Magnetism

Paul H.M. van Loosdrecht

pvl@ph2.uni-koeln.de

Website:

www.loosdrecht.net

Optical Condensed Matter Physics

Environment: crystal field

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 Quantum number
=> splitting of the 2L+1 orbital states
=> Quenching of the orbital angular momentum ($L_z \rightarrow 0$)

=> High spin – Low spin transitions
=> Jahn-Teller distortions
=> Orbital excitations (orbitons)

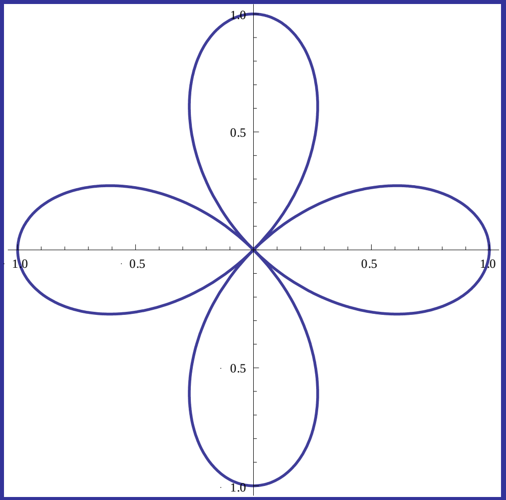
Anisotropy

Kramers degeneracy (local B-field probe)

Crystal field

Simple illustrative example:
2 dimensional p states in a two-fold crystal potential

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



p-states in 2D:

$$Y_{l,m}(\theta,\phi) = \cos(\theta)e^{im\phi} = e^{\pm i\phi}$$

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

2D p-states in a 2_z-potential

Only CF

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

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

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

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

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

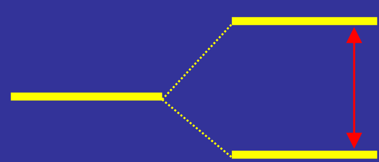
$H = H_0 + V_{CF}$

$$\begin{pmatrix} E_0 & Q & 0 & 0 \\ Q & E_0 & 0 & 0 \\ 0 & 0 & E_0 & Q \\ 0 & 0 & Q & E_0 \end{pmatrix} \cdot \begin{pmatrix} |p_{1,\uparrow}\rangle \\ |p_{-1,\uparrow}\rangle \\ |p_{1,\downarrow}\rangle \\ |p_{-1,\downarrow}\rangle \end{pmatrix} = E \cdot \begin{pmatrix} |p_{1,\uparrow}\rangle \\ |p_{-1,\uparrow}\rangle \\ |p_{1,\downarrow}\rangle \\ |p_{-1,\downarrow}\rangle \end{pmatrix}$$

$E = E_0 \pm Q$

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

$-: \; |p_{1\sigma}\rangle - |p_{-1\sigma}\rangle$



2Q

2D p-states in a 2_z-potential

With LS $\quad <\Psi\left|\vec{L}\cdot\vec{S}\right|\Psi> = \frac{\{J(J+1)-L(L+1)-S(S+1)\}}{2}$

$$<\mathrm{p}_{1,\uparrow}|\vec{L}\cdot\vec{S}|\mathrm{p}_{1,\uparrow}> = \frac{\frac{15}{4}-2-\frac{3}{4}}{2} = \frac{1}{2}$$

$$<\mathrm{p}_{-1,\uparrow}|\vec{L}\cdot\vec{S}|\mathrm{p}_{-1,\uparrow}> = \frac{\frac{3}{4}-2-\frac{3}{4}}{2} = -1$$

$$<\mathrm{p}_{1,\downarrow}|\vec{L}\cdot\vec{S}|\mathrm{p}_{1,\downarrow}> = -1$$

$$<\mathrm{p}_{-1,\downarrow}|\vec{L}\cdot\vec{S}|\mathrm{p}_{-1,\downarrow}> = \frac{1}{2}$$

$$\mathrm{H} = \mathrm{H}_0 + \mathrm{V}_{\mathrm{CF}} + \lambda\vec{L}\cdot\vec{S}$$

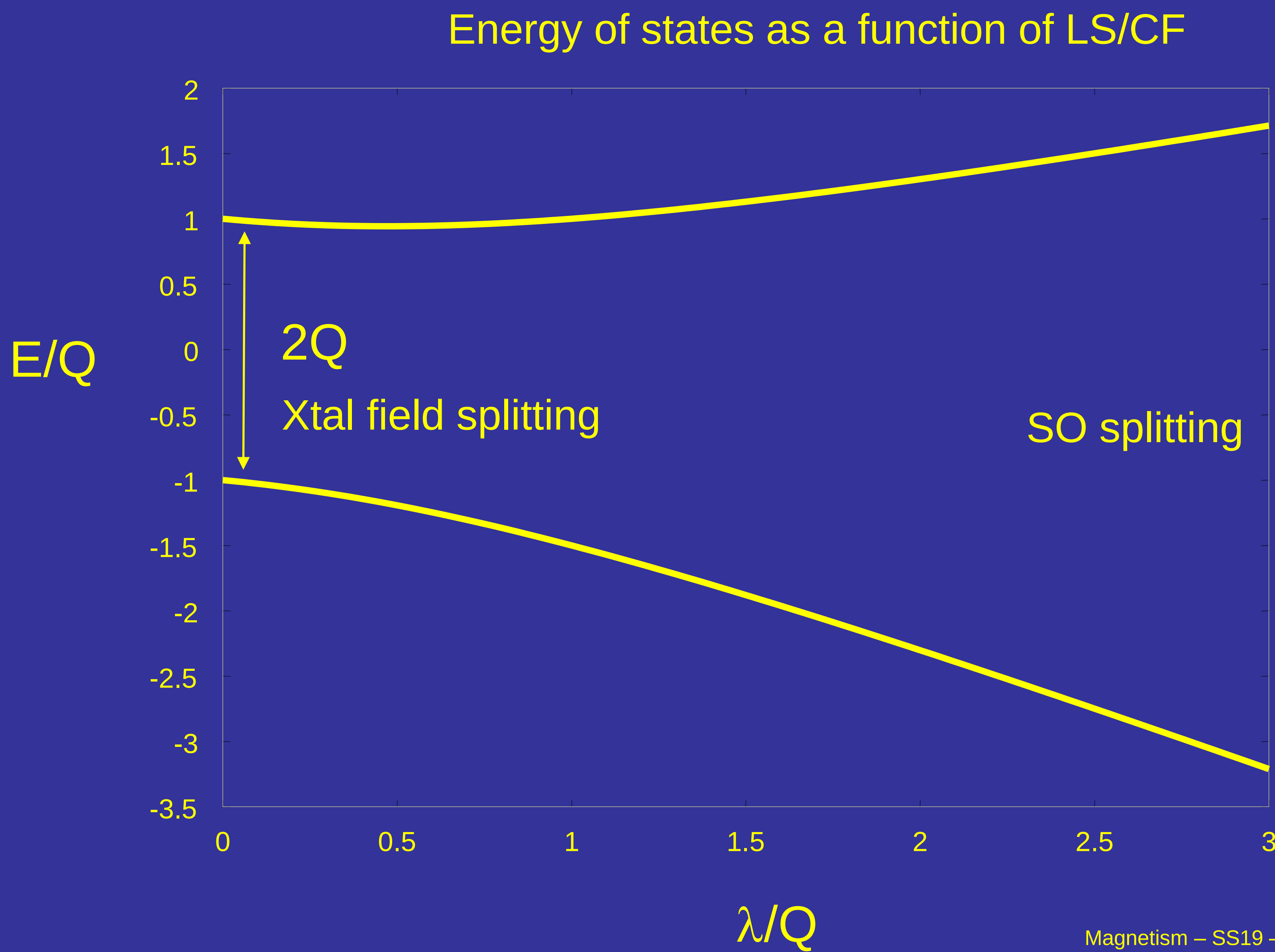
$$\begin{pmatrix} \lambda/2 & Q & 0 & 0 \\ Q & -\lambda & 0 & 0 \\ 0 & 0 & \lambda/2 & Q \\ 0 & 0 & Q & -\lambda \end{pmatrix} \cdot \begin{pmatrix} |p_{1\uparrow}\rangle \\ |p_{-1\uparrow}\rangle \\ |p_{-1\downarrow}\rangle \\ |p_{1\downarrow}\rangle \end{pmatrix} = E \cdot \begin{pmatrix} |p_{1\uparrow}\rangle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

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

$$+:\ u\left|p_{1\sigma}\right\rangle + v\left|p_{-1\sigma}\right\rangle \qquad u^2 = \frac{1}{2} + \frac{3\lambda/8}{\sqrt{9\lambda^2/16+Q^2}}$$

$$-:\ v\left|p_{1\sigma}\right\rangle - u\left|p_{-1\sigma}\right\rangle \qquad v^2 = \frac{1}{2} - \frac{3\lambda/8}{\sqrt{9\lambda^2/16+Q^2}}$$

2D p-states in a 2_z-potential



2D p-states in a 2_z-potential

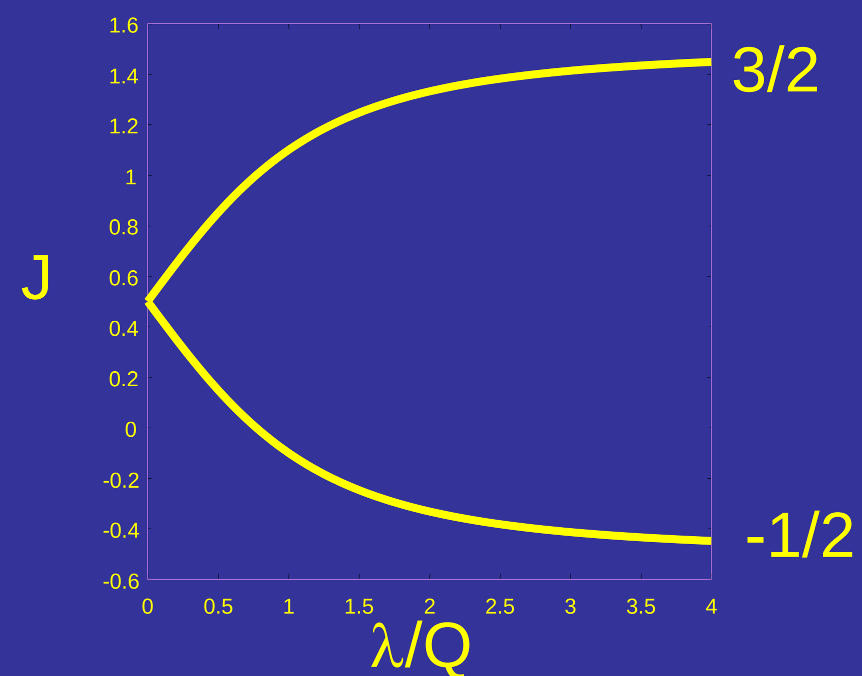
Angular moment of the states as a function of LS/CF

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

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

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

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



For strong crystal fields:
orbital moment completely quenched

2D p-states in a 2_z-potential

Magnetic moment of the states as a function of LS/CF

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

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

$$\Downarrow$$

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

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