4] Write down an expression for vibrational energy of a diatomic molecule taking it as a Simple Harmonic Oscillator. Sketch the vibrational energy levels of such a molecule.

→ The vibrational motion of nuclei of diatomic molecule is taken as equivalent to that of Simple Harmonic Oscillator.

Vibrational motion of a diatomic molecule.

∴ Vibrational energy $E_v = \left(v + \frac{1}{2}\right) h\nu_0$ ..... (1)

The energy absorbed in promoting a molecule from its lowest level to the next is given by

$$\Delta E = h\nu_0 \quad \text{.....} (2)$$

Acc. to Hook's law,

$$\nu_0 = \frac{1}{2\pi}\sqrt{k/\mu} \quad \text{.....} (3)$$

μ → reduced mass ; k → force constant.

Substituting eqn (3) in (2),

$$\Delta E = h \times \frac{1}{2\pi}\sqrt{k/\mu} \quad \text{.....} (4)$$

In terms of equilibrium vibrational frequency,

$$\boxed{E_v = \left(v + \frac{1}{2}\right) hc\omega_e} \quad \text{.....} (5)$$

putting $v = 0, 1, 2, 3 \ldots$ in eqn (5), it can be seen that vibrational energy levels of a harmonic oscillator are equally spaced.

The various vibrational energy levels are

diagrammatically Shown as follows.

→ For a lowest vibrational level, $\vartheta = 0$.

$$\therefore \boxed{E_0 = \frac{1}{2} hc\omega_e}$$

This energy is known as Zero point energy i.e) At absolute Zero, ~~when~~ all translational & rotational motion Stops in a crystal. But vibrational motion Still exists