L11: review

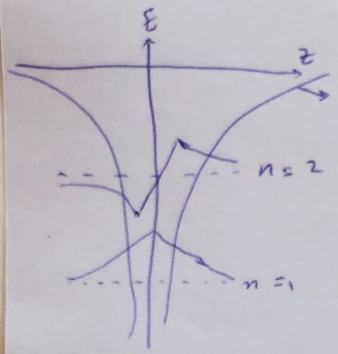
hydrogen atom

3 coordinates (x, y, z) cartesian
or
(r, θ, φ) polar

$\Rightarrow$ 3 quantum numbers n, l, m_l

Schrödinger eq.:

$$\left\{ -\frac{\hbar^2}{2m_e}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r} \right\}\psi = E_{n l m_l}\psi$$



$$V(z) = \frac{-e^2}{4\pi\varepsilon_0}\frac{1}{z}$$

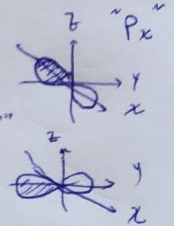
$$E_{n l m_l} = -R_H\left(\frac{1}{n^2}\right)$$

Rydberg constant $= 2.18 \times 10^{-18}$ J

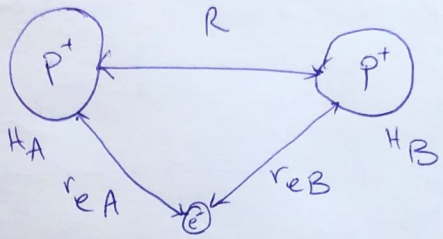
Solutions:

$n = 2, l = 1, m_l = 1$ (1,0)
$= -1$ (-1,0)
$= 0$ (0)

Linear combination



Today: H_2^+ molecule ion



Schrödinger equation:

$$\left\{ -\frac{\hbar^2}{2m_e}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) - \frac{Z_A e^2}{4\pi\varepsilon_0 r_{eA}} - \frac{Z_B e^2}{4\pi\varepsilon_0 r_{eB}} + \frac{Z_A Z_B e^2}{4\pi\varepsilon_0 R} \right\}\psi = E\psi$$

$$\downarrow$$

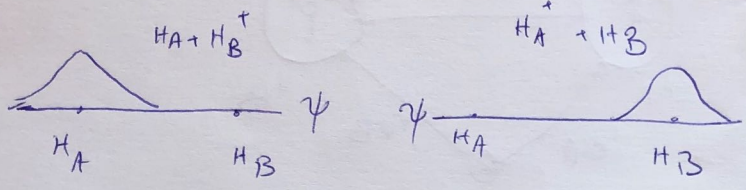
$$\psi_{n l m_l s}$$

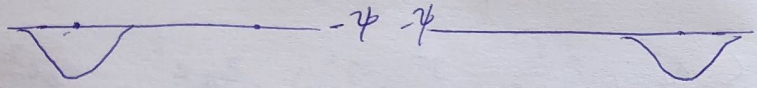
two features of the eq.:

(1) no nuclear kinetic energy; only the energy of electron is calculated

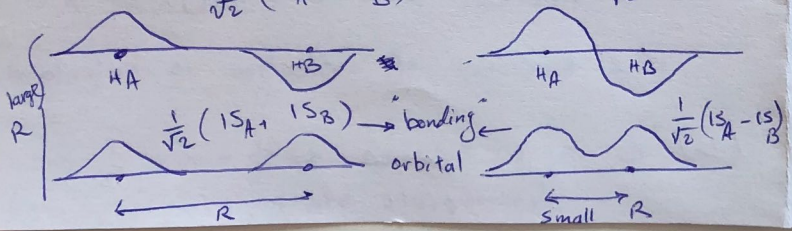
(2) no spin terms; $s = +\frac{1}{2}$ and $s = -\frac{1}{2}$ are degenerate states (similar energy)

* if ψ is a solution (eigen functions) then $-\psi$ is also a solution





instead of solving the exact schrödinger eq one can find an approximate solution by Linear Combination of Atomic Orbitals (LCAO) of free hydrogen atoms:



* There are softwares (e.g. IQmol) that can compute orbitals (wavefunctions) of a custom molecule by specifying the computation method and basis set. More on these later! Gopika showed a demo of IQmol for H_2^+ molecule.