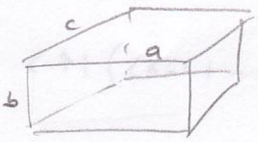
20.3. 2012 / prepis FKS vaje

VPLIV SKLOPITVE SPIN – TIR NA GIROMAGNETNO RAZMERJE – SPEKTROSKOPSKI FAKTOR

- obravnavamo p - orbitale v ortorombskem kristalu, računamo razcep v kristalnem polju

$$p_x = x\, f(r)$$
$$p_y = y\, f(r)$$
$$p_z = z\, f(r)$$



ortorombski kristal

Dodaten potencial, ki ga čuti atom : $V(r) = Ax^2 + By^2 - (A+B)z^2$

$\vec{L}^2, L_z \qquad l = 1 : \quad |11\rangle, \; |10\rangle, \; |1-1\rangle \;\Rightarrow\; |p_z\rangle = |10\rangle$

$$|p_x\rangle = \frac{|11\rangle + |1-1\rangle}{\sqrt{2}}$$

$$|p_y\rangle = \frac{|11\rangle - |1-1\rangle}{\sqrt{2}\, i}$$

$$H = H_{at} + V(\vec{r})$$

$\hookrightarrow \langle p_x | V(\vec{r}) | p_y \rangle = 0 \qquad (V(\vec{r})$ jinoda $, \; p_x \propto x \;, \; p_y \propto y)$

Neničelni so samo diagonalni elementi :

$$\langle p_x | V(\vec{r}) | p_x \rangle = \iiint x^2 f^2(\vec{r}) \left(Ax^2 + By^2 - (A+B)z^2\right) d\vec{r} = A(I_1 - I_2)$$

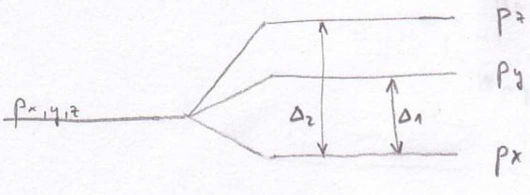
vpeljemo : $I_1 = \int f^2(\vec{r})\, x^4 \, dx\, dy\, dz$

$I_2 = \int f^2(\vec{r})\, x^2 y^2 \, dx\, dy\, dz$

in ekvivalentno :

$$\langle p_y | V(\vec{r}) | p_y \rangle = B(I_1 - I_2)$$
$$\langle p_z | V(\vec{r}) | p_z \rangle = (A+B)(I_2 - I_1)$$

V izoliranem atomu imajo $p_{x,y,z}$ enake energije. V ortorombskem kristalu smo izračunali razcep. Predpostavimo, da so A, B, I_1 in I_2 taki, da ima p_x najnižjo energijo !



$\Rightarrow$ efekt kristalnega polja

$\Rightarrow$ vsaka je 2x degenerirana zaradi spina

Sklopitev spin - tir : $H = H_{at} + V(\vec{r}) + \lambda \vec{L}\cdot\vec{S}$ Zanima nas, kaj se zgodi z energijo p_x

Računali bomo v najnižjem redu perturbacije za $|p_x \uparrow\rangle$

$$|n\rangle = |n\rangle^0 + \sum_{m \neq n} \frac{{}^0\langle m | \lambda \vec{L}\cdot\vec{S} | n\rangle^0}{E_n^0 - E_m^0} |m\rangle^0$$

za začetek: i.) $\vec{L}\cdot\vec{S} = L_x S_x + L_y S_y + L_z S_z \quad \left(= \frac{1}{2}(L_+ S_- + L_- S_+) + L_z S_z \right)$

$$L_x = \frac{1}{2}(L_+ + L_-) \qquad S_x = \frac{1}{2}(S_+ + S_-) \qquad L_y = \frac{1}{2i}(L_+ - L_-) \qquad S_y = \frac{1}{2i}(S_+ - S_-)$$

ii) $L_+|1\,-1\rangle = \sqrt{2}\hbar|1\,0\rangle$ $\qquad L_z|lm\rangle = \hbar m|lm\rangle$

$S_-|\uparrow\rangle = \hbar|\downarrow\rangle$

$$\vec{L}\cdot\vec{S}|p_x\uparrow\rangle = \vec{L}\vec{S}\,\frac{1}{\sqrt{2}}(|1\,1\rangle + |1\,-1\rangle) = \frac{1}{2}\frac{1}{\sqrt{2}}(L_+S_- + L_-S_+)(|1\,1\rangle+|1\,-1\rangle)|\uparrow\rangle + \frac{L_zS_z}{\sqrt{2}}(|1\,1\rangle+|1\,-1\rangle)|\uparrow\rangle =$$

$$= \frac{1}{2}\hbar^2|1\,0\rangle|\downarrow\rangle + \frac{\hbar^2}{2\sqrt{2}}(|1\,1\rangle - |1\,-1\rangle)|\uparrow\rangle = \frac{\hbar^2}{2}(|p_z\rangle|\downarrow\rangle + i|p_y\rangle|\uparrow\rangle)$$

$$|p_x\uparrow\rangle' = |p_x\uparrow\rangle + \frac{\langle p_y\uparrow|\lambda\vec{L}\vec{S}|p_x\uparrow\rangle}{-\Delta_1}|p_y\uparrow\rangle + \frac{\langle p_z\downarrow|\lambda\vec{L}\vec{S}|p_x\uparrow\rangle}{-\Delta_2}|p_z\downarrow\rangle =$$

$$= |p_x\uparrow\rangle - \frac{i\lambda\hbar^2}{2\Delta_1}|p_y\uparrow\rangle - \frac{\lambda\hbar^2}{2\Delta_2}|p_z\downarrow\rangle$$

Ekvivalentno: $|p_x\downarrow\rangle' = |p_x\downarrow\rangle + \frac{i\lambda\hbar^2}{2\Delta_1}|p_y\downarrow\rangle - \frac{\lambda\hbar^2}{2\Delta_2}|p_z\uparrow\rangle$

Damo v magnetno polje v z smeri: $\vec{B} = B_0\hat{e}_z$

$$-\vec{\mu}\vec{B} = \frac{\mu_B}{\hbar}(\vec{L} + 2\vec{S})\vec{B} = \frac{\mu_B}{\hbar}(L_z + 2S_z)B_0$$

$$'\langle p_x\uparrow|\frac{\mu_B}{\hbar}(L_z+2S_z)B_0|p_x\uparrow\rangle' = \frac{\mu_B B_0}{\hbar}\Big[\,'\langle p_x\uparrow|L_z|p_x\uparrow\rangle' + 2\underbrace{'\langle p_x\uparrow|S_z|p_x\uparrow\rangle'}_{=\frac{\hbar}{2}}\Big]$$

$$L_z|p_x\rangle = -i\hbar\frac{\partial}{\partial\varphi}x f(r) = -i\hbar\frac{\partial}{\partial\varphi}r\sin\vartheta\cos\varphi f(r) = i\hbar r\sin\vartheta\sin\varphi f(r) = i\hbar y f(r)$$

$$L_z|p_x\rangle = i\hbar|p_y\rangle$$

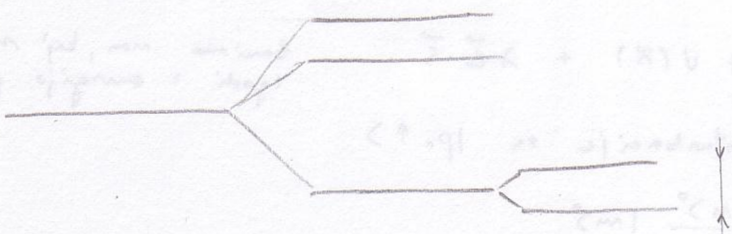
in $L_z|p_y\rangle = -i\hbar|p_x\rangle$, $\quad L_z|p_z\rangle = 0$

$$L_z|p_x\uparrow\rangle' = i\hbar|p_y\uparrow\rangle - \frac{\lambda\hbar^3}{2\Delta_1}|p_x\uparrow\rangle$$

$$\Rightarrow\ '\langle p_x\uparrow|L_z|p_x\uparrow\rangle' = -\frac{\lambda\hbar^3}{2\Delta_1} - \frac{\lambda\hbar^3}{2\Delta_1} = \frac{\lambda\hbar^3}{\Delta_1}$$

Vstavimo nazaj: $\Delta E_{p_x\uparrow} = B_0\mu_B\left(1 - \frac{\lambda\hbar^2}{\Delta_1}\right)$

analogno $\rightarrow$ $\Delta E_{p_x\downarrow} = -\Delta E_{p_x\uparrow}$



$\Delta E = 2\mu_0 B_0\left(1 - \frac{\lambda\hbar^2}{\Delta_1}\right)$

$$\boxed{g = 2\left(1 - \frac{\lambda\hbar^2}{\Delta_1}\right)}$$

spektroskopski faktor (popravek zaradi λ)