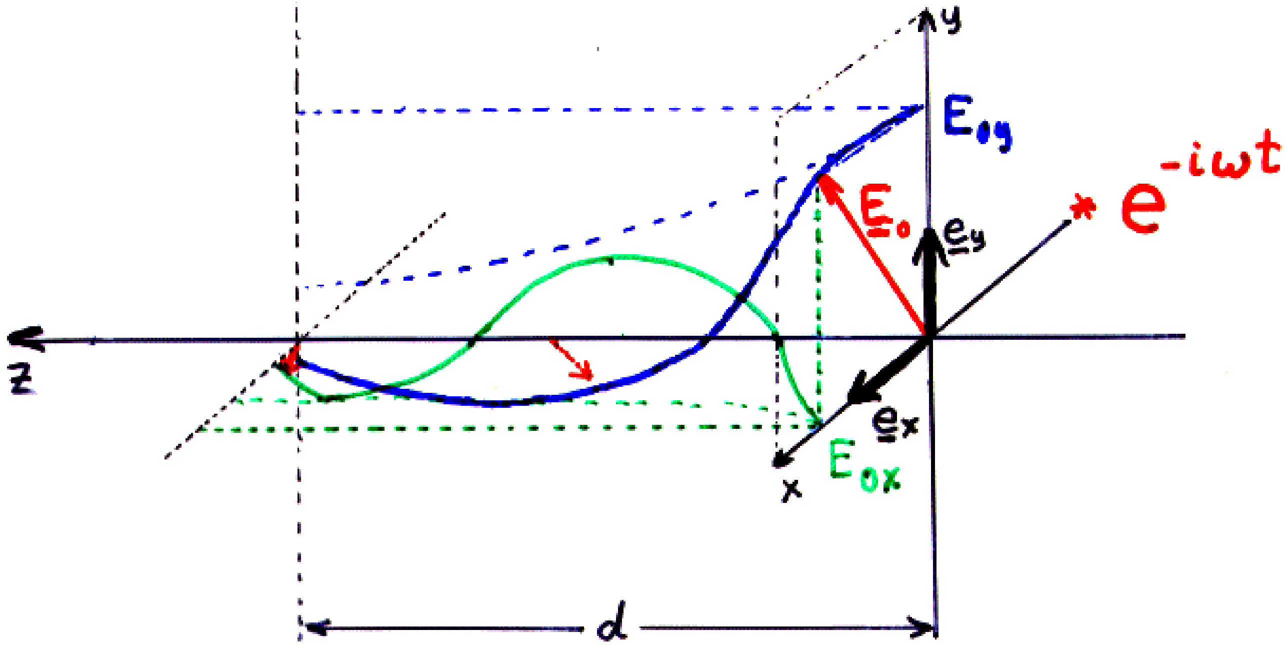
Die Absorption polarisierter Strahlung

(Klassische Optik)

Elektrisches Feld einer ebenen Welle:



$$\underline{E} = e^{i\underline{\underline{n}}kz}\,\underline{E}_0$$

$$\underline{\underline{n}} = \begin{pmatrix} n_{xx} & n_{xy} \\ n_{yx} & n_{yy} \end{pmatrix}$$

Im Allgemeinen ist $\underline{\underline{n}}$ nicht-Hermitsch und kann nicht diagonalisiert werden.

Wenn $\underline{\underline{n}}$ diagonal ist: $\quad \underline{\underline{n}} = \begin{pmatrix} n_x & 0 \\ 0 & n_y \end{pmatrix}$

$$E_x = e^{in_xkz}\,E_{0x}$$

$$E_y = e^{in_ykz}\,E_{0y}$$

$$e^{\begin{pmatrix} n_x & 0 \\ 0 & n_y \end{pmatrix}} = \begin{pmatrix} e^{n_x} & 0 \\ 0 & e^{n_y} \end{pmatrix}$$

Die Intensität der Strahlung:

$$I \sim |\underline{E}|^2 = \underbrace{\underline{E}^+ \underline{E}}$$

$$\Downarrow$$

$$(E_x^* \;\; E_y^*) \begin{pmatrix} E_x \\ E_y \end{pmatrix} = |E_x|^2 + |E_y|^2$$

$$I = I_0 \frac{\underline{E}^+ \underline{E}}{|\underline{E}_0|^2}$$

$$\underline{E}^+ \underline{E} = \left(e^{i\underline{n}kz} \underline{E}_0\right)^+ \left(e^{i\underline{n}kz} \underline{E}_0\right) =$$

$$= \left(\underline{E}_0^+ e^{-i\underline{n}^+ kz}\right)\left(e^{i\underline{n}kz} \underline{E}_0\right) =$$

$$Sp\left(e^{i\underline{n}kz} \underbrace{\underline{E}_0 \underline{E}_0^+}_{\underline{\underline{\rho}}_0 |\underline{E}_0|^2} e^{-i\underline{n}^+ kz}\right)$$

Dichtematrix:

$$\underline{\underline{\rho}}_0 := \frac{\underline{E}_0 \underline{E}_0^+}{\underline{E}_0^+ \underline{E}_0}$$

$$\boxed{I = I_0 \, Sp\left(e^{i\underline{n}kz} \underline{\underline{\rho}}_0 e^{-i\underline{n}^+ kz}\right)}$$

$$\underline{\underline{\rho}} := \frac{\underline{E}\,\underline{E}^+}{\underline{E}^+ \underline{E}}$$

$\underline{\underline{\rho}}$ ist Hermit'sch, weil

$$(\underline{E}\,\underline{E}^+)^+ = (\underline{E}^+)^+ \underline{E}^+ = \underline{E}\,\underline{E}^+$$

$$\boxed{Sp(\underline{\underline{\rho}}) = \frac{1}{\underline{E}^+ \underline{E}} \underbrace{Sp(\underline{E}\,\underline{E}^+)}_{\underline{E}^+ \underline{E}} = 1}$$

$$\boxed{\underline{\underline{\varrho}}^2 = \frac{\underline{E}\,\underline{E}^+\underline{E}\,\underline{E}^+}{(\underline{E}^+\underline{E})^2} = \frac{\underline{E}\,\underline{E}^+}{\underline{E}^+\underline{E}} = \underline{\underline{\varrho}}}$$

Die Dichtematrix (Kohärenzmatrix) einer vollständig polarisierten Strahlung ist idempotent (Projektions-matrix): $\underline{\underline{\varrho}}^2 = \underline{\underline{\varrho}}$.

Die Dichtematrix bei $z = d$:

$$\underline{\underline{\varrho}}(d) = \frac{\underline{E}(d)\,\underline{E}^+(d)}{\underline{E}^+(d)\,\underline{E}(d)} = \frac{e^{i\underline{\underline{n}}kd}\,\underbrace{\frac{\underline{E}_0\,\underline{E}_0^+}{\underline{E}_0^+\underline{E}_0}}_{\underline{\underline{\varrho}}_0}\,e^{-i\underline{\underline{n}}^+kd}}{} \;\; \frac{I_0}{I(d)}$$

$$\boxed{I(d)\,\underline{\underline{\varrho}}(d) = I_0\, e^{i\underline{\underline{n}}kd}\,\underline{\underline{\varrho}}_0\, e^{-i\underline{\underline{n}}^+kd}}$$

Kohärente Strahlung:

$$\underline{E} = E_x\,\underline{e}_x + E_y\,\underline{e}_y$$

$$E_x \Downarrow |E_x|\,e^{i\alpha_x} \qquad E_y \Downarrow |E_y|\,e^{i\alpha_y}$$

$$\underline{e}_i^+\underline{e}_k = \delta_{ik}$$

$$\underline{e}_x\,\underline{e}_x^+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\underline{e}_x\,\underline{e}_y^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \ldots$$

$$\cos^2\varphi = \frac{|E_x^2|}{|E_x|^2 + |E_y|^2}$$

$$\alpha = \alpha_y - \alpha_x$$

$\underline{\underline{\rho}}^2 = \underline{\underline{\rho}}$ gilt nur für vollständig polarisierte Strahlung.

$\underline{\underline{\rho}}$ ist Hermit'sch $\Rightarrow$ hat 2 reele Eigenwerte ρ_1 und ρ_2

Polarisationsgrad der Strahlung:

$$\xi = |\rho_1 - \rho_2| = \sqrt{1 - 4\,\mathrm{Det}(\underline{\underline{\rho}})}$$

Zirkulare Einheitsvektoren:

$$\underline{u}_{\pm 1} = \frac{1}{\sqrt{2}}(\underline{e}_x \pm i\,\underline{e}_y) \qquad \underline{u}_i^+ \underline{u}_k = \delta_{ik}$$

$$\underline{e}_x = \frac{1}{\sqrt{2}}(\underline{u}_{+1} + \underline{u}_{-1})$$

$$\underline{e}_y = \frac{-i}{\sqrt{2}}(\underline{u}_{+1} - \underline{u}_{-1})$$

$$\underline{E} = E_x \underline{e}_x + E_y \underline{e}_y =$$

$$= \underbrace{\frac{1}{\sqrt{2}}(E_x - iE_y)}_{E_{+1}} \underline{u}_{+1} + \underbrace{\frac{1}{\sqrt{2}}(E_x + iE_y)}_{E_{-1}} \underline{u}_{-1}$$

Dichtematrizen in zirkularem Basis:

Rechts- Links- polarisiert:

$$\underline{\underline{\rho}}_r = \begin{array}{c c} & \begin{array}{cc} +1 & -1 \end{array} \\ \begin{array}{c} +1 \\ -1 \end{array} & \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \end{array} \qquad \underline{\underline{\rho}}_l = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

Linearpolarisiert:

$\parallel x$ $\qquad$ $\parallel y$ $\qquad$ Richtung φ

$$\underline{\underline{\rho}}_x = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \qquad \underline{\underline{\rho}}_y = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \qquad \underline{\underline{\rho}}_\varphi = \frac{1}{2}\begin{pmatrix} 1 & e^{2i\varphi} \\ e^{-2i\varphi} & 1 \end{pmatrix}$$

Poincaré-Darstellung

$$\underline{\underline{1}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad \underbrace{\underline{\underline{\sigma}}_\xi = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \underline{\underline{\sigma}}_\eta = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \underline{\underline{\sigma}}_\zeta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\text{Pauli-Matrizen}}$$

kein Koeffizient, da $Sp(\underline{\underline{\rho}}) = 1$

$$\underline{\underline{\rho}} = \frac{1}{2}\left(\underline{\underline{1}} + \underline{P}\,\underline{\underline{\underline{\sigma}}}\right) \qquad \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{pmatrix}$$

Super-Vektor

(P_ξ, P_η, P_ζ)

reel, weil $\underline{\underline{\rho}}$ Hermit'sch

$\underline{P} = (\pm 1, 0, 0)$: $\left.\begin{matrix} x \\ y \end{matrix}\right\}$ linearpolarisiert

$\underline{P} = (0, 0, \pm 1)$: $\left.\begin{matrix} \text{links} \\ \text{rechts} \end{matrix}\right\}$ zirkularpolarisiert

Polarisationsgrad:

$$\xi = |\underline{P}|$$

Transformation der Dichtematrix $(\underline{u}_+, \underline{u}_-) \to (\underline{e}_x, \underline{e}_y)$

$$\underline{E} = \underbrace{\frac{1}{\sqrt{2}}\left(E_{+1} + E_{-1}\right)}_{E_x} \underline{e}_x + \underbrace{\frac{i}{\sqrt{2}}\left(E_{+1} - E_{-1}\right)}_{E_y} \underline{e}_y$$

$$\varrho_{xx} = \frac{1}{2}\left(\varrho_{11} + \varrho_{-1-1}\right) + \frac{1}{2}\left(\varrho_{1-1} + \varrho_{-11}\right)$$

$$\varrho_{yy} = \frac{1}{2}\left(\varrho_{11} + \varrho_{-1-1}\right) - \frac{1}{2}\left(\varrho_{1-1} + \varrho_{-11}\right)$$

$$\varrho_{xy} = \frac{i}{2}\left(\varrho_{11} - \varrho_{-1-1}\right) - \frac{i}{2}\left(\varrho_{1-1} - \varrho_{-11}\right)$$

$$\varrho_{yx} = -\frac{i}{2}\left(\varrho_{11} - \varrho_{-1-1}\right) - \frac{i}{2}\left(\varrho_{1-1} - \varrho_{-11}\right)$$

Linearpolarisierte Strahlung (Richtung φ):

in $(\underline{u}_1, \underline{u}_{-1})$ Basis

$$\underline{\varrho}_\varphi = \frac{1}{2}\begin{pmatrix} 1 & e^{2i\varphi} \\ e^{-2i\varphi} & 1 \end{pmatrix}$$

in $(\underline{e}_x, \underline{e}_y)$ Basis

$$\underline{\varrho}_\varphi = \frac{1}{2}\begin{pmatrix} 1+\cos 2\varphi & \sin 2\varphi \\ \sin 2\varphi & 1-\cos 2\varphi \end{pmatrix}$$

$$\underline{P}_\varphi = (\cos 2\varphi, -\sin 2\varphi, 0) \qquad \underline{P}_\varphi = (\sin 2\varphi, 0, \cos 2\varphi)$$

$$|\underline{P}_\varphi| = 1$$

Blume - Kistner - Formalismus:

$$\underline{\underline{n}}\, kz = a\,\underline{\underline{1}} + \underline{b}\,\underline{\underline{\sigma}} = a\,\underline{\underline{1}} + b_\xi \underline{\underline{\sigma}}_\xi + b_\eta \underline{\underline{\sigma}}_\eta + b_\zeta \underline{\underline{\sigma}}_\zeta$$

$a, b_\xi, b_\eta, b_\zeta$: komplexe Zahlen (da n nicht unbedingt Hermit'sch).

Die Intensität:

$$\boxed{\frac{I(d)}{I_0}} = Sp\left(e^{i\underline{\underline{n}}kz}\, \underline{\underline{\rho}}_0\, e^{-i\underline{\underline{n}}^+ kz}\right) =$$

$$= \frac{1}{2} Sp\left[e^{i(a\underline{\underline{1}} + \underline{b}\underline{\underline{\sigma}})}(\underline{\underline{1}} + \underline{P}_0 \underline{\underline{\sigma}})\, e^{-i(a^*\underline{\underline{1}} + \underline{b}^*\underline{\underline{\sigma}})}\right] = \ldots$$

$$\boxed{\ldots = e^{i(a-a^*)}\left[\cos b^* \cos b + \hat{\underline{b}}^* \hat{\underline{b}} \sin b^* \sin b + i\underline{P}_0\left(\hat{\underline{b}} \sin b \cos b^* - \hat{\underline{b}}^* \sin b^* \cos b + \hat{\underline{b}}^* \times \hat{\underline{b}} \sin b^* \sin b\right)\right]}$$

Der Poincaré - Vektor:

$$I(d)(\underline{\underline{1}} + \underline{P}(d)\underline{\underline{\sigma}}) = I_0\, e^{i\underline{\underline{n}}kd}(\underline{\underline{1}} + \underline{P}_0\underline{\underline{\sigma}})\, e^{-i\underline{\underline{n}}^+ kd}$$

$$\boxed{\begin{aligned}\frac{\underline{P}(d)\, I(d)}{I_0} = e^{i(a-a^*)}\Big[& i\left(\hat{\underline{b}} \sin b \cos b^* - \hat{\underline{b}}^* \sin b^* \cos b - \hat{\underline{b}}^* \times \hat{\underline{b}} \sin b^* \sin b\right) + \\ & + \underline{P}_0\left(\cos b^* \cos b - \hat{\underline{b}}^* \hat{\underline{b}} \sin b^* \sin b\right) + \\ & + \underline{P}_0 \times \left(\hat{\underline{b}} \sin b \cos b^* + \hat{\underline{b}}^* \sin b^* \cos b\right) + \\ & + \hat{\underline{b}}\,(\underline{P}_0 \hat{\underline{b}}^*) + \hat{\underline{b}}^*(\underline{P}_0 \hat{\underline{b}})\Big]\end{aligned}}$$

$$b = \sqrt{b_\xi^2 + b_\eta^2 + b_\zeta^2} \qquad \hat{\underline{b}} = \underline{b}/b$$

$\underline{\underline{\nu}} = ikd(\underline{\underline{n}}^+ - \underline{\underline{n}})$ ist Hermit'sch $\Rightarrow$ kann diagonalisiert werden:

$$\underbrace{\underline{\underline{\nu}}'}_{\text{diagonal}} = \underbrace{\underline{\underline{\mathcal{U}}}}_{\text{unitär}} \; \underbrace{\underline{\underline{\nu}}}_{\text{Hermit'sch}} \; \underline{\underline{\mathcal{U}}}^+$$

$$\underline{\underline{\rho}}_0' = \underline{\underline{\mathcal{U}}} \; \underline{\underline{\rho}}_0 \; \underline{\underline{\mathcal{U}}}^+$$

$$\boxed{I(d)} = I_0 \, \mathrm{Sp}\left\{ \underline{\underline{\rho}}_0 \, e^{-ikd(\underline{\underline{n}}^+ - \underline{\underline{n}})} \right\} =$$

(2)

$$= I_0 \, \mathrm{Sp}\left\{ \underline{\underline{\rho}}_0 \, e^{-\underline{\underline{\nu}}} \right\} = I_0 \, \mathrm{Sp}\left\{ \underline{\underline{\rho}}_0' \, \underbrace{e^{-\underline{\underline{\nu}}'}}_{\text{diagonal: } \begin{pmatrix} e^{-\nu'_{11}} & 0 \\ 0 & e^{-\nu'_{-1-1}} \end{pmatrix}} \right\} =$$

$$\boxed{= I_0 \sum_i \rho'_{0,ii} \, e^{-\nu'_{ii}}}$$

Für <u>unpolarisierten Strahl</u>:

$$\underline{\underline{\rho}}_0 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \Rightarrow \boxed{I(d) = \frac{I_0}{2}\left(e^{-\nu'_{11}} + e^{-\nu'_{-1-1}}\right)} \quad (1)$$

$$\boxed{\frac{I(d)\,\underline{\underline{\rho}}(d)}{I_0}} = e^{i\underline{\underline{n}}kd} \underbrace{\underline{\underline{\rho}}_0}_{\frac{1}{2}\underline{\underline{1}}} e^{-i\underline{\underline{n}}^+kd} = \frac{1}{2} e^{-ikd(\underline{\underline{n}}^+ - \underline{\underline{n}})} =$$

(3)

$$= \frac{1}{2} e^{-\underline{\underline{\nu}}} = \frac{1}{2} \underline{\underline{\mathcal{U}}}^+ e^{-\underline{\underline{\nu}}'} \underline{\underline{\mathcal{U}}} = \boxed{\frac{1}{2} \underline{\underline{\mathcal{U}}}^+ \begin{pmatrix} e^{-\nu'_{11}} & 0 \\ 0 & e^{-\nu'_{-1-1}} \end{pmatrix} \underline{\underline{\mathcal{U}}}}$$

Für mehrere "Grundzustände":

$$F_{pq} = \sum_{\alpha=1}^{2I_g+1} \frac{e^{-\frac{E_\alpha}{k_B T}}}{\sum_{\alpha'=1}^{2I_g+1} e^{-\frac{E_{\alpha'}}{k_B T}}} F_{pq}^{\alpha}$$

Für hyperfein aufgespaltenen Grundzustand bei $T \geq 1\,K$:

$$\boxed{F_{pq} = \frac{1}{2I_g+1} \sum_{\alpha=1}^{2I_g+1} F_{pq}^{\alpha}}$$

Für M1 Übergänge (z. B. ^{57}Fe):

$$a_p^{\alpha\beta}(\underline{\vartheta}) = 2\pi i\, M_1 \sqrt{\frac{\hbar c}{kV}} \sum_M V_{1M}^{\alpha\beta} D_{Mp}^{1}(\underline{\vartheta})$$

Reduziertes Matrixelement des M1 Übergangs

Euler-Winkel φ, ϑ, ψ der Drehung $S^E \to S^T$

$$V_{LM}^{\alpha\beta} = \sqrt{\frac{2L+1}{2I_e+1}} \sum_{m_e, m_g} e_{\beta m_e}^{*}\, g_{\alpha m_g} \left(I_g L m_g M \middle| I_e m_e\right)$$

Absorbermatrix:

$$\boxed{\tau_{pq}^{\alpha\beta}(\underline{\vartheta}) := \frac{Vk}{\hbar c M_1^2} \left[a_p^{\alpha\beta}(\underline{\vartheta})\right]^* a_q^{\alpha\beta}(\underline{\vartheta})}$$

Für E1 Übergang: $a_p^{\alpha\beta} \sim E_p\left(|I_e, e_\beta\rangle \to |I_g, g_\alpha\rangle\right)$

$$T_{pq}^{\alpha\beta} \sim \left(g_{0,pq}^{\alpha\beta}\right)^*$$

(gilt auch für M1)

Für mehrere nicht-equivalente Gitterplätze:

$$\underline{\underline{n}} = \underline{\underline{1}} - \frac{\sigma_0}{2k} \sum_j f_j(\underline{k})\, N_j \sum_{\alpha\beta} \underline{\underline{T}}_j^{\alpha\beta} \, \frac{\frac{\Gamma}{2}}{E-(E_\beta-E_\alpha)+i\frac{\Gamma}{2}} =$$

$$= \underline{\underline{1}} - \frac{\sigma_0}{2k} \sum_{\alpha\beta} \underbrace{\sum_j f_j(\underline{k})\, N_j\, \underline{\underline{T}}_j^{\alpha\beta}}_{N\,\bar{f}(k)\,\boxed{\bar{\underline{\underline{T}}}^{\alpha\beta}}} \, \frac{\frac{\Gamma}{2}}{E-(E_\beta-E_\alpha)+i\frac{\Gamma}{2}} =$$

$$N \leftarrow \sum_j N_j$$

$$\bar{f}(k) \leftarrow \underbrace{\frac{1}{N}\sum_j N_j f_j}_{\sum_j N_j f_j}$$

$$\bar{\underline{\underline{T}}}^{\alpha\beta} \leftarrow \boxed{\frac{1}{N\bar{f}} \sum_j f_j N_j \underline{\underline{T}}_j^{\alpha\beta}} = \frac{\sum_j N_j f_j \underline{\underline{T}}_j^{\alpha\beta}}{\sum_j N_j f_j}$$

$$= \underline{\underline{1}} - \frac{N\,\bar{f}(\underline{k})\,\sigma_0}{2k} \sum_{\alpha\beta} \bar{\underline{\underline{T}}}^{\alpha\beta} \, \frac{\frac{\Gamma}{2}}{E-(E_\beta-E_\alpha)+i\frac{\Gamma}{2}}$$

Effektive Dicke:

$$t(\underline{k}) := N d\, \bar{f}(\underline{k})\, \sigma_0$$

$N \approx 10^{26} \ldots 10^{28}\ m^{-3}$

$\sigma_0 \approx 10^{-22}\ m^2$

$\frac{1}{k} \approx 10^{-10}\ m$

$|n| \approx 1 - (10^{-6} \ldots 10^{-4})$

Winkel der Totalreflexion $\approx 10^{-3} \ldots 10^{-2} \approx 0.1° \ldots 1°$

Unter welchen Bedingungen ist $[n, n^+] = 0$?

$$[\underline{\underline{n}}, \underline{\underline{n}}^+] = -\frac{\sigma_0}{2k} N f \sum_{\alpha\alpha'\beta\beta'} [\underline{\underline{T}}^{\alpha\beta}, \underline{\underline{T}}^{\alpha'\beta'}] *$$

$$* \underbrace{\frac{\Gamma^2/4}{[E-(E_\beta - E_\alpha) + i\Gamma/2][E-(E_{\beta'} - E_{\alpha'}) - i\Gamma/2]}}_{G}$$

- $[\underline{\underline{T}}^{\alpha\beta}, \underline{\underline{T}}^{\alpha'\beta'}] = 0$

$$|G|^2 = [E-(E_\beta - E_\alpha)]^2 [E-(E_{\beta'} - E_{\alpha'})]^2 +$$
$$+ 2[E-(E_\beta - E_\alpha)][E-(E_{\beta'} - E_{\alpha'})](\Gamma^2/4) +$$
$$+ (\Gamma^2/4)\left[(\Gamma^2/4) + ((E_\beta - E_\alpha) - (E_{\beta'} - E_{\alpha'}))^2\right]$$

- $|(E_\beta - E_\alpha) - (E_{\beta'} - E_{\alpha'})| \gg \Gamma/2$

Das Mößbauer-Absorptionsspektrum

Quellenspektrum, Absorberspektrum aufgespalten.

Quelle (Linie i):

$$L_{si}(E, v) = \frac{(\Gamma^2/4)}{[E - E_{si}(1 + \frac{v}{c})]^2 + (\Gamma^2/4)}$$

- Dünner Absorber: $e^{i\underline{\underline{n}}kd} = 1 + i\underline{\underline{n}}kd$

$$SP(v) = \sum_{i,\alpha,\beta} SP(v)_i^{\alpha\beta}$$

$$SP(v)_i^{\alpha\beta} = f_s\, t\, I_{si}\, Sp\left(\underline{\underline{T}}^{\alpha\beta} \underline{\underline{\rho}}_{si}\right) \frac{\Gamma^2}{\left[E_{si}\frac{v}{c} - (E_\beta - E_\alpha)\right]^2 + \Gamma^2}$$

Fläche der Absorptionslinie (i, α, β):

$$\boxed{A_i^{\alpha\beta} = \int_{-\infty}^{\infty} SP_i^{\alpha\beta}(v)\, dv = f_s\, t\, \frac{\Gamma\pi}{2}\, Sp\left(\underline{\underline{T}}^{\alpha\beta} \underline{\underline{\rho}}_{si}\right)}$$

Für unpolarisierte Quelle: $\underline{\underline{\rho}}_{si} = \frac{1}{2}\underline{\underline{1}}$

$$\boxed{A^{\alpha\beta} = f_s\, t\, \frac{\Gamma\pi}{4}\, Sp\left(\underline{\underline{T}}^{\alpha\beta}\right)}$$

Gesamtfläche:

$$\sum_{\alpha\beta} A^{\alpha\beta} = f_s\, t\, \frac{\Gamma\pi}{2}$$

$$\sum_{\alpha\beta} Sp\left(\underline{\underline{T}}^{\alpha\beta}\right) = 2$$

$I_g = 1/2$, $I_e = 3/2$, M1-Übergang, reine Quadrupol-WW

$$I^{1,\alpha\beta}_{MM'} = V^{\alpha\beta\,*}_{1M}\, V^{\alpha\beta}_{1M'}$$

$$V^{\alpha\beta}_{1M} = \sqrt{3} \sum_{m_e m_g} e^{*}_{\beta m_e}\, \underbrace{g_{\alpha m_g}}_{\delta_{\alpha m_g}}\, (-1)^{m_e - \frac{1}{2}} \begin{pmatrix} 1/2 & 1 & 3/2 \\ m_g & M & -m_e \end{pmatrix}$$

$\delta_{\alpha m_g}$, da im Grundzustand keine Q-WW

$$e^{*}_{\beta m_e}: \quad \begin{array}{c|cccc} & 3/2 & 1/2 & -1/2 & -3/2 \\ \hline 1 & e_+ & 0 & e_- & 0 \\ 2 & 0 & e_- & 0 & e_+ \\ 3 & e_- & 0 & -e_+ & 0 \\ 4 & 0 & -e_+ & 0 & e_- \end{array}$$

$$e_\pm = \frac{1}{\sqrt{2}} \sqrt{1 \pm \frac{1}{\sqrt{1 + \frac{\eta^2}{3}}}}$$

$M = \quad 1 \qquad 0 \qquad -1$

$$V^{\frac{1}{2}1}_{1M} = \left(\frac{\sqrt{3}}{2} e_+,\ 0,\ \frac{1}{2} e_-\right) \qquad V^{-\frac{1}{2}1}_{1M} = \left(0,\ \frac{1}{\sqrt{2}} e_-,\ 0\right)$$

$$V^{\frac{1}{2}2}_{1M} = \left(0,\ \frac{1}{\sqrt{2}} e_-,\ 0\right) \qquad V^{-\frac{1}{2}2}_{1M} = \left(\frac{1}{2} e_-,\ 0,\ \frac{\sqrt{3}}{2} e_+\right)$$

$$V^{\frac{1}{2}3}_{1M} = \left(\frac{\sqrt{3}}{2} e_-,\ 0,\ -\frac{1}{2} e_+\right) \qquad V^{-\frac{1}{2}3}_{1M} = \left(0,\ -\frac{1}{\sqrt{2}} e_+,\ 0\right)$$

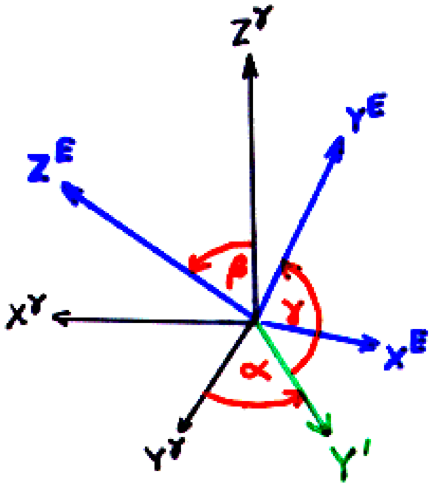
$$V^{\frac{1}{2}4}_{1M} = \left(0,\ -\frac{1}{\sqrt{2}} e_+,\ 0\right) \qquad V^{-\frac{1}{2}4}_{1M} = \left(-\frac{1}{2} e_+,\ 0,\ \frac{\sqrt{3}}{2} e_-\right)$$

$$I^{1,\frac{1}{2}1}_{MM'} = V^{\frac{1}{2}1\,*}_{1M}\, V^{\frac{1}{2}1}_{1M'} = \begin{pmatrix} \frac{3}{2} e_+^2 & 0 & \frac{\sqrt{3}}{4} e_+ e_- \\ 0 & 0 & 0 \\ \frac{\sqrt{3}}{4} e_+ e_- & 0 & \frac{1}{4} e_-^2 \end{pmatrix}, \quad \text{u.s.w.}$$

Textur

Die Systeme S^E sind verteilt : $T(\underline{\beta})\, d\underline{\beta}$

$$T(\underline{\beta}) = \sum_{L m' m} t^L_{m'm} D^L_{m'm}(\underline{\beta})$$



Axialsymmetrische Textur um die Z^γ-Achse:

keine α- Abhängigkeit $\rightarrow m' = 0$ $\quad (D^L_{m'm}(\underline{\beta}) \sim e^{im'\alpha})$.

Axialsymmetrische HFWW um die Z^E-Achse:

keine γ - Abhängigkeit $\rightarrow m = 0$ $\quad (D^L_{m'm}(\underline{\beta}) \sim e^{im\gamma})$

$$\frac{1}{8\pi^2} \int T(\underline{\beta}) \sin\beta \, d\alpha \, d\beta \, d\gamma = 1 \;\Rightarrow\; t^0_{00} = 1$$

Random Pulver: $\quad t^0_{00} = 1$

$\quad t^L_{mm'} = 0$ für $L \geq 1$

Für M1-Übergänge:

$$\underline{\underline{I}}^1(S^T) = \underline{\underline{D}}^1(\underline{\beta})\,\underline{\underline{I}}^1(S^E)\,\underline{\underline{D}}^{1^+}(\underline{\beta})$$

Mittlere Absorbermatrix in S^T:

$$\bar{\tau}_{pq} = \frac{1}{8\pi^2}\int T(\underline{\beta})\,\tau_{pq}(\underline{\beta})\,d\underline{\beta} =$$

$$= \bar{I}^1_{pq} = \frac{1}{8\pi^2}\int T(\underline{\beta})\,I^1_{pq}(S^T)\,d\underline{\beta} =$$

$$= \frac{1}{8\pi^2}\int \underbrace{T(\underline{\beta})}_{\Uparrow\ \sum\limits_{L m' m} t^L_{m'm} D^L_{m'm}(\underline{\beta})}\left[\underline{\underline{D}}^1(\underline{\beta})\,\underline{\underline{I}}^1(S^E)\,\underline{\underline{D}}^{1^+}(\underline{\beta})\right]_{pq} d\underline{\beta}$$

$$\frac{1}{8\pi^2}\int D^{L_1}_{m_1' m_1}(\underline{\beta})\,D^{L_2}_{m_2' m_2}(\underline{\beta})\,D^{L_3}_{m_3' m_3}(\underline{\beta})\,d\underline{\beta} =$$

$$= \begin{pmatrix} L_1 & L_2 & L_3 \\ m_1' & m_2' & m_3' \end{pmatrix}\begin{pmatrix} L_1 & L_2 & L_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

$$\boxed{\bar{I}^1_{pq} = \sum_{L' m' m j k} (-1)^{q+k}\begin{pmatrix} L' & 1 & 1 \\ m' & p & -q \end{pmatrix}\begin{pmatrix} L' & 1 & 1 \\ m & j & -k \end{pmatrix} I^1_{jk}(S^E)\,t^{L'}_{m'm}}$$

Für random Pulver:

$$\bar{I}^1_{pq} = \sum_{jk} (-1)^{q+k}\underbrace{\begin{pmatrix} 0 & 1 & 1 \\ 0 & p & -q \end{pmatrix}}_{\frac{1}{\sqrt{3}}(-1)^{p+1}\delta_{pq}}\begin{pmatrix} 0 & 1 & 1 \\ 0 & j & -k \end{pmatrix} I^1_{jk}(S^E) =$$

$$= \frac{1}{3} \sum_{jk} (-1)^{p+q+j+k} \delta_{pq} \delta_{jk} I^1_{jk}(S_E) =$$

$$= \frac{1}{3} \sum_{k} (-1)^{p+q} \delta_{pq} I^1_{kk}(S^E) = \frac{1}{3} Sp[\underline{\underline{I}}^1(S^E)] \delta_{pq}$$

$$\boxed{\bar{T}_{pq} = \frac{1}{3} Sp(\underline{\underline{I}}^1) \delta_{pq}}$$

Random Pulver-Absorber ändert nicht den Polarisationszustand der Strahlung.

Reine QWW:

$$Sp(\underline{\underline{I}}^{1\pi}) = Sp(\underline{\underline{I}}^{1\sigma}) = \frac{3}{2}$$

$$\boxed{\bar{T}^{\pi}_{pq} = \bar{T}^{\sigma}_{pq} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}}$$

Quadrupol-Spektren nicht-orientierter Proben sind symmetrisch

Für $3/2^- \rightarrow 1/2^-$ (M1) übergang:

$$\bar{T}^{\alpha\beta}_{11} = A^{\alpha\beta}_{00} + A^{\alpha\beta}_{20} \qquad (\alpha\beta) = \begin{cases} \pi \\ \sigma \end{cases}$$

$$\bar{T}^{\alpha\beta}_{1-1} = \sqrt{6}\, A^{\alpha\beta}_{2-2}$$

$$A^{\pi}_{00}{}^{\sigma} = 1/2$$

$$A^{\pi}_{2m}{}^{\sigma} = \pm \frac{1}{20\sqrt{6}} \left[\sqrt{6}\, t^2_{m0} + \eta (t^2_{m2} + t^2_{m-2})\right] \frac{1}{\sqrt{1 + \frac{\eta^2}{3}}}$$

5 Werte $\Rightarrow$ aus 5 unabhängigen Messungen
5 unabhängigen Textur-Parameter

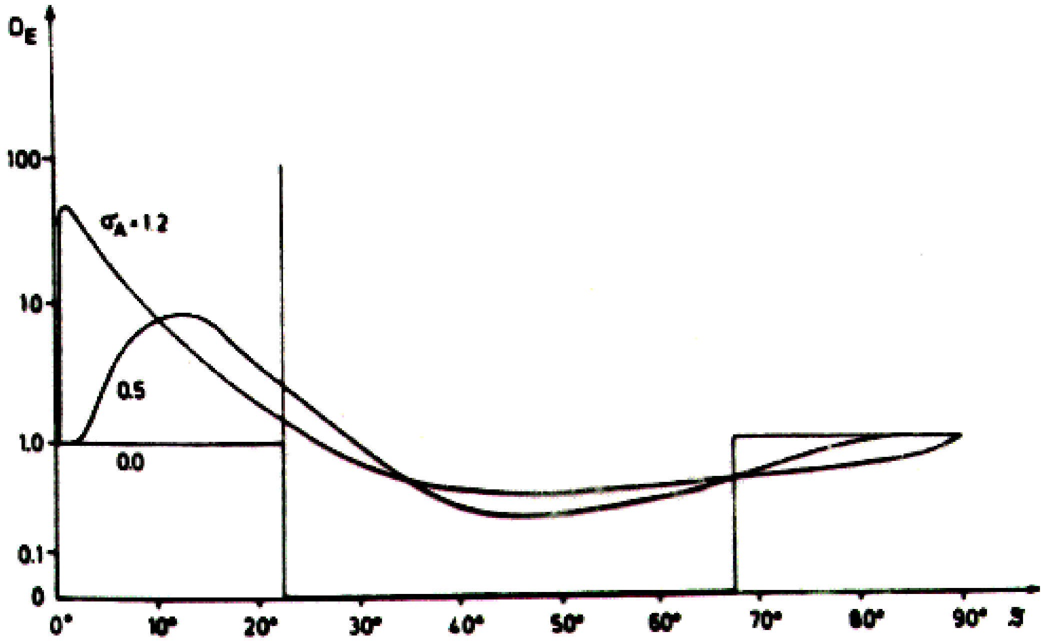


Fig. 6. The texture function $D_E(\vartheta)$ calculated with a logarithmic Gauss distribution of the critical field for some values of σ_A and a = 0·7056. (The ordinate is semilogarithmic so that it is proportional to $\log(D_E + 0{\cdot}1)$.)

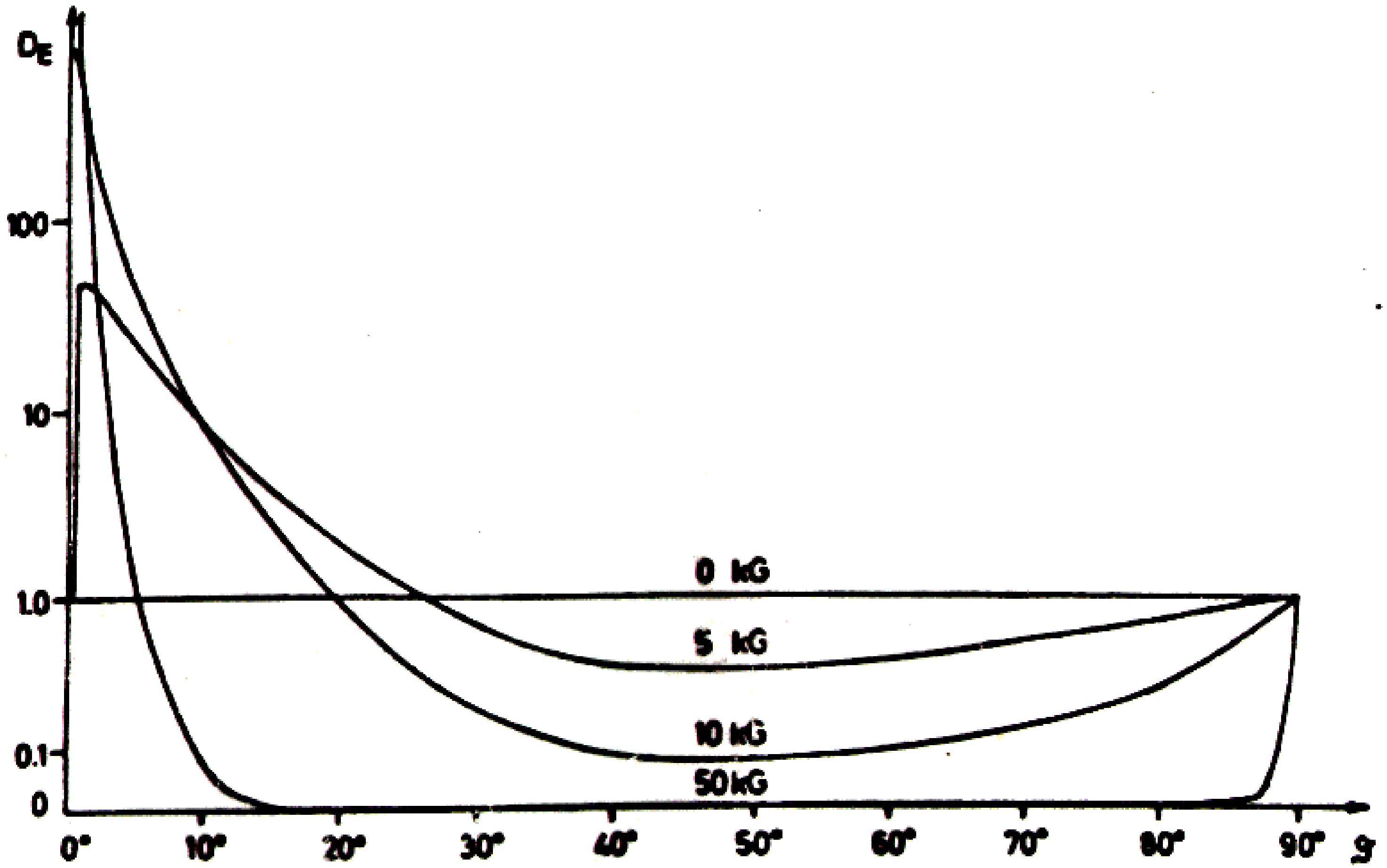


Fig. 9. The texture function $D_E(\vartheta)$ of polycrystalline $FeCO_3$ mixed with active carbon powder at 185 K after some applied fields H. (The ordinate is semilogarithmic so that it is proportional to $\log(D_E + 0{\cdot}1)$).

Goldanskii - Karyagin - Effekt

Die Gitterschwingungen sind anisotrop:

$$\langle x^2\rangle \neq \langle y^2\rangle \neq \langle z^2\rangle$$

$$\Downarrow$$

$$\underline{k} = k\,(\sin\vartheta\cos\varphi,\ \sin\vartheta\sin\varphi,\ \cos\vartheta)$$

$$f(\underline{k}) = e^{-k^2\left[(\cos^2\varphi\langle x^2\rangle + \sin^2\varphi\langle y^2\rangle)\sin^2\vartheta + \langle z^2\rangle\cos^2\vartheta\right]}$$

Super-Textur:

$$\Theta^L_{m'm}(\underline{\beta}) = t^L_{m'm}\ f(S^E, \underline{\beta})$$

$$\Uparrow$$

$$\underbrace{(0, \vartheta, \pi-\varphi)}$$

$$\Downarrow$$

$$= \sum_{Lm} f^L_m D^L_{0m}(\underline{\beta})$$

$$\tilde{A}_{L't} = \sum_{LL''mk} a^L_m \begin{pmatrix} L & L' & L'' \\ -q+p & q-p & 0 \end{pmatrix}\begin{pmatrix} L & L' & L'' \\ -m & k & m-k \end{pmatrix} t^{L'}_{tk} f^{L''}_{m-k}$$

$$\Downarrow$$

$$a^0_0 = \frac{1}{3}\,Sp\,(\underline{I}^1)$$

$$a^2_0 = \frac{1}{3}\,(I^1_{11} - I^1_{00})$$

$$a^2_{\pm 2} = \frac{1}{\sqrt{6}}\,I^1_{1-1}$$

$$f_{zz} = \frac{1}{2}(f_{xx} + f_{yy}) - \frac{\eta}{2}(f_{xx} - f_{yy})$$

Harmonische Näherung:

$$\underline{\underline{M}} = \begin{pmatrix} \langle x^2\rangle & 0 & 0 \\ 0 & \langle y^2\rangle & 0 \\ 0 & 0 & \langle z^2\rangle \end{pmatrix}$$

$$f(\underline{k}) = e^{-\underline{k}\underline{\underline{M}}\underline{k}}$$

$$f_m^L = (2L+1)\frac{1}{4\pi}\int f(\beta,\gamma)\left[D_{m0}^L(\beta,\gamma)\right]^+ \sin\beta \, d\beta \, d\gamma$$

$f_m^L = 0$ für L = ungerade

$f_m^L = f_{-m}^L$

Axialsymmetrie: $\langle x^2\rangle = \langle y^2\rangle \neq \langle z^2\rangle \Rightarrow f_m^L \sim \delta_{m0}$

Anisotropieparameter:

$$\varepsilon = k^2(\langle z^2\rangle - \langle x^2\rangle)$$

$$f_0^0 = e^{-k^2\langle x^2\rangle}\left(1 - \frac{1}{3}\varepsilon + \frac{1}{10}\varepsilon^2 + \dots\right)$$

$$f_0^2 = e^{-k\langle x^2\rangle}\,\varepsilon\left(-\frac{2}{3} + \frac{2}{7}\varepsilon + \dots\right)$$

$\vdots$ $\qquad\qquad$ $\vdots$

Unpolarisierte Quelle $(\underline{\underline{g}} = \frac{1}{2}\underline{\underline{1}})$, $3/2^- \to 1/2^-$ (M1)

Intensitätsverhältnis π/σ:

$$R = \frac{\frac{1}{2} + \tilde{A}^{\pi}_{20}}{\frac{1}{2} - \tilde{A}^{\pi}_{20}}$$

Axialsymmetrie: $f^2_2 = f^2_{-2} = 0$

$$R = \frac{\frac{1}{2} + \frac{1}{20}\frac{f^2_0}{f^0_0}}{\frac{1}{2} - \frac{1}{20}\frac{f^2_0}{f^0_0}} \approx 1 - \frac{2}{15}\varepsilon - \frac{337}{2625}\varepsilon^2 + \ldots \approx$$

$$\approx 1 - 0.133\,\varepsilon - 0.128\,\varepsilon^2 + \ldots$$

z.B. $R = 0.93 \Rightarrow \varepsilon \approx 0.4$ $\lambda = 0.086$ nm (^{57}Fe)

$$\Downarrow$$

$$\sqrt{\langle z^2\rangle - \langle x^2\rangle} = \frac{\sqrt{\varepsilon}}{k} = \frac{\sqrt{\varepsilon}\,\lambda}{2\pi} = 0.009 \text{ nm}$$

$$\varepsilon \sim k^2 \sim E_\gamma^2$$

$$\Downarrow$$

GKE kann bei höheren Energien besser beobachtet werden (z.B.: ^{119}Sn / 23.8 keV

^{151}Eu / 21.6 keV

^{156}Gd / 89 keV)

Intensitätstensor (nur für L = 1)

A_{2m} ist sphärischer Tensor 2-ter Stufe.

Cartesische Komponenten:

$$T_{xx} = -\frac{1}{2} A_{20} + \frac{\sqrt{6}}{4} \left(A_{22} + A_{2-2} \right)$$

$$T_{yy} = -\frac{1}{2} A_{20} - \frac{\sqrt{6}}{4} \left(A_{22} + A_{2-2} \right)$$

$$T_{zz} = A_{20}$$

$$T_{xy} = T_{yx} = -i \frac{\sqrt{6}}{4} \left(A_{22} - A_{2-2} \right)$$

$$T_{xz} = T_{zx} = -\frac{\sqrt{6}}{4} \left(A_{21} - A_{2-1} \right)$$

$$T_{yz} = T_{zy} = i \frac{\sqrt{6}}{4} \left(A_{21} + A_{2-1} \right)$$

Absorptionsfläche für unpolarisierte Quelle:

$$A^{\substack{\pi\\\sigma}} = f_0 \, t \, (\Gamma \pi / 2) \underbrace{r_{11}^{\substack{\pi\\\sigma}}}_{\Downarrow \;\; \frac{1}{2} + A_{20}^{\substack{\pi\\\sigma}}}$$

$$\boxed{T_{zz}^{\substack{\pi\\\sigma}} = A_{20}^{\substack{\pi\\\sigma}} = \frac{A^{\substack{\pi\\\sigma}}}{A^{\pi} + A^{\sigma}} - \frac{1}{2}}$$

Spezialfälle:

- **Random Pulver**

$$\underline{\underline{T}}^{\pi} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$T_{zz}(\vartheta) = \underline{e}_z^T \, \underline{\underline{0}} \, \underline{e}_z^T = 0$$

Quadrupolspektrum symmetrisch.

- **Axiale Textur**

$$\underline{\underline{T}}^{\pi} = \begin{pmatrix} d & 0 & 0 \\ 0 & d & 0 \\ 0 & 0 & -2d \end{pmatrix}$$

$$T_{zz}(\vartheta) = d \sin^2\vartheta - 2d \cos^2\vartheta =$$

$$= d\,(1 - 3\cos^2\vartheta)$$

$$T_{zz}(\vartheta) = 0 \text{ für } \begin{cases} d = 0 & \text{keine Textur} \\ \vartheta = 54.7^\circ & \text{magischer Winkel} \end{cases}$$

EFG

$$q = \frac{V_{zz}}{e}$$

$$\eta q = \frac{V_{xx} - V_{yy}}{e}$$

$$q = (1-R_s)\, q_{Ion} + (1-\gamma_\infty)\, q_{Gitter}$$

$$\eta q = (1-R_s)\, \eta_{Ion}\, q_{Ion} + (1-\gamma_\infty)\, \eta_{Gitter}\, q_{Gitter}$$

Sternheimersche Antiabschirmungsfaktoren

$0 \lesssim R_s \lesssim 1$ $\qquad -100 \lesssim \gamma_\infty \lesssim +100$

Punktladungsmodell:

$$q_{Gitter} = \frac{1}{e} \sum_i e_i \frac{3\cos^2\vartheta_i - 1}{r_i^3}$$

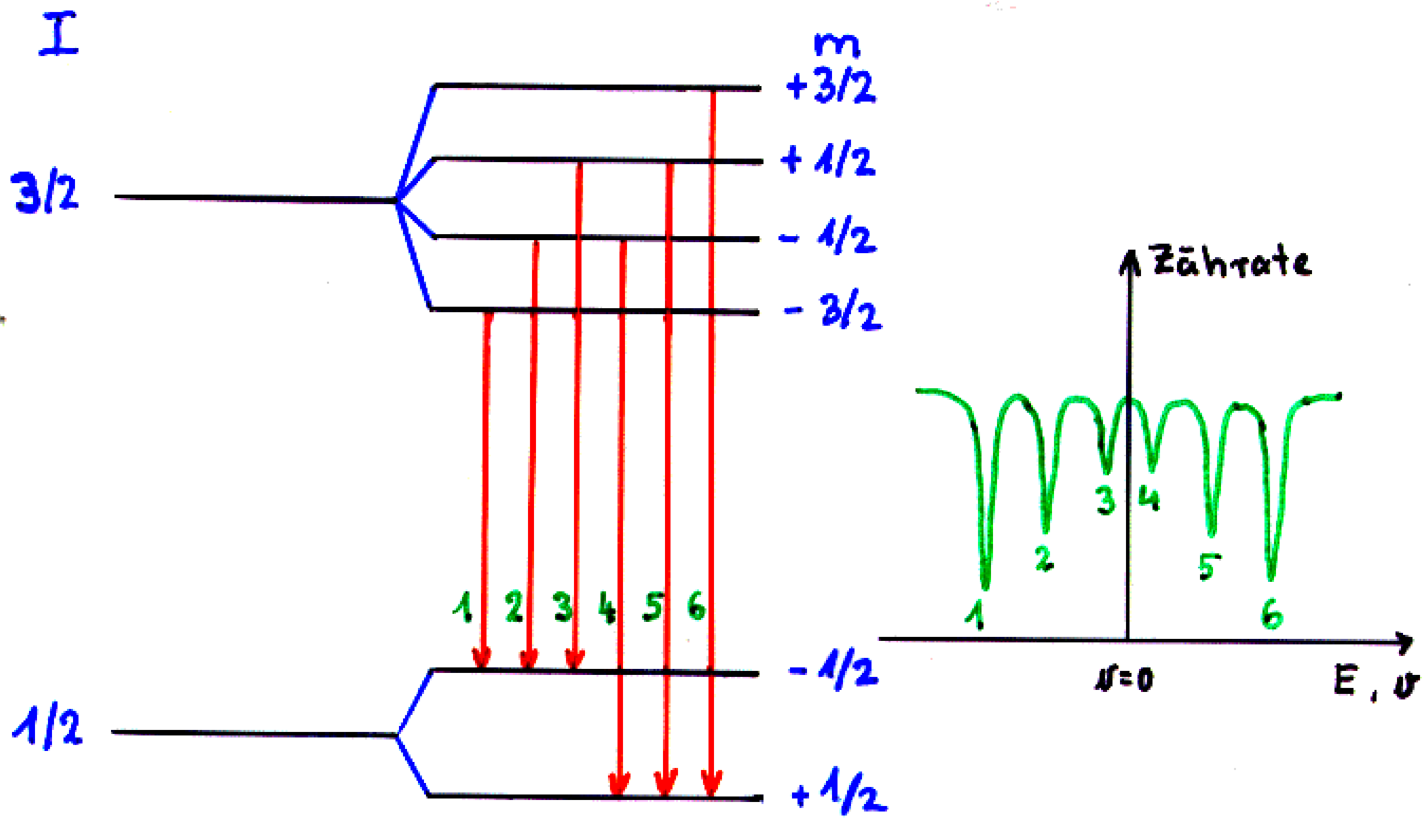
$$\eta_{Gitter}\, q_{Gitter} = \frac{1}{e} \sum_i e_i \frac{3\sin^2\vartheta_i \cos 2\varphi_i}{r_i^3}$$

Problem: effektive Ladungen

Magnetische Aufspaltung

$$|I, m\rangle : \qquad E_M = -g\mu_N H m$$

z.B.: $3/2^- \rightarrow 1/2^-$ (M1) $[{}^{57}Fe]$



$$H \sim v_6 - v_1$$

$$\underline{H} = \underline{H}_0 - D\underline{M} + \frac{4\pi}{3}\underline{M} + \underline{H}_d + \underline{H}_s + \underline{H}_L + \underline{H}_D$$

$\underline{H}_0$: Äußeres Feld

$-D\underline{M}$: Demagnetisierungsfeld

$\frac{4\pi}{3}\underline{M}$: Lorentz-Feld

$\underline{H}_d$: Dipolfeld äußerer Dipole

$\underline{H}_s$: Fermi-Kontaktfeld

$\underline{H}_L$: Bahndrehimpuls-Feld

$\underline{H}_D$: Spin-Dipolfeld

Klein für Proben ohne spontane Magnetisierung

$$H_s \sim \langle \underline{S} \rangle$$
$$H_L \sim \langle \underline{L} \rangle$$