Q1. $h\nu - W = \frac{1}{2} m v_{max}^2$

$\Rightarrow \frac{hc}{\lambda} - W = \frac{1}{2} m v_{max}^2$

$\Rightarrow \frac{6.626 \times 10^{-34} \times 3 \times 10^{8}}{3000 \times 10^{-10}} = \frac{1}{2} \times 9.1 \times 10^{-31} \times v^2 + 3.28\,eV.$

$\Rightarrow \frac{6.626 \times 10^{-34} \times 3 \times 10^{8}}{3000 \times 10^{-10}} J - 3.28\,eV = (KE)_{max}.$

$\Rightarrow \frac{6.626 \times 3}{3000} \times 10^{-34+8+10} J - 3.28\,eV = (KE)_{max}.$

$\Rightarrow \frac{6.626 \times 3}{3000} \times 10^{-16} J - 3.28\,eV = (KE)_{max}.$

$\Rightarrow \frac{0.006626 \times 10^{-16}}{1.602 \times 10^{-19}} eV - 3.28\,eV = (KE)_{max}.$

$\Rightarrow 0.00414 \times 10^{3}\,eV - 3.28\,eV = (KE)_{max}.$

$\Rightarrow (KE)_{max} = 4.14 - 3.28 = \underline{\underline{0.86\,eV}}$ ans.

Q2. Side length $= 20\ A^\circ = 20 \times 10^{-10}$ m

$\therefore$ Volume of cube $= a^3 = (20 \times 10^{-10})^3\ m^3$

$= 8000 \times 10^{-30}\ m^3$

$= 8 \times 10^{-21}\ cm^3$

Density of water $= 1\,g\,cc^{-1}$

mass of water molecules in the cube $= 8 \times 10^{-21}$ g

$\Rightarrow$ mass of single water molecule $= 18$ amu

$= 18 \times 1.66 \times 10^{-24}$ g

$\therefore$ No. of water molecules $= \dfrac{8 \times 10^{-21}}{18 \times 1.66 \times 10^{-24}}$

$= 0.2677 \times 10^3$

$\simeq \underline{268}$ ~~and~~ molecules.

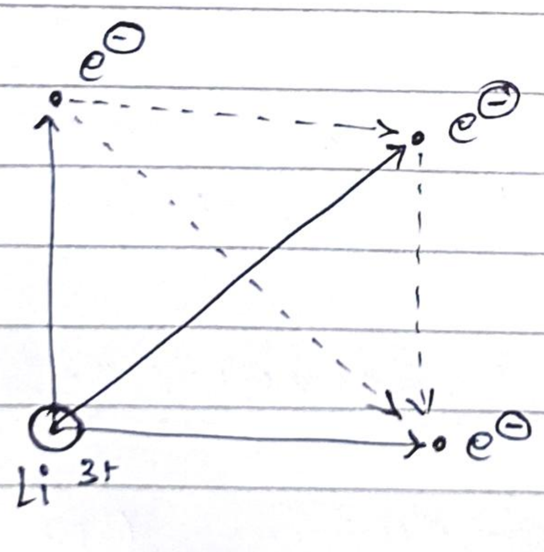
Q3. Li has 3 electrons at r_1, r_2 and r_3 respectively.

$$\therefore \hat{H} = -\frac{\hbar\nabla^2}{2m} - \frac{2e^2}{|r_1|} - \frac{2e^2}{|r_2|} - \frac{2e^2}{|r_3|} + \frac{e^2}{|r_1 - r_2|}$$

$$+ \frac{e^2}{|r_2 - r_3|} + \frac{e^2}{|r_3 - r_1|}$$

Thus, potential energy is,

$$-\frac{2e^2}{|r_1|} - \frac{2e^2}{|r_2|} - \frac{2e^2}{|r_3|} + \frac{e^2}{|r_1 - r_2|} + \frac{e^2}{|r_2 - r_3|} + \frac{e^2}{|r_3 - r_1|}$$



Q4. a). In Born - Oppenheimer approximation, the nuclear motion is assumed to be fixed wrt the electronic motion.

b) For multielectron systems, there is a PE term in the Hamiltonian due to the interaction b/w the electrons themselves. Taking into account this repulsive potential, it is not possible to solve exactly a multi-electron quantum system.

c) (i) Mean-Field Approximation or Hartree-Fock Method

(ii) Born- Oppenheimer Approximation