INITIAL STATES

→ zeige Begleit-Folien vor den Rechnungen...

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$$\boxed{2p_{1/2} \quad , \quad j = \tfrac{1}{2}}$$

$$\left|\tfrac{1}{2},\tfrac{1}{2}\right> = \frac{1}{\sqrt{3}}\Big(-\underbrace{|1,0>}_{l,\,m_l} \cdot \underbrace{|\tfrac{1}{2},\tfrac{1}{2}>}_{s,\,m_s} + \sqrt{2}\,\underbrace{|1,1>}_{l,\,m_l} \cdot \underbrace{|\tfrac{1}{2},-\tfrac{1}{2}>}_{s,\,m_s} \Big)$$

$$\left|\tfrac{1}{2},-\tfrac{1}{2}\right> = \frac{1}{\sqrt{3}}\Big(-\sqrt{2}\,|1,-1> \cdot |\tfrac{1}{2},\tfrac{1}{2}> + |1,0>\,|\tfrac{1}{2},-\tfrac{1}{2}> \Big)$$

sei spin ↑ sei spin ↓

$$\boxed{2p_{3/2} \quad , \quad j = \tfrac{3}{2}}$$

$$\left|\tfrac{3}{2},\tfrac{3}{2}\right> = |1,1> \cdot |\tfrac{1}{2},\overset{\uparrow}{\tfrac{1}{2}}>$$

$$\left|\tfrac{3}{2},\tfrac{1}{2}\right> = \frac{1}{\sqrt{3}}\Big(\sqrt{2}\,|1,0> \cdot |\tfrac{1}{2},\overset{\uparrow}{\tfrac{1}{2}}> + |1,1> \cdot |\tfrac{1}{2},\overset{\downarrow}{-\tfrac{1}{2}}> \Big)$$

$$\left|\tfrac{3}{2},-\tfrac{1}{2}\right> = \frac{1}{\sqrt{3}}\Big(|1,-1> \cdot |\tfrac{1}{2},\overset{\uparrow}{\tfrac{1}{2}}> + \sqrt{2}\,|1,0>\,|\tfrac{1}{2},\overset{\downarrow}{-\tfrac{1}{2}}> \Big)$$

$$\left|\tfrac{3}{2},-\tfrac{3}{2}\right> = |1,-1> \cdot |\tfrac{1}{2},\overset{\downarrow}{-\tfrac{1}{2}}>$$

FINAL STATES

d-Orbitale in atomarer Basis $\Rightarrow l = 2$

$m_l = -2, -1, 0, 1, 2$

$$\Rightarrow |f> = \{ |2,-2>, \ |2,-1>, \ |2,0>, \ |2,1>, \ |2,2> \}$$

a) L_2 - Kante : $2p_{1/2} \longrightarrow 3d$

Dipolnäherung, d.h. $\Delta m_s = 0$, Spin ist bei Übergängen erhalten! D.h. Übergänge werden jeweils nur aus den Zuständen mit passendem Spin getriggert $\vec{M} \parallel \vec{S}$

- RCP: $\Delta m_l = +1$, $\vec{M} = \uparrow$, $\Delta m_s = 0$

$$I^{\uparrow} = \sum_{i,f} \left|\langle f | C^1_{\Delta m} | i \rangle\right|^2 =$$

$$= \frac{1}{3}\left|\langle 2,1|^{\uparrow} C^1_{+1} |1,0\rangle^{\uparrow}\right|^2 + \frac{2}{3}\left|\langle 2,0|^{\uparrow} C^1_{+1} |1,-1\rangle^{\uparrow}\right|^2$$

$$= \frac{1}{3} \cdot \frac{(1+0+2)(1+0+1)}{2(2\cdot1+3)(2\cdot1+1)} + \frac{2}{3}\,\frac{(1-1+2)(1-1+1)}{2(2\cdot1+3)(2\cdot1+1)}$$

$$= \frac{1}{3} \cdot \frac{6}{30} + \frac{2}{3} \cdot \frac{2}{30} = \underline{\underline{\frac{1}{9}}}$$

$\Delta m_l = +1$, $\vec{M} = \downarrow$, $\Delta m_s = 0$

$$I^{\downarrow} = \sum_{i,f} \left|\langle f | C^1_{\Delta m} | i \rangle\right|^2 =$$

$$= \frac{2}{3}\left|\langle 2,2|^{\downarrow} C^1_{+1} |1,1\rangle^{\downarrow}\right|^2 + \frac{1}{3}\left|\langle 2,1|^{\downarrow} C^1_{+1} |1,0\rangle^{\downarrow}\right|^2$$

$$= \frac{2}{3}\,\frac{(1+1+2)(1+1+1)}{2(2\cdot1+3)(2\cdot1+1)} + \frac{1}{3}\,\frac{(1+0+2)(1+0+1)}{2(2\cdot1+3)(2\cdot1+1)}$$

$$= \frac{2}{3} \cdot \frac{12}{30} + \frac{1}{3} \cdot \frac{6}{30} = \underline{\underline{\frac{1}{3}}}$$

• **LCP:** $\Delta m_l = -1$, $\vec{M} = \uparrow$, $\Delta m_s = 0$

$$I^{\uparrow} = \sum_{i,f} \left| \langle f | C^1_{\Delta m} | i \rangle \right|^2 =$$

$$= \frac{1}{3} \left| \langle 2,-1|^{\uparrow} C_{-1} |1,0\rangle^{\uparrow} \right|^2 + \frac{2}{3} \left| \langle 2,-2|^{\uparrow} C^1_{-1} |1,-1\rangle^{\uparrow} \right|^2$$

$$= \frac{1}{3} \frac{(1-0+2)(1-0+1)}{2(2\cdot1+3)(2\cdot1+1)} + \frac{2}{3} \frac{(1+1+2)(1+1+1)}{2(2\cdot1+3)(2\cdot1+1)}$$

$$= \frac{1}{3} \cdot \frac{6}{30} + \frac{2}{3} \cdot \frac{12}{30} = \underline{\underline{\frac{1}{3}}}$$

$\Delta m_l = -1$, $\vec{M} = \downarrow$, $\Delta m_s = 0$

$$I^{\downarrow} = \sum_{i,f} \left| \langle f | C^1_{-1} | i \rangle \right|^2 =$$

$$= \frac{2}{3} \left| \langle 2,0|^{\downarrow} C^1_{-1} |1,1\rangle^{\downarrow} \right|^2 + \frac{1}{3} \left| \langle 2,-1|^{\downarrow} C^1_{-1} |1,0\rangle^{\downarrow} \right|^2$$

$$= \frac{2}{3} \frac{(1-1+2)(1-1+1)}{2(2\cdot1+3)(2\cdot1+1)} + \frac{1}{3} \cdot \frac{(1-0+2)(1-0+1)}{2\cdot(2\cdot1+3)(2\cdot1+1)}$$

$$= \frac{2}{3} \cdot \frac{2}{30} + \frac{1}{3} \cdot \frac{6}{30} = \underline{\underline{\frac{1}{9}}}$$

b) L_2 - Kante:

$$\bullet \quad \frac{I^{\uparrow}_{RCP}}{I^{\uparrow}_{RCP} + I^{\downarrow}_{RCP}} = \frac{1/9}{1/9 + 1/3} = 1/4 \mathrel{\hat{=}} \underline{\underline{25\,\%}}$$

$$\frac{I^{\downarrow}_{RCP}}{I^{\downarrow}_{RCP} + I^{\uparrow}_{RCP}} = \frac{1/3}{1/3 + 1/9} = 3/4 \mathrel{\hat{=}} \underline{\underline{75\,\%}}$$

$$\frac{I^{\uparrow}_{LCP}}{I^{\uparrow}_{LCP} + I^{\downarrow}_{LCP}} = \frac{1/3}{1/3 + 1/9} = 3/4 \mathrel{\hat{=}} \underline{\underline{75\,\%}}$$

$$\frac{I^{\downarrow}_{LCP}}{I^{\downarrow}_{LCP} + I^{\uparrow}_{LCP}} = \frac{1/9}{1/3 + 1/9} = 1/4 \mathrel{\hat{=}} \underline{\underline{25\,\%}}$$

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L_3 - Kante : $\quad 2p_{3/2} \longrightarrow 3d$

RCP: $\Delta m_\ell = +1$, $\vec{M} = \uparrow$, $\Delta m_s = 0$

$$I^\uparrow = \sum_{i,f} |\langle f | C_{+1}^1 | i \rangle|^2 =$$

$$= |\langle 2,2|^\uparrow C_{+1}^1 | 1,1\rangle^\uparrow|^2 + \frac{2}{3} |\langle 2,1|^\uparrow C_{+1}^1 | 1,0\rangle^\uparrow|^2$$

$$+ \frac{1}{3} |\langle 2,0|^\uparrow C_{+1}^1 | 1,-1\rangle^\uparrow|^2$$

$$= \frac{12}{30} + \frac{6}{30} \cdot \frac{2}{3} + \frac{2}{30} \cdot \frac{1}{3} = \underline{\underline{\frac{5}{9}}}$$

$\Delta m_\ell = +1$, $\vec{M} = \downarrow$, $\Delta m_s = 0$

$$I^\downarrow = \sum_{i,f} |\langle f | C_{+1} | i \rangle|^2 =$$

$$= \frac{1}{3} |\langle 2,2|^\downarrow C_{+1}^1 | 1,1\rangle^\downarrow|^2 + \frac{2}{3} |\langle 2,1|^\downarrow C_{+1}^1 | 1,0\rangle|^2$$

$$+ |\langle 2,0|^\downarrow C_{+1}^1 | 1,-1\rangle|^2$$

$$= \frac{1}{3} \cdot \frac{12}{30} + \frac{2}{3} \cdot \frac{6}{30} + \frac{2}{30} = \underline{\underline{1/3}}$$

LCP: $\Delta m_\ell = -1, \quad \vec{M} = \uparrow, \quad \Delta m_s = 0$

$$I^\uparrow = \sum_{i,f} \left| \langle f | C_{-1} | i \rangle \right|^2 =$$

$$= \left| \langle 2,0|^\uparrow C^1_{-1} | 1,1 \rangle^\uparrow \right|^2 + \frac{2}{3} \left| \langle 2,-1|^\uparrow C^1_{-1} | 1,0 \rangle \right|^2$$

$$+ \frac{1}{3} \left| \langle 2,-2|^\uparrow C^1_{-1} | 1,-1 \rangle \right|^2$$

$$= \frac{2}{30} + \frac{2}{3} \cdot \frac{6}{30} + \frac{1}{3} \cdot \frac{12}{30} = \underline{\underline{\frac{1}{3}}}$$

$\Delta m_\ell = -1, \quad \vec{M} = \downarrow, \quad \Delta m_s = 0$

$$I^\downarrow = \sum_{i,f} \left| \langle f | C_{-1} | i \rangle \right|^2$$

$$= \frac{1}{3} \left| \langle 2,0|^\downarrow C_{-1} | 1,1 \rangle^\downarrow \right|^2 + \frac{2}{3} \left| \langle 2,-1|^\downarrow C_{-1} | 1,0 \rangle^\downarrow \right|^2$$

$$+ \left| \langle 2,-2|^\downarrow C_{-1} | 1,-1 \rangle \right|^2$$

$$= \frac{1}{3} \cdot \frac{2}{30} + \frac{2}{3} \cdot \frac{6}{30} + \frac{12}{30} = \underline{\underline{\frac{5}{9}}}$$

b) L_3 - Kante:

$$\frac{I_{RCP}^{\uparrow}}{I_{RCP}^{\uparrow} + I_{RCP}^{\downarrow}} = \frac{5/9}{5/9 + 1/3} = \frac{5}{8} \mathrel{\hat{=}} \underline{\underline{62{,}5\,\%}}$$

$$\frac{I_{RCP}^{\downarrow}}{I_{RCP}^{\downarrow} + I_{RCP}^{\uparrow}} = \frac{1/3}{1/3 + 5/9} = \frac{3}{8} \mathrel{\hat{=}} \underline{\underline{37{,}5\,\%}}$$

$$\frac{I_{LCP}^{\uparrow}}{I_{LCP}^{\uparrow} + I_{LCP}^{\downarrow}} = \frac{1/3}{1/3 + 5/9} = \frac{3}{8} \mathrel{\hat{=}} \underline{\underline{37{,}5\,\%}}$$

$$\frac{I_{LCP}^{\downarrow}}{I_{LCP}^{\downarrow} + I_{RCP}^{\uparrow}} = \frac{5/9}{5/9 + 1/3} = \frac{5}{8} \mathrel{\hat{=}} \underline{\underline{62{,}5\,\%}}$$

$$I^{\uparrow\downarrow\,(RCP\ M\downarrow)} = \frac{1}{3}\cdot\frac{1}{5} + \frac{2}{3}\cdot\frac{2}{5} = 1/3$$

Notation:

$I^{\vec{L}_{1},\,\vec{M}}$

b)

	$I^{\uparrow\uparrow}$	$I^{\uparrow\downarrow}$	$I^{\downarrow\uparrow}$	$I^{\downarrow\downarrow}$
L_2	$1/9$	$1/3$	$1/3$	$1/9$
L_3	$5/9$	$1/3$	$1/3$	$5/9$

L_2 total : $I^{\uparrow\uparrow} + I^{\downarrow\uparrow} = 1/9 + 1/3 = \frac{4}{9}$

L_3 total : $I^{\uparrow\uparrow} + I^{\downarrow\uparrow} = 1/3 + 5/9 = \frac{8}{9}$

$$\frac{I_{L_3}}{I_{L_2}} = 2:1 \quad ✓$$

c) XMCD

$L_2: \Delta I = I^{\uparrow\uparrow} - I^{\downarrow\uparrow} = 1/1 - \frac{1}{3} = \frac{2}{3}$

$L_3: \Delta I = I^{\uparrow\uparrow} - I^{\downarrow\uparrow} = \frac{1}{1} - \frac{5}{3} = -\frac{2}{3}$

$$\frac{\Delta I_{L_3}}{\Delta I_{L_2}} = -1 : 1$$