DIATOMIC MOLECULES

(NO STRUCTURE)

LCAO – MO

→ ENERGY LEVELS

↓

MOLECULAR PROPERTIES

HOMONUCLEAR 

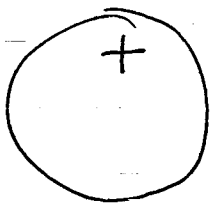
HETERONUCLEAR 

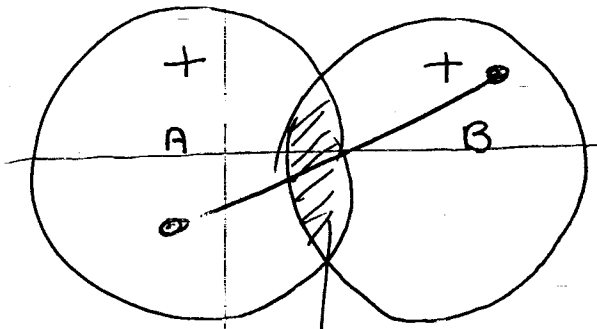
MIXING

— SIMILAR ENERGY

— Overlap

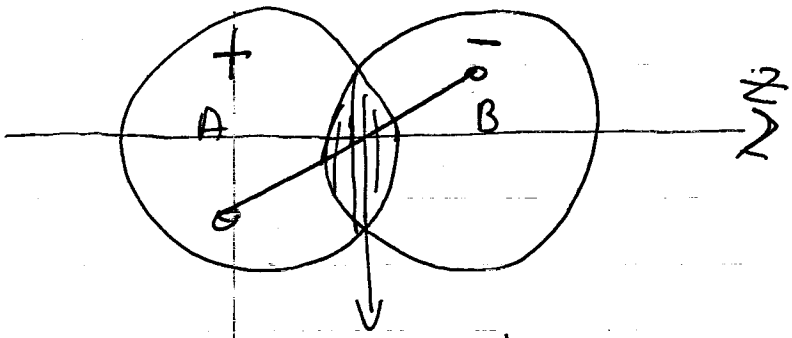
LCAO – MO

1s ↔ 



$$\Psi_{\sigma_g 1s} = C_1 \phi^A_{1s} + C_1 \phi^B_{1s}$$

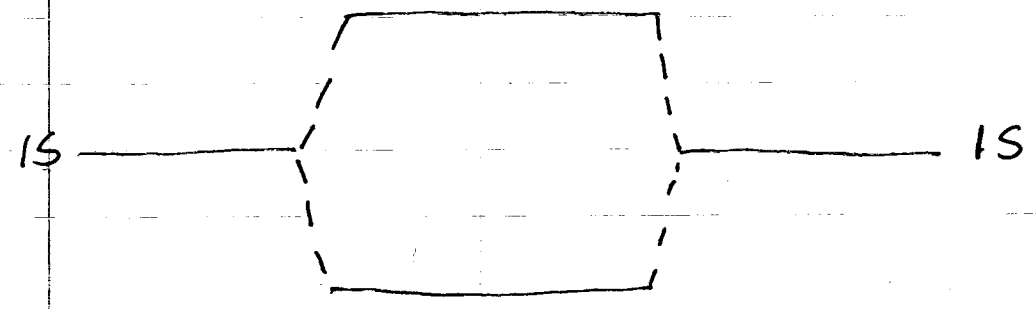
OVERLAP ⟶ bonding

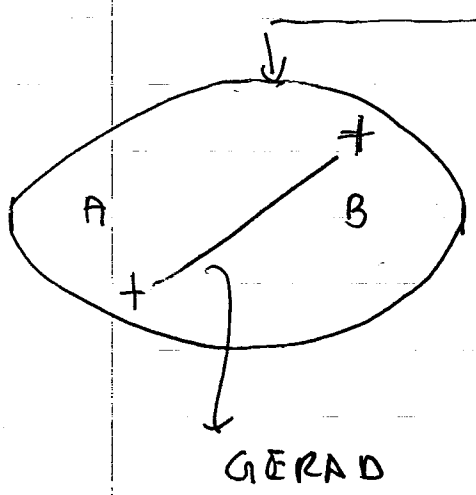


$$\Psi_{\sigma_u 1s} = C_2 \phi^A_{1s} - C_2 \phi^B_{1s}$$

Cancelation ⟶ antibonding

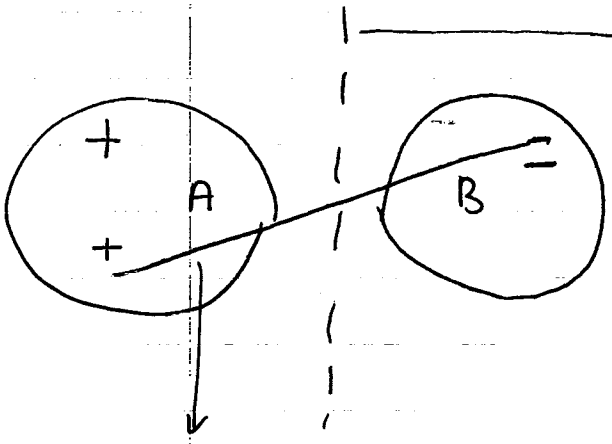
A B





BONDING

$$\left|\Psi_{\sigma_{gls}}\right|^2 = \left\{ |\phi_{1s}^A|^2 + |\phi_{1s}^B|^2 + \phi_{1s}^A \phi_{1s}^B \right\} |C_1|^2$$



antibonding → *

$$\left|\Psi_{\sigma^*_{uls}}\right|^2 = \left\{ |\phi_{1s}^A|^2 + |\phi_{1s}^B|^2 - \phi_{1s}^A \phi_{1s}^B \right\} |C_2|^2$$

ungerad

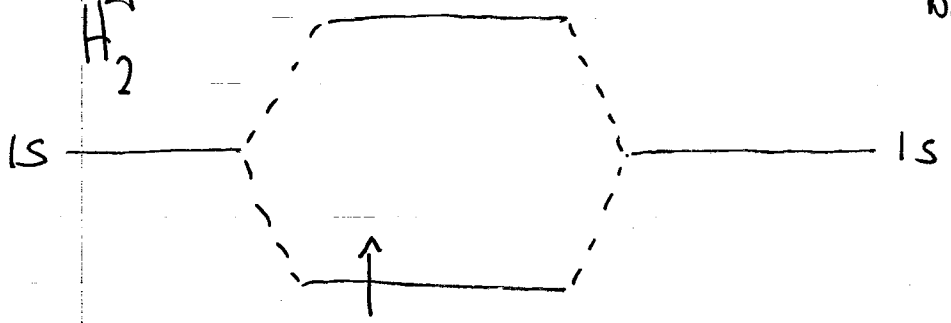
GERAD → $\Psi_{\sigma^*_{gls}}(-x,-y,-z) = \Psi_{\sigma_{gls}}(x,y,z)$

UNGERAD → $\Psi_{\sigma^*_{uls}}(-x,-y,-z) = -\Psi_{\sigma^*_{uls}}(x,y,z)$

H_2^+, H_2, He_2^+, He_2

1 2 3 4 electrons

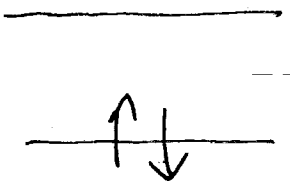
H_2^+



$bo = \frac{1}{2}[1-0] = \frac{1}{2}$

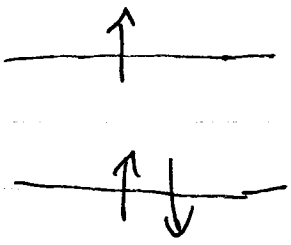
BOND ORDER

H_2

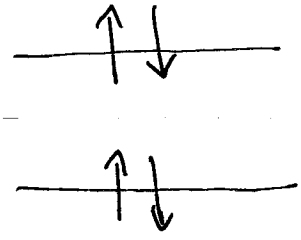


$bo = \frac{1}{2}[2-0] = 1$

He_2^+



$bo = \frac{1}{2}[2-1] = \frac{1}{2}$



He_2

$bo = \frac{1}{2}[2-2] = 0$

NO He_2

HOMONUCLEAR DIATOMICS

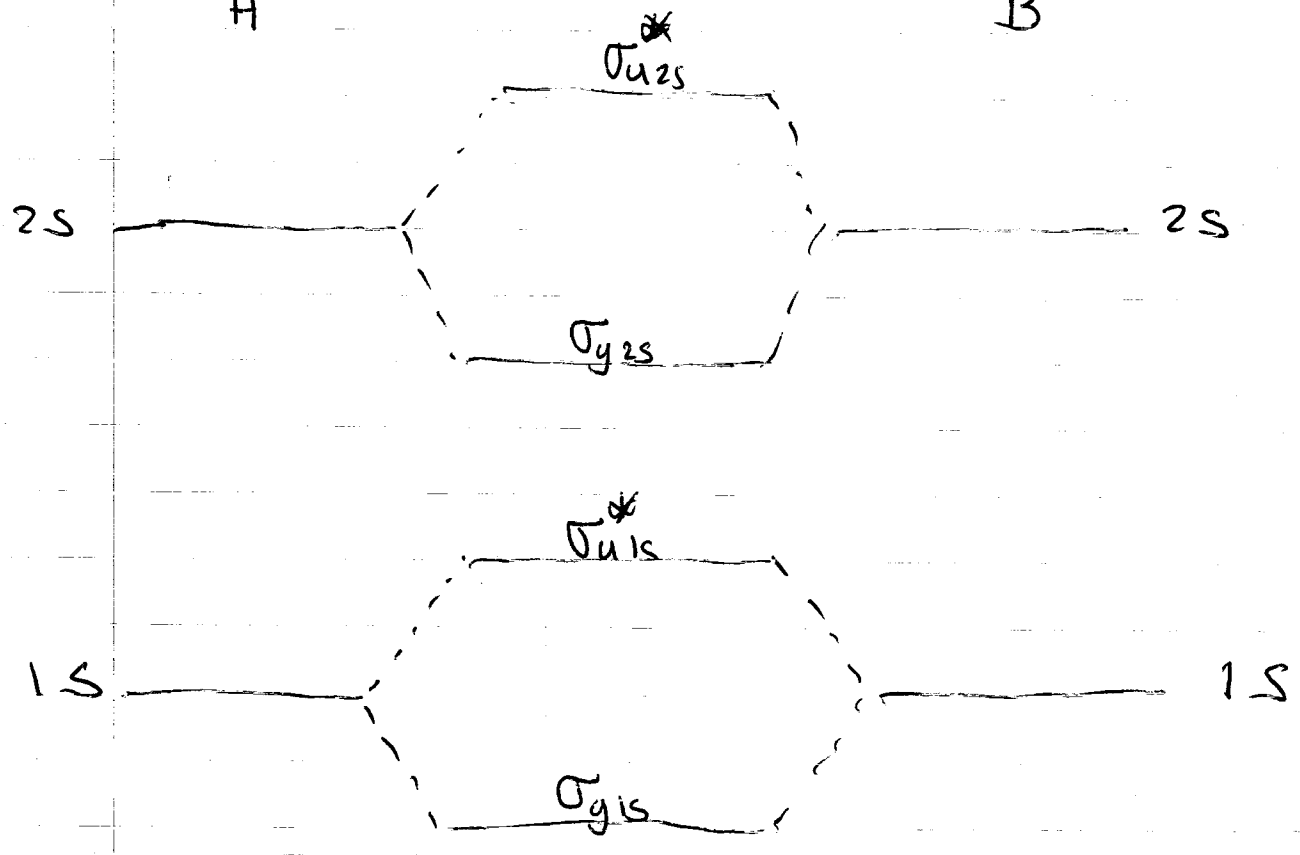
A B

2S ——— ——— 2S

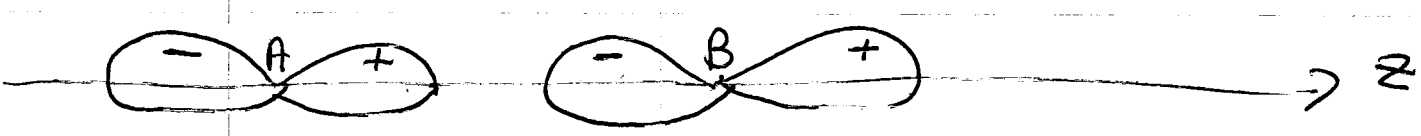
1S ——— ——— 1S

$$\Phi = C_1 \phi_{1S}^{A} + C_2 \phi_{1S}^{B} + C_3 \phi_{2S}^{A} + C_4 \phi_{2S}^{B}$$

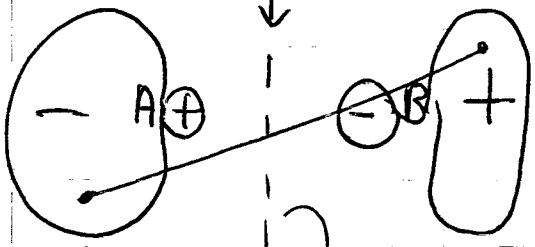
A B



p_z^A p_z^B

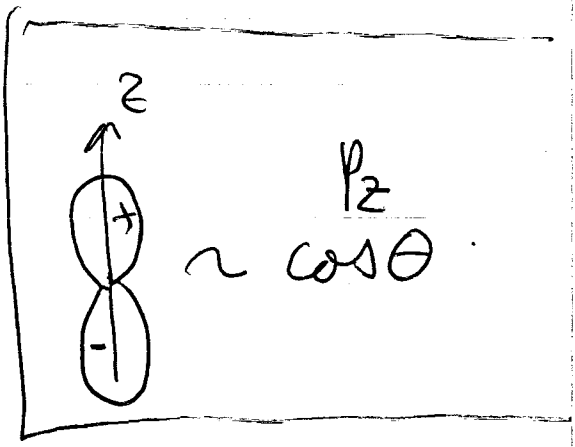


$\phi_{2p_z^A} + \phi_{2p_z^B}$



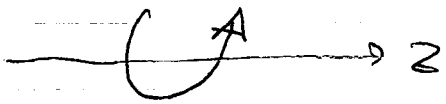
$\sigma^*_{u\,2p_z}$

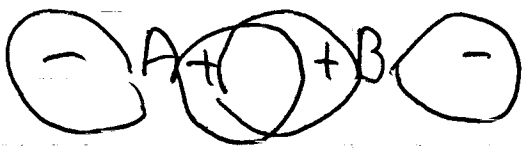
↳ ANTIBONDING

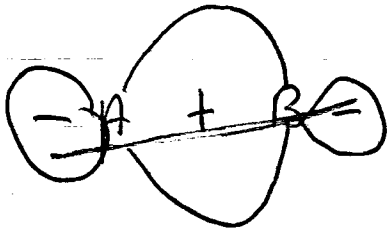


$\phi_{2p_z^A} - \phi_{2p_z^B}$

σ → cylindrical symmetry







$\sigma_{g\,2p_z}$