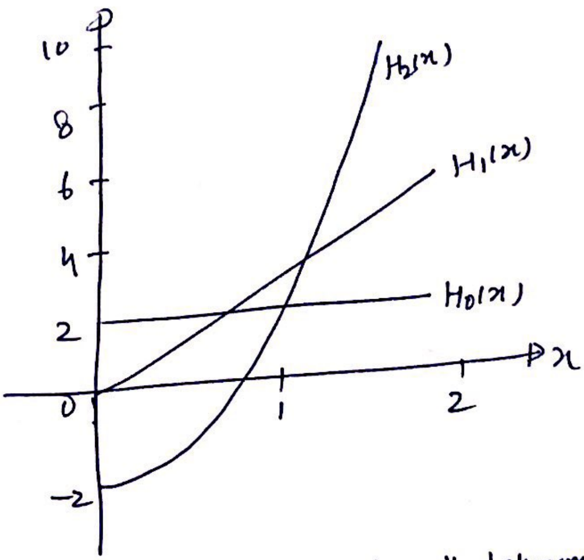
$$H_n(z) = \frac{n!}{2\pi i} \oint e^{-t^2+2tz} \, t^{-n-1} \, dt$$

$H_0(x) = 1$

$H_1(x) = 2x$

$H_2(x) = 4x^2 - 2$

$H_3(x) = 8x^3 - 12x$



Fig→ Hermite polynomials.