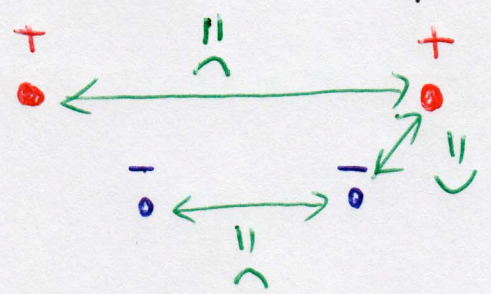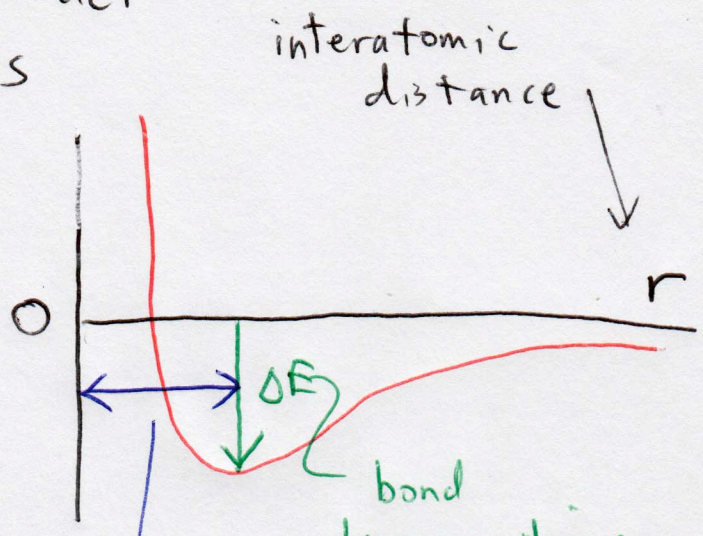classical bonding model
quantum bonding model
Sigma + pi bonds

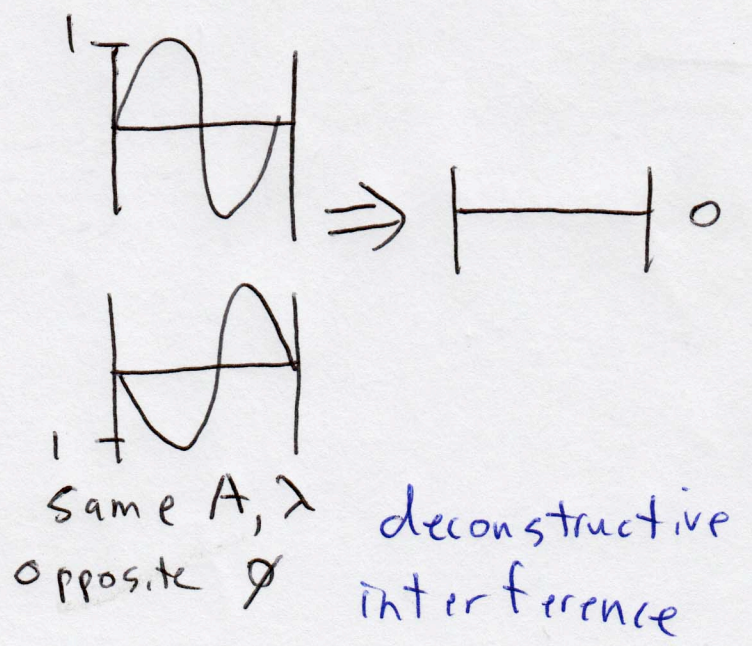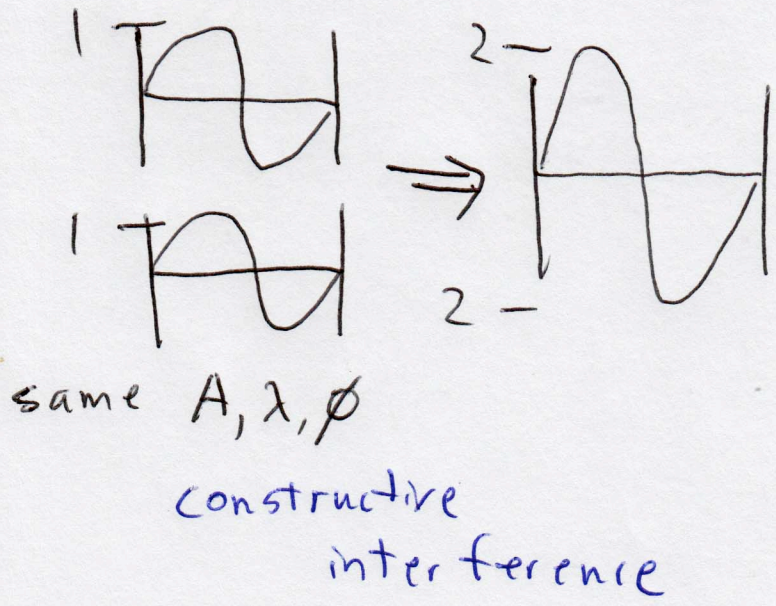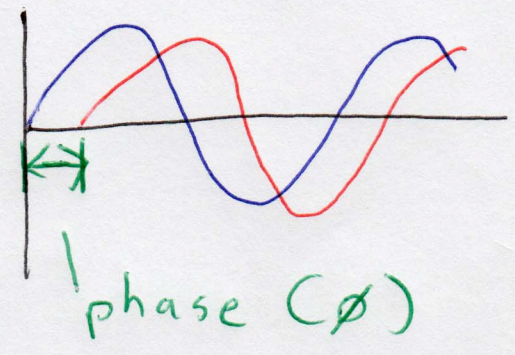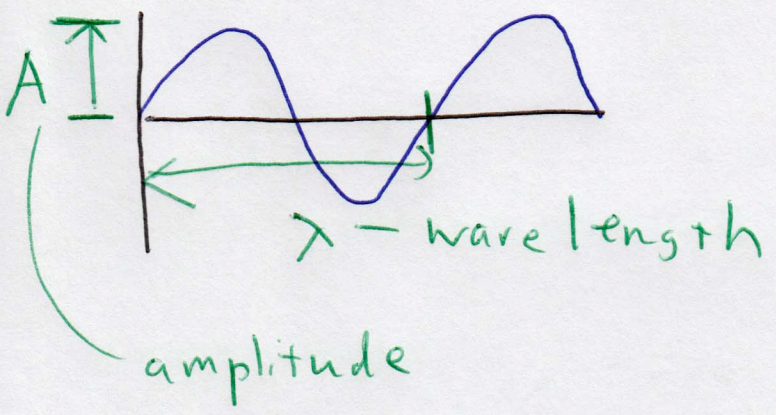interatomic distance
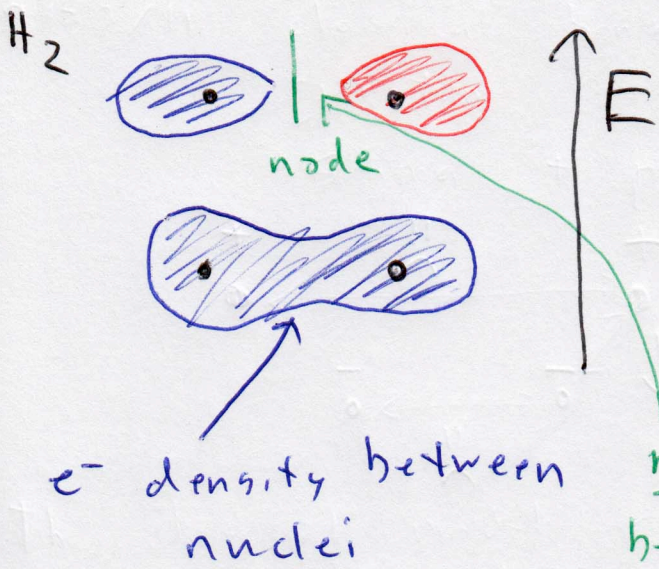

This classical model can be used to describe H_2, but fails to describe He_2. This is because the electrons are treated as particles, ignoring their wave behavior.
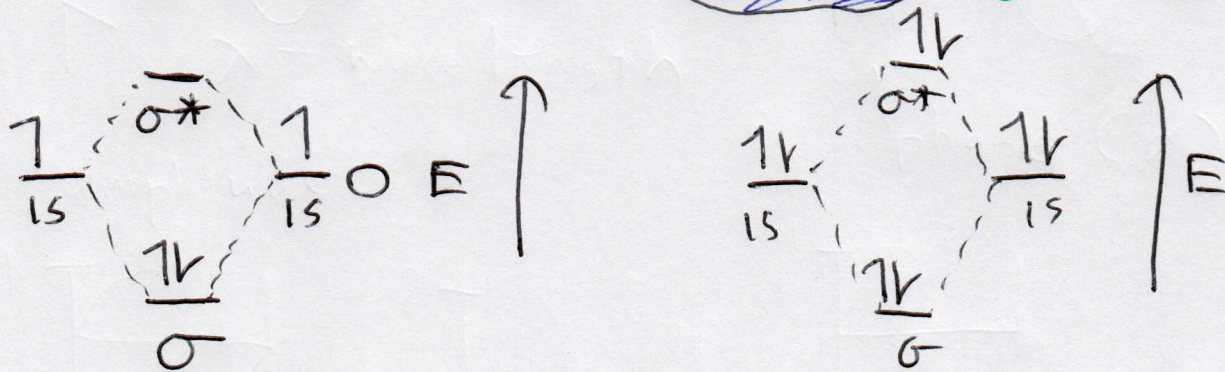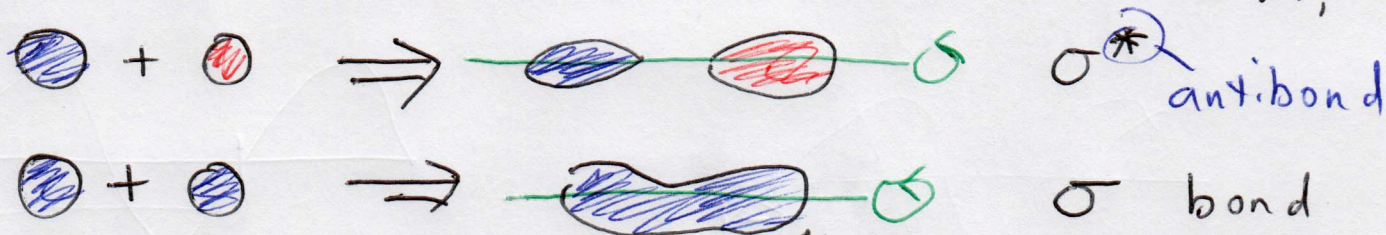
bond length

ΔE

bond dissociation energy

A — amplitude

λ — wavelength

phase (ϕ)

same A, λ, ϕ

constructive interference

same A, λ opposite ϕ

deconstructive interference

H_2

node

e⁻ density between nuclei

no e⁻ density between nuclei

This orbital is an **antibond** because its energy is <u>higher</u> than the energy of the two atoms if they had not interacted

This orbital is a **bond** because the energy is <u>lower</u> than the isolated atoms.

E

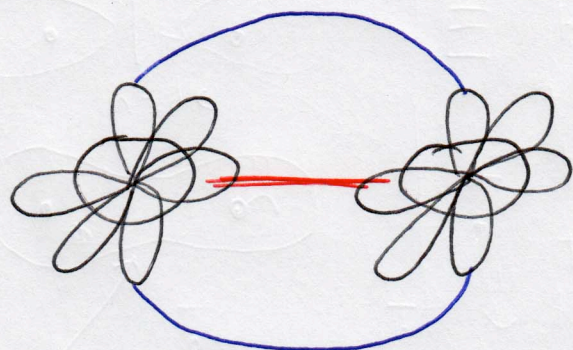LCAO- linear combination of atomic orbitals - atomic orbitals are added + subtracted in such a way as to estimate molecular orbitals (MO) such as bonds + antibonds.
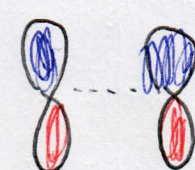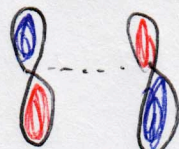
$\bigcirc$ + $\bigcirc$ ⟹ ⬭⬭ σ ⟲ σ^* **antibond**

$\bigcirc$ + $\bigcirc$ ⟹ ⬭ σ ⟲ σ **bond**

σ^*
1S — — 1S   OE ↑ E
σ

H_2

σ^*
1S — — 1S   ↑ E
σ

Bond order = $\dfrac{\#\ bonding\ e^- - \#\ antibond\ e^-}{2}$

Each antibonding e⁻ causes a destabilization (increase in energy) that negates the stabilization (decrease in energy) provided by a bonding electron.
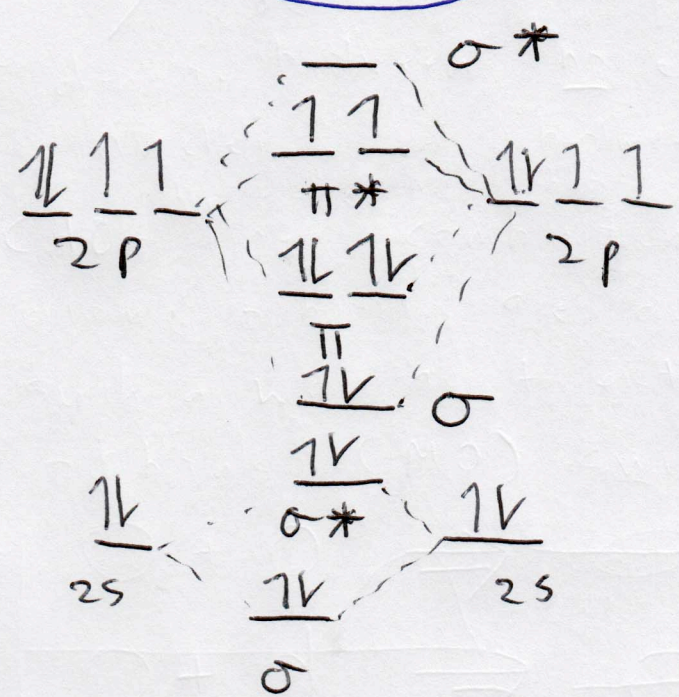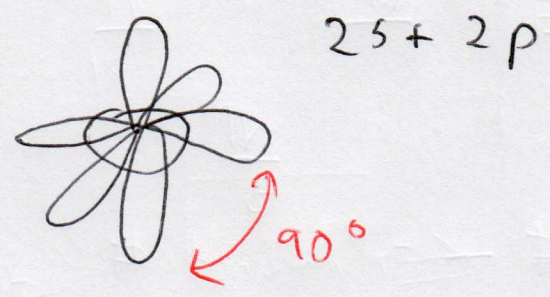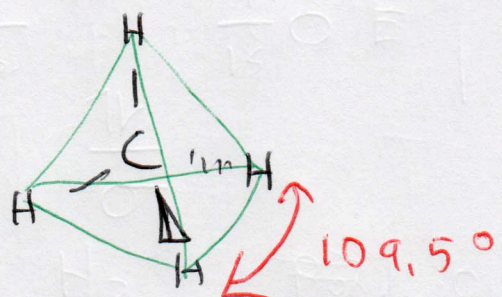
π bonds

π* bond

π bond

no node between atoms

$$B.O. = \frac{8-4}{2} = 2$$

(MO diagram, left to right:)

2p: ↑↓ ↑ ↑
2p: ↑↓ ↑ ↑

σ* (empty)

π*: ↑ ↑

π: ↑↓ ↑↓

π: ↑↓

σ: ↑↓

σ*: 2s ↑↓ ... ↑↓ 2s

σ: ↑↓

---

methane CH_4

109.5°

2s + 2p

90°

The atomic orbitals of carbon cannot be used directly to describe the molecule methane since the geometry of the orbitals does not match and the energy of the orbitals is not the same. To describe methane, a set of hybrid orbitals are created by adding + subtracting orbitals on the same atom.