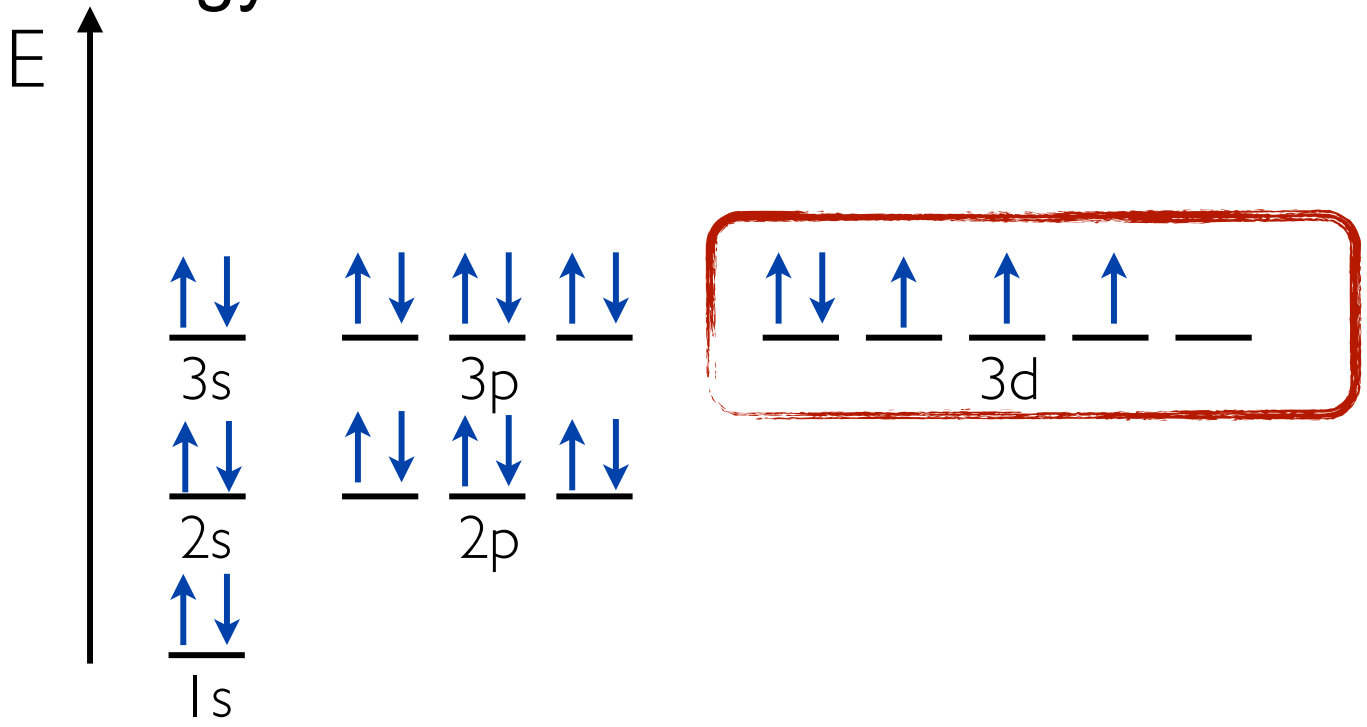
- Magnetism
  - Always an interaction effect (otherwise all states doubly occupied or empty)
  - Simplest to understand in very strongly interacting systems where electrons are localized - almost always this has at least some truth to it in practice
- Plan:
  - Magnetism: atomic limit
  - Exchange
  - Ordering
  - Collective modes - spin waves
  - Frustrated magnets etc.
  - Itinerant magnetism: Kondo, heavy fermions

- We start with a picture of atomic magnetism: why should local moments form in “isolated” atoms
  - By isolated we are thinking along the lines of the Mott picture/Hubbard model where Coulomb repulsion is large enough that hopping of electrons on/off the ion is a perturbation
  - Our problem consists of a Hamiltonian with the Coulomb potential from the nucleus and electron kinetic energy, plus several perturbations: e-e interactions, potentials from other charges outside the atom, SOC, and hopping away from the atom
  - We want to take that last effect as smaller than the e-e one.

$$H = H_{kin} + V + H'_C + H'_{SOC} + H'_{hop}$$

$$H = H_{kin} + V_0 + V_{cf} + H'_C + H'_{SOC} + H'_{hop}$$

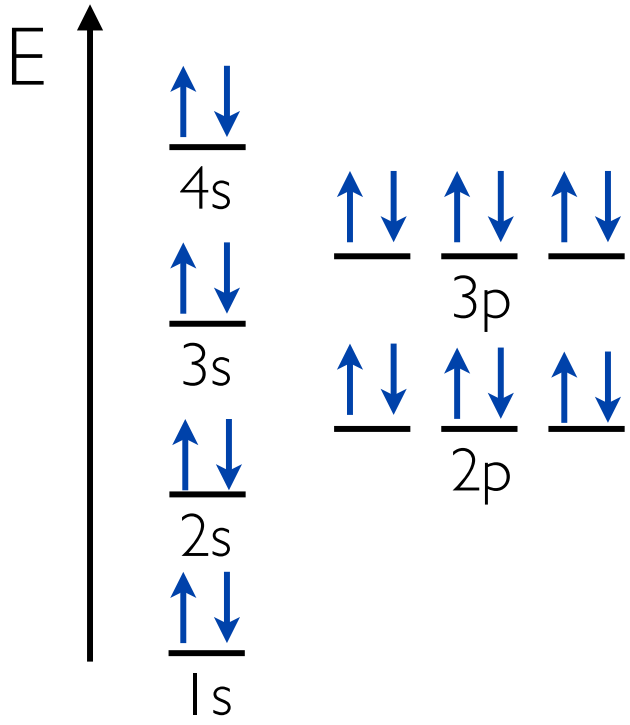
- Hydrogen atom $V_0 = -k/r$ $E_n = -\dfrac{\mathrm{Ry}}{n^2}$
- Level degeneracy: magnetism w/o kinetic energy cost

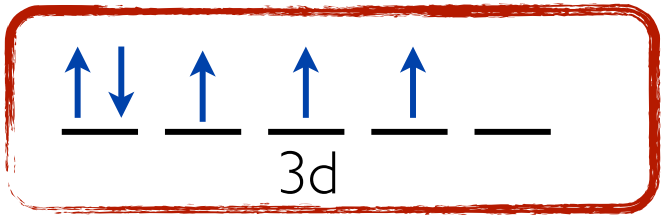


$$H = H_{kin} + V_0 + V_{cf} + H'_C + H'_{SOC} + H'_{hop}$$

$$V_0 = v(r)$$

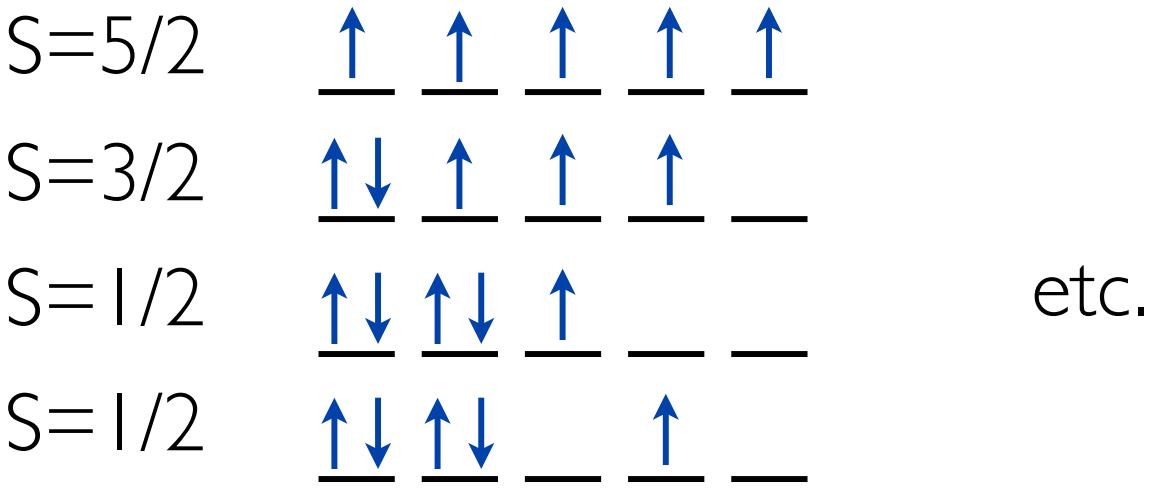
- Due to screening by inner electrons, potential is not 1/r, so degeneracy of different l states is lifted, and $E_{2s}<E_{2p}$, $E_{3s}<E_{3p}<E_{3d}$ etc





- 2L+1 degeneracy is required by spherical symmetry
- Generally d and f electrons are most isolated - more localized - from other atoms because they are "protected" inside higher shell s states
- Most magnetism involves *transition metals* or *rare earths*

- A partially filled shell has a lot of possible states



- Without considering interactions *between* electrons in these shells, all are degenerate

- Note: when # of electrons is odd, there is always at least a 2-fold Kramer's degeneracy

- Claim: there is a strong tendency for states with local moments to be selected

- General problem:

  - Some set of orbital states a=1..p which are low energy

  - Expand Coulomb in this basis $c_\alpha(r) = \sum_a \phi_a(r) c_{a\alpha}$

$$H_C = \int_{r,r'} \frac{U(r-r')}{2} c^\dagger_\alpha(r) c^\dagger_\beta(r') c_\beta(r') c_\alpha(r)$$

$$= \frac{1}{2} \sum_{abcd} U_{abcd}\, c^\dagger_{a\alpha} c^\dagger_{b\beta} c_{c\beta} c_{d\alpha}$$

where $$U_{abcd} = \int_{r,r'} \frac{U(r-r')}{2} \phi^*_a(r) \phi^*_b(r') \phi_c(r') \phi_d(r)$$

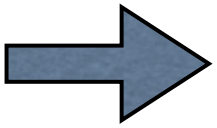
- Hartree-Fock (like) approximation:
  - assume states are products of orbitals

$$|\psi\rangle = \sum_{\alpha\beta\ldots} f_{\alpha\beta\ldots} c^\dagger_{a\alpha} c^\dagger_{b\beta} \cdots |0\rangle$$

  - Then to first order in Coulomb, Hamiltonian must preserve set (ab...) of occupied orbitals

$$\langle\psi|H|\psi\rangle = \langle\psi|H_{HF}|\psi\rangle$$

$$H = \frac{1}{2}\sum_{abcd} U_{abcd}\, c^\dagger_{a\alpha} c^\dagger_{b\beta} c_{c\beta} c_{d\alpha}$$



c=b, d=a: "Hartree"

c=a, d=b: "Fock"

- Some manipulations

$$H_{HF} = U \sum_a n_{a\uparrow} n_{a\downarrow} + \frac{1}{2} \sum_{a \neq b} \left[U_{abba}\, c^\dagger_{a\alpha} c^\dagger_{b\beta} c_{b\beta} c_{a\alpha} + U_{abab}\, c^\dagger_{a\alpha} c^\dagger_{b\beta} c_{a\beta} c_{b\alpha} \right]$$

$$= H_U + \frac{1}{2} \sum_{a \neq b} \left[U_{abba}\, n_a n_b - U_{abab}\, c^\dagger_{a\alpha} c_{a\beta} c^\dagger_{b\beta} c_{b\alpha} \right]$$

"Hubbard U": favors single occupancy

just classical electro-static energy

Fock = "exchange"

- A useful identity $\quad c^\dagger_{a\alpha} c_{a\beta} = \frac{n_a}{2} \delta_{\alpha\beta} + \vec{S}_a \cdot \vec{\sigma}_{\beta\alpha}$

$$H_F = -\frac{1}{2} \sum_{ab} U_{abab} \mathrm{Tr} \left[\left(\frac{n_a}{2} I + \vec{S}_a \cdot \vec{\sigma} \right) \left(\frac{n_b}{2} I + \vec{S}_b \cdot \vec{\sigma} \right) \right]$$

$$-\frac{1}{2} \sum_{ab} U_{abab} \left(\frac{n_a n_b}{2} + 2 \vec{S}_a \cdot \vec{S}_b \right)$$

Favors aligning spins on different orbitals