Multi-electron atoms

Similarities / Differences to H:

- Individual orbitals identical in shape to H
- orbitals lower in energy (stronger bound) than H orbitals because of stronger core potential

Example: $n=2 \rightarrow n'=1$ transition

H $\quad Ly\,\alpha = 121\,nm = 10.2\,eV$ (UV)

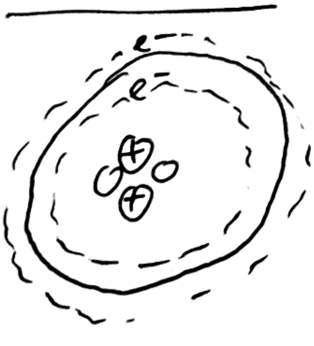
Cu $\quad K\,\alpha = 0.15\,nm = 8.04\,keV$ (x-rays)

- Ionization energies differ because of shielding and Coulomb repulsion

$$H = \frac{p_1^2}{2m} - \frac{Ze^2}{r_1} + \frac{p_2^2}{2m} - \frac{Ze^2}{r_2} + \frac{e^2}{|r_1 - r_2|}$$

shielding: - inner e^- shield nuclear charge

$\rightarrow Z_{eff}$



two extreme cases:

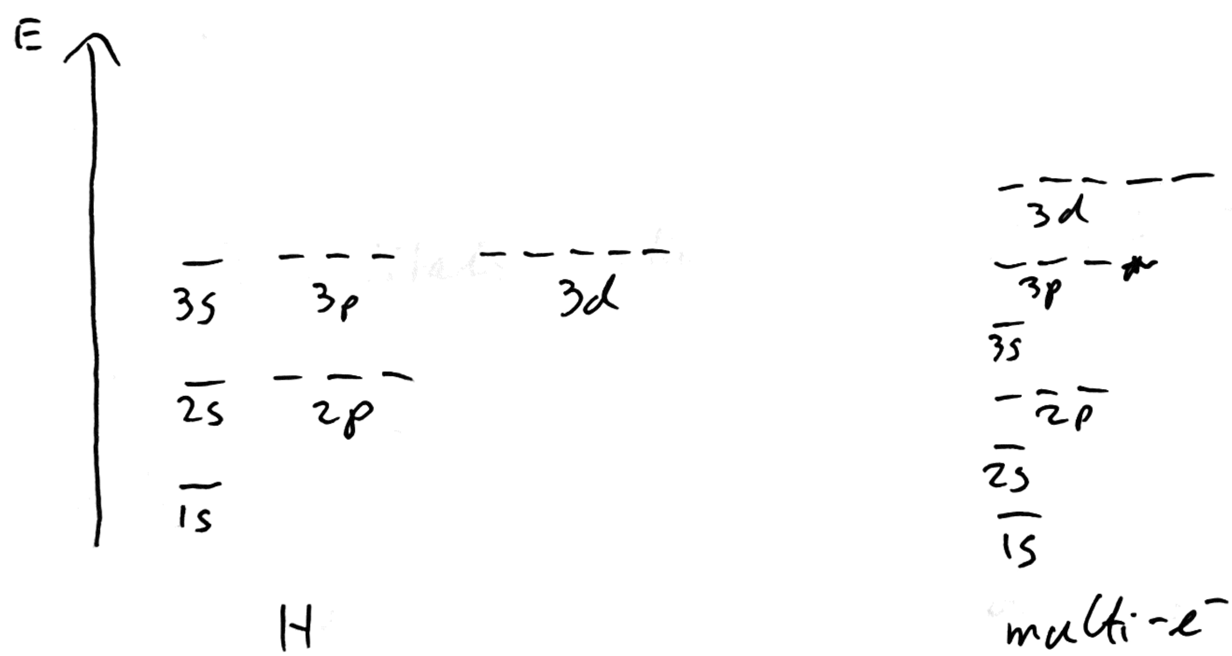
- no shielding: $Z_{eff} = Z$
- max shielding: $Z_{eff} = Z + (N-1)q_e$ $\quad N = \#e$

In Reality, usually in between both cases because of orbital overlap

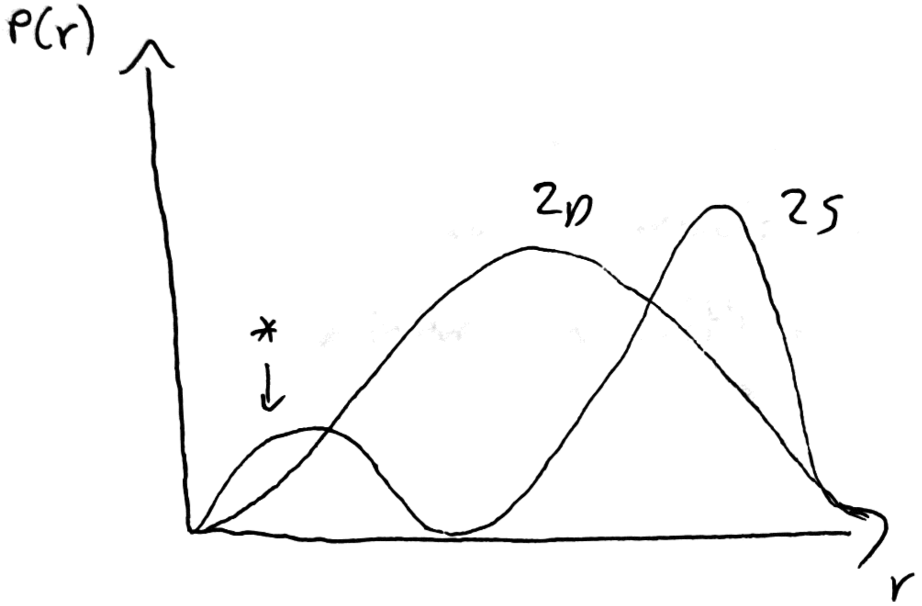
Example: $E_1^{exp} = 3.94 \cdot 10^{-18}\,J \rightarrow Z_{eff} = 1.34$

$\rightarrow$ effective potential („pseudo-potential")

$\rightarrow$ n no longer sole factor for E. Now n, l because radial distributions matter



Why $E_{ns} < E_{np} < E_{nd} < E_{nf}$?



* higher probability to find e^- near nucleus
  -> less shielding

Electron configurations / Periodic table

Now: - need to consider spin!

-> fill orbitals starting with lowest E

AND

follow these rules

1) Pauli exclusion principle: two or more identical particles with half-integer spin cannot occupy the same quantum state (same n, l, m_l, m_s)

2) Hund's rules

2.1 Maximize $S = \sum s_i$ (spins align if they can)

Reason: aligned spins require different orbit

→ Coulomb repulsion is minimized

→ interaction with nucleus is maximized