Announcements:

- error in Act. #9, p.78 – should be $-\frac{\hbar^2}{2m_e}\left(\nabla_1^2+\nabla_1^2\right)-\ldots$

- Assignment #7 due next Monday

- Next few classes:
  - Wed. Linux exercises
  - Fri. beginning Gaussian03
  - Mon. Huckel (Act. #14/15)

- begin reading Cramer Ch. 4

Today:

- quick quiz
- recap of ME atoms

$$E_{1e}(Z,n) = -\frac{1}{2}\underbrace{\left(\frac{m_e e^4}{(4\pi\varepsilon_0)^2\hbar^2}\right)}_{\text{atomic unit of energy} = E_h}\left(\frac{Z}{n}\right)^2 = -\tfrac{1}{2}E_h\left(\frac{Z}{n}\right)^2 = -(13.6\text{ eV})\left(\frac{Z}{n}\right)^2$$

TABLE A.8 Wavefunctions for Hydrogen-like Atoms.

$$\Psi_{1s} = \Psi_{100} = \frac{1}{\pi^{1/2}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$$

$$\Psi_{2s} = \Psi_{200} = \frac{1}{4(2\pi)^{1/2}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2-\frac{Zr}{a_0}\right) e^{-Zr/2a_0}$$

$$\Psi_{210} = \Psi_{2p_z} = \frac{1}{4(2\pi)^{1/2}}\left(\frac{Z}{a_0}\right)^{5/2} r\, e^{-Zr/2a_0}\cos\theta$$

Multi-Electron Atoms

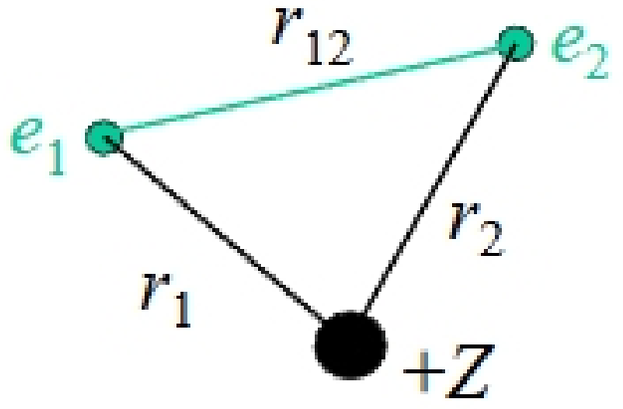
(in atomic units: m_e, $4\pi\varepsilon_0$, $\hbar$, $e = 1$)

1e atom:

$$\hat{H} = -\frac{1}{2}\nabla^2 - \frac{Z}{r} = \hat{h}(1)$$

all coords. of e #1

$$\Psi_{n,l,m_l}(r,\theta,\varphi) = \Psi(1)$$



2e atom:

$$\hat{H} = \underbrace{\left(-\frac{1}{2}\nabla_1^2 - \frac{Z}{r_1}\right)}_{\hat{h}(1)} + \underbrace{\left(-\frac{1}{2}\nabla_2^2 - \frac{Z}{r_2}\right)}_{\hat{h}(2)} + \underbrace{\frac{1}{r_{12}}}_{V_{ee}(1,2)} \qquad r_{12} = |\vec{r}_1 - \vec{r}_2|$$

$$\Psi(\vec{r}_1,\vec{r}_2) = \Psi(1,2)$$

even for only 2 e, exact solutions are impossible due to V_{ee} term