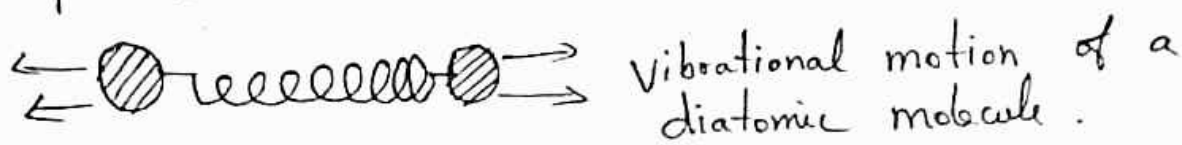


4] Write down an expression for vibrational energy of a diatomic molecule taking it as a Simple Harmonic Oscillator. Sketch the vibrational energy levels of such a molecule.

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



∴ Vibrational energy  $E_v = (v + \frac{1}{2}) h \nu_0 \dots \dots \textcircled{1}$

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

Acc. to Hook's law,  $\Delta E = h \nu_0 \dots \dots \textcircled{2}$

$\nu_0 = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} \dots \dots \textcircled{3}$

$\mu \rightarrow$  reduced mass ;  $k \rightarrow$  force constant.  
Substituting eqn (3) in (2),

$\Delta E = h \times \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} \dots \dots \textcircled{4}$

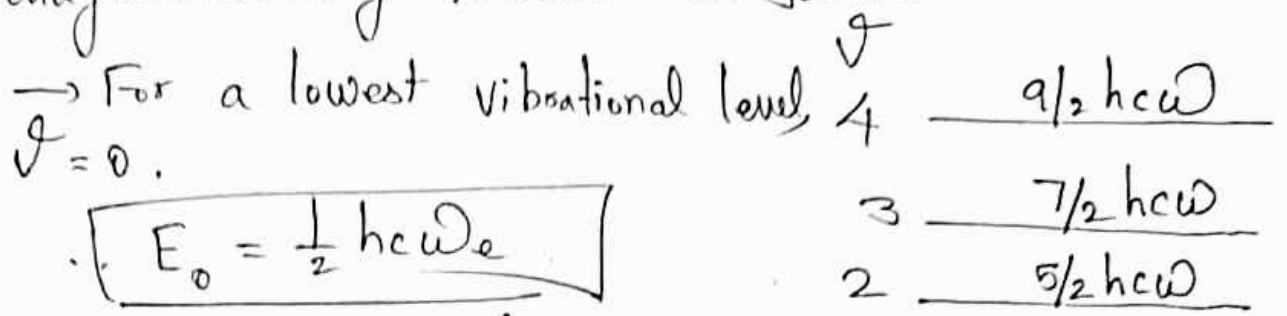
In terms of equilibrium vibrational frequency,

$E_v = (v + \frac{1}{2}) h c \omega_e \dots \dots \textcircled{5}$

Putting  $v = 0, 1, 2, 3, \dots$  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.



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.