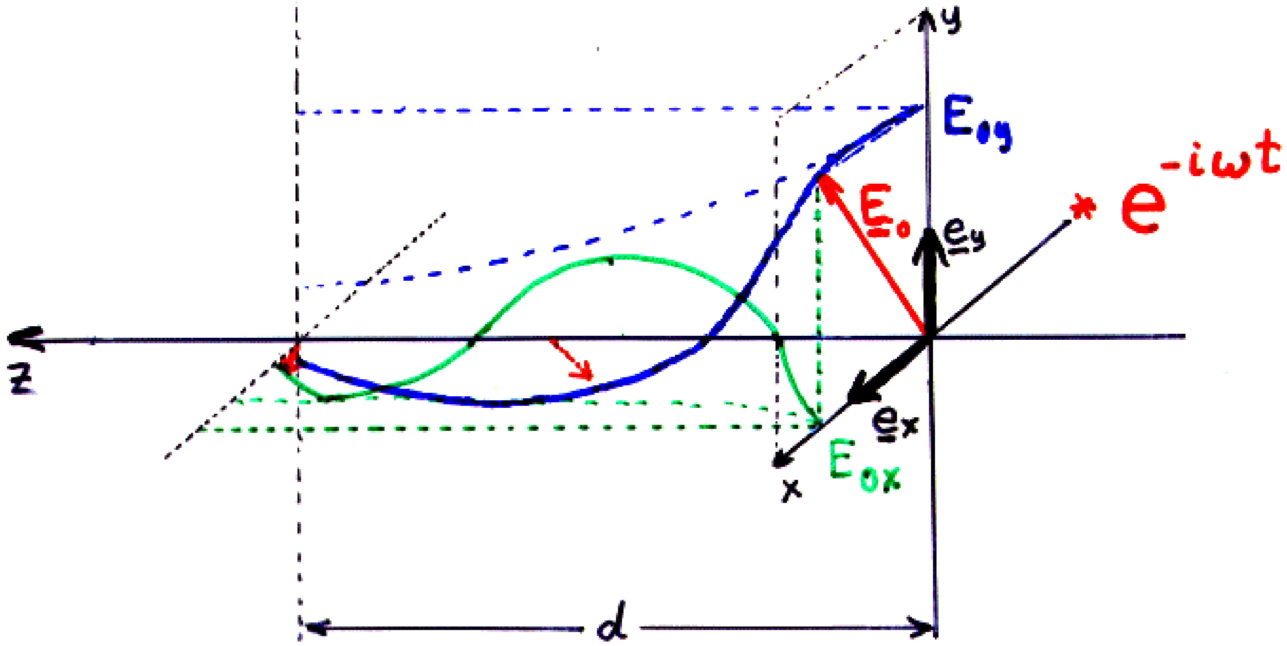
Die Absorption polarisierter Strahlung

(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-Hermitisch 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:

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

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

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

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

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

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

Dichtematrix:

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

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

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

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

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

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

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

Die Dichtematrix (Kohärenzmatrix) einer vollständig polarisierten Strahlung ist idempotent (Projektionsmatrix): $\underline{\underline{\rho}}^2 = \underline{\underline{\rho}}$.

Die Dichtematrix bei $z = d$:

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

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

Kohärente Strahlung:

$$\underline{E} = \underbrace{E_x}_{\Downarrow\ |E_x|e^{i\alpha_x}}\,\underline{e}_x + \underbrace{E_y}_{\Downarrow\ |E_y|e^{i\alpha_y}}\,\underline{e}_y$$

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

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

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

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

$\alpha = \alpha_y - \alpha_x$

$$\underline{\underline{\rho}} = \begin{pmatrix} \cos^2\varphi & \frac{1}{2}\sin 2\varphi\, e^{i\alpha} \\ \frac{1}{2}\sin 2\varphi\, e^{-i\alpha} & \sin^2\varphi \end{pmatrix}$$

$$\underline{\underline{\rho}}^2 = \underline{\underline{\rho}} \qquad\qquad Sp(\underline{\underline{\rho}}) = 1$$

Inkohärente Strahlung:

Unkorrelierte Wellen: $\underline{E}_1, \underline{E}_2, \dots \underline{E}_\nu, \dots \underline{E}_N$

$$I_\nu \sim |\underline{E}_\nu|^2$$

$$I = \sum_{\nu=1}^{N} I_\nu = \sum_{\nu=1}^{N} I_{\nu 0}\, Sp\left(e^{i\underline{\underline{n}}kz}\, \underline{\underline{\rho}}_{\nu 0}\, e^{-i\underline{\underline{n}}^+ kz}\right) =$$

$$= Sp\left(e^{i\underline{\underline{n}}kz} \underbrace{\sum_{\nu=1}^{N} I_{\nu 0}\, \underline{\underline{\rho}}_{\nu 0}}_{\bar{\underline{\underline{\rho}}}_0 \sum_{\nu=1}^{N} I_{\nu 0}} e^{-i\underline{\underline{n}}^+ kz}\right)$$

$$\boxed{\bar{\underline{\underline{\rho}}}_0 := \frac{\sum_{\nu=1}^{N} I_{\nu 0}\, \underline{\underline{\rho}}_{\nu 0}}{\sum_{\nu=1}^{N} I_{\nu 0}}}$$

Annahme (RPA): φ, α sind random verteilt und es gibt keine Korrelation zwischen ν, φ und α.

$$\bar{\underline{\underline{\rho}}}_0 = \langle \underline{\underline{\rho}}_{\nu 0} \rangle = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

$$\bar{\underline{\underline{\rho}}}_0^2 = \begin{pmatrix} 1/4 & 0 \\ 0 & 1/4 \end{pmatrix} \neq \bar{\underline{\underline{\rho}}}_0 \qquad\qquad Sp(\bar{\underline{\underline{\rho}}}_0) = 1$$

$\underline{\underline{\rho}}^2 = \underline{\underline{\rho}}$ 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:

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

Linearpolarisiert:

$\parallel x$ | $\parallel y$ | 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 $Sp(\underline{\underline{\rho}}) = 1$

$$\underline{\underline{\rho}} = \frac{1}{2}\left(\underline{\underline{1}} + \underline{P}\,\underline{\underline{\sigma}}\right)$$

Super-Vektor $\begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{pmatrix}$

(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 $(\underline{u}_+, \underline{u}_-) \Rightarrow (\underline{e}_x, \underline{e}_y)$

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

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

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

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

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

Linearpolarisierte Strahlung (Richtung φ):

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

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

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

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

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

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

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

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:

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

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

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

Der Poincaré-Vektor:

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

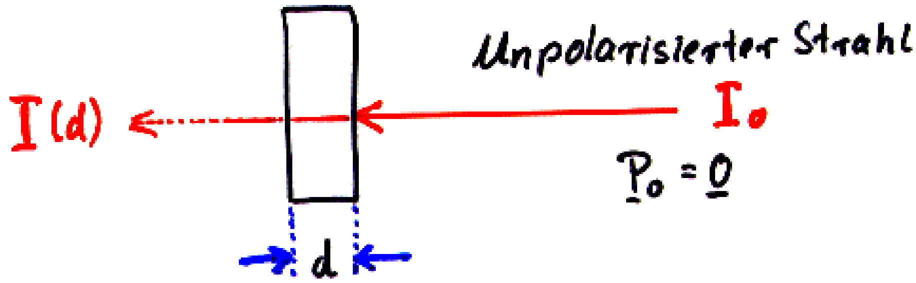
$$\Downarrow$$

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

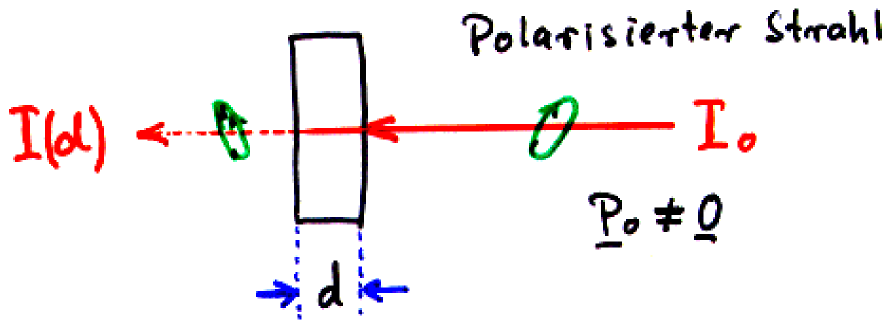
$b = \sqrt{b_\xi^2 + b_\eta^2 + b_\zeta^2}$ $\qquad$ $\hat{\underline{b}} = \underline{b}/b$

Wichtige Spezialfälle:

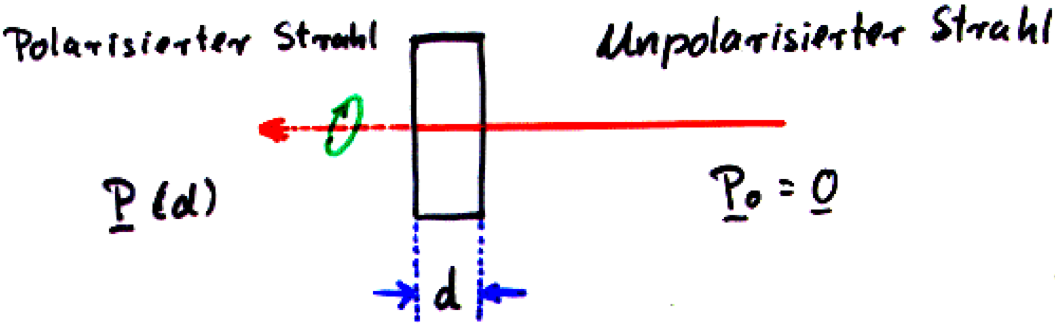
1.



2.



3.



Vereinfachung, wenn $[n, n^+] = 0$:

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

$$= I_0 \, Sp\left(\underline{\underline{\rho}}_0 \, \underbrace{e^{-i\underline{\underline{n}}^+kd} \, e^{i\underline{\underline{n}}kd}}_{e^{-ikd(\underline{\underline{n}}^+ - \underline{\underline{n}})}}\right) =$$

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

$i(\underline{\underline{n}}^+ - \underline{\underline{n}})$ ist Hermit'sch: $[i(\underline{\underline{n}}^+ - n)]^+ = -i(\underline{\underline{n}} - \underline{\underline{n}}^+) = i(\underline{\underline{n}}^+ - \underline{\underline{n}})$

$\underline{\underline{\nu}} = ikd(\underline{\underline{n}}^+ - \underline{\underline{n}})$ 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 unpolarisierten Strahl:

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

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

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

3

Brechungsindex

Annahmen:
- schwache Absorption ($n \sim 1$)
- random verteilte Streuzentren

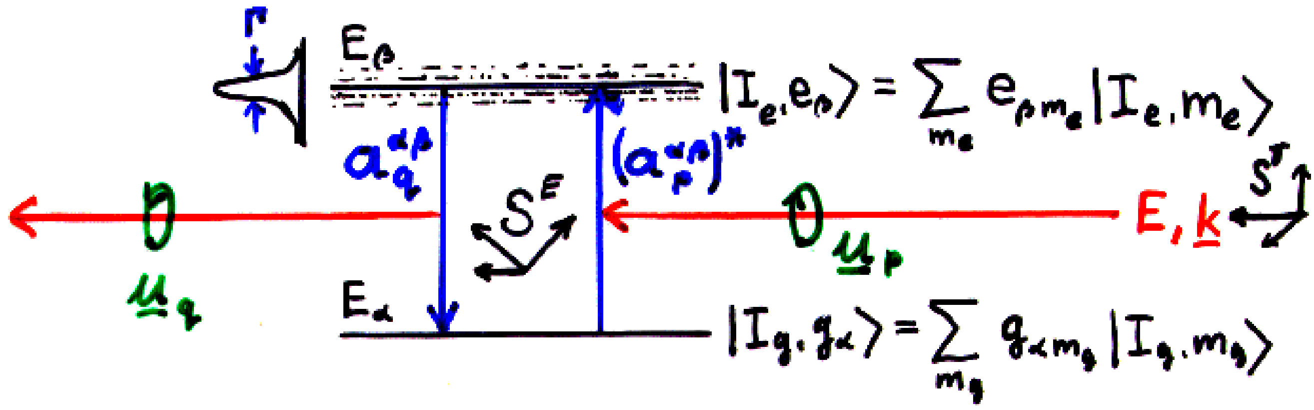
$$\boxed{n_{pq} = \delta_{pq} - \frac{2\pi}{k^2} N F_{pq}}$$

Polarisation

Streuamplitude der kohärenten Vorwärtsstreuung

Anzahl der Streuzentren / Volumen

- nur Mößbauer-Streuung
  (keine Photoelektrische Absorption)



Für mehrere angeregte Zustände:

$$\boxed{F_{pq}^{\alpha} = \left(\frac{kV}{2\pi \hbar c}\right) f(\underline{k}) \sum_{\beta} \frac{(a_p^{\alpha\beta})^* (a_q^{\alpha\beta})}{E - (E_\beta - E_\alpha) + i\frac{\Gamma}{2}}}$$

V: Normierungsvolumen

Mößbauer-Lamb-Faktor

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 $T \gtrsim 1\,K$:

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

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 Matrix-element des M1 Übergangs

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

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

Absorbermatrix:

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

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

maximaler Wirkungsquerschnitt

$$\sigma_0 = \frac{4 M_1^2}{(2I_g+1)k\Gamma}$$

$$\tau_{pq}^{\alpha\beta}(\underline{\vartheta}) = \sum_{M,M'} D_{pM}^{1+}(\underline{\vartheta})\, \underbrace{V_{1M}^{\alpha\beta *}\, V_{1M'}^{\alpha\beta}}_{I_{MM'}^{1,\alpha\beta}}\, D_{M'q}^{1}(\underline{\vartheta})$$

Intensitätsmatrix

Intensitätsmatrix bei allgemeiner Multipolarität:

$$I_{MM'}^{L\alpha\beta} := V_{LM}^{\alpha\beta *}\, V_{LM'}^{\alpha\beta}$$

Transformation von $V_{LM}^{\alpha\beta}$:

$$V_{LM}^{\alpha\beta}(S^\vartheta) = \sum_{M'} V_{LM'}^{\alpha\beta}(S^E)\, D_{M'n}(\underline{\vartheta})$$

Transformation von $I_{MM'}^{L,\alpha\beta}$:

$$I_{pq}^{L,\alpha\beta}(S^\vartheta) = \sum_{M,M'} D_{pM}^{L+}(\underline{\vartheta})\, I_{MM'}^{L,\alpha\beta}(S^E)\, D_{M'q}^{L}(\underline{\vartheta})$$

Für M 1:

$$\boxed{\tau_{pq}^{\alpha\beta} = I_{pq}^{1,\alpha\beta}}$$

($\underline{\underline{\tau}}^{\alpha\beta} \neq \underline{\underline{I}}^{1,\alpha\beta}$, da $\underline{\underline{\tau}}^{\alpha\beta}$ (2×2) während $\underline{\underline{I}}^{1,\alpha\beta}$ (3×3) Matrix)

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:

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

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

$$N = \sum_j N_j$$

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

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

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

Effektive Dicke:

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

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

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

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

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

Winkel der Totalreflexion $\approx 10^{-3} \dots 10^{-2} \approx 0.1^\circ \dots 1^\circ$

$$\boxed{\underline{\underline{n}}\,k\,d = k\,d\,\underline{\underline{1}} - \frac{1}{2}t \sum_{\alpha\beta} \overline{\underline{\underline{T}}}^{\alpha\beta} \frac{\frac{\Gamma}{2}}{E-(E_\beta - E_\alpha)+i\frac{\Gamma}{2}}}$$

$$\alpha = (\alpha', i_{\alpha'}) \qquad \beta = (\beta', j_{\beta'})$$

$i_{\alpha'}$: Index des Zustandes innerhalb des entarteten Multipletts

α': Index des entarteten Mutipletts

$$\sum_{\alpha\beta} \overline{\underline{\underline{T}}}^{\alpha\beta} \frac{\Gamma/2}{E-(E_\beta-E_\alpha)+i(\Gamma/2)} =$$

$$= \sum_{\alpha'\beta'} \underbrace{\sum_{i_{\alpha'} j_{\beta'}} \overline{\underline{\underline{T}}}^{(\alpha', i_{\alpha'})(\beta', j_{\beta'})}}_{:= \overline{\underline{\underline{T}}}^{\alpha'\beta'}} \frac{\Gamma/2}{E-(E_{\beta'}-E_{\alpha'})+i(\Gamma/2)}$$

Mittlere Intensitätsmatrix: (M1)

$$\overline{\underline{\underline{I}}}^1(S^\uparrow) = \frac{1}{N\bar{f}(k)} \sum_j f_j(\underline{k})\, N_j\, \underline{\underline{D}}^{1^+}(\underline{\vartheta}_j)\, \underline{\underline{I}}^1(S_j^E)\, \underline{\underline{D}}^1(\underline{\vartheta}_j)$$

Wenn $f_j(\underline{k}) = \bar{f}(\underline{k}) = \bar{f} = \text{const}$ (kein Goldanskii-Karyagin-Effekt):

$$\boxed{\overline{\underline{\underline{I}}}^1(S^\uparrow) = \frac{1}{N} \sum_j N_j\, \underline{\underline{D}}^{1^+}(\underline{\vartheta}_j)\, \underline{\underline{I}}^1(S_j^E)\, \underline{\underline{D}}^1(\underline{\vartheta}_j) = \underline{\underline{D}}^{1^+}(\underline{\vartheta})\, \overline{\underline{\underline{I}}}^1(S^A)\, \underline{\underline{D}}^1(\underline{\vartheta})}$$

Absorber-System

Intensität der Linie i: I_{si} $\sum_i I_{si} = 1$

Dichtematrix der Linie i: $\underline{\underline{\rho}}_{si}$

Dichtematrix der Quelle bei Energie E und Geschwindigkeit v:

$$\underline{\underline{S}}(E,v) = \sum_i I_{si}\, \underline{\underline{\rho}}_{si}\, L_{si}(E,v)$$

Gesamtintensität hinter dem Absorber (Dicke d):

$$\boxed{I(d,E,v) = Sp\left[e^{i\underline{\underline{n}}kd}\, \underline{\underline{S}}(E,v)\, e^{-i\underline{\underline{n}}^+kd}\right]}$$

Zählrate hinter dem Absorber:

$$\boxed{N(d,v) = N(d,\infty)\left[1-\underbrace{f_s\left(1-\frac{2}{\Gamma\pi}\int_{-\infty}^{\infty} I(d,E,v)\,dE\right)}_{SP(v)}\right]}$$

Mößbauer-Lamb-Faktor der Quelle

Spezialfälle:

- Unpolarisierte Einzellinien-Quelle:

$$SP(v) = f_s\left\{1-\frac{1}{\Gamma\pi}\int_{-\infty}^{\infty} L_s(E,v)\, Sp\left(e^{i\underline{\underline{n}}kd}\, e^{-i\underline{\underline{n}}^+kd}\right) dE\right\}$$

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

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

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

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

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

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

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:

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

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

Die Intensitätsmatrix eines einzelnen Überganges

Summenregeln

	Allgemein	für $L=1,\ I_g=1/2,\ I_e=3/2$
$\sum_\alpha Sp(\underline{\underline{I}}^L)^{\alpha\beta} =$	$\dfrac{2L+1}{2I_e+1}$	$= \dfrac{3}{4}$
$\sum_\beta Sp(\underline{\underline{I}}^L)^{\alpha\beta} =$	$\dfrac{2L+1}{2I_g+1}$	$= \dfrac{3}{2}$
$\sum_{\alpha\beta} (\underline{\underline{I}}^L)^{\alpha\beta}_{MM'} =$	$\delta_{MM'}$	$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

$$\sum_{\alpha\beta} T^{\alpha\beta}_{pq} = \delta_{pq} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$\uparrow$

Eine Einzellinie kann den Polarisationszustand nicht ändern

Symmetrieeigenschaften für reine Quadrupol-WW

$I^L_{MM'}$ ist reel

$I^L_{MM'} = 0$ für $M + M' =$ *ungerade* (Schachbrett-Regel)

$I^L_{MM'} = I^L_{M'M}$

$I^L_{MM'} = I^L_{-M\,-M'}$

$$\begin{pmatrix} I_{11} & 0 & I_{1-1} \\ 0 & I_{00} & 0 \\ I_{1-1} & 0 & I_{11} \end{pmatrix}$$

$I_g = 1/2$, $I_e = 3/2$, 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

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

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

M = 1 0 -1

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

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

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

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

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