

---

## Problem Set 7

### Hund's rules

---

Consider an atom with many electrons  $i$  in states characterized by the orbital angular momentum  $\mathbf{l}_i$  and the spin  $\mathbf{s}_i$  (in units of  $\hbar$ ). We define the total orbital angular momentum  $\mathbf{L} = \sum_i \mathbf{l}_i$ , the total spin  $\mathbf{S} = \sum_i \mathbf{s}_i$ , and the total angular momentum  $\mathbf{J} = \mathbf{L} + \mathbf{S}$ .

According to Hund's rules (1925), for the case of a partially filled shell, the lowest energy values are found in the following way:

- (1) Maximize  $S = |\mathbf{S}|$ , respecting the Pauli exclusion principle.
- (2) Maximize  $L = |\mathbf{L}|$ , respecting the Pauli exclusion principle and rule (1).
- (3)  $J = |\mathbf{J}| = L + S$  when the shell is more than half filled and  $J = |L - S|$  when the shell is less than half filled.

The *term symbol* of the resulting configuration is  $(^{2S+1})L_J$ , where the orbital angular momentum is usually given by a letter following the convention

$L$	0	1	2	3	4	5	6
symbol	S	P	D	F	G	H	I

Apply Hund's rules to determine the ground state angular momenta for the following cases:

- (a) O in the configuration  $1s^2 2s^2 2p^4$
- (b) V in the configuration  $[\text{Ar}] 3d^3 4s^2$
- (c)  $\text{Eu}^{2+}$  in the configuration  $[\text{Xe}] 4f^7$
- (d)  $\text{Dy}^{3+}$  in the configuration  $[\text{Xe}] 4f^9$