10.1 Landé g-factor

Considering the two expressions of the total magnetic moment, find the expression of g_J

$$\boldsymbol{\mu} = -\frac{\mu_B}{\hbar}(\boldsymbol{L} + 2\boldsymbol{S})$$

$$\boldsymbol{\mu} = -\frac{\mu_B}{\hbar} g_J \boldsymbol{J}$$

$$g_J = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

Hints:

1) Multiply both sides of both equations by $\boldsymbol{J}$
2) Remember that the eigenvalue of $\boldsymbol{S}^2$ is $S(S+1)\hbar^2$, of $\boldsymbol{L}^2$ is $L(L+1)\hbar^2$ and of $\boldsymbol{J}^2$ is $J(J+1)\hbar^2$
3) Use the expressions of the type $\boldsymbol{L}^2 = (\boldsymbol{J} - \boldsymbol{S})^2$ to rewrite the expressions found in 1)
4) Find the expression of g_J

10.1 Landé g-factor - Solution

$$\boldsymbol{\mu}\cdot\boldsymbol{J} = -\frac{\mu_B}{\hbar} g_J\, \boldsymbol{J}\cdot\boldsymbol{J} = -\frac{\mu_B}{\hbar} g_J\, \boldsymbol{J}^2 \quad\rightarrow\quad -\mu_B g_J J\,(J+1)$$

$$\boldsymbol{\mu}\cdot\boldsymbol{J} = -\frac{\mu_B}{\hbar}(\boldsymbol{L}+2\boldsymbol{S})\cdot\boldsymbol{J} = -\frac{\mu_B}{\hbar}(\boldsymbol{L}\cdot\boldsymbol{J}+2\boldsymbol{S}\cdot\boldsymbol{J}) =$$

$$\boldsymbol{L}^2 = (\boldsymbol{J}-\boldsymbol{S})^2 = \boldsymbol{J}^2+\boldsymbol{S}^2-2\boldsymbol{S}\cdot\boldsymbol{J} \quad\rightarrow\quad \boldsymbol{S}\cdot\boldsymbol{J} = \frac{1}{2}\left(\boldsymbol{J}^2-\boldsymbol{L}^2+\boldsymbol{S}^2\right) \quad\rightarrow\quad \frac{1}{2}\left(J(J+1) - L(L+1) + S(S+1)\right)$$

$$\boldsymbol{S}^2 = (\boldsymbol{J}-\boldsymbol{L})^2 \quad\rightarrow\quad \boldsymbol{L}\cdot\boldsymbol{J} = \frac{1}{2}\left(\boldsymbol{J}^2+\boldsymbol{L}^2-\boldsymbol{S}^2\right) \quad\rightarrow\quad \frac{1}{2}\left(J(J+1) + L(L+1) - S(S+1)\right)$$

$$g_J J(J+1) = \frac{1}{2}\left(J(J+1)+L(L+1)-S(S+1)\right) + \left(J(J+1)-L(L+1)+S(S+1)\right) = \frac{3}{2}J(J+1) + \frac{1}{2}\left(S(S+1) - L(L+1)\right)$$

$$g_J = \frac{3}{2} + \frac{S(S+1)-L(L+1)}{2J(J+1)}$$

10.2 Magnetic moments

We want to evaluate the magnetic moment of atoms in different environments. We apply an external magnetic field B along the z direction and for simplicity we assume $T = 0$ K.

1) Calculate the magnetic moment of a free-standing Co ([Ar] $3d^7$ $4s^2$) , Sm ([Xe] $4f^6$ $6s^2$) and Dy ([Xe] $4f^{10}$ $6s^2$) atom.

2) Calculate the magnetic moment of a Co atom in bulk Co knowing that $n_{3d}(\downarrow) = 5.0$, $n_{3d}(\uparrow) = 3.3$, $n_{4s}(\downarrow) = 0.35$, $n_{4s}(\uparrow) = 0.35$ where n_{3d} and n_{4s} the number of electrons with spin down/up in the respective band.

3) Consider the alloys $SmCo_5$ and $DyCo_5$. In both composites the magnetic moment of the Co atoms is anti-parallel to the magnetic moment of the rare earth element. Assume for Co the electronic configuration $n_{3d}(\downarrow) = 5.0$, $n_{3d}(\uparrow) = 3.0$, $n_{4s}(\downarrow) = 0.35$, $n_{4s}(\uparrow) = 0.35$. For the rare earth assume the standard ([Xe] $4f^{N-1}$ $5d^1$ $6s^2$) configuration and note that the electron in the 5d state occupies the orbital with $M_L = 0$. What is the magnetic moment per unit formula?

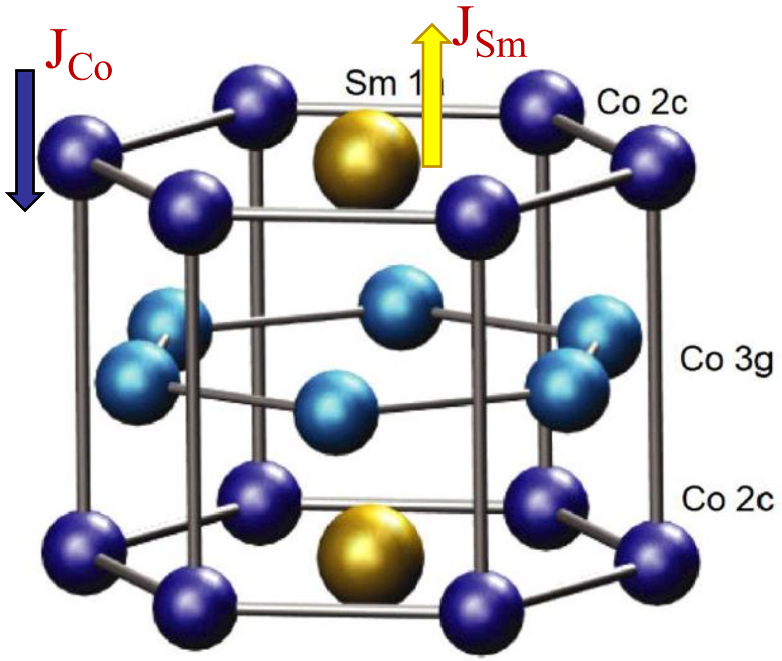
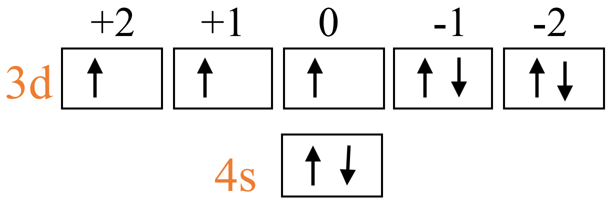


FIG. 1. Unit cell of the hexagonal intermetallic $SmCo_5$.

Adapted from : B. Das *et al.,* Phys. Rev. B **100**, 024419 (2019) DOI: 10.1103/PhysRevB.100.024419

1)

Ground state of Co ([Ar] $3d^7$ $4s^2$)

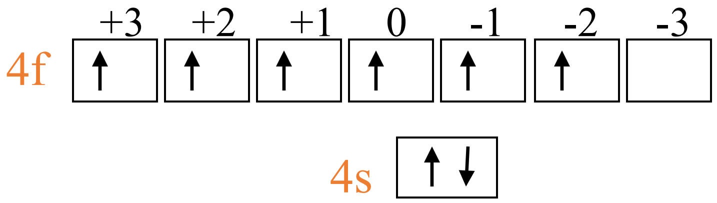


$S = 3/2 \quad L = 3 \quad J = 9/2$

$g_J = 4/3$

$\mu = g_J J\ \mu_B = \frac{4}{3}\frac{9}{2}\mu_B = 6\ \mu_B$

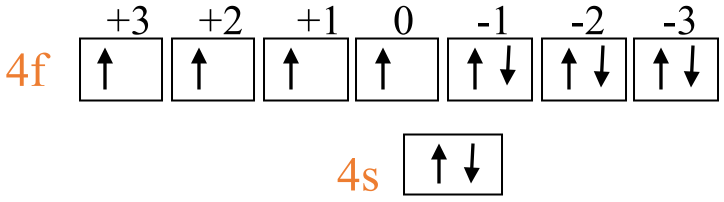
Ground state of Sm ([Xe] $4f^6$ $6s^2$)



$S = 3 \quad L = 3 \quad J = 0$

$\mu = g_J J\ \mu_B = 0$

Ground state of Dy ([Xe] $4f^{10}$ $6s^2$)



$S = 2 \quad L = 6 \quad J = 8$

$g_J = 5/4$

$\mu = \frac{5}{4} 8\ \mu_B = 10\ \mu_B$

2) In bulk the orbital moment is quenched; therefore $L = 0$

Using the occupation number $n_{3d}(\downarrow) = 5.0$, $n_{3d}(\uparrow) = 3.3$, $n_{4s}(\downarrow) = 0.35$, $n_{4s}(\uparrow) = 0.35$, for the spin we obtain these contributions:

from the d band: $\mu_S = g_s\, S\, (5.0 - 3.3)\ \mu_B = 2\ ½\ 1.7\ \mu_B = 1.7\ \mu_B$

from the 4s band: $\mu_S = 0$

Thus, $\mu = 1.7\ \mu_B$

10.2 Magnetic moments - Solution

EPFL

3) Co contribution: in bulk the orbital moment is quenched thus $L = 0$

Using the occupation number $n_{3d}(\downarrow) = 5.0$, $n_{3d}(\uparrow) = 3.0$, $n_{4s}(\downarrow) = 0.35$, $n_{4s}(\uparrow) = 0.35$, for the spin we obtain these contributions:

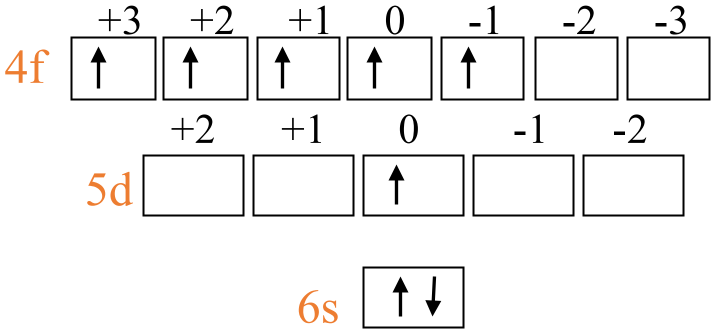
from the d band: $\mu_S = 2\ ½\ 2\ \mu_B = 2.0\ \mu_B$

from the 4s band: $\mu_S = 0$

Thus, $\mu_{Co} = 2\ \mu_B$ in both alloys

Rare earth contribution can be calculated with Hund's rules

Ground state of Sm ([Xe] $4f^5\ 5d^1\ 6s^2$)



$$4f\!: S = 5/2, L = 5, J = 5/2$$
$$\mu_{4f} = g_J J\ \mu_B = 2/7 \cdot 5/2\ \mu_B = 5/7\ \mu_B$$

$$5d\!: S = 1/2, L = 0, J = 1/2$$
$$\mu_{5d} = g_J J\ \mu_B = 2 \cdot ½\ \mu_B = 1\ \mu_B$$

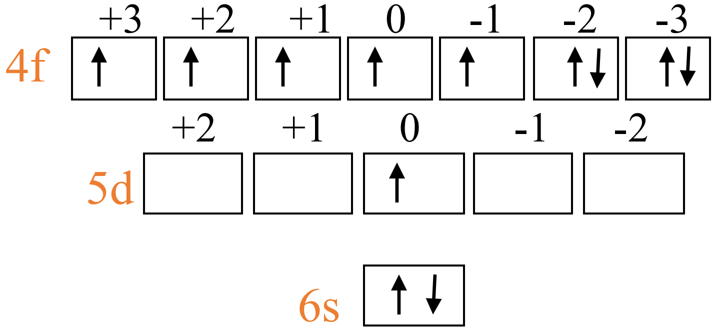
$$\mu_{6s} = g_J J\ \mu_B = 0\ \mu_B$$

$$\mu_{Sm} = 2/7 \mu_B$$

$$\mu_{u.f.} = 5\ \mu_{Co} - \mu_{Sm} = 68/7\ \mu_B \approx 10\ \mu_B$$

S_{5d} is parallel to S_{4f} (exchange coupling).
Since $L_{4f} > S_{4f}$,
J_{4f} is parallel to L_{4f} and antiparallel to S_{4f}.
So S_{5d} is antiparallel to J_{4f}

Ground state of Dy ([Xe] $4f^9\ 5d^1\ 6s^2$)



$$4f\!: S = 5/2, L = 5, J = 15/2$$
$$\mu_{4f} = g_J J\ \mu_B = 4/3 \cdot 15/2\ \mu_B = 10\ \mu_B$$

$$5d\!: S = 1/2, L = 0, J = 1/2$$
$$\mu_{5d} = g_J J\ \mu_B = 1\ \mu_B$$

$$\mu_{6s} = g_J J\ \mu_B = 0\ \mu_B$$

$$\mu_{Dy} = 11\ \mu_B$$

$$\mu_{u.f.} = 5\ \mu_{Co} - \mu_{Dy} = -1\ \mu_B$$