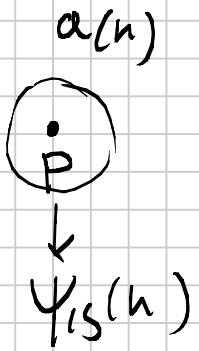
LECTURE #8

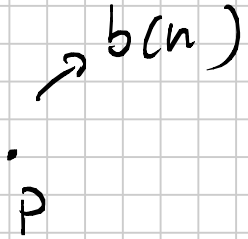
Note Title 9/26/2007

Monday → Dr. Grochol

Last time: Molecular Orbital

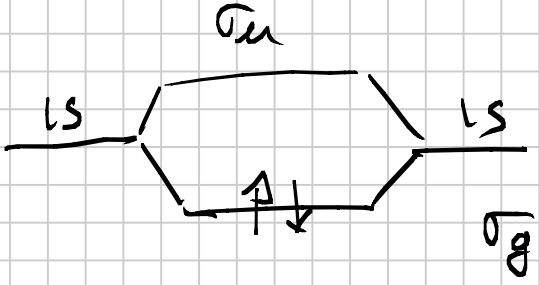
H_2 built MO

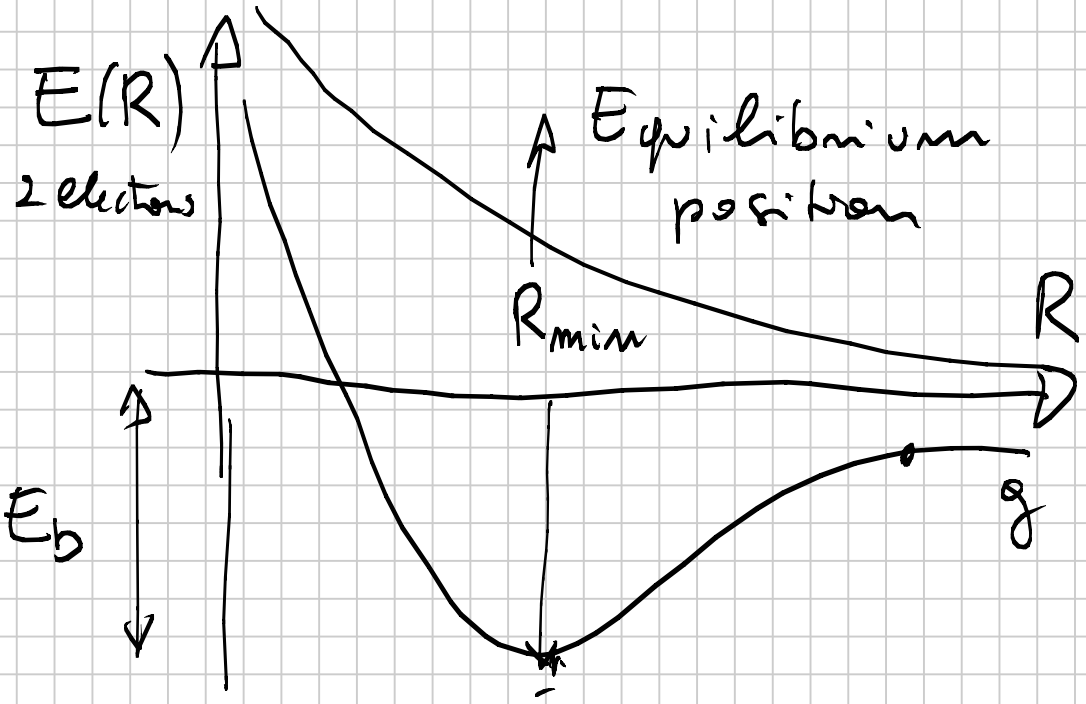


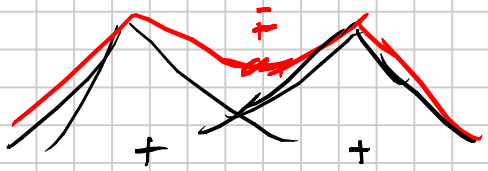


$(\sigma_g 1s) \sim a(n) + b(n)$

$(\sigma_u 1s) \sim a(n) - b(n)$







COVALENT BONDING

$E_b \sim 2.65 <$ Real ~ 4 eV

Heitler - London

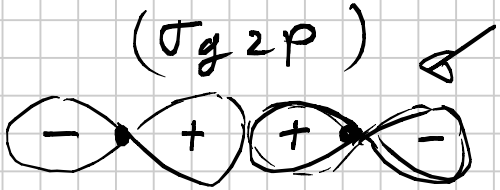
$$\psi_{MO} \sim (a(r_1) + b(r_1))(a(r_2) + b(r_2))$$

(σ_g 1s) (σ_g 1s)

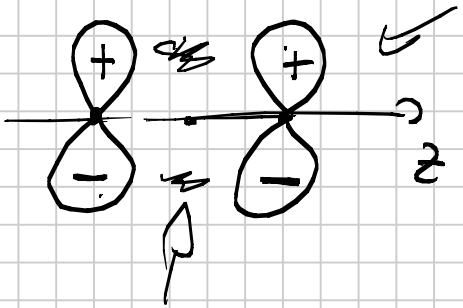
$$\psi_{HL} \sim a(r_1)\,b(r_2) + a(r_2)\,b(r_1)$$

Still MO is a good picture

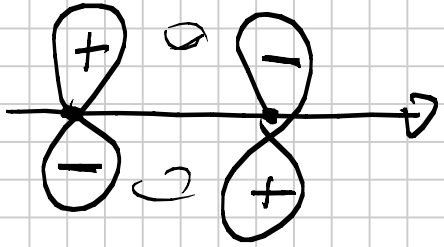
Use it for <u>diatomic molecules</u>



$\ell_z = 0$

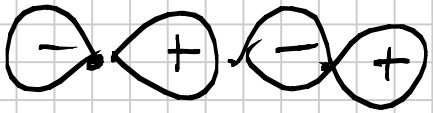


$(\pi_u 2p)$
UNGERADE
$\ell_z = \pm 1$
DOUBLY DEGENERATE

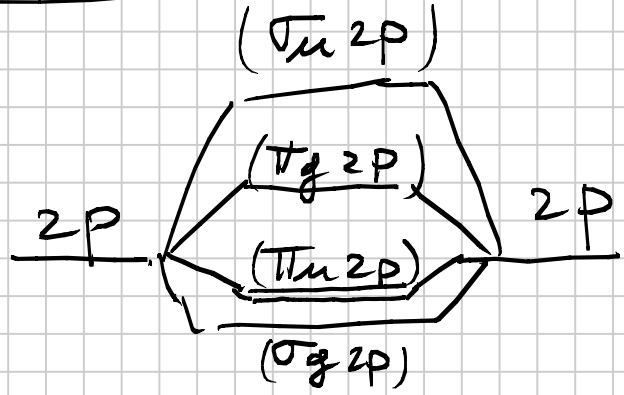


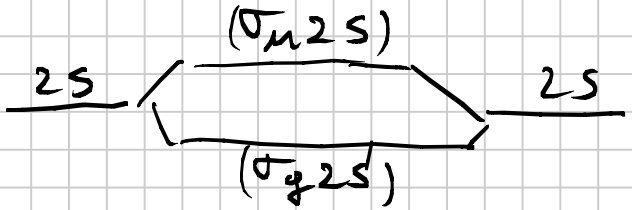
$(\pi_g 2p)$
GERADE

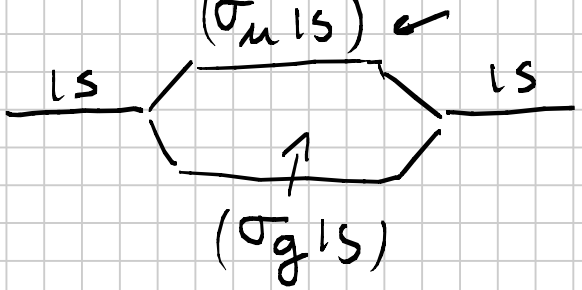
ℓ_x, ℓ_y



σ_v

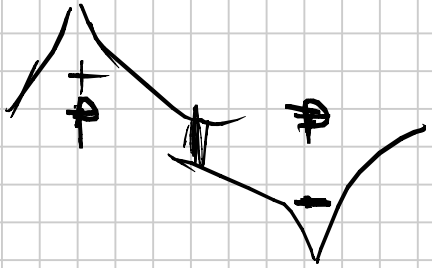






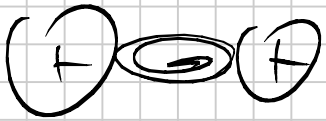
GERADE (σ_g 1S)

BONDING ORBITAL



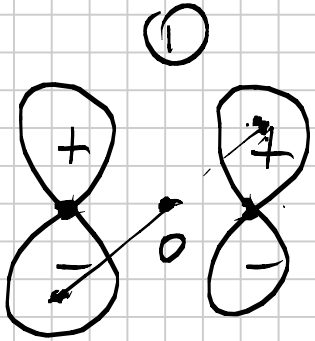
UNGERADE

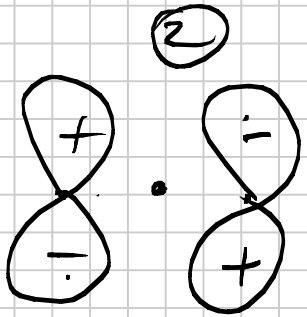
$a - b$



GERADE

UNGERADE





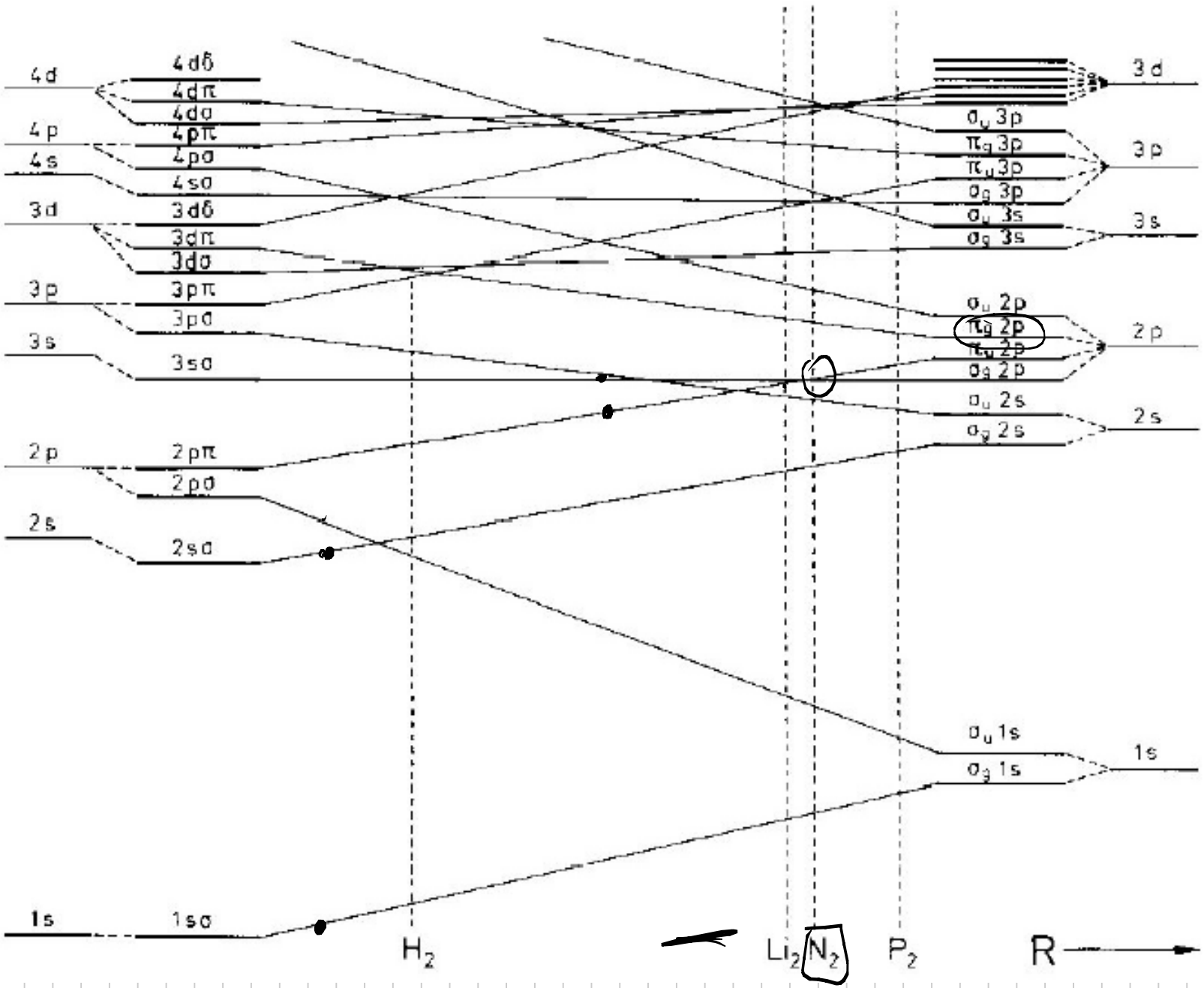
$H_2 \longrightarrow He$

$(\sigma_g 1s)^2 \longrightarrow (1s)^2$ Ground state

$(\sigma_g 1s)(\sigma_g 2s) \qquad (1s)(\underline{2s})$

$\sigma_g 2s$ fills before the $(\sigma_u 1s)$

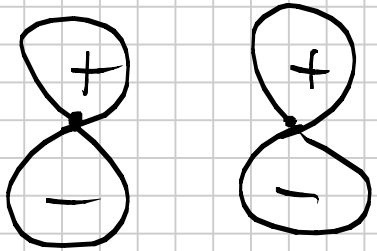
σ UNGERADE



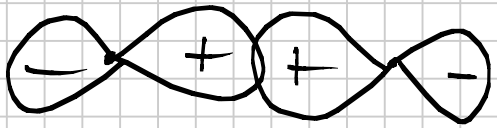
H_2^+

$(\pi_u 2p) < (\sigma_g 2p)$

For Nitrogen



Stronger than



He_2

$(\sigma_g 1s)^2 (\sigma_u 1s)^2$ Non stable

Excited state for He_2 $(\sigma_g 1s)^2 (\sigma_u 1s)(\sigma_g 2s)$ ← BONDING

BOUND EXCIMER (Good for lasers)

Li_2 $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$

$(\sigma_g 1s)^2 (\sigma_u 1s)^2 (\sigma_g 2s)^2$

Be_2

$\uparrow\downarrow$ $(\sigma_g 1s)^2$ $\uparrow\downarrow$ $(\sigma_u 1s)^2$ $\uparrow\downarrow$ $(\sigma_g 2s)^2$ $\uparrow\downarrow$ $(\sigma_u 2s)^2$

Not stable

$^1\Sigma_g$

VAN DER WAALS

$V \propto \frac{1}{R^6}$

HUND'S RULE

$l_z = 1$ $l_z = -1$

$\uparrow$ $\uparrow$ $(\pi_u 2p)^2$

B_2

$\uparrow\downarrow$ $(\sigma_g 1s)^2$ $\uparrow\downarrow$ $(\sigma_u 1s)^2$ $\uparrow\downarrow$ $(\sigma_g 2s)^2$ $\uparrow\downarrow$ $(\sigma_u 2s)^2$

$\downarrow$

PARAMAGNETIC

$\downarrow$

$[Be_2]$

$\uparrow$ $\uparrow$ $^3\Sigma_g$

$B = B$

$l_z = 0$

$(\sigma_g 2p)$ $l_z = 0$

π $l_z = 1$, $l_z = -1$

$N_2 =$ [Be$_2$] 8

$l_z=1$ ↑↓	$l_z=-1$ ↑↓

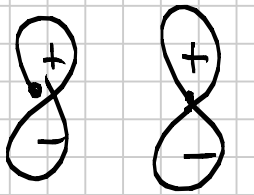
$(\pi_u 2p)^4$

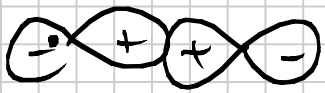
$l_z=0$ ↑↓

$(\sigma_g 2p)^2$

3 Bonding orbitals

$N \equiv N$





$O_2 =$ [Be] 8

↑↓	↑↓

$(\pi_u 2p)^4$

↑↓

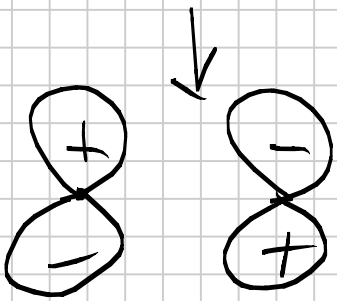
$(\sigma_g 2p)^2$

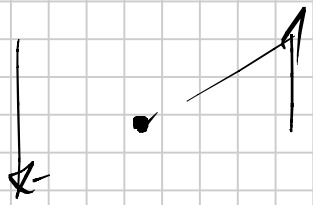
$l_z=1$ ↑	$l_z=-1$ ↑

$(\pi_g 2p)^2$

→ PARAMAGNETIC

$^3\Sigma_g$





σ_u → GERADE

B_2^+ - $[Be_2]$ $(\pi_u 2p)$ $^2\Pi_u$