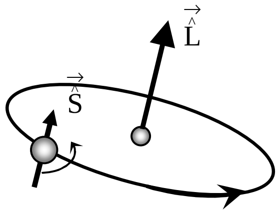
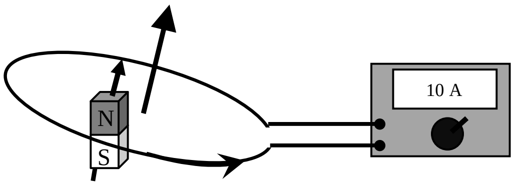
<u>Spin-Orbit Coupling</u>





light elements-perturbation: $\mathcal{H}_o + \mathcal{H}'_{so}$

spin-orbit interaction: $\mathcal{H}'_{so} = \xi\, \vec{\hat{L}} \cdot \vec{\hat{S}}$

$\vec{J} = \vec{L} + \vec{S}$ $\qquad \hat{J}^2 = \vec{J} \cdot \vec{J} = (\vec{\hat{L}} + \vec{\hat{S}}) \cdot (\vec{\hat{L}} + \vec{\hat{S}}) = \vec{\hat{L}} \cdot \vec{\hat{L}} + \vec{\hat{S}} \cdot \vec{\hat{S}} + 2\vec{\hat{L}} \cdot \vec{\hat{S}} = \hat{L}^2 + \hat{S}^2 + 2\, \vec{\hat{L}} \cdot \vec{\hat{S}}$

$\vec{\hat{L}} \cdot \vec{\hat{S}} = ½\, (\hat{J}^2 - \hat{L}^2 - \hat{S}^2)$

$\Psi_{J,m_J} = \Psi_{L,m_L}\, \Psi_{S,m_S}$ $\qquad \hat{L}^2\, \Psi_{L,m_L} = \hbar^2\, L(L + 1)\, \Psi_{L,m_L}$ $\qquad \hat{S}^2\, \Psi_{S,m_S} = \hbar^2\, S(S + 1)\, \Psi_{S,m_S}$

$|\, \vec{\hat{L}} \cdot \vec{\hat{S}}\, | = ½\, \hbar^2\, [J(J+1) - L(L+1) - S(S+1)]$

$E_{so} = ½\, \mathcal{A}hc\, [J(J+1) - L(L+1) - S(S+1)]$

$\mathcal{A}$ in cm^{-1} and $\mathcal{A}hc = \xi\hbar^2$

Example:Spin-orbit splitting of the $^2P_{3/2}$ and $^2P_{½}$ terms for the sodium atom p^1 configuration.

$E_{so}\, (J = {}^3/_2) = ½\, \mathcal{A}hc\, [{}^3/_2({}^3/_2 + 1) - 1(1+1) - ½(½+1)] = ½\, \mathcal{A}hc\, [{}^{15}/_4 - {}^8/_4 - {}^3/_4] = ½\, \mathcal{A}hc$

$E_{so}\, (J = ½) = ½\, \mathcal{A}hc\, [½(½ + 1) - 1(1+1) - ½(½+1)] = ½\, \mathcal{A}hc\, [{}^3/_4 - {}^8/_4 - {}^3/_4] = -1\, \mathcal{A}hc$

$\Delta E_{so} = -½\, \mathcal{A}hc =$ $\qquad \Delta E_{so} = -½\, \mathcal{A} = -17\ cm^{-1}$

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