

1/19

LECTURE 19/36 OCT/23/02

H_2^+ MOLECULE

HOMO NUCLEAR MOLECULES

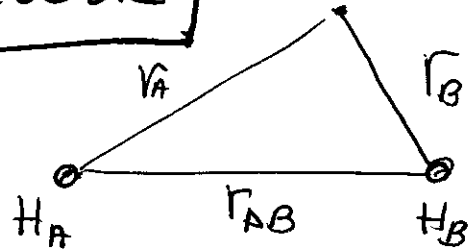
HETERO NUCLEAR DIATOMIC MOLECULES

BACKGROUND: OUBRY CH16

READ: TODAY'S LEC CH3

NEXT LEC CH9

H_2^+ MOLECULE



THE HAMILTONIAN

$$\hat{H} = -\frac{\hbar^2 \nabla^2}{2M} - \frac{|e|^2}{4\pi\epsilon_0 r_A} - \frac{|e|^2}{4\pi\epsilon_0 r_B} + \frac{|e|^2}{4\pi\epsilon_0 r_{AB}}$$

INSTEAD OF SOLVING THE SE. WE
CONSIDER A LINEAR COMBINATION OF
ATOMIC ORBITAL MOLECULAR ORBITAL
(LCAO-MO)

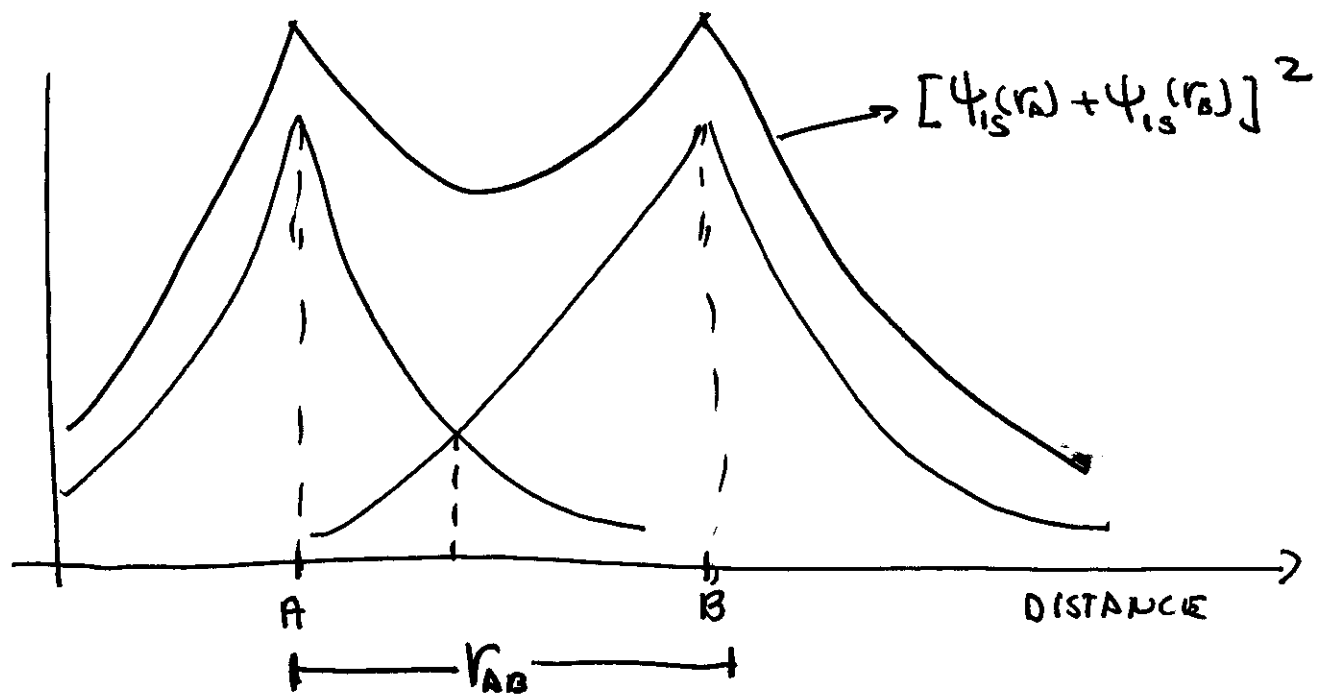
$$\psi_{\pm} = c(\psi_{1sA} \pm \psi_{1sB})$$

AND ASSUME THAT IS AN APPROXIMATION
OF THE WAVE FUNCTION. THUS

$$E_{\pm}(r_{AB}) = \frac{\int dV \psi_{\pm}^* \hat{H} \psi_{\pm}}{\int dV \psi_{\pm}^* \psi_{\pm}}$$

H_2^+ HYDROGEN MOLECULE

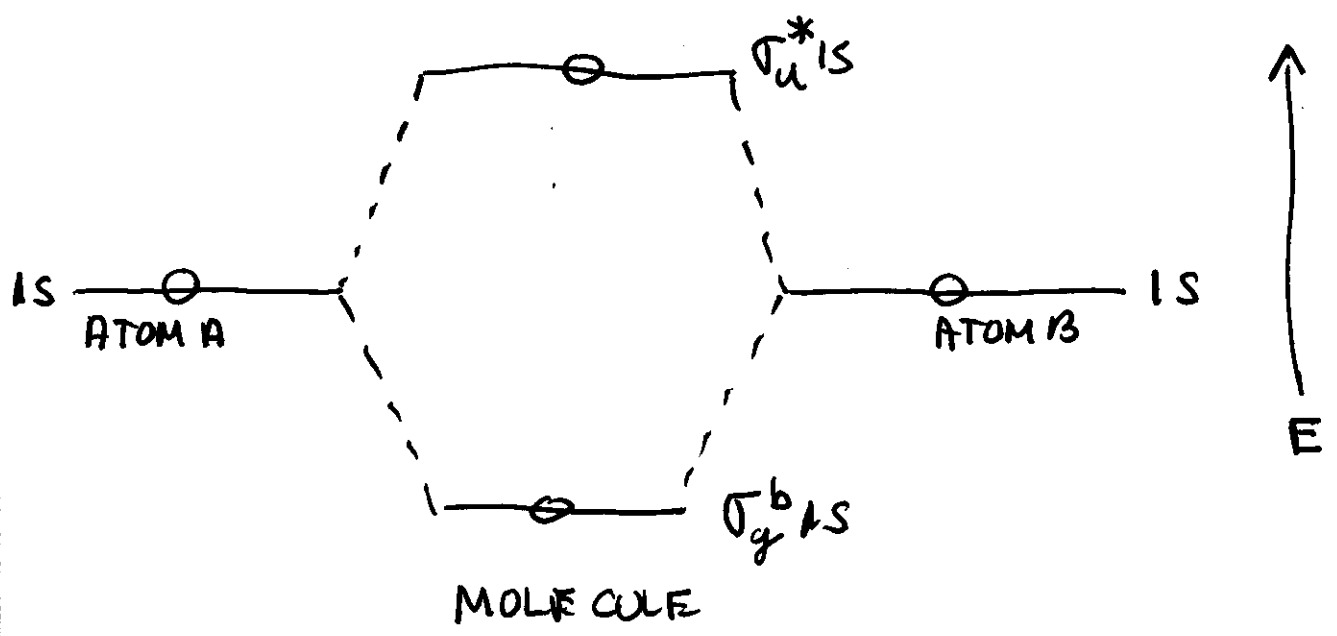
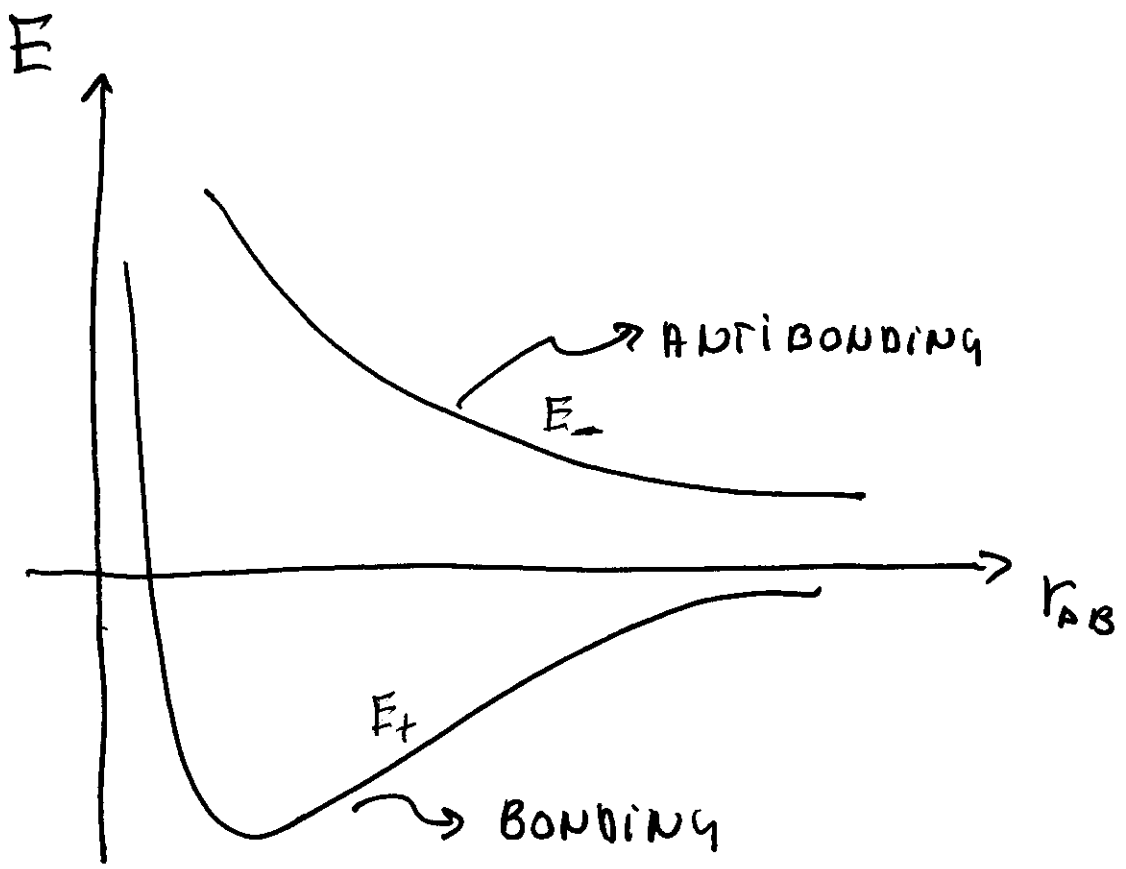
WE CONSIDER THE ψ_{1s} ORBITAL FOR EACH HYDROGEN ATOM



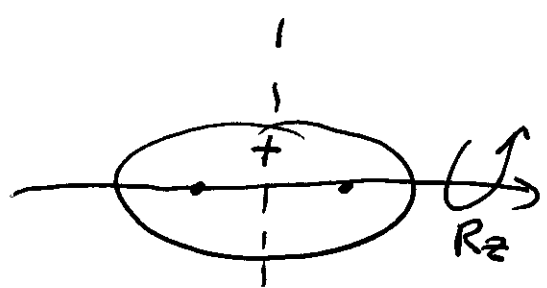
WE CAN CONSIDER TWO LINEAR COMBINATIONS

$$\psi_{\sigma^b} = \frac{1}{\sqrt{2}} [\psi_{1s}(r_A) + \psi_{1s}(r_B)]$$

$$\psi_{\sigma^a} = \frac{1}{\sqrt{2}} [\psi_{1s}(r_A) - \psi_{1s}(r_B)]$$

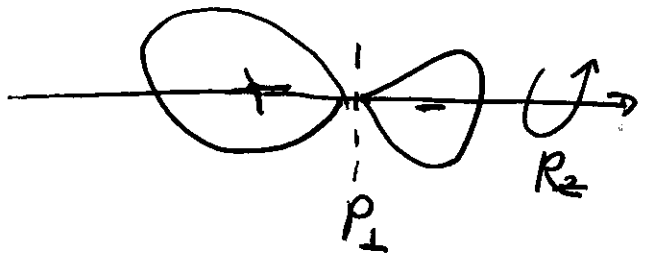


ψ_+



σ SYMMETRY

ψ_-



σ SYMMETRY

$$R_z \psi_+ = \psi_+ \Rightarrow \sigma$$

$$R_z \psi_- = \psi_- \Rightarrow \sigma$$

REFLEXION $P_{\perp} + R_z = INV$

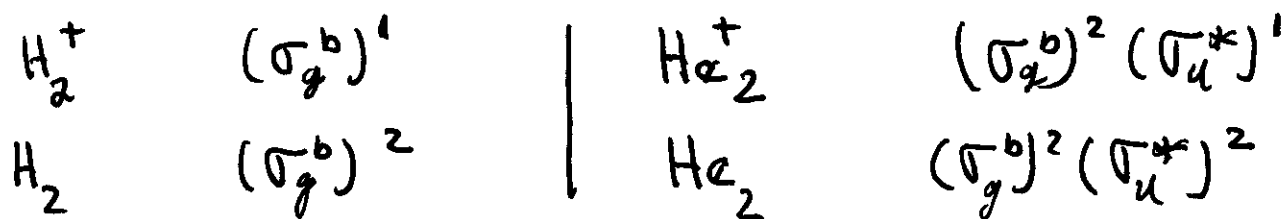
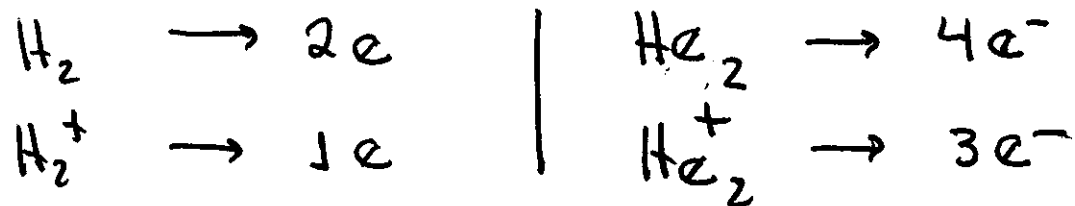
$$INV \psi_+ = \psi_+ \quad \text{GERADE (EVEN)} \quad g$$

$$INV \psi_- = -\psi_- \quad \text{UNGERADE (ODD)} \quad u$$

ψ_+ BONDING σ_g σ_g^b $\sigma_g^b IS$

ψ_- ANTIBONDING σ_u σ_u^* $\sigma_u^* IS$

WE CAN USE THIS DESCRIPTION TO DESCRIBE H_2 , H_2^+ , He_2^+ AND He_2 .



FOR H_2^+ AND He_2^+ \rightarrow ONE BONDING ELEC.
 H_2 \rightarrow TWO BONDING e^-
 He_2 \rightarrow ZERO BONDING e^-
 \Rightarrow NO MOLECULE

AND H_2^+ AND He_2^+ \rightarrow PARAMAGNETIC
 H_2 \rightarrow DIAMAGNETIC