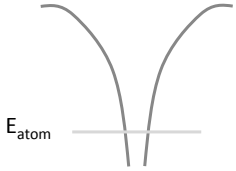
4.1 Hydrogen molecule

Q1. Sketch the potential V(r) of an electron due to a single proton (as in a hydrogen atom).

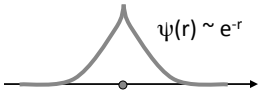
Q2. Sketch the ground state wave function ψ(r) of the electron in Q1.

Q1. Sketch the potential V(r) of an electron due to a single proton.

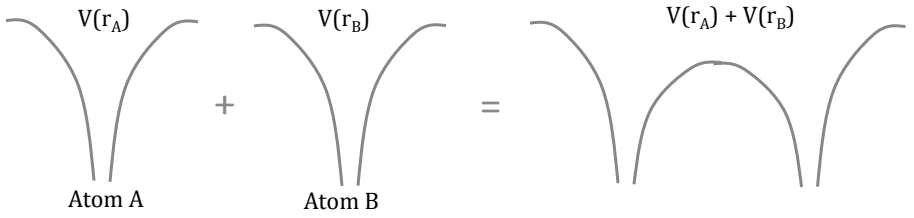
$V = -ke^2/r$



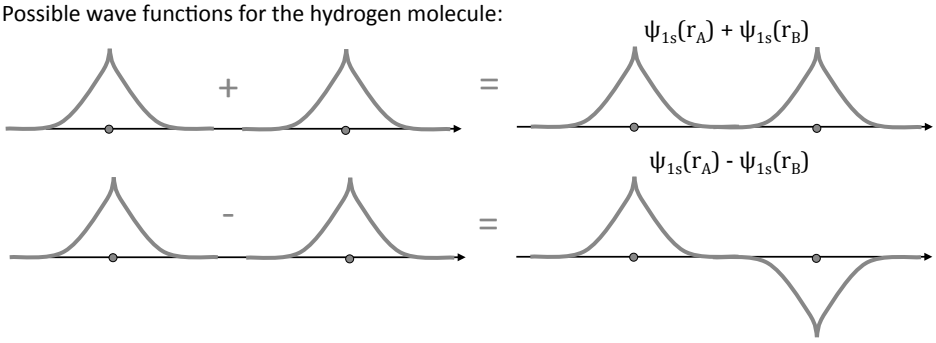
Q2. Sketch the ground state wave function ψ(r) of the electron in Q1.

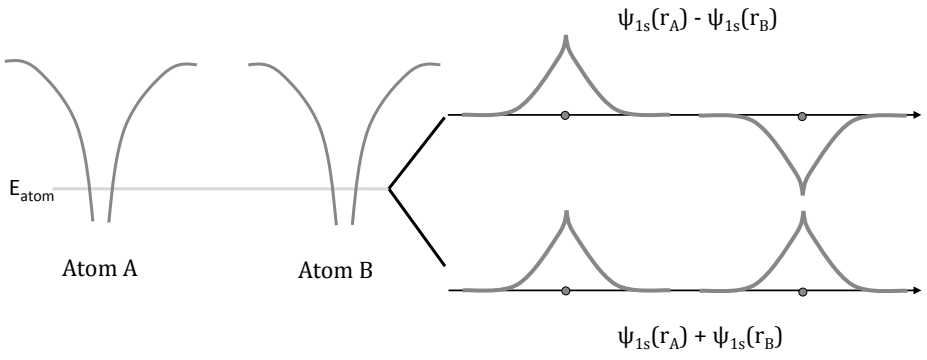


Potential:



Possible wave functions for the hydrogen molecule:

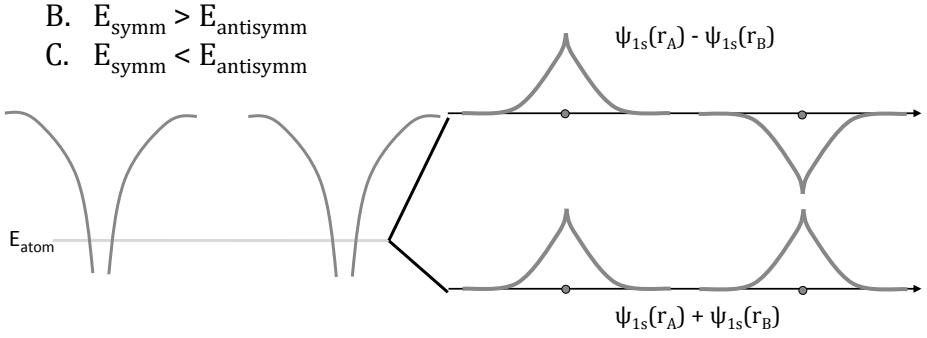




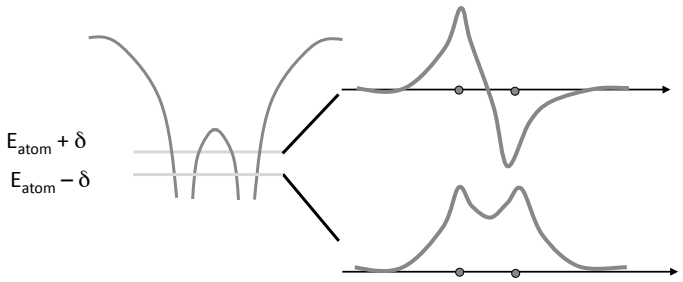
As the proton gets closer, how does the energy of the symmetric wave function $\psi_{1s}(r_A) + \psi_{1s}(r_B)$ compare to that of the antisymmetric wave function $\psi_{1s}(r_A) - \psi_{1s}(r_B)$?

Hint: Think about what the probability density looks like for each.

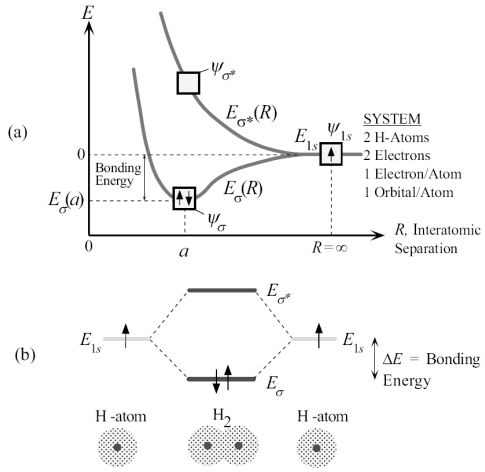
A. $E_{symm} = E_{antisymm}$
B. $E_{symm} > E_{antisymm}$
C. $E_{symm} < E_{antisymm}$



C. $E_{symm} < E_{antisymm}$



As separation decreases, energy splitting δ increases.



(a) Energy of *symmetric* ψ_σ and *antisymmetric* ψ_{σ^*} vs. the interatomic separation *R*.
(b) Schematic diagram showing the changes in the electron energy as two isolated H atoms, far left and far right, come together to form a hydrogen molecule.

From *Principles of Electronic Materials and Devices, Third Edition*, S.O. Kasap (© McGraw-Hill, 2005)

Example: A hypothetical molecule consisting of three H atoms.

a. Using the LCAO (linear combination of atomic orbitals) principle, sketch the possible molecular orbitals.
b. Sketch the associated probability density distributions.
c. Order the energies of the molecular orbitals.