Condensed Matter Physics I

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Previously

Intro magnetism
- Diamagnetism: induced moments, no interaction
- Paramagnetism: needs moments, no interaction
- Ordered magnetism: needs moments & interaction

Magnetism

Diamagnetism:

- No magnetic moments
- No magnetic interaction
- Response due to induced currents
- Magnetization <u>opposite</u> to field

- Water
- Ideal gases
- Superconductors

Paramagnetism:

- Magnetic moments (spin, orbit)
- Weak magnetic interactions
- Response due to orientation
- Magnetization in field direction

- Metals
- ‘odd electron’ systems
- O_2, biradicals

Ordered magnetism:

- Magnetic moments
- Strong magnetic interactions
- Response due to polarization
- Ferro-, antiferro-, ferrimagnetic

- Fe, Ni, Co
- Cr, high-T_c (CuO systems)

Today

Non-ordered magnetism

Magnetic moments

Crystal field effects

Magnetization and susceptibility

Magnetization at T=0: $M(H) = -\frac{\partial E_o}{\partial H}$

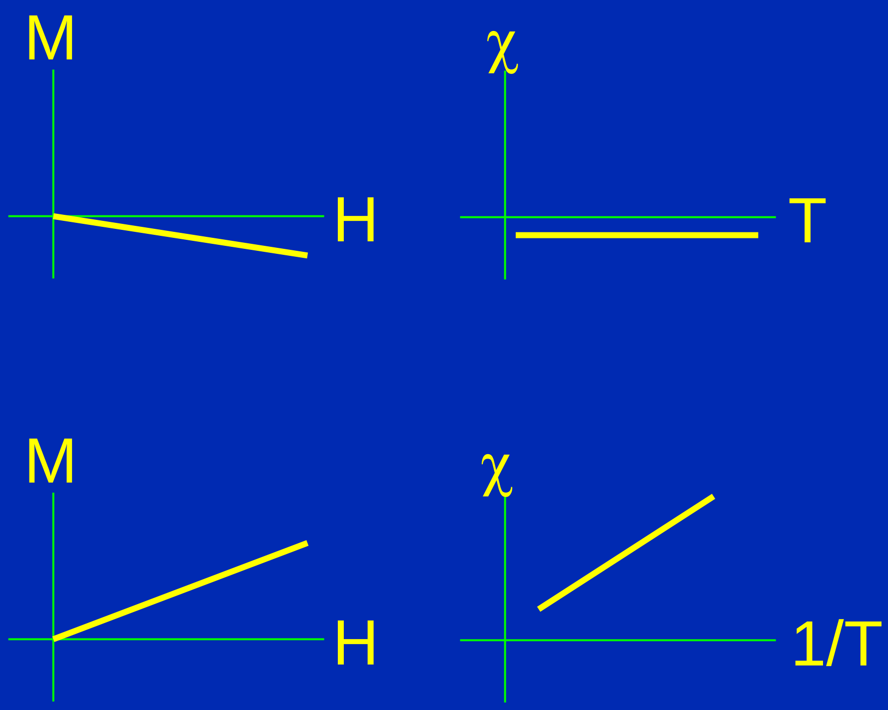
at finite T: $M(H) = \frac{\sum_n M_n(H) e^{-E_n/kT}}{\sum_n e^{-E_n/kT}}$

Magnetic susceptibility: $\chi = \frac{\partial M}{\partial H}$

Only ground state (low T): $\chi = -\frac{\partial^2 E_o}{\partial H^2}$

Dia- & paramagnetism

$M = \chi H$



Diamagnetism
Temperature independent

Paramagnetism
1/T dependence

QM treatment: orbit

Inclusion of the field in the motion: $\vec{p} \to \vec{p} + \frac{e}{c}\vec{A}$

Uniform H-field: $\vec{A} = -\frac{1}{2}\vec{r} \times \vec{H}$ Gauge: $\vec{\nabla} \cdot \vec{A} = 0;$

$$H = T + V \qquad \hbar\vec{L} = \sum_i \vec{r} \times \vec{p}_i$$

$$T = \frac{1}{2m}\sum_i \left[\vec{p}_i + \frac{e}{c}\vec{A}_i\right]^2 = \frac{1}{2m}\sum_i \left[\vec{p}_i - \frac{e}{2c} r_i \times \vec{H}_i\right]^2$$

$$= T_o + \mu_B \vec{L} \cdot \vec{H} + \frac{e^2}{8mc^2}\sum_i (x_i^2 + y_i^2) H^2$$

H//z

QM treatment: spin

Inclusion spin moment: $g_o \mu_B \vec{H} \cdot \vec{S} = g_o \mu_B H S_z$

$$\mathcal{H} = T_o + \mu_B (\vec{L} + g_o \vec{S}) \cdot \vec{H} + \frac{e^2}{8mc^2} \sum_i (x_i^2 + y_i^2) H^2 = T_0 + \mathcal{H}_B$$

$$E_n = E_{n,o} + E_B$$

$$E_B = \langle n | H_B | n \rangle + \sum_{n \neq n'} \frac{\langle n | H_B | n' \rangle^2}{E_n - E_{n'}}$$

$$\approx \mu_B \vec{H} \cdot \langle n | \vec{L} + g_o \vec{S} | n \rangle + \sum_{n \neq n'} \frac{\left[\mu_B \vec{H} \cdot \langle n | \vec{L} + g_o \vec{S} | n' \rangle \right]^2}{E_n - E_{n'}} + \frac{e^2}{8mc^2} H^2 \left\langle n \left| \sum_i \left(x_i^2 + y_i^2 \right) \right| n \right\rangle$$

⮱ Curie ⮱ Van vleck ⮱ Langevin

•Everything is (dia)magnetic

•Langevin diamagnetism: 'shielding' effect (Lenz law)

•Meissner effect in superconductors $\chi = -1$

•QM: inclusion of field

Orbit $\vec{p} \rightarrow \vec{p} + \frac{e}{c}\vec{A}$

Spin $g_o \mu_B \vec{H} \cdot \vec{S} = g_o \mu_B H S_z$

$$H = T_0 + H_B$$

$$H_B = \mu_B(\vec{L} + g_o \vec{S}) \cdot \vec{H} + \frac{e^2}{8mc^2} H^2 \sum_i (x_i^2 + y_i^2)$$

Magnetism

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Langevin <u>dia</u>magnetism

$$E_B \approx \mu_B \vec{H}\cdot\left\langle n\middle|\vec{L}+g_o\vec{S}\middle|n\right\rangle + \sum_{n\neq n'}\frac{\left[\mu_B\vec{H}\cdot\left\langle n\middle|\vec{L}+g_o\vec{S}\middle|n'\right\rangle\right]^2}{E_n - E_{n'}} + \frac{e^2}{8mc^2}H^2\left\langle n\middle|\sum_i\left(x_i^2+y_i^2\right)\middle|n\right\rangle$$

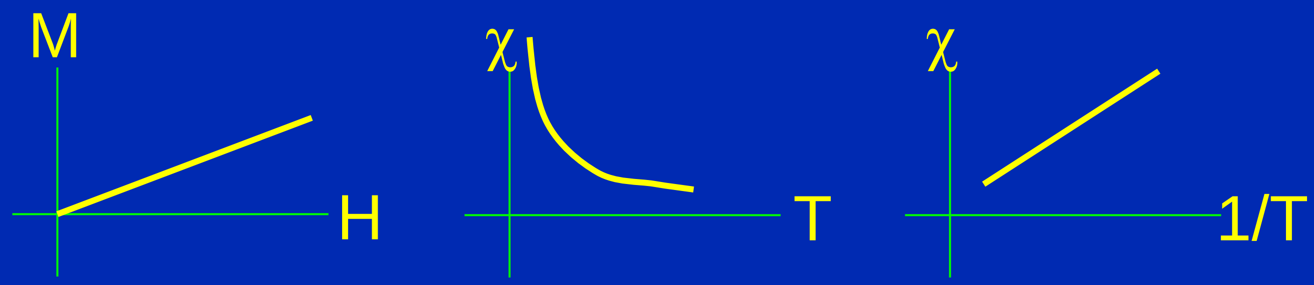
Low temperature, filled shell ions ($J|0\rangle = L|0\rangle = S|0\rangle = 0$)

$$E_B \approx \frac{e^2}{12mc^2}H^2\left\langle 0\middle|\sum_i r_i^2\middle|0\right\rangle$$

$$\chi = -n\frac{\partial^2 E_B}{\partial H^2} = -n\frac{e^2}{6mc^2}\left\langle 0\middle|\sum_i r_i^2\middle|0\right\rangle = -nZ\frac{e^2}{6mc^2}\left\langle r^2\right\rangle$$

(SI: $\chi = -nZ\frac{\mu_o e^2}{6m}\left\langle r^2\right\rangle$)

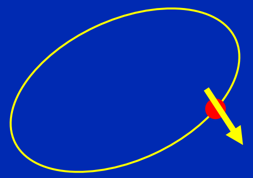
Paramagnetism



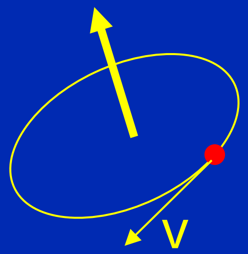
- alignment of weakly interacting magnetic moments in a magnetic field
- Curie law $\chi = \theta/T$
- Magnetic moments = spin, orbit
- Ground state splitting (Curie)
- Low lying excited states (van Vleck)
- Density of states effects (Pauli magnetism)

First: Coupling between L and S: Russel-Saunders

Spin-Orbit interaction (qualitative)



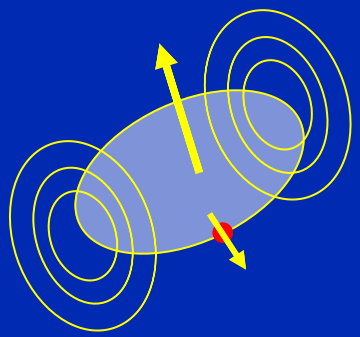
Magnetic moment electron spin: $\vec{\mu} = -g_o \mu_B \vec{S}$



Current of the electron in orbit:

$$I = \frac{v\,e}{2\pi R} = \frac{e(\vec{R}\times\vec{p})/m}{2\pi R^2} = \frac{eL}{2\pi m R^2}$$

$$B = I/2\pi R = \frac{eL}{4\pi^2 m R^3}$$



Energy of the spin in the field of the orbit:

$$U = -\vec{m}\cdot\vec{B} = g_o \mu_B \vec{S}\cdot\frac{e}{4\pi^2 m R^3}\vec{L} = \lambda \vec{L}\cdot\vec{S}$$

Partially filled shells

1. Russel-Saunders coupling L,S and J commute with Hamiltonian. Quantum numbers L,L_z, S,S_z,J,J_z describe electronic state

2. Hund's rules for n electrons in $2(2\ell+1)$ states (Maximization anti-symmetry + Pauli)

   I. Lowest state has highest S
   II. Lowest state has highest L$(= \sum \ell_z)$
   III. Lowest state has minimized LS interaction
      L+S for more than half filled (L,S opposite)
      |L-S| for less than half filled (L,S parallel)

States are characterized by $|L\,S\,J\,J_z\rangle$

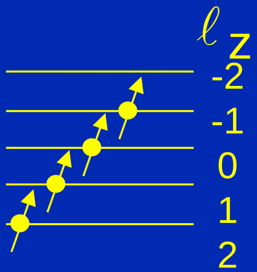
Hund's rules

Spectroscopic notation

$$^{2S+1}X_J$$

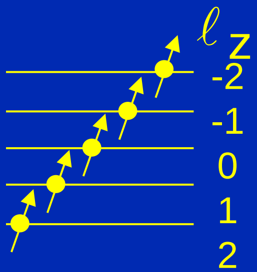
L =	0	1	2	3	4	5	6
X =	S	P	D	F	G	H	I

d-shell ($\ell = 2$), 4 electrons
Mn^{3+},Cr^{2+}



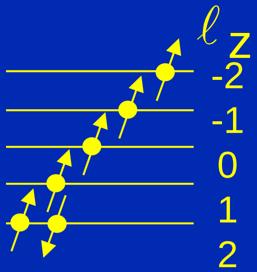
S=2
L=2 => $^5D_0$
J=0

d-shell ($\ell = 2$), 5 electrons
Fe^{3+},Mn^{2+}



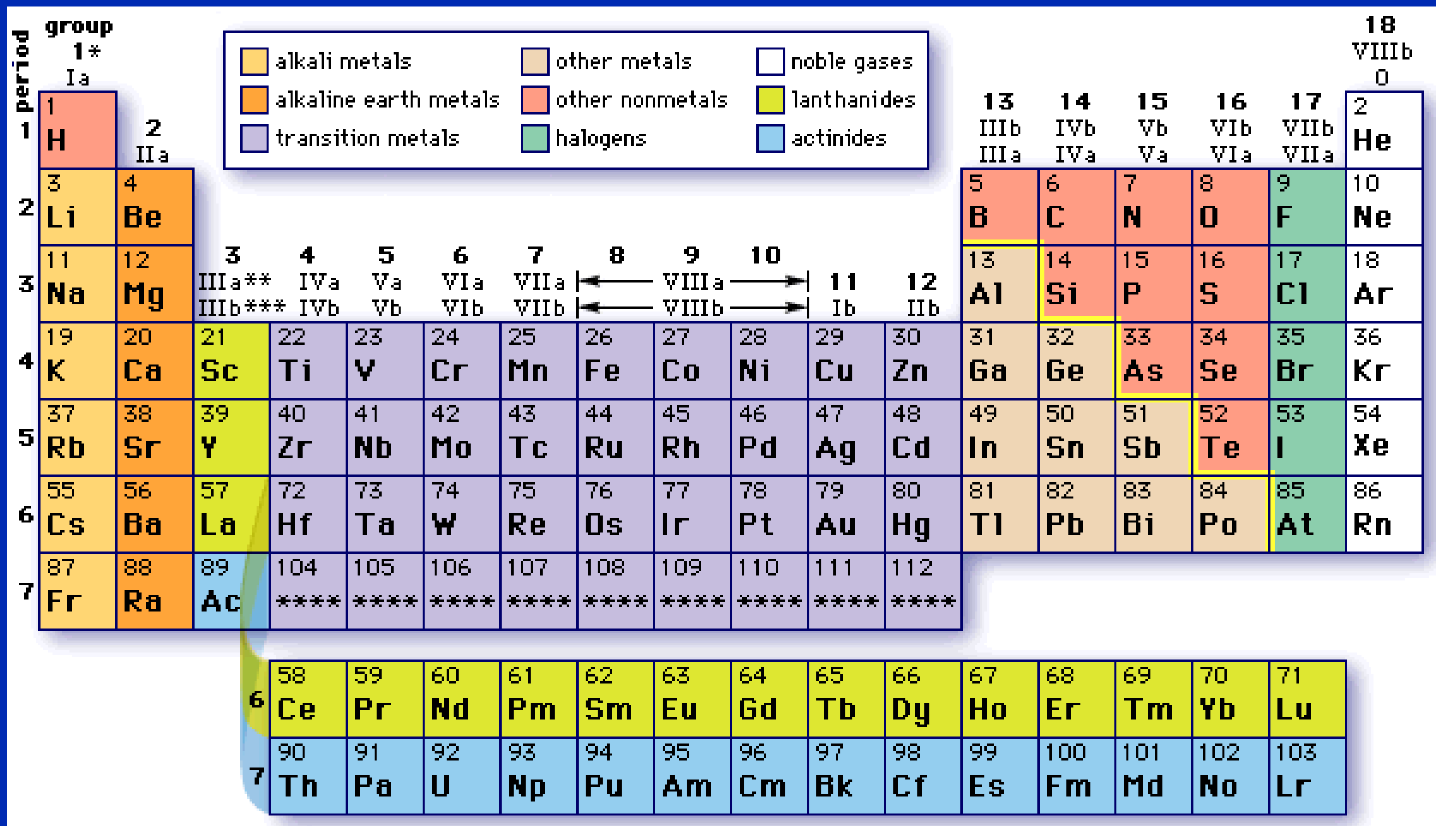
S=5/2
L=0 => $^6S_{5/2}$
J=5/2

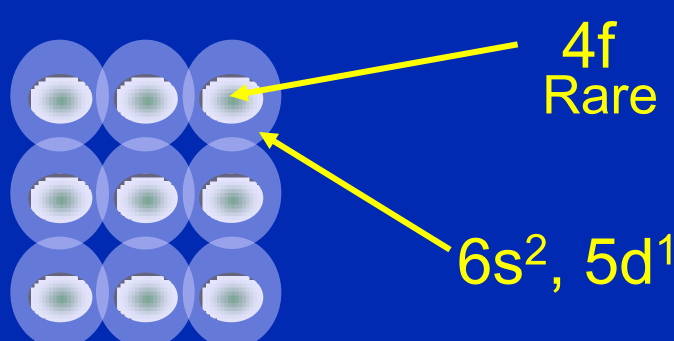
d-shell ($\ell = 2$), 6 electrons
Fe^{2+}



S=2
L=2 => $^5D_4$
J=4

Rare earth elements

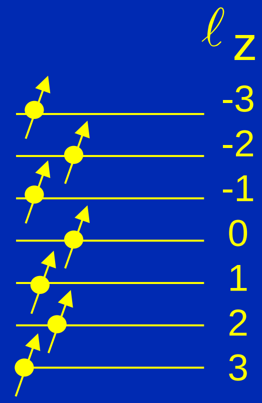




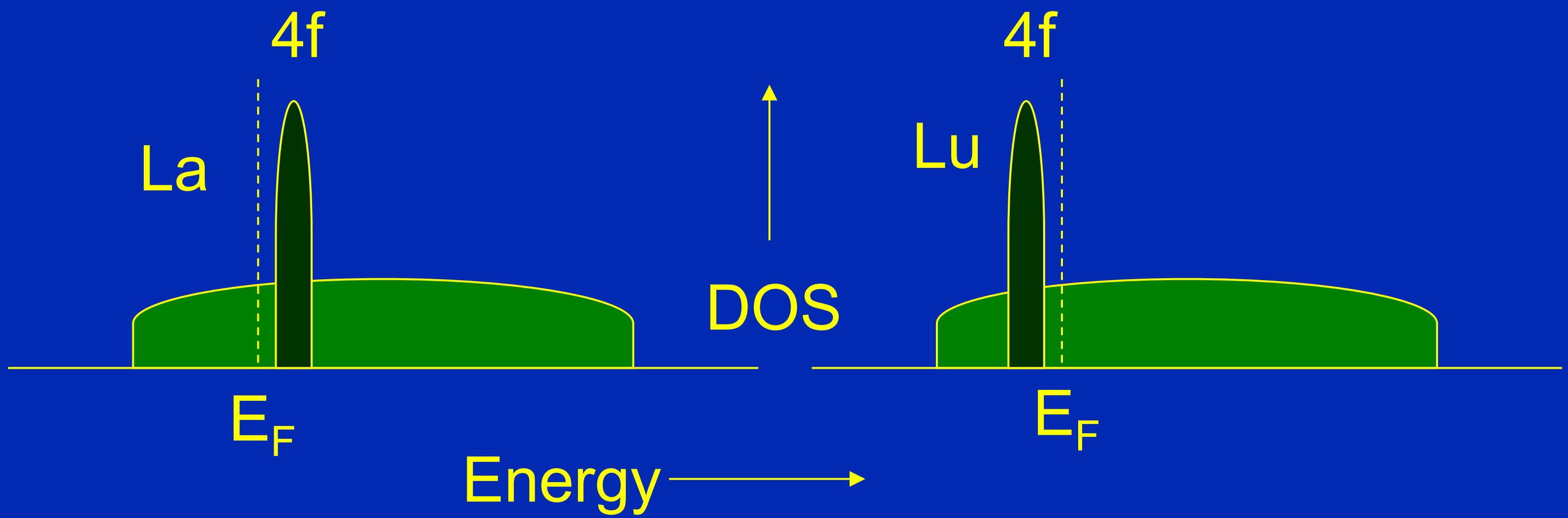
Rare earth elements:
Ce-Lu

Rare earth elements

f-shell ($\ell = 3$), 7 electrons
Gd^{3+}



S=7/2
L=0 => $^8S_{7/2}$
J=7/2



Spectroscopic splitting factor
Level splitting in a field

$$H'_B = \mu_B(\vec{L} + g_o\vec{S})\cdot\vec{H} \equiv g_j\,\mu_B\,\vec{J}\cdot\vec{H}$$

$$(\vec{L} + g_o\vec{S}) = g_j\,\vec{J}$$

$$(\vec{L} + g_o\vec{S})\cdot\vec{J} = g_j\,\vec{J}\cdot\vec{J}$$

$$\vec{L}\cdot\vec{L} + (1 + g_o)\vec{L}\cdot\vec{S} + g_o\vec{S}\cdot\vec{S} = g_j\; j(j+1)$$

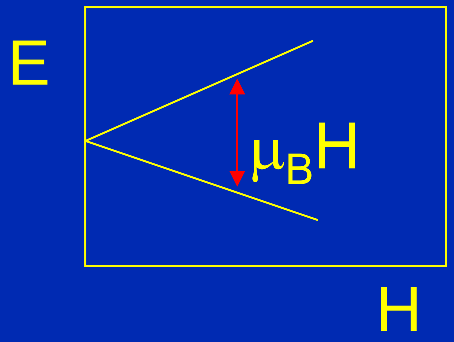
$$\vec{L}\cdot\vec{S} = (\vec{J}\cdot\vec{J} - \vec{L}\cdot\vec{L} - \vec{S}\cdot\vec{S})/2$$

$$g_j = \frac{(1+g_o)\,j(j+1) + (1-g_o)\,l(l+1) - (1-g_o)\,s(s+1)}{2j(j+1)}$$

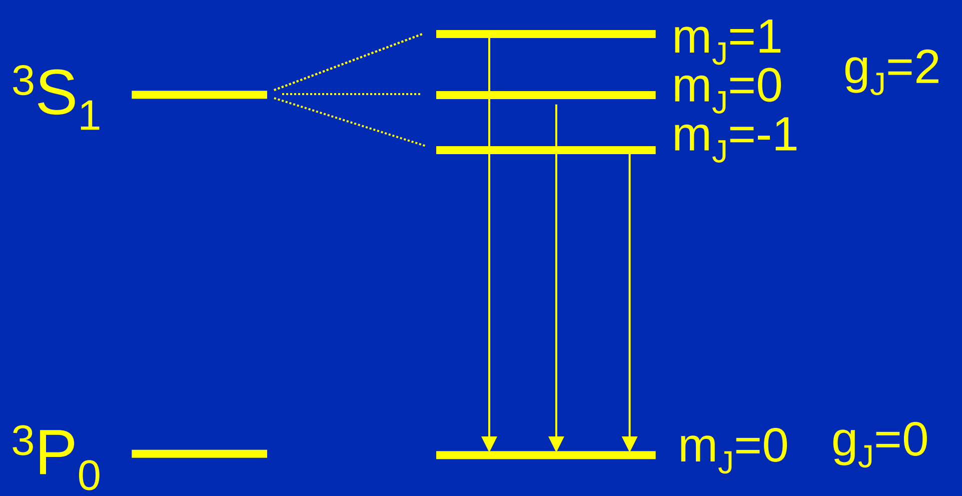
Spectroscopic splitting

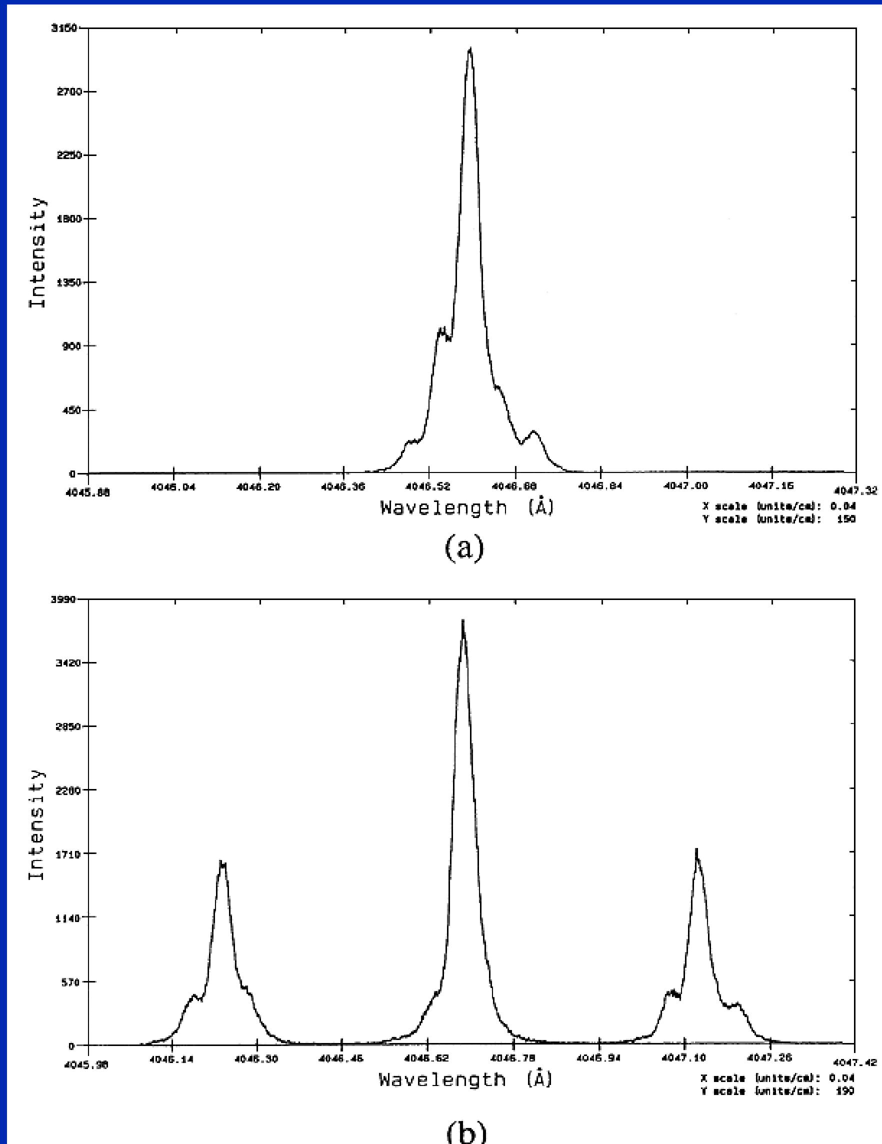
s shell, 1 electron:

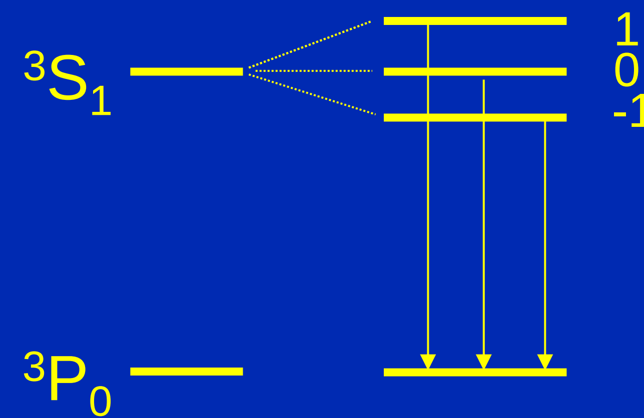
$^2S_{1/2}$ (S=1/2,L=0,J=1/2) => $g_j=g_o=2$



Mercury $^3S_1$ – $^3P_0$ transition ($6s^1 7s^1$ – $6s^1 6p^1$, G.S. $6s^2 5d^{10}$)







Experimental spectrum of the 4046.6 Å, 7 $^3S_1$ --> 6 $^3P_0$ transitions of atomic Hg with
(a) zero magnetic field
(b) a magnetic field B = 29.0 kG.

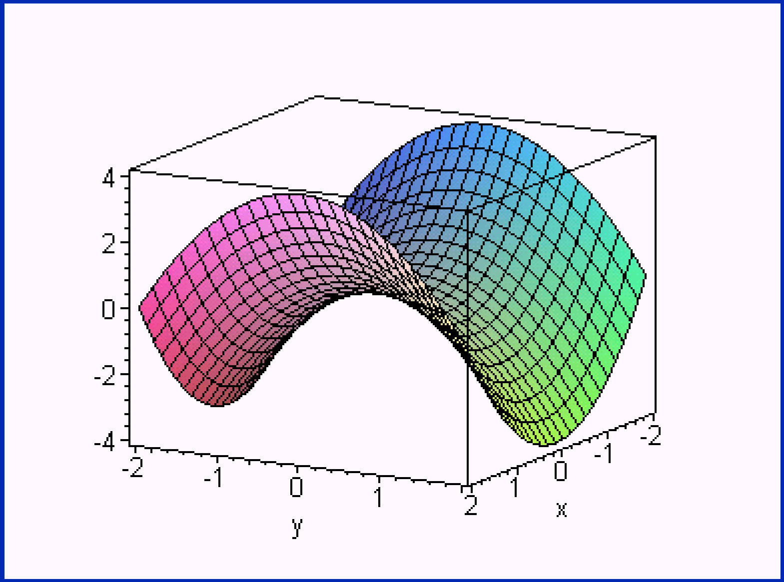
Crystal field splitting

Rare earth's: 4f shell's small ('inner' electrons)
Iron group: 3d shell's on the outside

=> decoupling of L and S, J no longer good QN
=> splitting of the 2L+1 orbital states
=> Quenching of the orbital angular momentum ($L_z \rightarrow 0$)

2D p states in a 2 fold potential

$V_{CF} = Q\cos(2\phi)$



p-states in 2D: $Y_{l,m}(\theta,\phi) = \cos(\theta)e^{im\phi} = e^{\pm i\phi}$

$p_{\pm 1,\sigma} = R(r)e^{\pm i\theta}\chi_\sigma \qquad \sigma = \uparrow \text{ or } \downarrow$

$$\langle p_{1,\sigma} | V_{CF} | p_{1,\sigma} \rangle = \int d\phi \, e^{-i\phi} \cdot Q \cos(2\phi) \cdot e^{i\phi} = 0$$

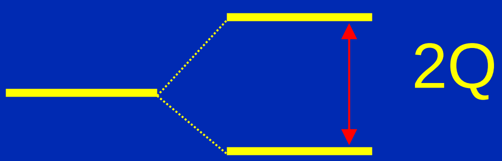
$$\langle p_{-1,\sigma} | V_{CF} | p_{-1,\sigma} \rangle = \int d\phi \, e^{i\phi} \cdot Q \cos(2\phi) \cdot e^{-i\phi} = 0$$

$$\langle p_{-1,\sigma} | V_{CF} | p_{1,\sigma} \rangle = \int d\phi \, e^{i\phi} \cdot Q \cos(2\phi) \cdot e^{i\phi} = Q$$

$$\langle p_{1,\sigma} | V_{CF} | p_{-1,\sigma} \rangle = \int d\phi \, e^{-i\phi} \cdot Q \cos(2\phi) \cdot e^{-i\phi} = Q$$

$$H = H_o + V_{CF} \qquad \begin{pmatrix} E_o & Q & 0 & 0 \\ Q & E_o & 0 & 0 \\ 0 & 0 & E_o & Q \\ 0 & 0 & Q & E_o \end{pmatrix} \cdot \begin{pmatrix} |p_{1,\uparrow}\rangle \\ |p_{-1,\uparrow}\rangle \\ |p_{1,\downarrow}\rangle \\ |p_{-1,\downarrow}\rangle \end{pmatrix} = E \cdot \begin{pmatrix} |p_{1,\uparrow}\rangle \\ |p_{-1,\uparrow}\rangle \\ |p_{1,\downarrow}\rangle \\ |p_{-1,\downarrow}\rangle \end{pmatrix}$$

$$E = E_0 \pm Q \qquad \begin{aligned} +: &\; |p_{1\sigma}\rangle + |p_{-1\sigma}\rangle \\ -: &\; |p_{1\sigma}\rangle - |p_{-1\sigma}\rangle \end{aligned}$$



With LS coupling

$$\left\langle \Psi \middle| \vec{L}\cdot\vec{S} \middle| \Psi \right\rangle = \{J(J+1) - L(L+1) - S(S+1)\}/2$$

$$\left\langle p_{1,\uparrow} \middle| \vec{L}\cdot\vec{S} \middle| p_{1,\uparrow} \right\rangle = (15/4 - 2 - 3/4)/2 = 1/2$$

$$\left\langle p_{-1,\downarrow} \middle| \vec{L}\cdot\vec{S} \middle| p_{-1,\downarrow} \right\rangle = 1/2$$

$$\left\langle p_{1,\downarrow} \middle| \vec{L}\cdot\vec{S} \middle| p_{1,\downarrow} \right\rangle = (3/4 - 2 - 3/4)/2 = -1$$

$$\left\langle p_{1,\downarrow} \middle| \vec{L}\cdot\vec{S} \middle| p_{1,\downarrow} \right\rangle = (3/4 - 2 - 3/4)/2 = -1$$

$$H = H_o + V_{CF} + \lambda \vec{L}\cdot\vec{S}$$

$$\begin{pmatrix} \lambda/2 & Q & 0 & 0 \\ Q & -\lambda & 0 & 0 \\ 0 & 0 & \lambda/2 & Q \\ 0 & 0 & Q & -\lambda \end{pmatrix} \cdot \begin{pmatrix} |p_{1,\uparrow}\rangle \\ |p_{-1,\uparrow}\rangle \\ |p_{1,\downarrow}\rangle \\ |p_{-1,\downarrow}\rangle \end{pmatrix} = E \cdot \begin{pmatrix} |p_{1,\uparrow}\rangle \\ |p_{-1,\uparrow}\rangle \\ |p_{1,\downarrow}\rangle \\ |p_{-1,\downarrow}\rangle \end{pmatrix}$$

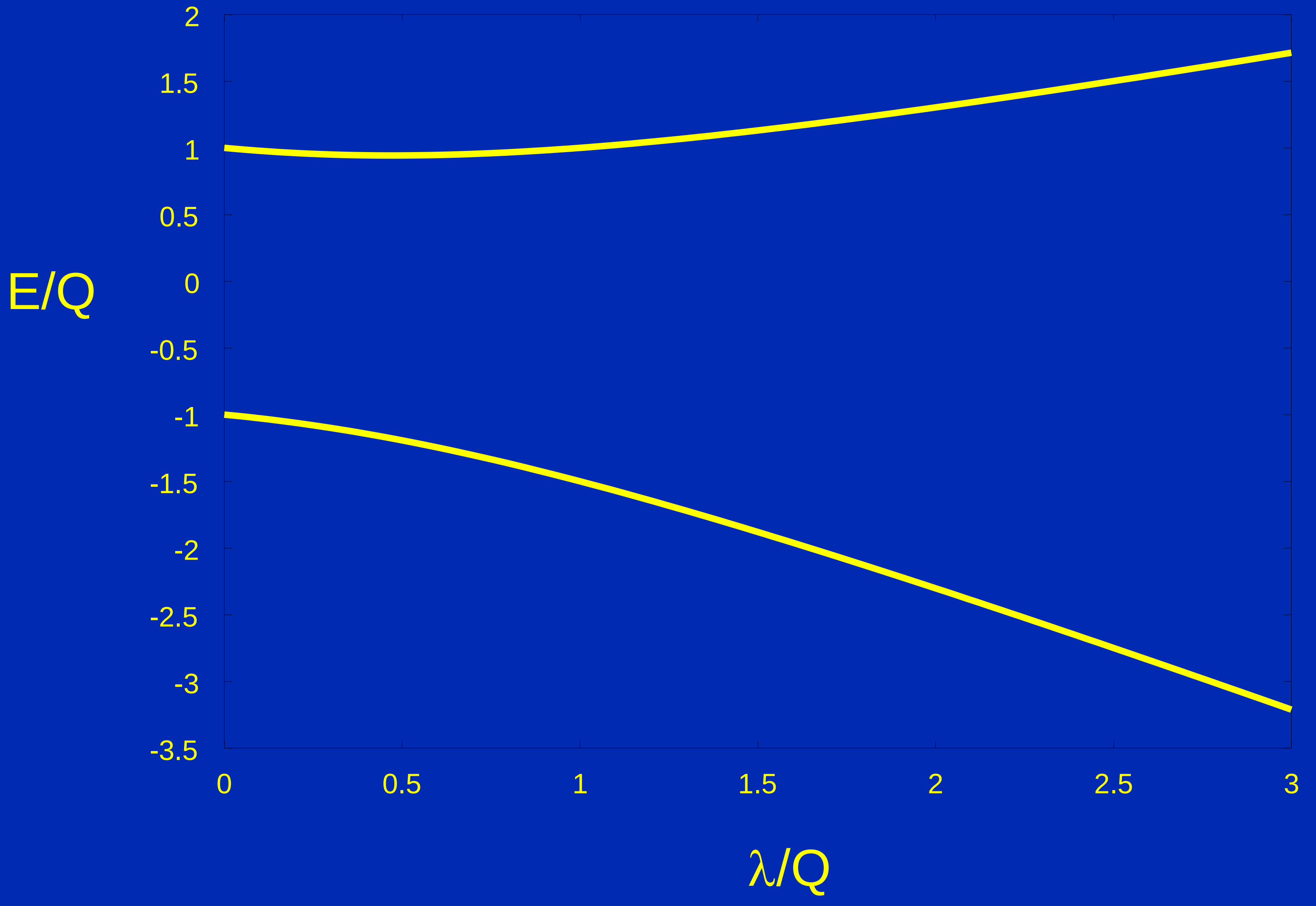
$$E_{\pm} = -\lambda/4 \pm \sqrt{9\lambda^2/16 + Q^2}$$

$$+:\ u|p_{1\sigma}\rangle + v|p_{-1\sigma}\rangle$$

$$-:\ v|p_{1\sigma}\rangle - u|p_{-1\sigma}\rangle$$

$$u^2 = \frac{1}{2} + \frac{3\lambda/8}{\sqrt{9\lambda^2/16 + Q^2}}$$

$$v^2 = \frac{1}{2} - \frac{3\lambda/8}{\sqrt{9\lambda^2/16 + Q^2}}$$


E/Q
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
-3
-3.5
0
0.5
1
1.5
2
2.5
3
λ/Q

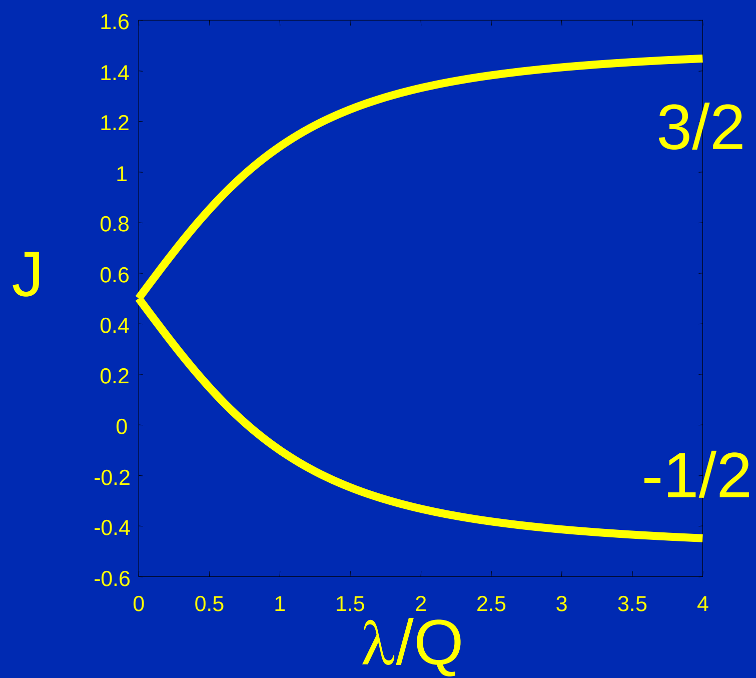
Angular momentum

$$\left\langle \phi_{+,\uparrow} \middle| J \middle| \phi_{+,\uparrow} \right\rangle = u^2 \cdot \left\langle p_{1,\uparrow} \middle| J \middle| p_{1,\uparrow} \right\rangle + v^2 \cdot \left\langle p_{-1,\uparrow} \middle| J \middle| p_{-1,\uparrow} \right\rangle$$

$$= \left\{ \frac{1}{2} + \frac{3\lambda/8}{\sqrt{9\lambda^2/16 + Q^2}} \right\} \cdot \frac{3}{2} + \left\{ \frac{1}{2} - \frac{3\lambda/8}{\sqrt{9\lambda^2/16 + Q^2}} \right\} \cdot \frac{-1}{2}$$

$$= \frac{1}{2} + \frac{3\lambda/4}{\sqrt{9\lambda^2/16 + Q^2}}$$

$$\left\langle \phi_{+,\downarrow} \middle| J \middle| \phi_{+,\downarrow} \right\rangle = \frac{1}{2} - \frac{3\lambda/4}{\sqrt{9\lambda^2/16 + Q^2}}$$



Magnetic moment

$$\langle p_{1,\uparrow}|m_z|p_{1,\uparrow}\rangle = (L_z + gS_z)\mu_B = (1+2\cdot\frac{1}{2})\mu_B = 2\mu_B$$

$$\langle p_{1,\downarrow}|m_z|p_{1,\downarrow}\rangle = (L_z - gS_z)\mu_B = (1-2\cdot\frac{1}{2})\mu_B = 0$$

$$\Downarrow$$

$$\langle \phi_{+,\uparrow}|m_z|\phi_{+,\uparrow}\rangle = u^2\cdot\langle p_{1,\uparrow}|m_z|p_{1,\uparrow}\rangle + v^2\cdot\langle p_{-1,\uparrow}|m_z|p_{-1,\uparrow}\rangle = \left\{1+\frac{3\lambda/4}{\sqrt{9\lambda^2/16+Q^2}}\right\}\cdot\mu_B$$

$$\langle \phi_{+,\downarrow}|m_z|\phi_{+,\downarrow}\rangle = \left\{1-\frac{3\lambda/4}{\sqrt{9\lambda^2/16+Q^2}}\right\}\cdot\mu_B$$