

# Problem Sheet 11

## Ex. 11.1: Internal magnetic fields

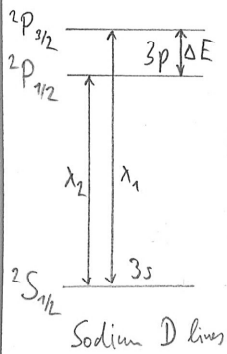
a)  $\lambda_1 = 588,995 \text{ nm}$   
 $\lambda_2 = 589,592 \text{ nm}$

$$E = h \cdot \nu = \frac{hc}{\lambda} \rightarrow \Delta E_\lambda = -\frac{hc}{\lambda^2} \Delta \lambda$$

$$= 2,13 \text{ meV}$$

$$\Delta \lambda = \lambda_1 - \lambda_2 = -0,597 \text{ nm}$$

$$\bar{\lambda} = \frac{\lambda_1 + \lambda_2}{2} = 589,294 \text{ nm}$$



$$E_B = -\vec{\mu} \cdot \vec{B} = 2 \cdot \mu_B \cdot (\pm 1/2) \cdot |\vec{B}|$$

with  $\vec{\mu}_s = -g_s \mu_B \frac{\vec{S}}{\hbar}$

$g_s \approx 2$   
 $\vec{S} \rightarrow S_z = \pm 1/2 \hbar$   
 $(\vec{B} \text{ field dictates quantization axis})$

$$\Delta E_B = 2 \cdot E_B = 2 \mu_B \cdot B = \Delta E_\lambda$$

$$B = \frac{\Delta E_\lambda}{2 \mu_B} = 18,4 \text{ T}$$

$$\mu_B = \frac{e}{2m_e} \hbar = 9,274 \cdot 10^{-24} \frac{\text{J}}{\text{T}}$$

b) instead of Na ( $Z=11$ )  $\rightarrow$  K ( $Z=19$ ): repeat a) but with  
 (Sodium) (Potassium)

$$\lambda_1 = 766,41 \text{ nm}$$

$$\lambda_2 = 769,90 \text{ nm}$$

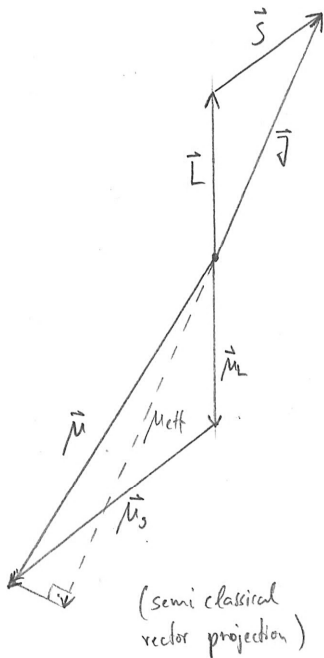
$$\Delta \lambda = \lambda_1 - \lambda_2 = -3,49 \text{ nm}$$

$$\bar{\lambda} = \frac{\lambda_1 + \lambda_2}{2} = 768,155 \text{ nm}$$

$$\Delta E_\lambda = -\frac{hc}{\lambda^2} \Delta \lambda = 7,33 \text{ meV} \quad B = \frac{\Delta E_\lambda}{2 \mu_B} = 63,3 \text{ T}$$

## Ex. 11.2: The Landé factor

a)



$$\vec{\mu} = -g_J \mu_B \frac{\vec{J}}{\hbar} \quad \text{with} \quad g_J = \frac{3}{2} + \frac{s(s+1) - l(l+1)}{2j(j+1)} \quad \begin{cases} s=0 \rightarrow g_J = 1 \\ l=0 \rightarrow g_J = 2 \end{cases}$$

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

$$b) \quad \mu_{\text{eff}} = \frac{|\vec{\mu} \cdot \vec{J}|}{|\vec{J}|} = -\mu_B \frac{(\vec{L} + 2\vec{S}) \cdot \vec{J}}{\hbar |\vec{J}|} = -\mu_B \frac{\vec{J} \cdot \vec{J} + \vec{S} \cdot \vec{J}}{\hbar |\vec{J}|} = -\mu_B \sqrt{j(j+1)} g_J$$

$$g_J = \frac{|\vec{J}|^2 + \frac{1}{2}(|\vec{L}|^2 + |\vec{S}|^2 - |\vec{L}|^2)}{\hbar |\vec{J}|} = \frac{|\vec{J}|^2}{\hbar |\vec{J}|} g_J$$

$$g_J = \frac{3}{2} + \frac{\frac{1}{2}(|\vec{S}|^2 - |\vec{L}|^2)}{2|\vec{J}|^2}$$

$$= \frac{3}{2} + \frac{s(s+1) - l(l+1)}{2j(j+1)}$$

\*  $\vec{L} = \vec{J} - \vec{S} \quad |\vec{L}|^2$

$$|\vec{L}|^2 = \vec{J} \cdot \vec{J} - 2 \cdot \vec{J} \cdot \vec{S} + \vec{S} \cdot \vec{S}$$

$$\vec{J} \cdot \vec{S} = \frac{1}{2}(|\vec{J}|^2 + |\vec{S}|^2 - |\vec{L}|^2)$$

$$|\vec{J}|^2 = j(j+1) \hbar^2$$

$$|\vec{L}|^2 = l(l+1) \hbar^2$$

$$|\vec{S}|^2 = s(s+1) \hbar^2$$

Ex. 11.3: Hexagonal lattice

$$\vec{a}_1 = \begin{pmatrix} \sqrt{3}/2 \\ 1/2 \\ 0 \end{pmatrix} a \quad \vec{a}_2 = \begin{pmatrix} -\sqrt{3}/2 \\ 1/2 \\ 0 \end{pmatrix} a \quad \vec{a}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} c$$

a) Volume of unit cell given by:  $V_{\text{cell}} = \vec{a}_1 (\vec{a}_2 \times \vec{a}_3)$  "Spatprodukt"

$$V_{\text{cell}} = \begin{pmatrix} \sqrt{3}/2 \\ 1/2 \\ 0 \end{pmatrix} \cdot \left[ \begin{pmatrix} -\sqrt{3}/2 \\ 1/2 \\ 0 \end{pmatrix} \times \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right] a^2 c$$

$$= \begin{pmatrix} \sqrt{3}/2 \\ 1/2 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 1/2 & -0 \\ 0 & -(-\sqrt{3}/2) \\ 0 & 0 \end{pmatrix} a^2 c = \left( \frac{\sqrt{3}}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} \right) a^2 c = \underline{\underline{\frac{\sqrt{3}}{2} a^2 c}}$$

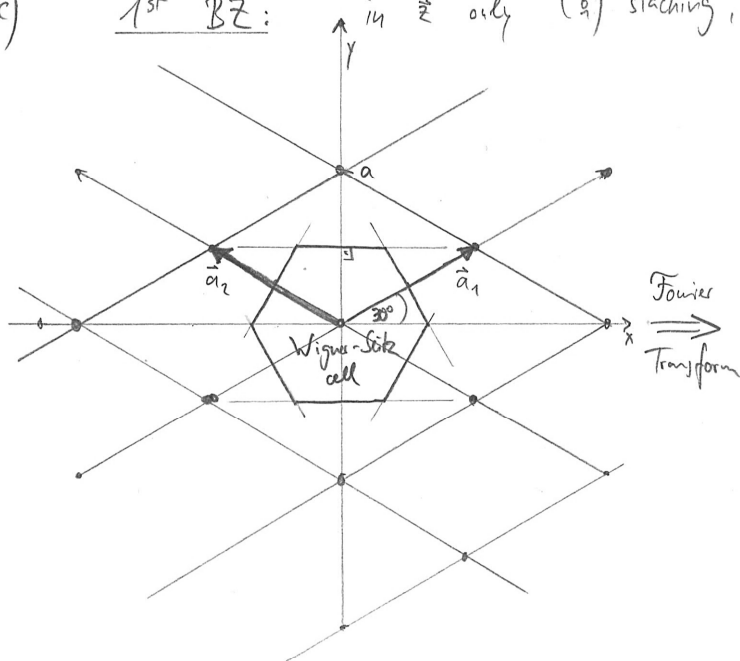
b) The primitive translation vectors of reciprocal space are given by all cyclic permutations of:

$$\vec{b}_1 = \frac{2\pi}{V_{\text{cell}}} (\vec{a}_2 \times \vec{a}_3) = \frac{2\pi a c}{\frac{\sqrt{3}}{2} a^2 c} \left[ \begin{pmatrix} -\sqrt{3}/2 \\ 1/2 \\ 0 \end{pmatrix} \times \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right] = \frac{2\pi}{\sqrt{3}/2 a} \begin{pmatrix} 1/2 \\ \sqrt{3}/2 \\ 0 \end{pmatrix} = \underline{\underline{\frac{2\pi}{a} \begin{pmatrix} 1/\sqrt{3} \\ 1 \\ 0 \end{pmatrix}}}$$

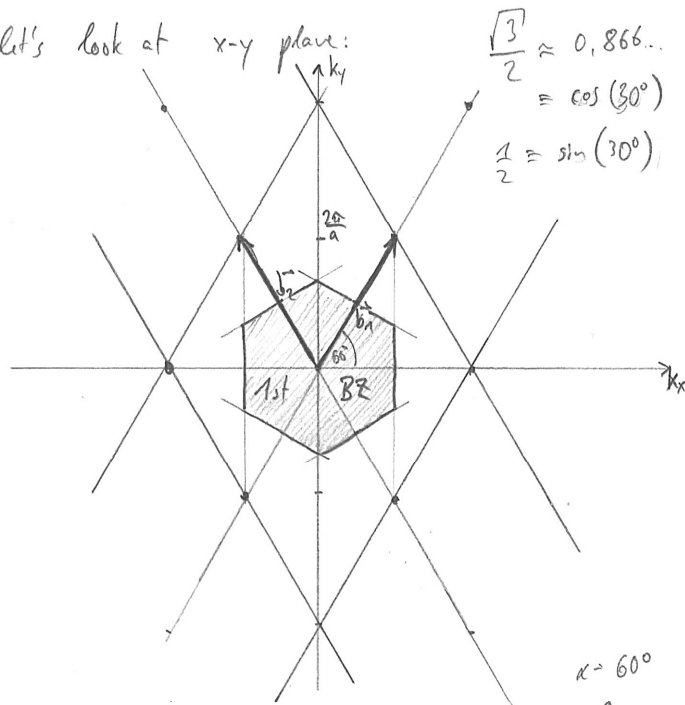
$$\vec{b}_2 = \frac{2\pi}{V_{\text{cell}}} (\vec{a}_3 \times \vec{a}_1) = \frac{2\pi a c}{\frac{\sqrt{3}}{2} a^2 c} \left[ \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \times \begin{pmatrix} \sqrt{3}/2 \\ 1/2 \\ 0 \end{pmatrix} \right] = \frac{2\pi}{\sqrt{3}/2 a} \begin{pmatrix} -1/2 \\ \sqrt{3}/2 \\ 0 \end{pmatrix} = \underline{\underline{\frac{2\pi}{a} \begin{pmatrix} -1/\sqrt{3} \\ 1 \\ 0 \end{pmatrix}}}$$

$$\vec{b}_3 = \frac{2\pi}{V_{\text{cell}}} (\vec{a}_1 \times \vec{a}_2) = \frac{2\pi a^2}{\frac{\sqrt{3}}{2} a^2 c} \left[ \begin{pmatrix} \sqrt{3}/2 \\ 1/2 \\ 0 \end{pmatrix} \times \begin{pmatrix} -\sqrt{3}/2 \\ 1/2 \\ 0 \end{pmatrix} \right] = \frac{2\pi}{\frac{\sqrt{3}}{2} c} \begin{pmatrix} 0 \\ 0 \\ \sqrt{3}/4 + \sqrt{3}/4 \end{pmatrix} = \underline{\underline{\frac{2\pi}{c} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}}}$$

c) 1st BZ: in  $\vec{z}$  only ( $\frac{2}{3}$ ) stacking, so let's look at x-y plane:



Fourier Transform



$$\alpha = 60^\circ$$

$$\begin{pmatrix} 1/\sqrt{3} \\ 1 \\ 0 \end{pmatrix}$$

$$\tan \alpha = \frac{y}{x}$$