

LECTURE # 9

Note Title

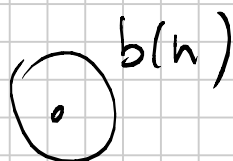
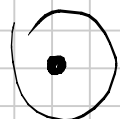
9/24/2008

RMS + RM6 +
Ch 32 ASHROFT-MERMIN
(672-682)

MOLECULAR ORBITALS

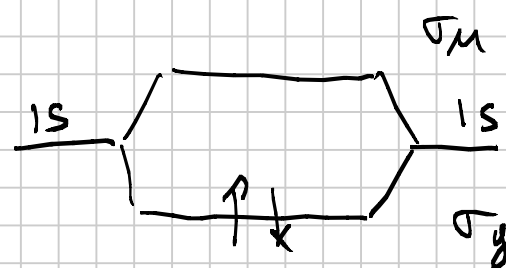
H₂

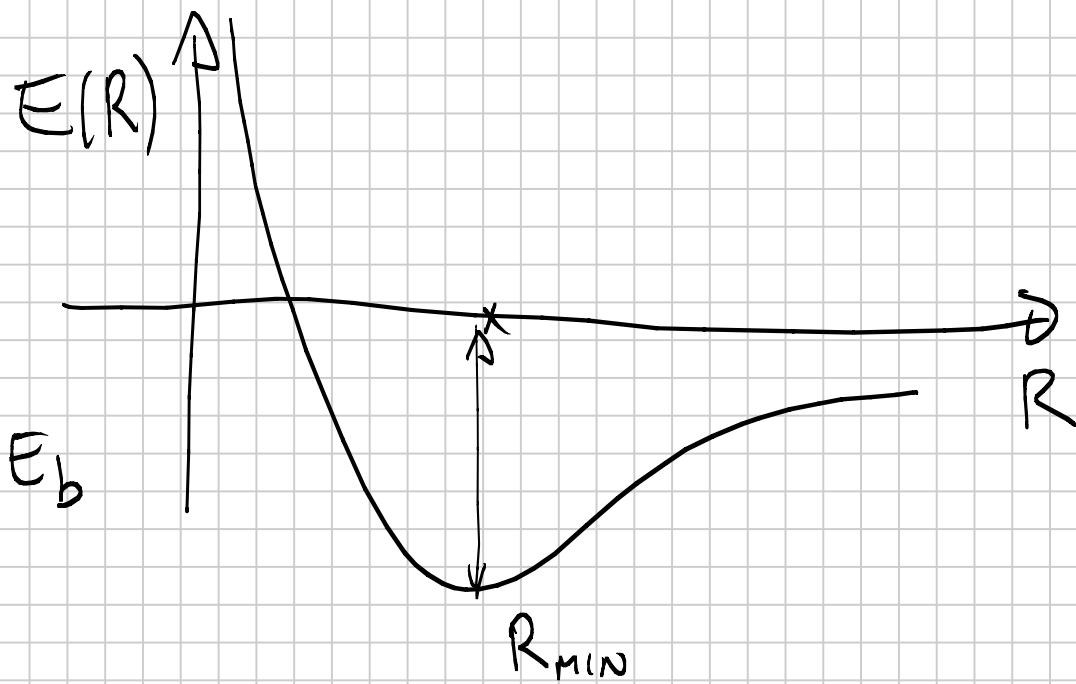
$a(r) \sim (1s)$ ORBITAL



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

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





$$E_b^{MO} \sim 2.7 \text{ eV}$$

$$E_b^{EXP} \sim 4.7 \text{ eV}$$

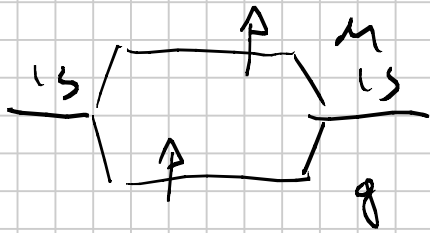
HEITLER-LONDON

APPROXIMATION

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

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

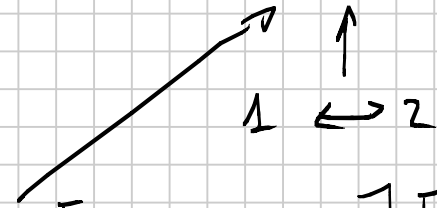
EXCITED H_2



• MAXIMIZE SPIN

$$(\sigma_g 1s) (\sigma_u 1s) \sum_M^3$$

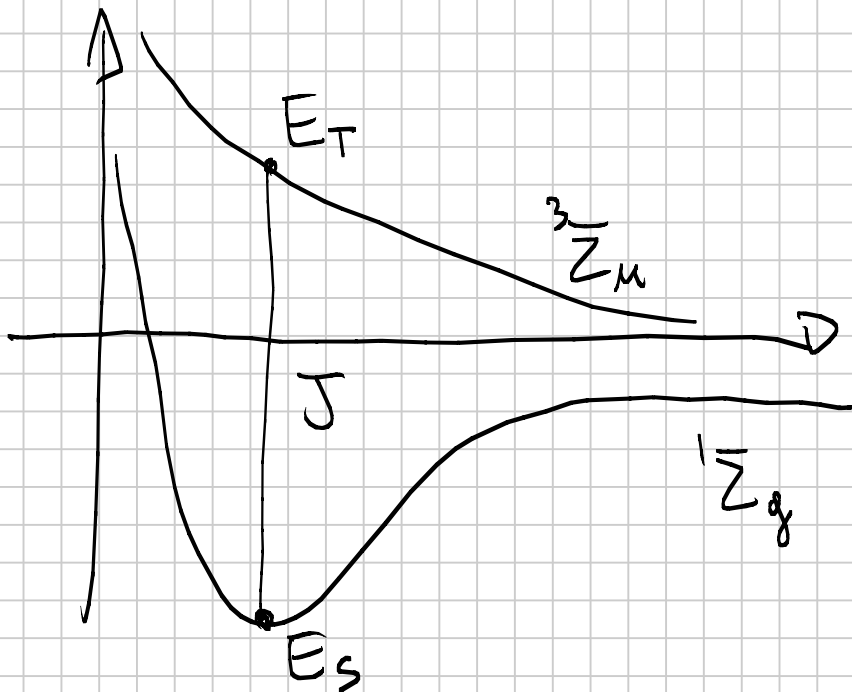
ANTISYMMETRIZATION



$$[a(r_1) + b(r_1)] [a(r_2) - b(r_2)] - [a(r_2) + b(r_2)] [a(r_1) - b(r_1)]$$

$$= 2 [a(r_2)b(r_1) - a(r_1)b(r_2)]$$

ALREADY
OF H_2 TYPE



H_2 CAN BE SEEN

AS 2 INTERACTING H

WITH A SPIN-DEPENDENT

INTERACTION

$$J = E_S - E_T$$



DEFINE EFFECTIVE HAMILTONIAN

$$H_{\text{EFF}} = -J \vec{S}_1 \cdot \vec{S}_2$$

HEISENBERG
HAMILTONIAN

$$\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2} \left[(\vec{S}_1 + \vec{S}_2)^2 - \vec{S}_1^2 - \vec{S}_2^2 \right]$$

SINGLET $-\frac{3}{4}$
TRIPLET $+\frac{1}{4}$

$J < 0$ FOR H_2 MEANS TWO H

INTERACT WITH ANTI-FERROMAGNETIC

COUPLING $\Rightarrow S_1$ AND S_2 LIKE

TO BE ANTI PARALLEL $\uparrow \downarrow$

IF $J > 0$
 $\uparrow \uparrow$

THE HEISENBERG HAMILTONIAN
DESCRIBES A FERROMAGNETIC
INTERACTION BETWEEN ATOMS

$$(S) = \uparrow \downarrow - \downarrow \uparrow$$

$$(\uparrow \uparrow)$$

MAGNETISM IN MOLECULES/SOLIDS HAS TO DO

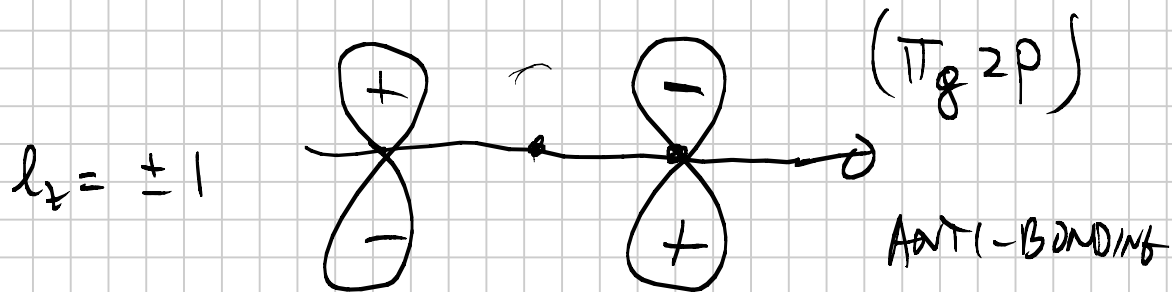
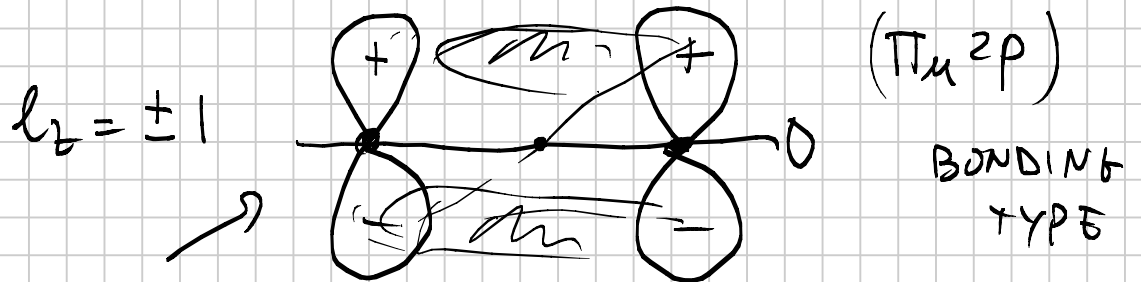
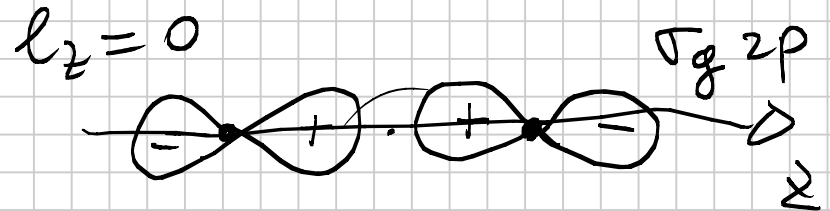
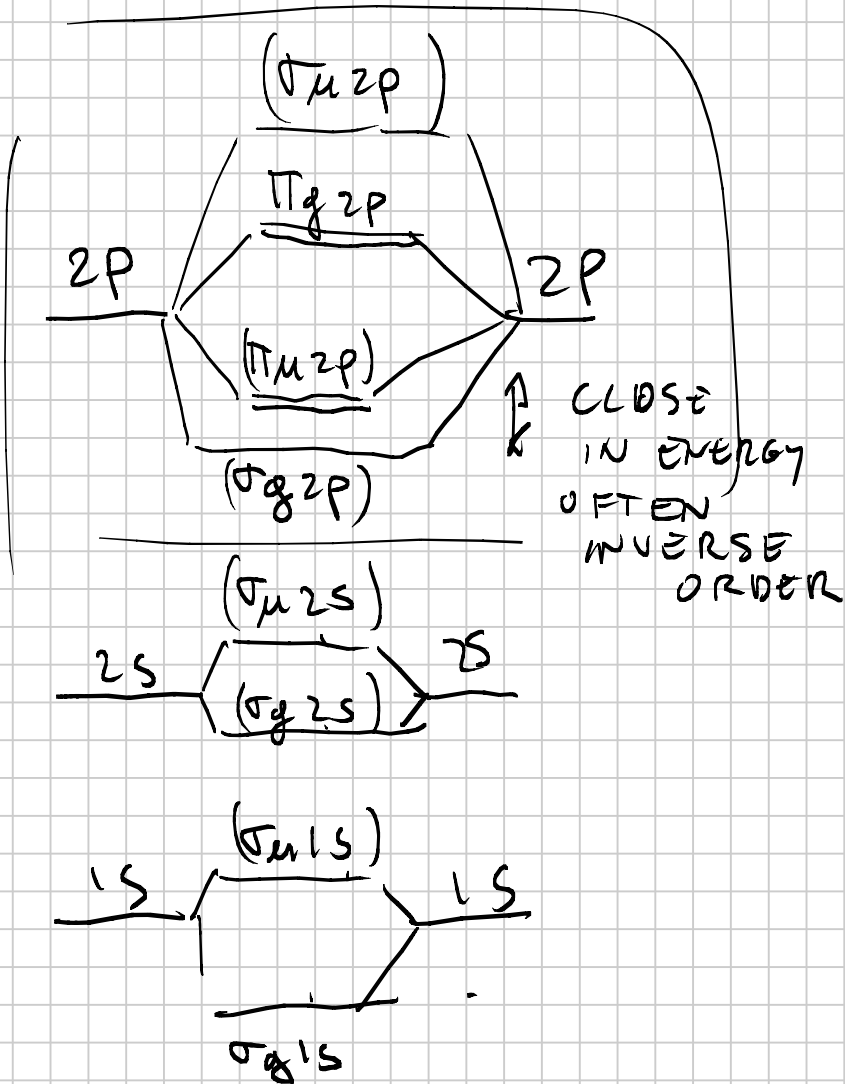
WITH COULOMB EFFECTS BETWEEN INTERACTING
ELECTRONS

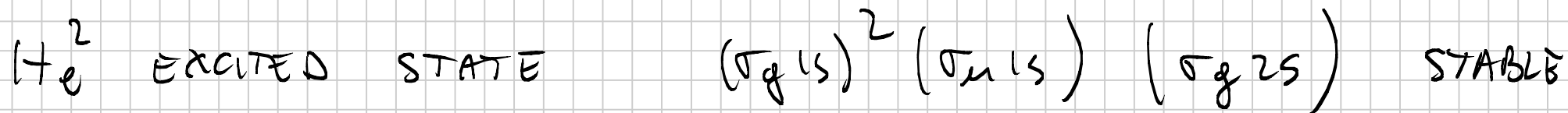
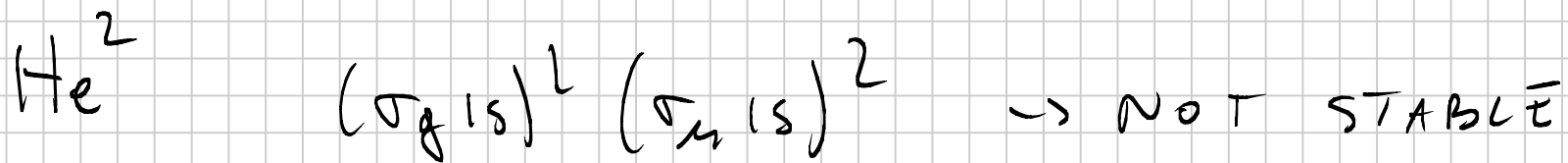


$$I \sim \frac{(\vec{\mu}_1 \cdot \vec{\mu}_2) - 3(\vec{\mu}_1 \cdot \vec{R})(\vec{\mu}_2 \cdot \vec{R})}{R^3}$$

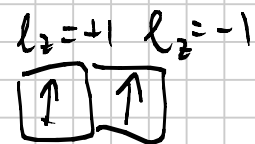
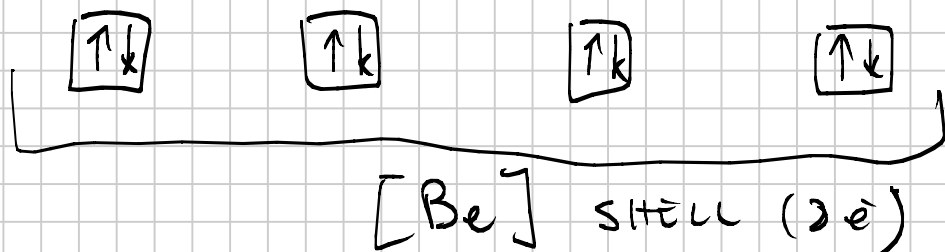
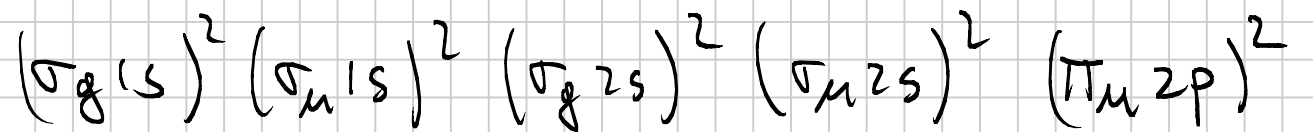
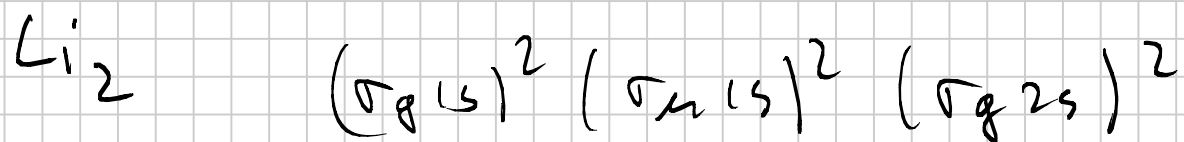
DIPOLE - DIPOLE INTERACTION \ll COULOMB EXCHANGE J

II MOLECULAR ORBITALS





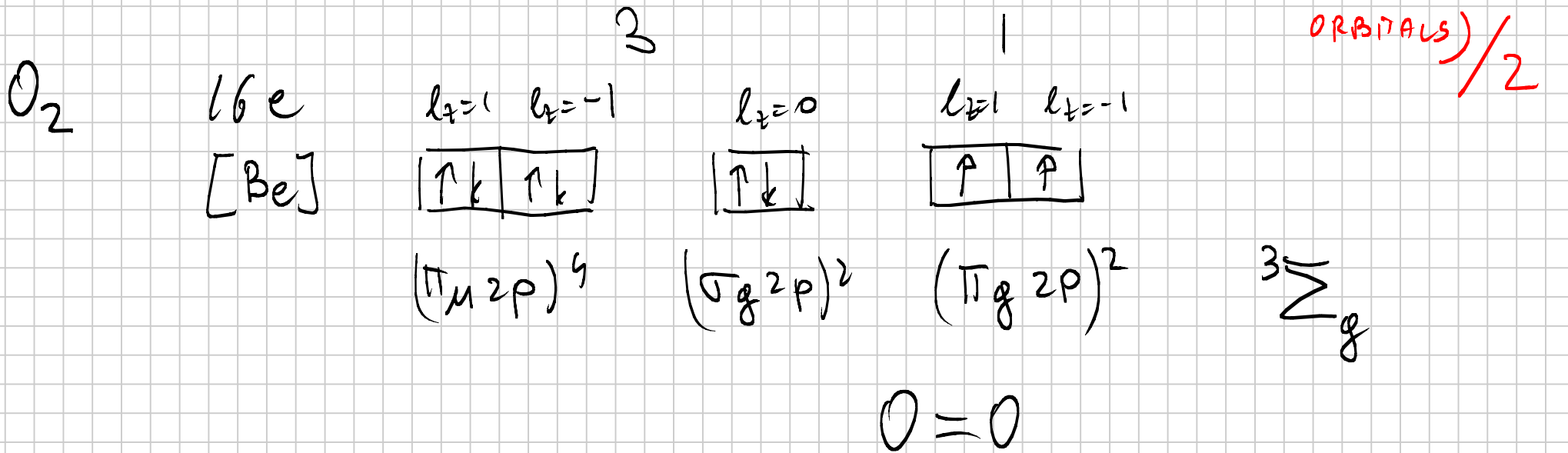
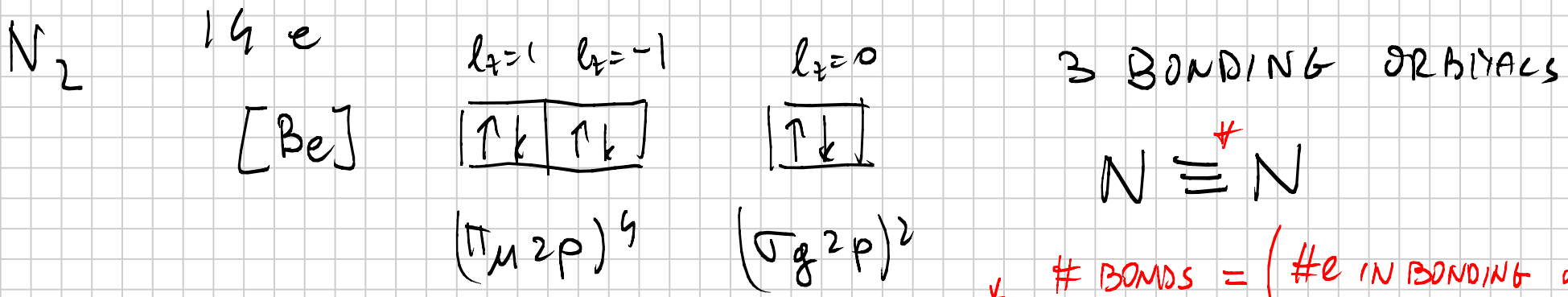
EXCIMER (GOOD FOR LASERS)



B - B

m_l = l_z

3 Σ_g



O_2 IS A PARAMAGNETIC GAS