Die Übergänge

$$\tfrac{1}{2} \to 1 \qquad \tfrac{1}{2} \to 2 \qquad -\tfrac{1}{2} \to 1 \qquad -\tfrac{1}{2} \to 2$$

sind entartet.

$$\underline{\underline{I}}^{\pi} = \underline{\underline{I}}^{\frac{1}{2}1} + \underline{\underline{I}}^{\frac{1}{2}2} + \underline{\underline{I}}^{-\frac{1}{2}1} + \underline{\underline{I}}^{-\frac{1}{2}2}$$

$$\underline{\underline{I}}^{\sigma} = \underline{\underline{1}} - \underline{\underline{I}}^{\pi}$$

$$\underline{\underline{I}}^{\pi} = \begin{pmatrix} \frac{3}{4}e_+^2 + \frac{1}{4}e_-^2 & 0 & \frac{\sqrt{3}}{2}e_+e_- \\ 0 & e_-^2 & 0 \\ \frac{\sqrt{3}}{2}e_+e_- & 0 & \frac{3}{4}e_+^2 + \frac{1}{4}e_-^2 \end{pmatrix}$$

$$\underline{\underline{\tau}}^{\pi} = \begin{pmatrix} \frac{3}{4}e_+^2 - \frac{1}{4}e_-^2 & \frac{\sqrt{3}}{2}e_+e_- \\ \frac{\sqrt{3}}{2}e_+e_- & \frac{3}{4}e_+^2 + \frac{1}{4}e_-^2 \end{pmatrix}$$

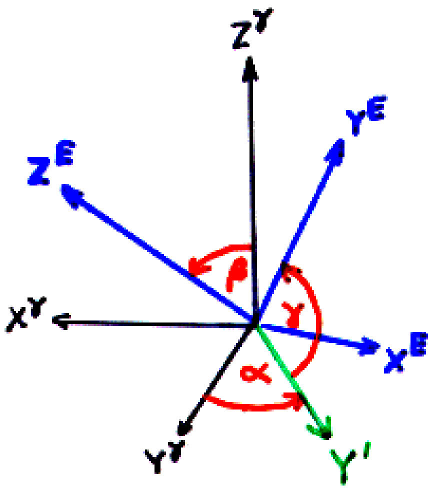
$$\underline{\underline{\tau}}^{\sigma} = \underline{\underline{1}} - \underline{\underline{\tau}}^{\pi} \Rightarrow [\underline{\underline{\tau}}^{\pi}, \underline{\underline{\tau}}^{\sigma}] = 0 \Rightarrow [\underline{\underline{n}}, \underline{\underline{n}}^+] = 0$$

$$\underline{\underline{n}}kd = kd \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \frac{1}{2}t \left[\begin{pmatrix} \frac{3}{4}e_+^2 - \frac{1}{4}e_-^2 & \frac{\sqrt{3}}{2}e_+e_- \\ \frac{\sqrt{3}}{2}e_+e_- & \frac{3}{4}e_+^2 + \frac{1}{4}e_-^2 \end{pmatrix} \frac{\Gamma/2}{E - E_\pi + i(\Gamma/2)} + \begin{pmatrix} \frac{1}{4}e_+^2 - \frac{3}{4}e_-^2 & -\frac{\sqrt{3}}{2}e_+e_- \\ -\frac{\sqrt{3}}{2}e_+e_- & \frac{1}{4}e_+^2 - \frac{3}{4}e_-^2 \end{pmatrix} \frac{\Gamma/2}{E - E_\sigma + i(\Gamma/2)} \right]$$

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: $t^0_{00} = 1$

$t^L_{mm'} = 0$ 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:

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

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

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

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

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

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

Für random Pulver:

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

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

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

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

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:

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

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

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

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

5 Werte $\Rightarrow$ aus 5 unabhängigen Messungen

5 unabhängigen Textur-Parameter

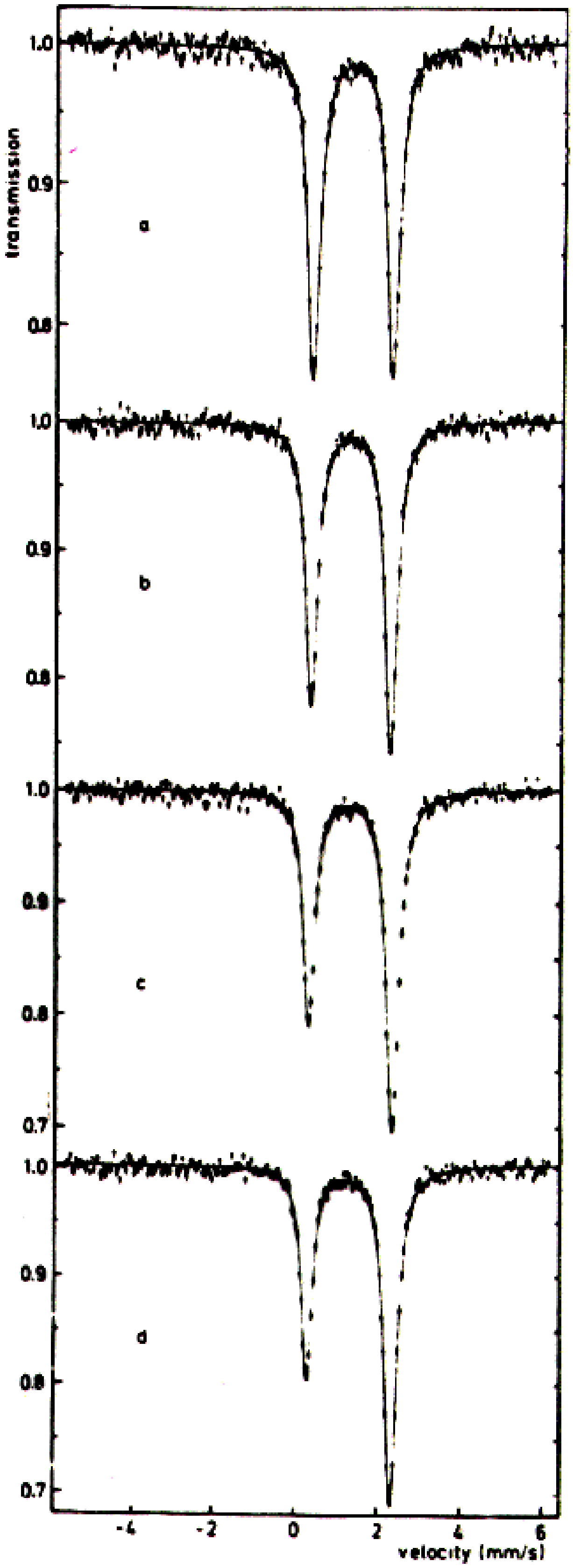


Fig. 3. Temperature dependence of the field-induced asymmetry of the Mössbauer spectrum of polycrystalline $FeCO_3$ mixed with active carbon powder. (a) Original spectrum at 185 K, (b) spectrum at 185 K after 5 kG at 185 K, (c) spectrum at 60 K after 5 kG at 60 K, (d) spectrum at 60 K after 7·5 kG at 60 K.

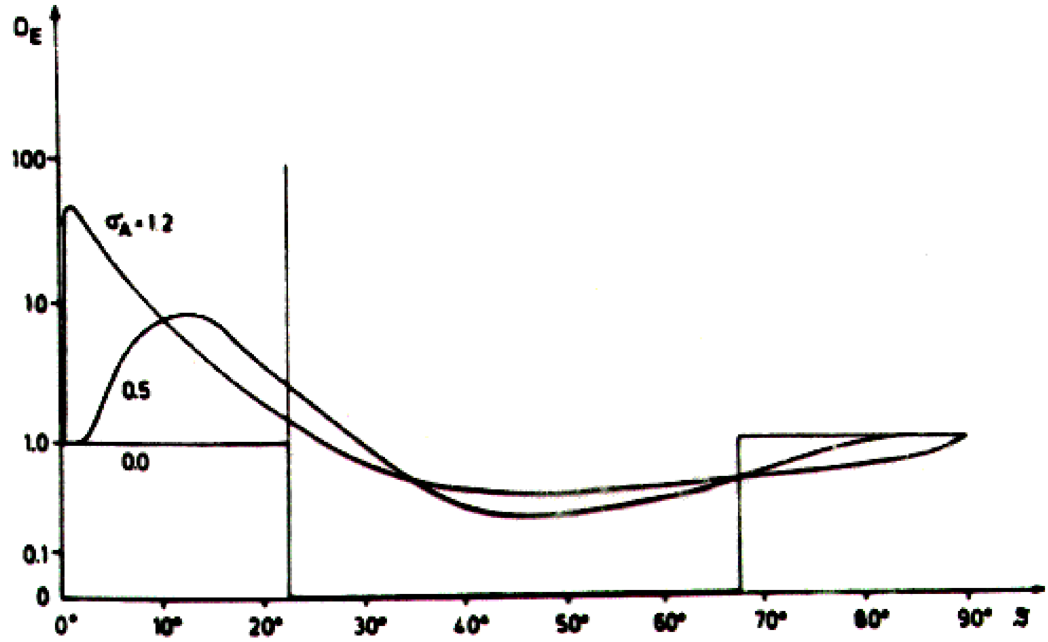


Fig. 6. The texture function $D_E(\vartheta)$ calculated with a logarithmic Gauss distribution of the critical field for some values of σ_A and $a = 0{\cdot}7056$. (The ordinate is semilogarithmic so that it is proportional to $\log(D_E + 0{\cdot}1)$.)

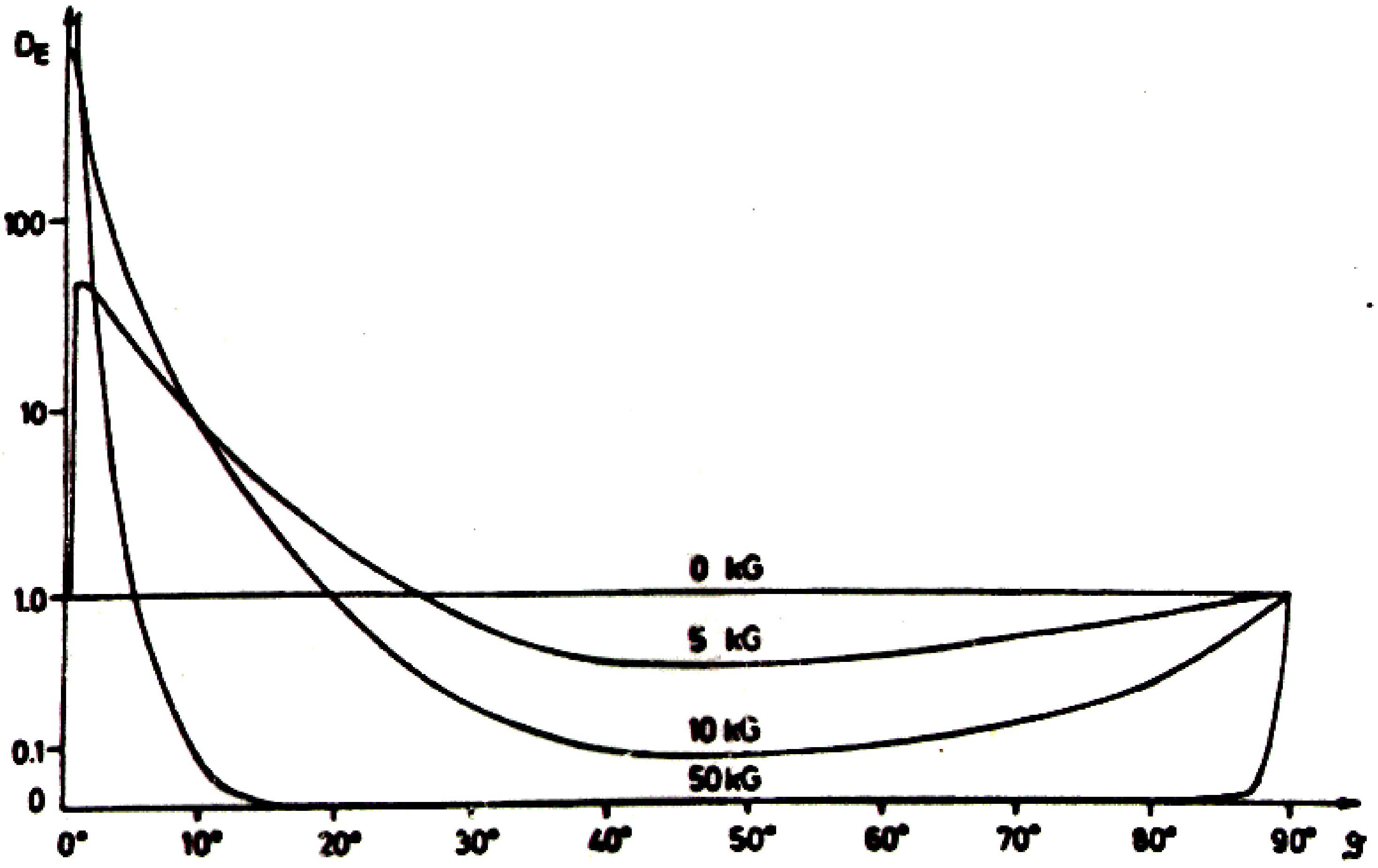


Fig. 9. The texture function $D_E(\vartheta)$ of polycrystalline $FeCO_3$ mixed with active carbon powder at 185 K after some applied fields H. (The ordinate is semilogarithmic so that it is proportional to $\log(D_E + 0{\cdot}1)$.

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:

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

$$\Uparrow$$

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

$$\Downarrow$$

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

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

$$\Downarrow$$

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

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

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

$3/2^- \to 1/2^-$ (M1) Übergang:

Random Pulver: $t^L_{m'm} = \delta_{L0}$

$$\tilde{T}^{\alpha\beta}_{11} = \tilde{A}^{\alpha\beta}_{00} + \tilde{A}^{\alpha\beta}_{20} = \tilde{T}^{\alpha\beta}_{-1-1} \qquad (\alpha\beta) = \begin{cases} \pi \\ \sigma \end{cases}$$

$$\tilde{T}^{\alpha\beta}_{1-1} = 0$$

$$\tilde{A}^{\pi}_{0\,\sigma} = 1/2$$

$$\tilde{A}^{\pi}_{20\,\sigma} = \pm\left\{\frac{1}{20\sqrt{6}}\left[\sqrt{6}\, f^2_0 + \eta\left(f^2_2 + f^2_{-2}\right)\right] \frac{1}{\sqrt{1+\frac{\eta^2}{3}}}\right\} \frac{1}{f^0_0}$$

Eigenschaften:

- $\tau^{\pi}_{pq\,\sigma} \sim \delta_{pq}$

$\Downarrow$

Die Intensitäten hängen nicht von der γ-Richtung ab

- $\tau^{\pi}_{pq} \neq \tau^{\sigma}_{pq}$

$\Downarrow$

Quadrupol-Spektren sind auch ohne Textur nicht unbedingt symmetrisch.

Gilt nicht umgekehrt:

Wenn $\sqrt{6}\, f^2_0 + \eta\left(f^2_2 + f^2_{-2}\right) = 0$, dann

$$\tau^{\pi}_{pq} = \tau^{\sigma}_{pq}$$

auch wenn $f^2_0 \neq 0,\ f^2_2 \neq 0,\ f^2_{-2} \neq 0$.

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

Harmonische Näherung:

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

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

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

$f^L_m = 0$ für L = ungerade

$f^L_m = f^L_{-m}$

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

Anisotropieparameter:

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

$$f^0_0 = e^{-k^2 \langle x^2 \rangle}\left(1 - \frac{1}{3}\varepsilon + \frac{1}{10}\varepsilon^2 + \dots\right)$$

$$f^2_0 = e^{-k\langle x^2 \rangle}\,\varepsilon\left(-\frac{2}{3} + \frac{2}{7}\varepsilon + \dots\right)$$

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

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. $R = 0.93 \Rightarrow \varepsilon \approx 0.4$ $\qquad \lambda = 0.086\ \text{nm}$ (^{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)

^{57}Fe

$3/2^- \rightarrow 1/2^-$

$E_\gamma = 14.4\ keV$

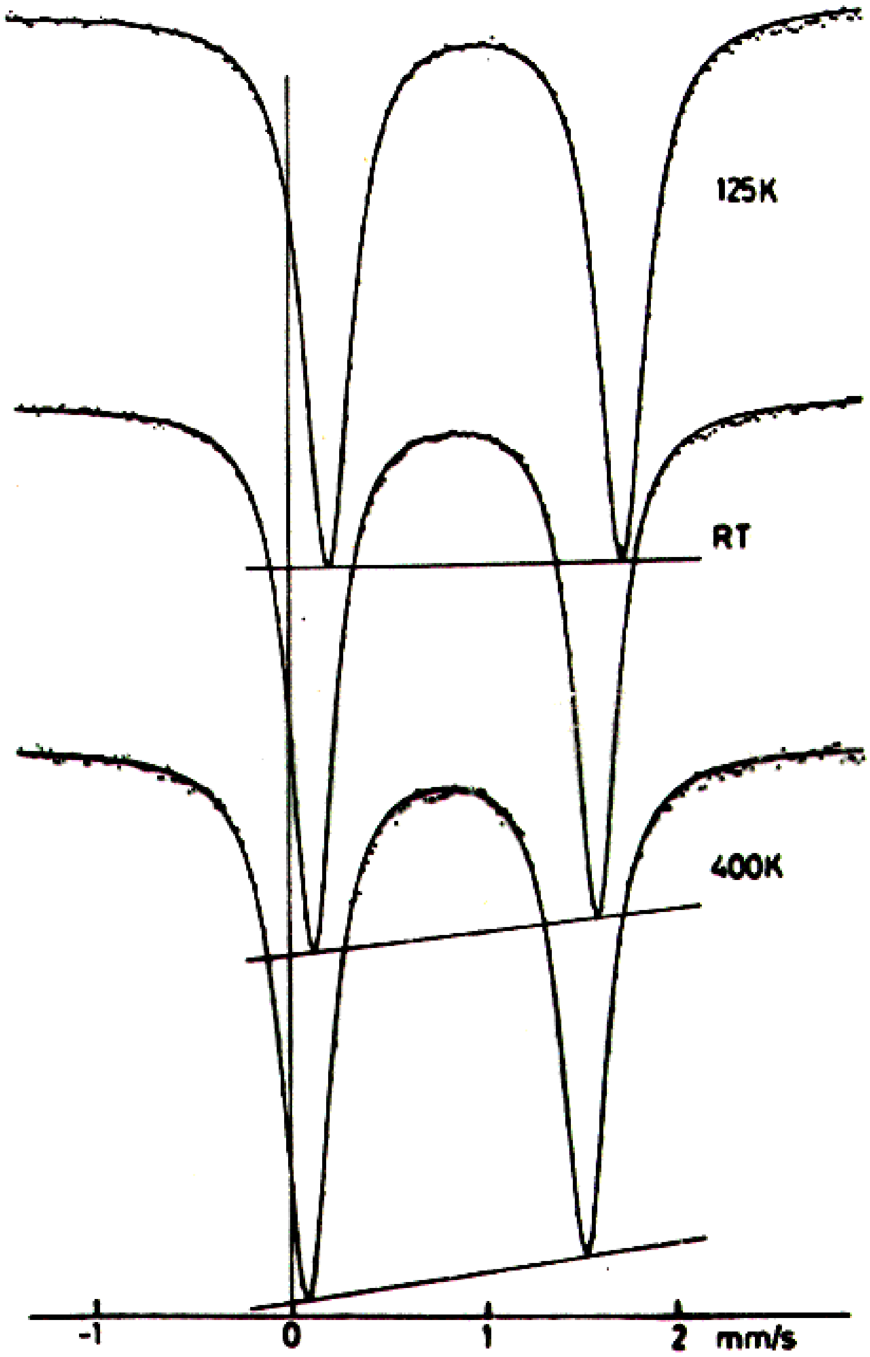
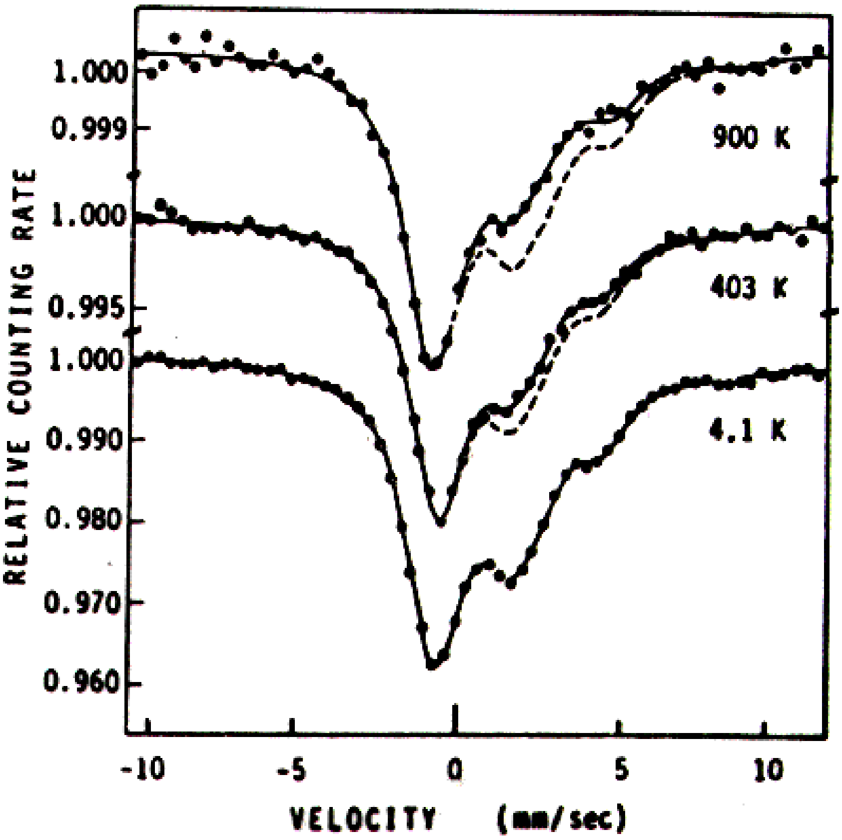


FIGURE 7. Mössbauer spectra of $FePS_3$ recorded at 125 K, room temperature, and 400 K. The asymmetry is visualized by straight lines through the peak positions (from Reference 38).

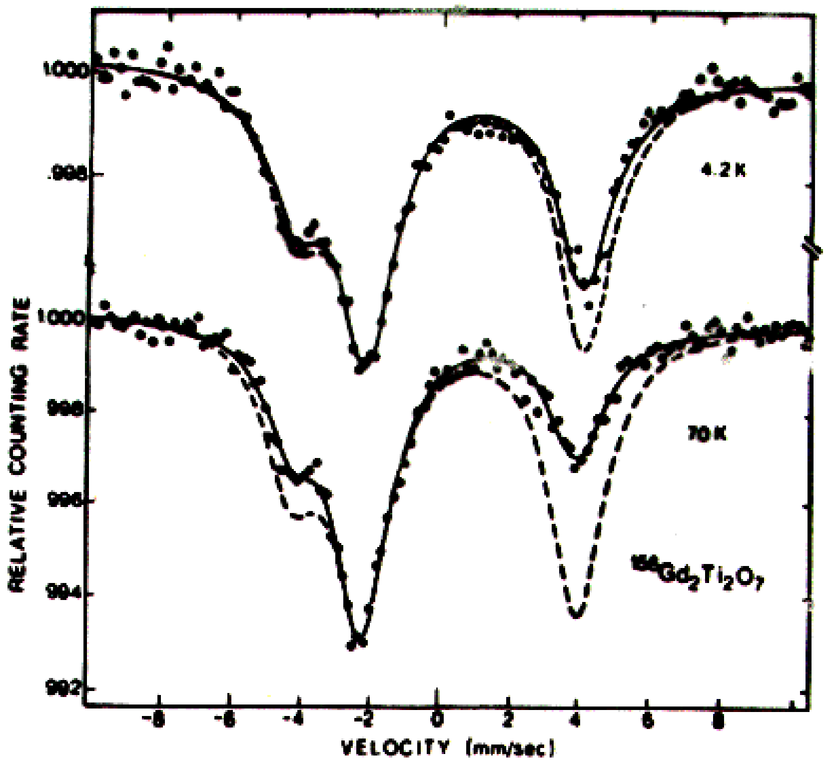


^{151}Eu

$5/2^+ \rightarrow 7/2^+$

$E_\gamma = 21.6$ keV

FIGURE 8. Recoilless absorption spectra of the 21.6-keV gamma rays of ^{151}Eu in $Eu_2Ti_2O_7$. The solid lines are the theoretical spectra obtained from least-squares computer fits to the experimental spectra, taking into account an anisotropic absorption fraction. The dashed lines are theoretical spectra obtained with isotropic absorption fraction (from Reference 41).



^{156}Gd

$2^+ \rightarrow 0^+$

$E_\gamma = 89$ keV

FIGURE 9. Recoilless absorption spectra of the 89-keV gamma rays of ^{156}Gd in $Gd_2Ti_2O_7$ at 4.2 and 70 K. The solid lines are the theoretical spectra obtained from a least-squares fit to the experimental spectra, taking into account an anisotropic absorption fraction. The dashed curves are the theoretical spectra obtained with an isotropic absorption fraction (from Reference 42).

Intensitätstensor (nur für $L = 1$)

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

Cartesische Komponenten:

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

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

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

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

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

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

Absorptionsfläche für unpolarisierte Quelle:

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

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

Asymmetrie der Intensität in Richtung $\underline{\vartheta}$:

$$T_{zz}(\underset{\overset{\Uparrow}{S^\gamma}}{\underline{\vartheta}}) = \Big[\underset{\Downarrow}{\underline{\underline{R}}}\;\underline{\underline{T}}(\underset{\overset{\Uparrow}{S^c}}{\underline{0}})\;\underline{\underline{R}}^{-1}\Big]_{zz}$$

$$\sum_i R_{ik}\,\underline{e}_i^c = \underline{\underline{R}}\,\underline{e}_k^c = \underline{e}_k^\gamma$$

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

Für einen Gitterplatz:

$$T^\pi_{pq} = \frac{1}{4\sqrt{1+\frac{\eta^2}{3}}}\begin{pmatrix} -\frac{1-\eta}{2} & 0 & 0 \\ 0 & -\frac{1+\eta}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$T^\sigma = -T^\pi$$

$$\boxed{e\,Q\,V_{pq} = 8\,\Delta E_Q\,\mathrm{sign}(V_{zz})\,T^\pi_{pq} = 8\,\Delta E_Q\,T^h_{pq}}$$

2. Invariante: $\phi_{II}(T^{\pi}_{\sigma\,pq})$

$$\boxed{T_\Delta = 64\,\phi_{II}(T^{\pi}_{\sigma\,pq}) = \begin{cases} 1 & \text{für einen Gitterplatz} \\ <1 & \text{für mehrere Gitterplätze} \end{cases}}$$

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**

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

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

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

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

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

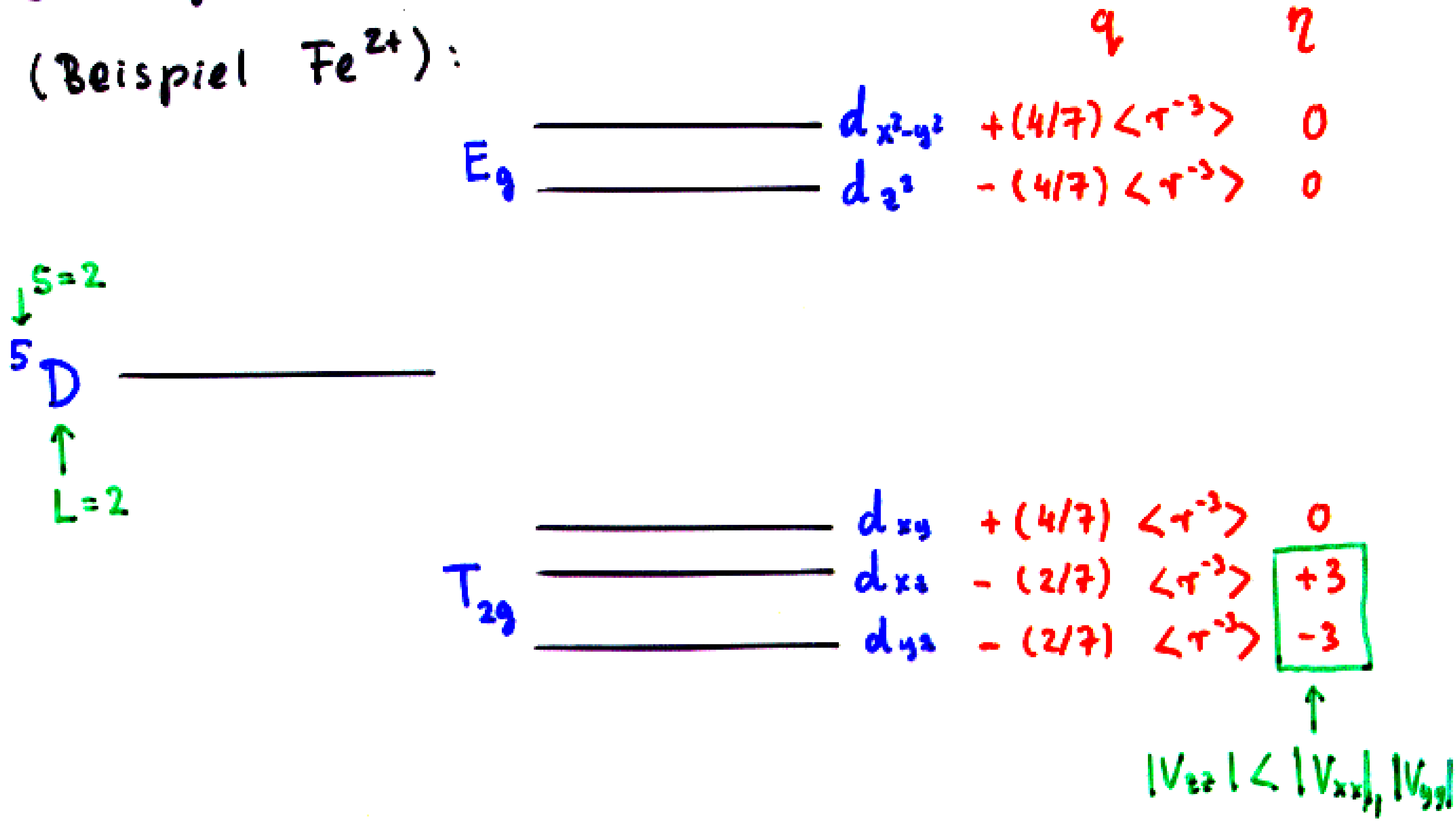
$$q_{Ion} = -\sum_i \int \Psi^*(r_1,\dots,r_z)\, \frac{3\cos^2\vartheta_i - 1}{r_i^3}\, \Psi(r_1,\dots,r_z)\, d^3r_1 \dots d^3r_z$$

$$\eta_{Ion}\, q_{Ion} = -\sum_i \int \Psi^*(r_1,\dots,r_z)\, \frac{3\sin^2\vartheta_i \cos 2\varphi_i}{r_i^3}\, \Psi(r_1,\dots,r_z)\, d^3r_1 \dots d^3r_z$$

Es genügt, das Integral nur für nicht-abgeschlossene Schalen zu bestimmen.

Beiträge der einzelnen elektronischen Zuständen:

(Beispiel Fe^{2+}):



Schnelle Relaxation: thermisches Mittelwert.

$\Downarrow$

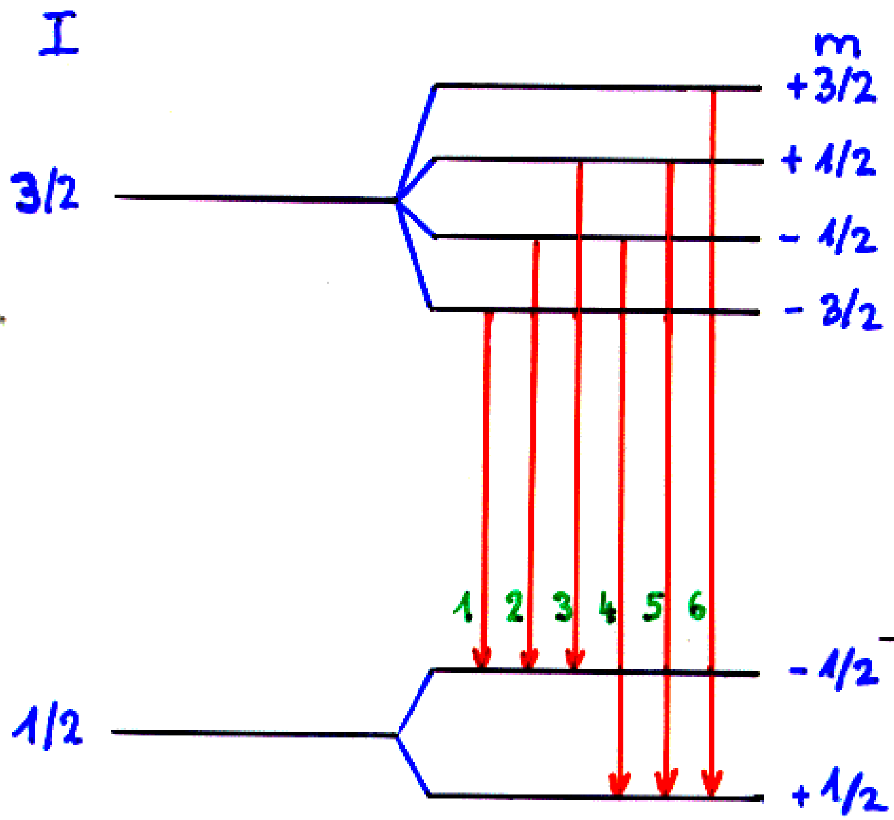
EFG temperaturabhängig.

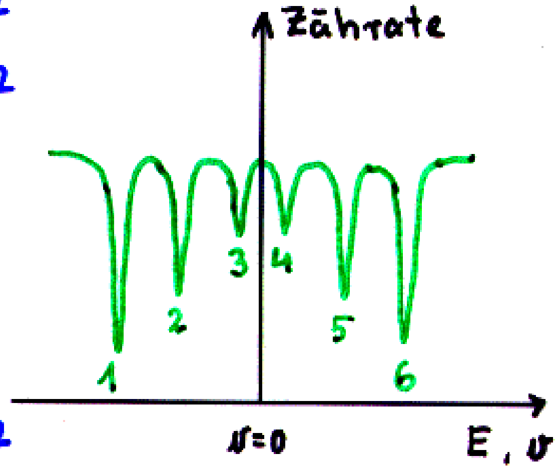
(Nicht der einzige Grund für ein temperaturabhängiges EFG!)

Magnetische Aufspaltung

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

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





$$H \sim v_6 - v_1$$

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

$\underline{H}_0$: 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

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