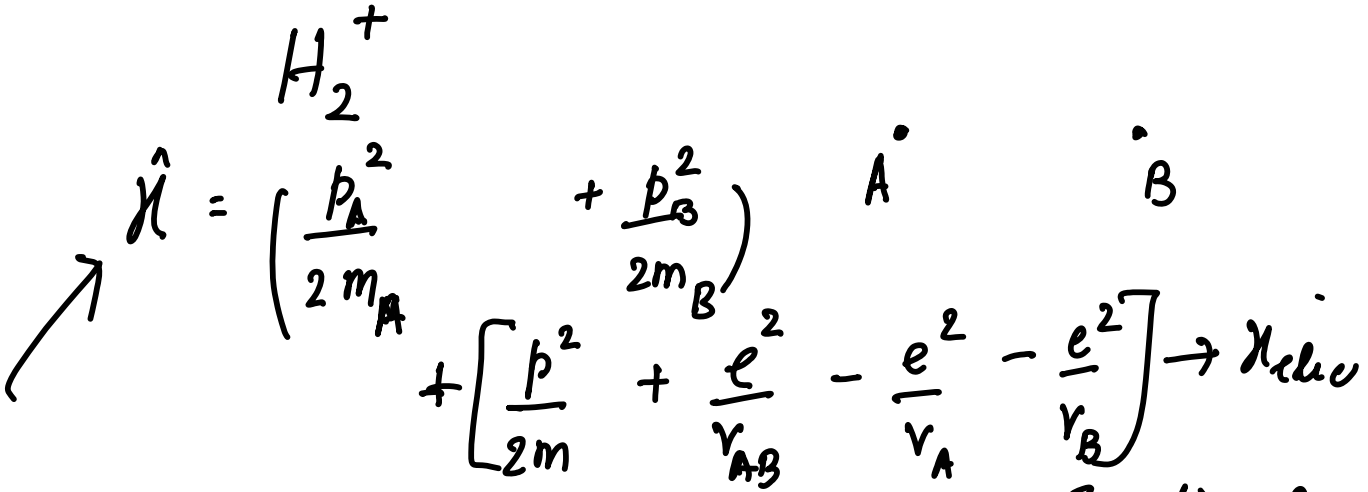
Bonding in molecules

H_2^+



$$\hat{\mathcal{H}} = \left(\frac{p_A^2}{2m_A} + \frac{p_B^2}{2m_B}\right) + \left[\frac{p^2}{2m} + \frac{e^2}{r_{AB}} - \frac{e^2}{r_A} - \frac{e^2}{r_B}\right] \rightarrow \mathcal{H}_{elec}$$

$$\hat{\mathcal{H}}\psi = E\psi(\vec{r}, \vec{R})$$

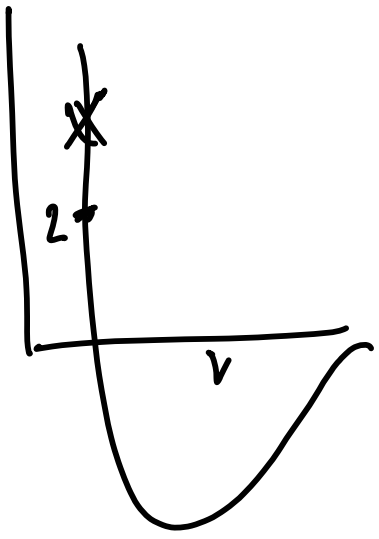
Function of electron & nuclear coordinates

$$\frac{m_N}{m_e} \gg 1$$

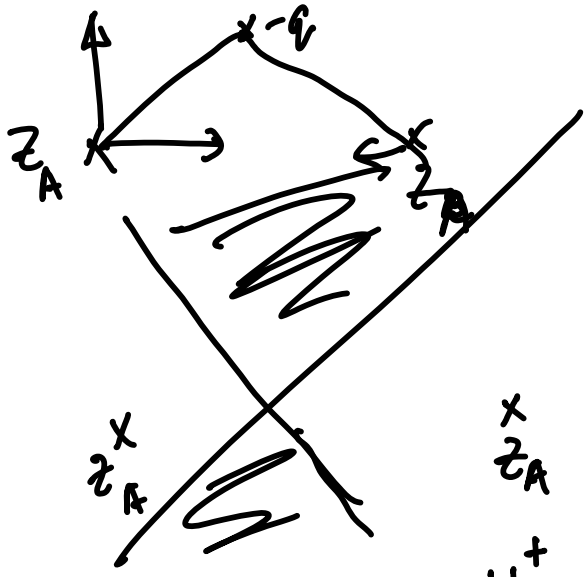
$$\psi = \boxed{\psi_{elec}(\vec{r}; \vec{R})} \times \psi_{nucl}$$

ψ_{tot}

"Born-Oppenheimer approximation"



$$V_{AB} = \frac{(Z_A e)^2}{r_{AB}^2}$$

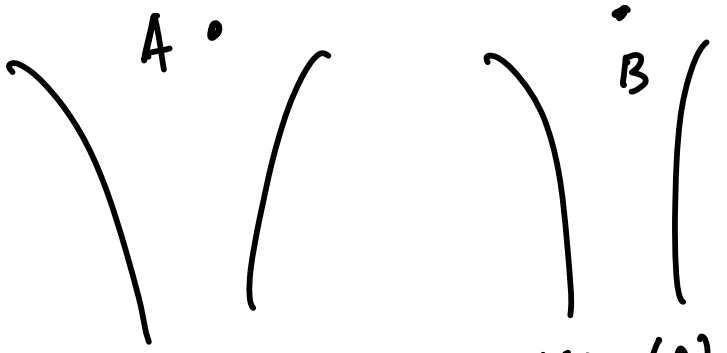


Z_A^x

$H_2^+ \rightarrow H_A + H_B^+$

$\hookrightarrow H_A^+ + H_B$

$R = \infty$

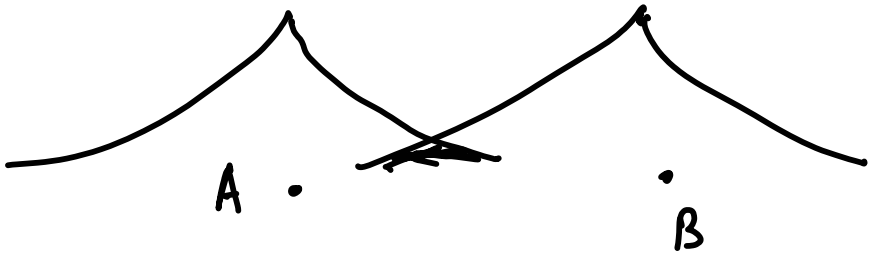


$\psi \sim 1s_A$

$1s_B$

$\psi_{100}(A) = 1s_A$

$\psi = c_A(1s_A + c_B 1s_B$



$\int 1s_A^* \, 1s_B \, dz = S$

overlap integral

One electron Ψ_f

$H_2^+ \rightarrow H_2$

$\psi_+(1)\ \psi_+(2)$

LCAO - Molecular Orbital Theory