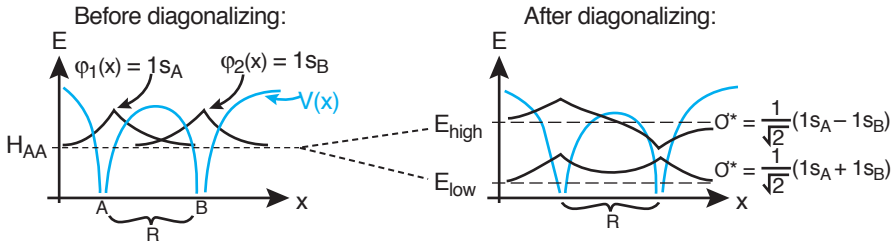
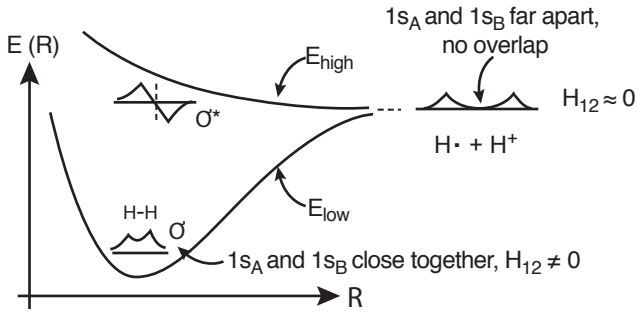
A symmetric 1-electron system: H_2^+



The energy E(R) depends to the distance R between the nuclei.
If R ∞, then E=H_{AA}, the energy of a hydrogen atom plus the proton.
If R gets smaller, the lowest energy is E_{low} and the electron occupies the σ state.
If R gets too short, the nuclear repulsion increases the energy again.
The lowest energy E(R_{eq}) at R=R_{eq} is the equilibrium bond energy of H_2^+:



Diagonalizing the minimal basis (2x2) matrix for an asymmetric 1-electron system, HeH^{++}