Last Lecture before MSE

Modern QM → SE → 1 e⁻ Atom (H-atom) Exactly Solvable

Structure → Time integrated picture

Eigenvalue Eigenf^n soln.

$\hat{H}\psi = E\psi$

Solve assuming Central force ← Potential. $l > 0$

V_{eff} = Coulomb + $\frac{\hbar^2 l(l+1)}{2I}$

ψ → {Radial ← Angular

L

Rydberg atoms ← H-like

multielectron Problem

neglect $e^- - e^-$ repulsion

He

Li

Be

etc.

Recipe

↳ Write $\hat{H}$

SE → Solve

SE

↳ Spatial soln. (n, l, m_l) 3 quantum #

→ Antisymm. of wavefn → Pauli Exclusion Principle → Spin quantum #

4th quantum #

n, l, m_l, m_s

$$\Psi_{Total} = \Psi_{Space}\ \Psi_{Spin}$$

Aufbau Principle

Hunds Rule

H

He

Li

Be

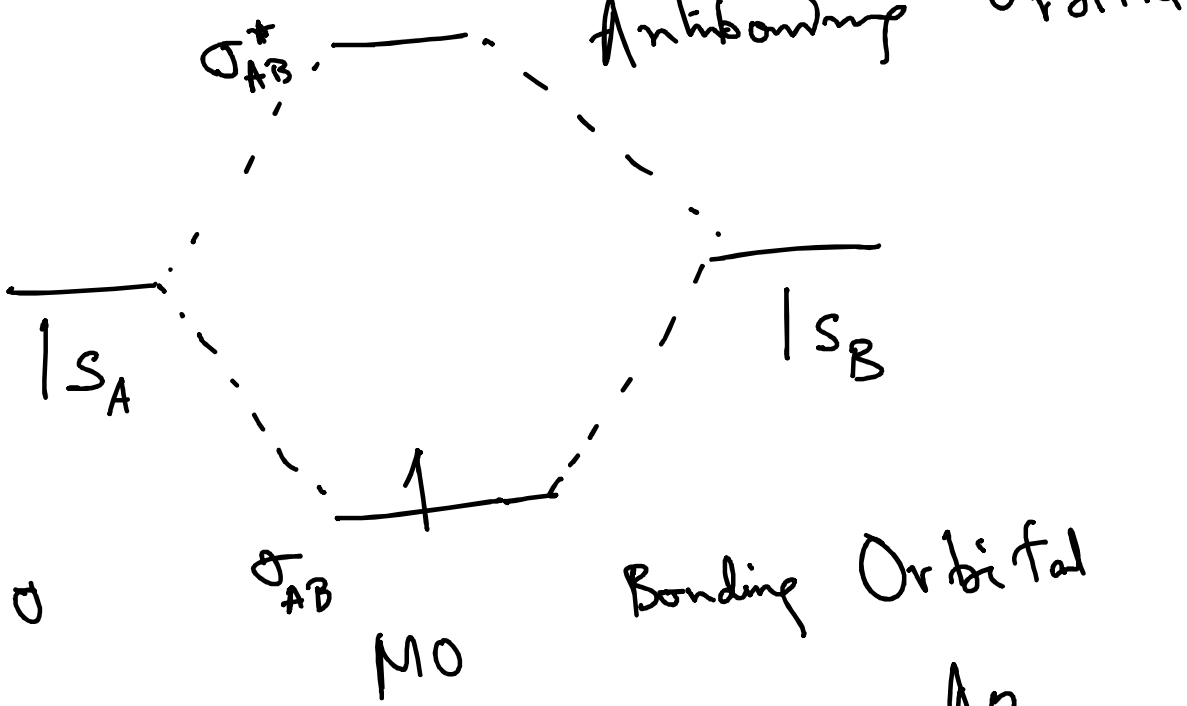
Atomic Orbitals

1e wavefn.

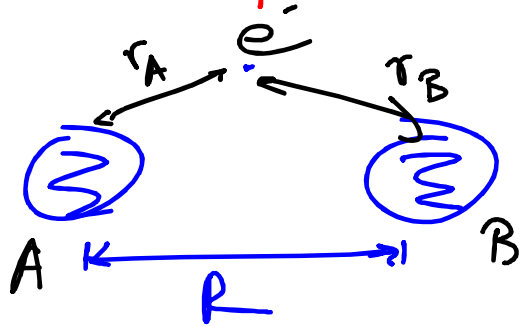
1e⁻ Molecule ion

H_2^+

LCAO — MO Theory

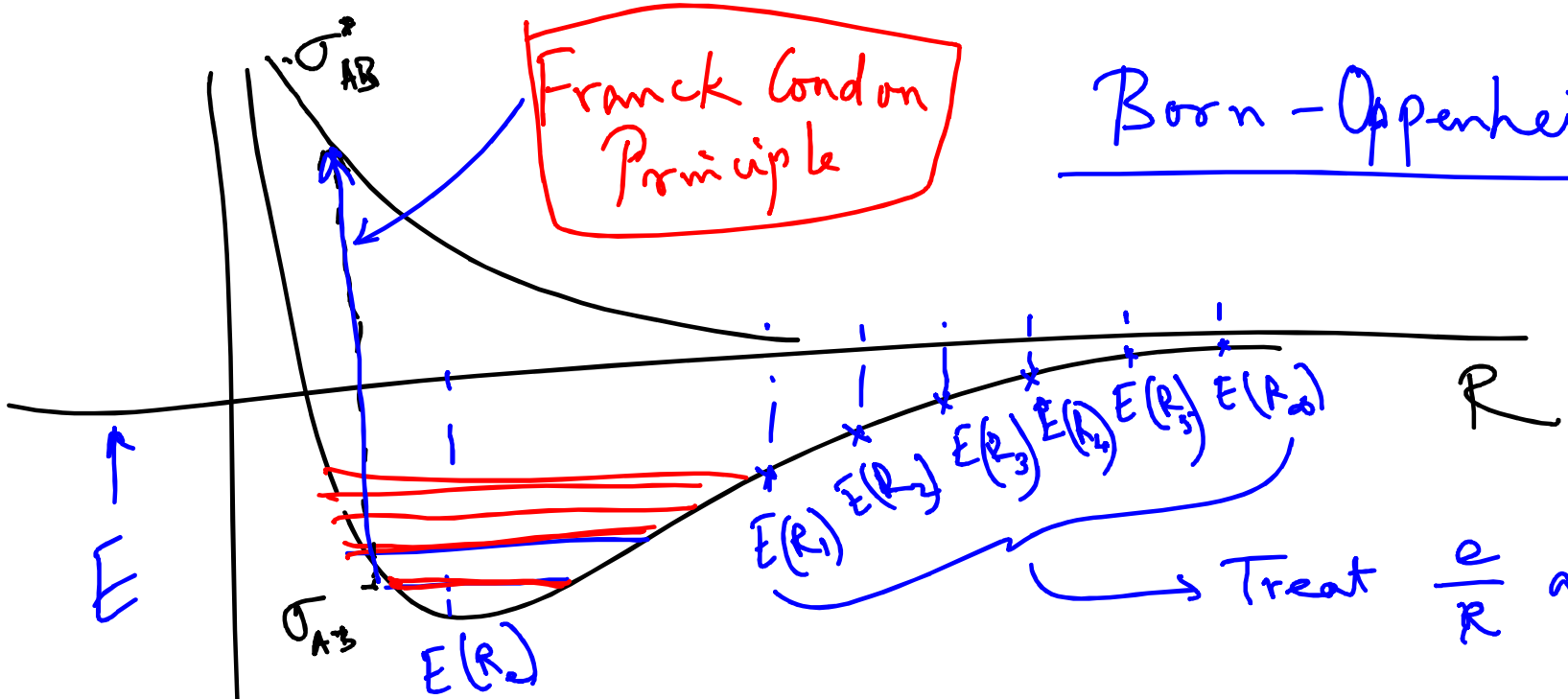


Constant Inter nuclear Separation



$$\hat{H}\Psi = E\Psi$$

$$-\frac{\hbar^2}{2m_e}\nabla^2 - \frac{e^2}{r_A} - \frac{e^2}{r_B} + \underbrace{\frac{e^2}{R}}_{\text{Const}}$$



Franck Condon Principle

Born - Oppenheimer Approx.^{n}

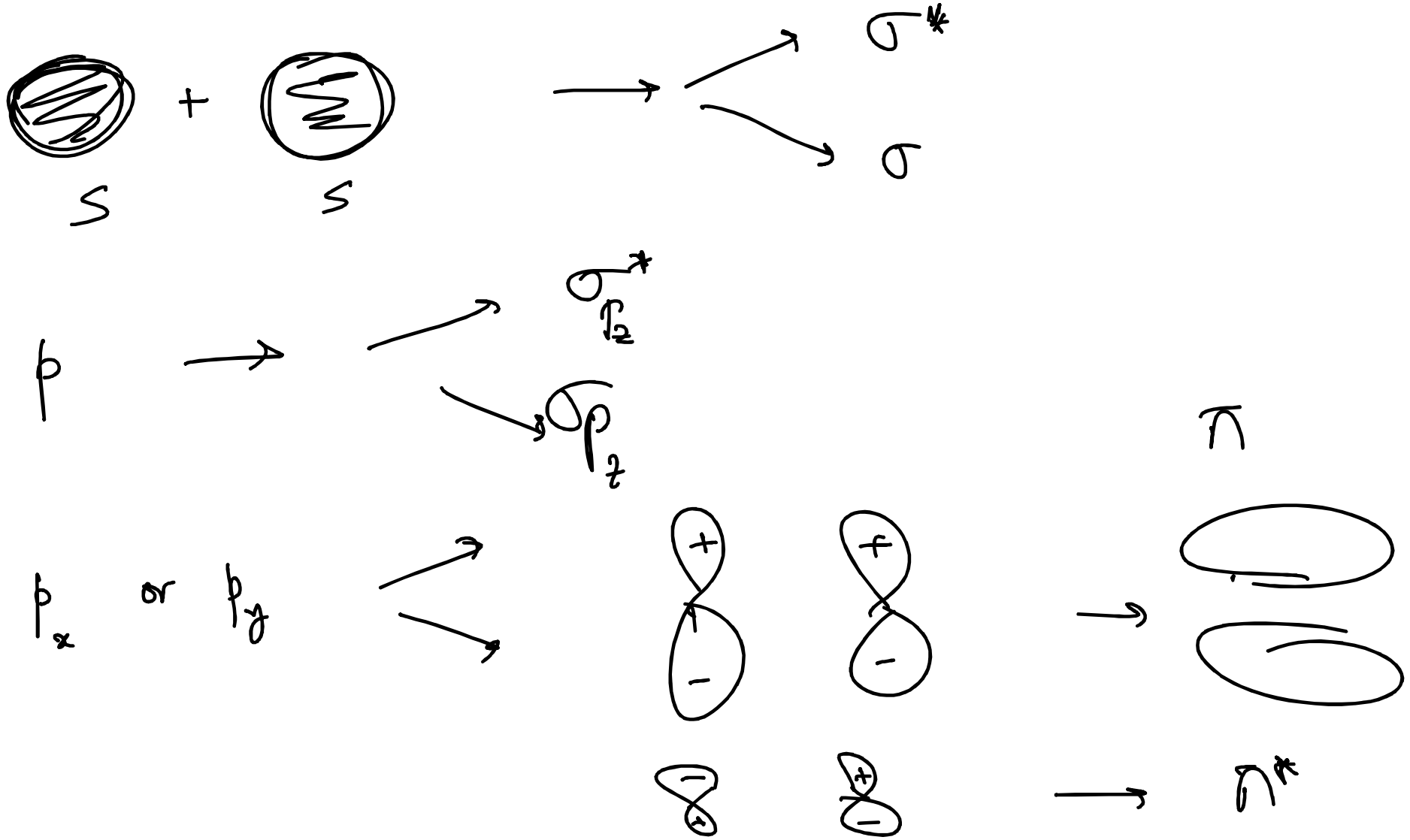
→ Treat $\frac{e}{R}$ as const.

Internal energy

$$E = E_{vib} + E_{rot} + E_{el}$$

Spectroscopy

Light - matter interaction


s
+
s
σ*
σ
p
σ*
p_z
p_x or p_y
+
−
+
−
π
π*

O_2 molecule → Triplet

HOMO — Highest occupied MO

LUMO — lowest unoccupied MO

LUMO ——

HOMO ——

$$\text{Bond Order} = \frac{1}{2}\left(N_B - N_{AB}\right)$$

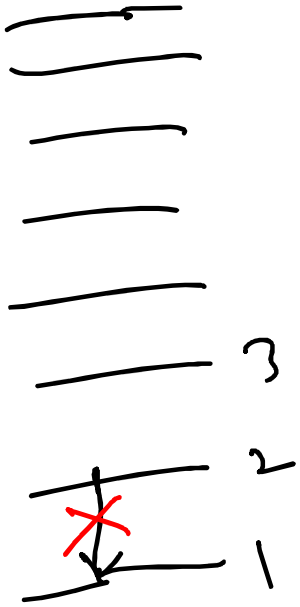
Non bonding electrons

Sp - hybridization

HF

$$\psi = c_1\phi_1 + c_2\phi_2$$

Selection Rule



S

$\ell = 0$

P

$\ell = 1$

D

$\ell = 2$

...

$\Delta m = \pm 1, 0$ ✓

$\Delta \ell = \pm 1$ ✓

$\Delta \ell \neq 0$