Q → Give the valence bond wavefunction $\psi_{AB}$ for $H_2$ molecule.

Ans :- $H_2$ Molecule :-

Suppose, $H_A$ & $H_B$ Two atoms.

$e^\ominus$ of $H_A$ = (1)

$e^\ominus$ of $H_B$ = (2)


Nucleus of $H_A$ = A

Nucleus of $H_B$ = B

When they close together -

① Attractive forces → A ⟷ (1) (2)

B ⟷ (1) (2)

② Repulsive forces → A ⟷ B

(1) ⟷ (2)

A bond (covalent) is formed when - attractive forces is equal to repulsive forces. The distance between the two nucleus is called equilibrium distance ($r_0$).

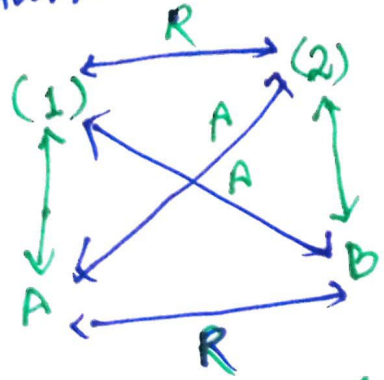


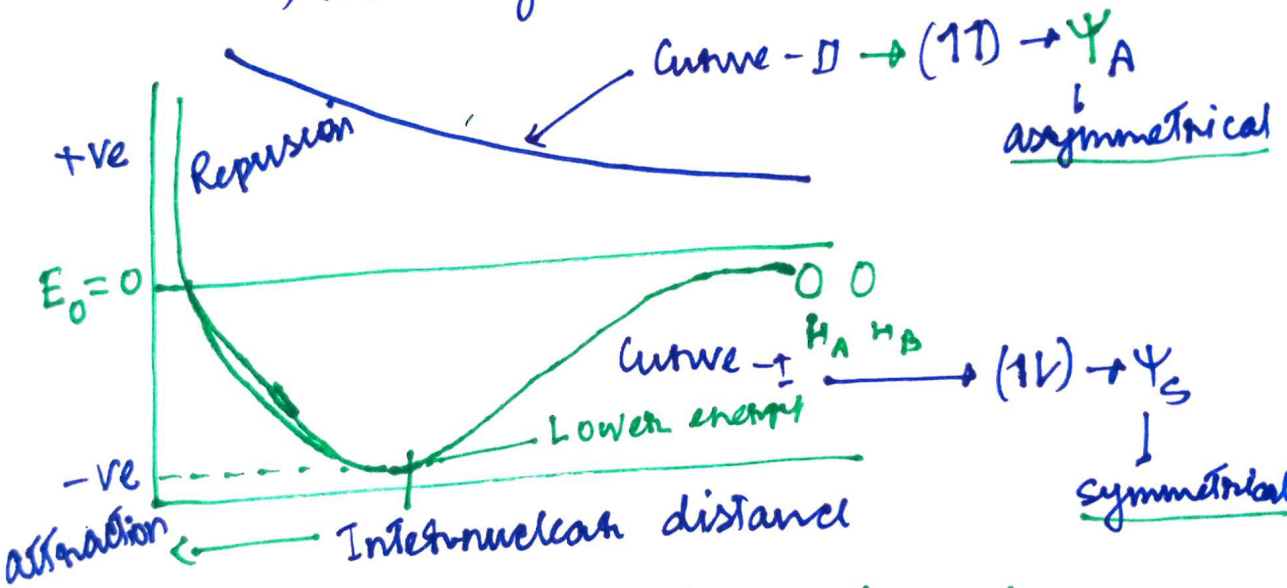

Fig. Attraction & Repulsion when Two H-atoms come closer.

⊛ Redistribution of $e^{\ominus}$ occurs –

Two conditions occur –

① (11) → same direction, same spin, so, repulsion occurs, energy increases, ∴ stability decreases.

② (1↓) → opposite spin, so attraction occurs, bond is formed, energy minimum, so, stability increases.




When $e^{\ominus}$s mix, two covalent structures formed – Here, after mixing, identity of $e^{\ominus}$s lost.

I

$H_A(1) \cdot H_B(2)$

II

$H_A(2) \cdot H_B(1)$

Now, we will write wavefunctions for both cases –

$$\Psi_I = \Psi_A(1) \cdot \Psi_B(2)$$

$$\Psi_2 = \Psi_A(2) \cdot \Psi_B(1) \ .$$

Total wave function of $H_2$ molecule —

$$\psi = \psi_I + \psi_{II}$$

$$\psi = c_1 \psi_I + c_2 \psi_{II} \rightarrow c_1 \& c_2 \text{ mixing coefficient.}$$

$$\psi_{AB} = c_1 \psi_A(1) \cdot \psi_B(2) + c_2 \psi_A(2) \cdot \psi_B(1) \quad \text{—— (1)}$$

For $H_2$ molecule —

$$\boxed{c_1 = \pm c_2} \quad \text{if } c_1 = 1, \text{ then, } c_2 = \pm 1$$

eqn (1) $\Rightarrow (\psi_{AB})_S = \psi_A(1) \cdot \psi_B(2) + \psi_A(2) \cdot \psi_B(1)$ . $\rightarrow c_1 = 1, c_2 = 1$

and $\Rightarrow (\psi_{AB})_A = \psi_A(1) \cdot \psi_B(2) - \psi_A(2) \cdot \psi_B(1) \rightarrow c_1 = 1, c_2 = -1$