IMPORTANT ANNOUNCEMENT RELATED TO ETE

LAB COMPONENT: 10 MARKS

- A TOTAL OF 16 QUESTIONS WILL BE THERE. YOU SHOULD ATTEMPT 10.
- 2 COMPULSORY QUESTIONS + ATTEMPT ANY 8 OUT OF 14 (2 QUESTIONS FROM EACH EXPERIMENT)
- THERE WILL BE MULTIPLE CORRECT ANSWERS IN EACH QUESTION

  (YOU NEED TO MARK ALL CORRECT ANSWERS TO SCORE)
- ONLY THE FIRST 10 QUESTIONS WILL BE EVALUATED. THEREFORE, ANSWER ONLY 10

ETE: 40 MARKS (10 MARKS FROM PRE MTE SYLLABUS

+ 30 MARKS FROM POST MTE SYLLABUS)

- **MODE OF ETE: LIKE MTE**

NOTE :

IF YOU DO NOT WRITE YOUR NAME, ENROLLMENT NUMBER, AND QUESTION SET NUMBER IN THE ORS SHEET AND IN THE WORKBOOKLET, YOUR PAPER WILL NOT BE EVALUATED.

!! PLEASE DO NOT BRING ANY EXCUSES AFTERWARD FOR NOT FOLLOWING THE INSTRUCTIONS!!

QUANTUM HARMONIC OSCILLATOR

- Harmonic motion occurs when a system vibrates about an equilibrium configuration.
- The condition for harmonic motion is the presence of a restoring force that acts to return the system to its equilibrium configuration when it is disturbed.
- In simple harmonic motion, the **restoring force *F*** on a particle of **mass *m*** is **linear** ➔ $F \propto x$ from its equilibrium position and in the opposite direction.

$$F = -kx$$ Hooke's law

From the second law of motion, $F = ma$,

$$-kx = m\frac{d^2x}{dt^2}$$

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

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

There are various ways to write the solution; a common one is

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

where

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

Frequency of harmonic oscillator

A is their amplitude.
ϕ is the phase angle, which depends on what x is at the time t = 0 and on the direction of motion at that time.

The importance of SHO in both Classical and Modern Physics lies in the fact that these restoring forces reduce to Hooke's law for small displacements *x*.

To verify this important point, we note that any restoring force, which is a function of x, can be expressed in a Maclaurin series about the equilibrium position $x = 0$ as

$$F(x) = F_{x=0} + \left(\frac{dF}{dx}\right)_{x=0} x + \frac{1}{2}\left(\frac{d^2F}{dx^2}\right)_{x=0} x^2 + \frac{1}{6}\left(\frac{d^3F}{dx^3}\right)_{x=0} x^3 + \cdots$$

$$F(x) = F_{x=0} + \left(\frac{dF}{dx}\right)_{x=0} x + \frac{1}{2}\left(\frac{d^2F}{dx^2}\right)_{x=0} x^2 + \frac{1}{6}\left(\frac{d^3F}{dx^3}\right)_{x=0} x^3 + \cdots$$

Since $x = 0$ is the equilibrium position, $F_{x=0} = 0$. For small x the values of $x^2, x^3, \ldots$ are very small compared with x, so the third and higher terms of the series can be neglected. The only term of significance when x is small is therefore the second one.

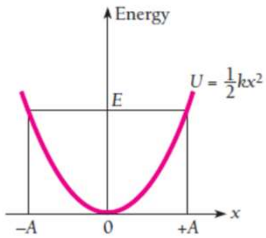
$$F(x) = \left(\frac{dF}{dx}\right)_{x=0} x$$

which is Hooke's law when $(dF/dx)_{x=0}$ is negative

The conclusion is that *all* oscillations are simple harmonic in character when their amplitudes are sufficiently small.

The potential-energy function

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



The amplitude A of the motion is determined by the total energy E of the oscillator, **which classically can have any value.**

$$E = \tfrac{1}{2}kA^2$$

We can anticipate three quantum mechanical modifications to this classical picture:

- ❖ The allowed energies will not form a continuous spectrum, but instead a discrete spectrum of certain specific values only.
- ❖ The lowest allowed energy will not be $E = 0$, rather some definite minimum energy, $E = E_0$.
- ❖ There will be a certain probability that the particle can penetrate the potential well it is in and go beyond the limits of -A and +A.

Schrödinger's equation for the harmonic oscillator is, with $U = \frac{1}{2}kx^2$,

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

Let us simplify the equation by introducing the dimensionless quantities:

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

and

$$\alpha = \frac{2E}{\hbar}\sqrt{\frac{m}{k}} = \frac{2E}{h\nu}$$

We changed the units for x and E from meters and joules, respectively, to dimensionless units.

In terms of y and α Schrödinger's equation becomes

$$\frac{d^2\psi}{dy^2} + (\alpha - y^2)\psi = 0$$

The acceptable solutions to this equation are limited by the **condition that $\psi \to 0$ as $y \to \pm\infty$** so that

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

$$\frac{d^2\psi}{dy^2} + (\alpha - y^2)\psi = 0$$

The mathematical properties of this equation are such that the condition will be fulfilled only when

$$\alpha = 2n + 1 \qquad n = 0, 1, 2, 3, \ldots$$
$$= 2E/h\nu$$

The energy levels of a harmonic oscillator whose classical frequency of oscillation is ν are given by the formula

$$E_n = (n + \tfrac{1}{2})h\nu \qquad n = 0, 1, 2, 3, \ldots$$

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

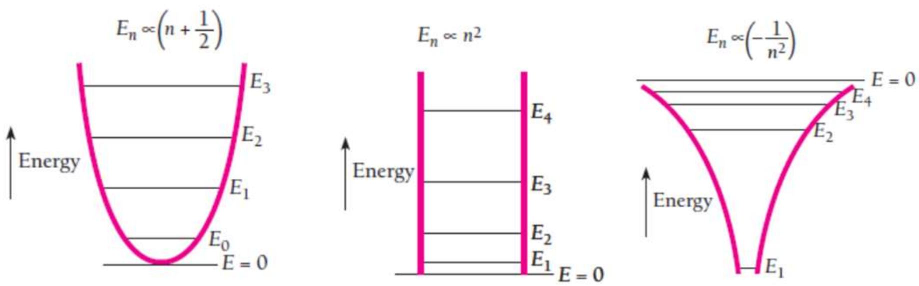
We note that when $n = 0$,

$$\boxed{E_0 = \tfrac{1}{2}h\nu}$$ **Called Zero-point Energy**

$$\boxed{E_n = (n + \tfrac{1}{2})h\nu \qquad n = 0, 1, 2, 3, \ldots}$$

$$\boxed{E_0 = \tfrac{1}{2}h\nu}$$

- ➔ The lowest value of energy of the oscillator.
- ➔ This value is called the **zero-point energy** because a harmonic oscillator in equilibrium with its surroundings would approach an energy of $E = E_0$, not $E = 0$ as the temperature approaches 0K.



harmonic oscillator: a particle in a box: a hydrogen atom:

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 $e^{-y^2/2}$, and a numerical coefficient which is needed for ψ_n to meet the normalization condition

$$\alpha = 2n + 1 \qquad n = 0, 1, 2, 3, \ldots$$
$$= 2E/h\nu$$

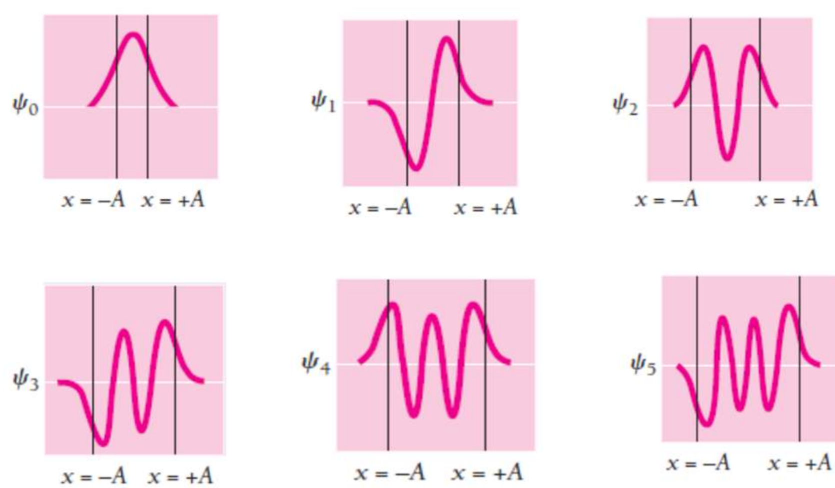
$$\int_{-\infty}^{\infty} |\psi_n|^2 \, dy = 1 \qquad n = 0, 1, 2 \ldots$$

The general formula for the n^{th} wave function is

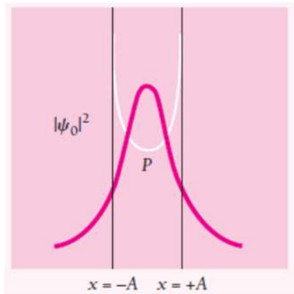
$$\psi_n = \left(\frac{2m\nu}{\hbar}\right)^{1/4} (2^n n!)^{-1/2} H_n(y) e^{-y^2/2}$$

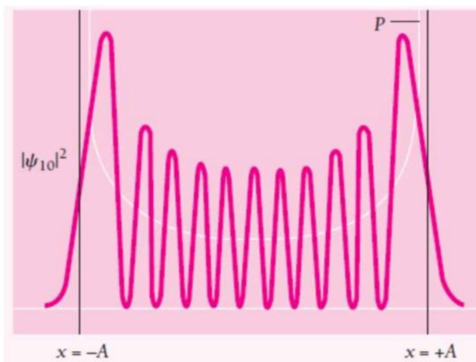
The first six Hermite polynomials $H_n(y)$ are listed

n	$H_n(y)$	α_n	E_n
0	1	1	$\frac{1}{2}h\nu$
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	$\frac{11}{2}h\nu$



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.





- ✓ Probability densities for the n = 0 and n = 10 states of a quantum-mechanical harmonic oscillator.
- ✓ The probability densities for classical harmonic oscillators with the same energies are shown in white.
- ✓ In the n = 10 state, the wavelength is shortest at x = 0 and longest at x = ± A.

Example 5.7

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

Solution The general formula for $\langle x\rangle$ is $$\langle x\rangle = \int_{-\infty}^{\infty} x\,|\psi|^2\,dx$$

In calculations such as this it is easier to begin with y in place of x and afterward use

$$y = \left(\frac{1}{\hbar}\sqrt{km}\right)^{1/2} x = \sqrt{\frac{2\pi m\nu}{\hbar}}\,x$$ to change to x.

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

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

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

$$n = 0: \int_{-\infty}^{\infty} y|\psi_0|^2\, dy = \int_{-\infty}^{\infty} ye^{-y^2}\, dy = -\left[\frac{1}{2}e^{-y^2}\right]_{-\infty}^{\infty} = 0$$

$$n = 1: \int_{-\infty}^{\infty} y|\psi_1|^2\, dy = \int_{-\infty}^{\infty} y^3e^{-y^2}\, dy = -\left[\left(\frac{1}{4} + \frac{y^2}{2}\right)e^{-y^2}\right]_{-\infty}^{\infty} = 0$$

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.

Another representation: $U_s = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$ $\quad \omega = \sqrt{k/m}$

$$E = K + U_s = \tfrac{1}{2}kA^2 = \tfrac{1}{2}m\omega^2A^2$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \tfrac{1}{2}m\omega^2x^2\psi = E\psi$$

We take as our guess the following wave function: $\psi = Be^{-Cx^2}$

Test if this guess solution satisfies the Schrodinger Equation !

$$C = \frac{m\omega}{2\hbar} \quad \text{and} \quad E = \tfrac{1}{2}\hbar\omega$$

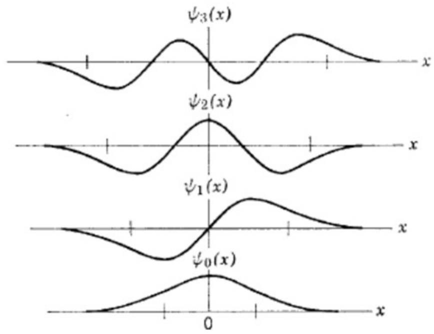
It turns out that the solution we have guessed corresponds to the ground state of the system, which has an energy $\frac{1}{2}\hbar\omega$..

Because $C = m\omega/2\hbar$, the wave function for this state is

$$\psi = Be^{-(m\omega/2\hbar)x^2}$$

where B is a constant to be determined from the normalization condition.

The remaining solutions that describe the excited states are more complicated, but all solutions include the exponential factor e^{-Cx^2}.



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