Line Shape Analysis of Spin Echo Signals in Cubic Solids

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In the case of static magnetic dipolar and electric quadrupolar interactions (inhomogenous broadening) the dependency of the spin echo height at time $t=2\tau$ after a $\pi/2$-τ-β pulse sequence on the rotation angle β of the second rf-pulse is calculated for the spins $I=3/2$, 5/2, 7/2, 9/2. For each spin I an optimum rotation angle β_{opt} is found out for which the spin echo signal has a maximum. From the measured spin echo lineshape the distribution function of the quadrupole distortion in a solid can be determined. The mean quadrupole distortion can be obtained from the echo width. Detailed calculations in the case of Gaussian and Lorentzian distribution functions are presented.

In cubic crystals the effect of static magnetic dipole and electric quadrupole interactions on the line shape of spin echo signals was demonstrated by SOLOMON [1], FLETT and RICHARDS [2], BUTTERWORTH [3], BONERA and GALIMBERTI [4]. In a cubic crystal, the echo width at time $t=2\tau$ after a $\pi/2$-τ-β pulse sequence is determined by the magnetic dipole and static quadrupole interactions. The latter are produced by lattice defects. Simultaneously the echo height depends strongly on the rotation angle β of the second rf-pulse. Starting from the results in the papers mentioned above, this work aimes at the determination of the spin echo line shape in the presence of both types of interactions for the nuclear spins $I=3/2$, 5/2, 7/2, 9/2. Furthermore an instruction in detail will be given to calculate the quadrupole line function and the coresponding mean quadrupole distortion from the measured spin echo signal. The Fourier-transform of the quadrupole part represents the distribution function of the quadrupole perturbation in the sample. It is correlated with the number, type, and distribution of the lattice defects in the crystal, and so one can obtain information about the defects by means of spin echo measurements. In a proceeding paper [5] such an analysis was made by the authors in the case of point defects and dislocations respectively.

I. NMR Signals after a $\pi/2$-τ-β Pulse Sequence

Let us consider in a cubic lattice a system of identical spins $I>1/2$ with a gyromagnetic ratio γ in a frame (x, y, z) rotating with the frequency $\omega_z=-\omega_0=-\gamma H_0$ relative to the laboratory frame (X, Y, Z). Here the Z, z-directions are represented by the static magnetic field H_0 and the y-direction by the rf-field H_1 respectively. The system shall have magnetic dipolar perturbation b with a distribution function $p(b)$ and an electric quadrupole perturbation a with a distribution function $p(a)$. The perturbation frequencies

$$b=\gamma\cdot H_{\mathrm{D}z} \qquad (1)$$

($H_{\mathrm{D}z}$: Component of the local dipolar field at the site of a given nucleus in the direction of the external magnetic field H_0) and

$$a=\frac{3\,e\,Q}{4\,I(2\,I-1)\,\hbar}\,V_{zz} \qquad (2)$$

(Q: Electrical quadrupole moment of the corresponding nucleus, V_{zz}: Component of the electric field gradient (EFG) tensor $\mathbf{V}$ in the direction of the external field H_0) are assumed to be small compared with the Zeeman frequency $\omega_0=\gamma\cdot H_0$ and the rotation frequency $\omega_1=\gamma\cdot H_1$ of the rf-field H_1 during a rf-pulse. The distribution functions are normalized to one:

$$\int_{-\infty}^{+\infty} p(a)\,\mathrm{d}a=\int_{-\infty}^{+\infty} p(b)\,\mathrm{d}b=1. \qquad (3)$$

The nmr signal $E_x(t)$ following an rf-pulse is easily obtained by

$$E(t)=\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} E_x(t)\,p(a)\,p(b)\,\mathrm{d}a\,\mathrm{d}b \qquad (4)$$

[1] I. SOLOMON, Phys. Rev. **110**, 61 [1958].
[2] A. FLETT and J. RICHARDS, Proc. Phys. Soc. London **86**, 171 [1965].
[3] J. BUTTERWORTH, Proc. Phys. Soc. London **86**, 297 [1965].
[4] G. BONERA and M. GALIMBERTI, Rend., Ist. Lombardo Sci. Lettere **A 100**, 617 [1966].
[5] M. MEHRING and O. KANERT, Z. Naturforsch. **24 a**, 332 [1969].

where the free precession signal $E_x(t)$ is defined by

$$E_x(t) = \langle I_x(t) \rangle / \langle I_x(0) \rangle . \quad (5)$$

With $I_\pm = I_x \pm i\, I_y$ Eq. (5) can be rewritten as

$$E_x(t) = (\langle I_+(t) \rangle + \langle I_-(t) \rangle) / \langle I_x(0) \rangle . \quad (6)$$

The average $\langle I \rangle$ of the spin operators I_x, $I_\pm$ can be calculated by means of the spin density matrix ϱ using the general relation:

$$\langle I \rangle = \mathrm{Tr}(\varrho I) \quad \text{(see: TER HAAR [6])}.$$

Assuming that

1) the spin system obeys to a Boltzmann distribution,
2) the perturbation frequencies a, b are small compared to the rotation frequency ω_0,
3) the average of the Spin Hamiltonian $\langle \mathcal{H} \rangle \ll k\,T$ (high temperature approximation)

one obtains for the spin dependent part of the density matrix at time $t=0$ after the first $\pi/2$ pulse

$$\varrho(0) = K \cdot I_x \quad (7)$$

where

$$K = \gamma \hbar H_0 / [(2I+1)\, k\,T] .$$

Substituing Eqs. (5) and (7) into Eq. (4) the nmr signal becomes

$$E(t) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{\mathrm{Tr}\{\varrho(t) \cdot I_x\}}{K \cdot \mathrm{Tr}\{I_x^2\}}\, p(a)\, p(b)\, \mathrm{d}a\, \mathrm{d}b . \quad (8)$$

In this equation the density matrix $\varrho(t)$ is given by the general transformation

$$\varrho(t) = U(t)\, \varrho(0)\, U(t)^{-1} \quad (9)$$

with

$$U(t) = \exp\{-(i/\hbar)\, \mathcal{H} \cdot t\} \quad (10)$$

if the Hamiltonian $\mathcal{H}$ is time independent. In the case discussed here (static inhomogenous magnetic dipole und electric quadrupole broadening) the truncated Hamiltonian $\mathcal{H}$ in the rotating frame has the form (BUTTERWORTH [3]):

$$\mathcal{H} = b\,\hbar\, I_z + a\,\hbar\, I_z^2. \quad (11)$$

At the presence of a strong rf-field ($H_1 \gg a, b$) acting in the y-direction of the rotating frame the Hamiltonian $\mathcal{H}_1$ is given by

$$\mathcal{H}_1 = -\gamma\, H_1\, \hbar\, I_y \quad (12)$$

which causes a rotation of the spin system around the y-direction with the rotating frequency $\omega_1 = \gamma \cdot H_1$. Consequently the rotation angle β after an rf-pulse of time t_p is

$$\beta = \gamma\, H_1\, t_\mathrm{p} . \quad (13)$$

Now the desnity matrix $\varrho(t-\tau)$ after a $\pi/2 - \tau - \beta$ pulse sequence can be written by using Eqs. (9), (10) as

$$\varrho(t-\tau) = L\, \varrho(0)\, L^{-1} \quad (14)$$

with $L = U(t-\tau) \cdot P(\beta) \cdot U(\tau)$ where

a) the operator $P(\beta)$ describes the rotation of the spin ensemble by the rf-field H_1

$$P(\beta) = \exp(i\,\beta\, I_y) \quad \text{and} \quad (15)$$

b) the operator U transforms the spin system to time τ and $t-\tau$ respectively:

$$U(^{\tau}_{t-\tau}) = \exp[-(i/\hbar)\, \mathcal{H}(^{\tau}_{t-\tau})] .$$

To determine the nmr signal $E(t-\tau)$ according to Eq. (4) one has to compute:

$$\mathrm{Tr}\{\varrho(t-\tau)\, I_\pm\} = \sum_{m=-I}^{I} \langle m \,|\, \varrho(t-\tau)\, I_\pm \,|\, m \rangle . \quad (16)$$

Supposing a pulse spacing $\tau \gg 2\pi/\langle b \rangle$ ($\langle b \rangle$: mean value of dipole interaction) a straight-forward calculation yields the result (BUTTERWORTH [3]):

$$\mathrm{Tr}\{\varrho(t-\tau)\, I_+\} = K \cdot \sum_{m,m',m''} [I(I+1) - m(m+1)]^{1/2} \langle m \,|\, P(\beta) \,|\, m' \rangle \cdot \langle m' \,|\, I_x \,|\, m'' \rangle \langle m'' \,|\, P(\beta)^{-1} \,|\, m+1 \rangle \cdot \exp[i\{(t-\tau)[(2m+1)\, a + b] + \tau[(m''+m')\, a + b](m''-m')\}] . \quad (17)$$

The same calculation shows, that

$$\mathrm{Tr}\{\varrho(t-\tau)\, I_-\} = [\mathrm{Tr}\{\varrho(t-\tau)\, I_+\}]^* .$$

Therefore the signal $E_x(t)$ can be expressed by the real part of $\mathrm{Tr}\{\varrho I_+\}$. Thus

$$E_x(t) = \mathrm{Re}[\mathrm{Tr}\{\varrho(t)\, I_+\} / \mathrm{Tr}\{\varrho(0)\, I_x\}] . \quad (18)$$

[6] D. TER HAAR, Resonance in Magnetic Systems, Scot. Univ. Sumer School 1961, Oliver & Boyd, London 1961.

The trace in Eq. (17) leads to maximum nmr signal, if the argument of the exponential function vanishes. From this one gets the relation

$$\frac{t-\tau}{\tau} = \frac{(m''+m')\, a + b}{(2m+1)\, a + b} (m' - m'') \quad (19)$$

which defines the positions in time of the multiple spin echoes primarily observed by SOLOMON [1]. In the case discussed here, only the main echo at time

$t=2\pi$ is of interest, for which the spin quantum numbers (m, m', m'') satisfy the conditions

$$m''=m \quad \text{and} \quad m'=m+1. \tag{20}$$

With $\quad \mathrm{Tr}\{I_x^2\}=\frac{1}{3}(2I+1)\,I(I+1)$

$$\langle m+1|I_x|m\rangle=\tfrac{1}{2}[I(I+1)-m(m+1)]^{1/2}$$

and the symmetric relation (see: EDMONDS [7])

$$\langle m'|P(\beta)|m\rangle=(-1)^{m'-m}\langle m'|P(\beta)^{-1}|m\rangle$$

the shape $E(t-2\tau)$ of the main spin echo at time $t=2\tau$ after a $\pi/2-\tau-\beta$ pulse sequence is obtained from Eqs. (8), (17), (20) as

$$E(t-2\tau)=\mathrm{Re}\left[\sum_{m=-I}^{I-1} C_m^I \int_{-\infty}^{\infty} p(a)\,p(b)\,\exp\{i(t-2\tau)[(2m+1)a+b]\}\,db\,da\right].$$

Here the amplitude C_m^I of the transition $m\rightarrow m+1$ is given by

$$C_m^I=-\tfrac{3}{2}\,\frac{I(I+1)-m(m+1)}{I(I+1)(2I+1)}\,\langle m|P(\beta)|m+1\rangle^2 \tag{22}$$

where the matrix elements according to EDMONDS [6] are

$$\langle m'|P(\beta)|m\rangle=\left[\frac{(I+m')!\,(I-m')!}{(I+m)!\,(I-m)!}\right]^{1/2}\sum_\sigma\binom{I+m}{I-m'-\sigma}\cdot\binom{I-m}{\sigma}\cdot(-1)^{I-m'-\sigma}[\cos(\beta/2)]^{2\sigma+m'+m}\cdot[\sin(\beta/2)]^{2I-2\sigma-m'-m}. \tag{23}$$

Using the symmetry relation $C_m^I=C_{-(m+1)}^I$ and with a time base transformation $t-2\tau\rightarrow t$ the echo can be rewritten as

$$E(t)=C_{-1/2}^{\mathrm{I}}D(t)+\sum_{m=\frac{1}{2}}^{I-1}2\,C_m^I\,D(t)\,Q((2m+1)\,t) \tag{24}$$

where the dipolar function

$$D(t)=\int_{-\infty}^{\infty}p(b)\cos b\,t\,db \tag{25}$$

and the quadrupolar function

$$Q((2m+1)\,t)=\int_{-\infty}^{\infty}p(a)\cos((2m+1)\,a\,t)\,da \tag{26}$$

are the cosine Fourier transforms of the distribution function $p(b)$ and $p(a)$ respectively. Both functions are normalized to

$$D(0)=Q(0)=1. \tag{27}$$

Therefore the spin echo amplitude $E(0)$ is determined only by the coefficients C^I

$$E(0)=E_M+\sum_m E_Q(m) \tag{28}$$

where $E_M=C_{-1/2}^{\mathrm{I}}$ and $E_Q(m)=2\,C_m^I$. The echo amplitudes E_M (central transition) and $E_Q(m)$ (satellite transition) have been computed for spins $I=3/2$, $5/2$, $7/2$, $9/2$ as a function of the rotation angle β caused by the second rf-pulse. Results of such calculations are plotted in Figs. 1 – 6 showing that the

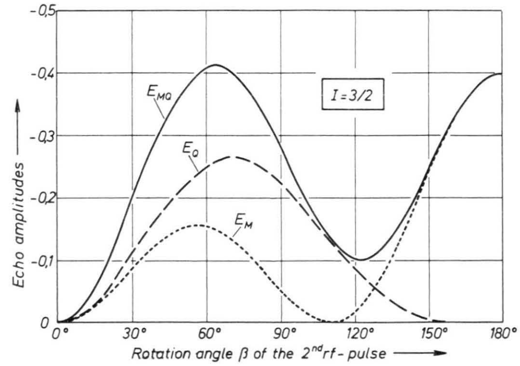


Fig. 1. Computed echo amplitudes E_M (central transition), E_Q (satellite transition) and the total amplitude $E_{MQ}=E_M+E_Q$ for spin $I=3/2$ versus rotation angle β of the 2nd rf-pulse.

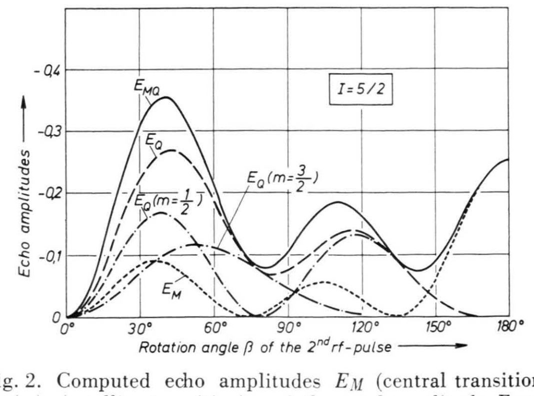


Fig. 2. Computed echo amplitudes E_M (central transition), $E_Q(m)$ (satellite transition) and the total amplitude $E_{MQ}=E_M+E_Q$ for spin $I=5/2$ versus rotation angle β of the 2nd rf-pulse.

[7] A. R. EDMONDS, Drehimpulse in der Quantenmechanik, BI Hochschultaschenbücher 53/53a.

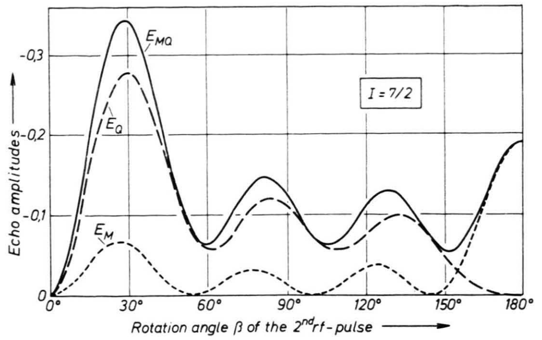


Fig. 3. Computed echo amplitudes E_M (central transition), E_Q (satellite transition) and the total amplitude $E_{MQ}=E_M+E_Q$ for spin $I=7/2$ versus rotation angle β of the 2nd rf-pulse.

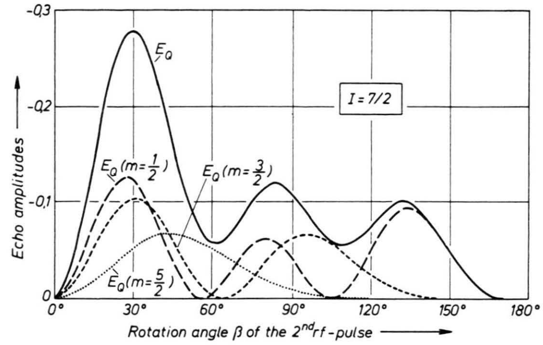


Fig. 4. Computed echo amplitudes $E_Q(m)$ (satellite transition) and the total satellite amplitude $E_Q=\sum E_Q(m)$ for spin $I=7/2$ versus rotation angle β of the 2nd rf-pulse.

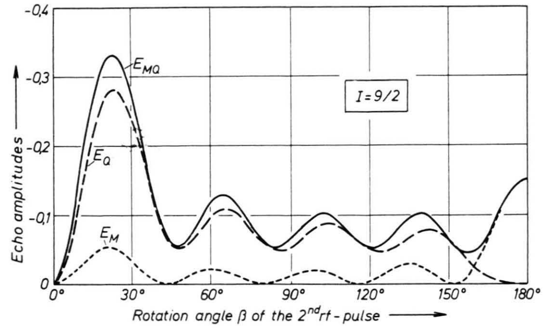


Fig. 5. Computed echo amplitudes E_M (central transition), E_Q (satellite transition) and the total amplitude $E_{MQ}=E_M+E_Q$ for spin $I=9/2$ versus rotation angle β of the 2nd rf-pulse.

spin echo amplitude $E(0)$ is a complex mixture of the central and the different satellite transitions.

For a spin echo anlaysis as done in the case of RbBr single crystals by Mehring and Kanert [5] one has to take into account the different parts of several transitions on the rotation angle β. An interesting point of view is that the maximum echo height is

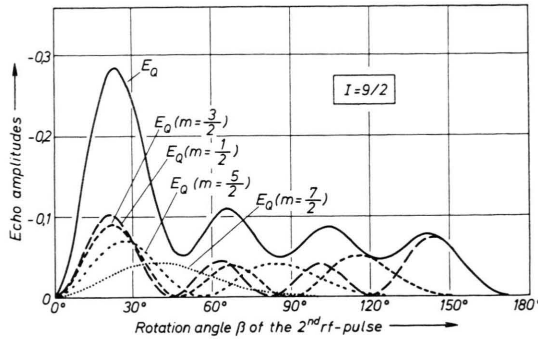


Fig. 6. Computed echo amplitudes $E_Q(m)$ (satellite transitions) and the total satellite amplitude $E_Q=\sum E_Q(m)$ for spin $I=9/2$ versus rotation angle β of the 2nd rf-pulse.

not obtained for $\beta=\pi$, but in all cases at a smaller value of $\beta_{opt} \leqq 64^{\circ}$ as stated earlier by Solomon [1] and Butterworth [3]. The optimum rotation angle β_{opt} for maximum echo height decreases for increasing spin I as shown in Table 1. For $\beta=\pi$ all amplitudes $E_Q(m)$ of the satellite transitions vanish, whereas the amplitude E_M of the central transition has a maximum value. Thus for a $\pi/2-\tau-\pi$ pulse sequence the spin echo is determined by the central transition only. An experimental verification of the theory in the case of spin $I=3/2$ is given in Fig. 7.

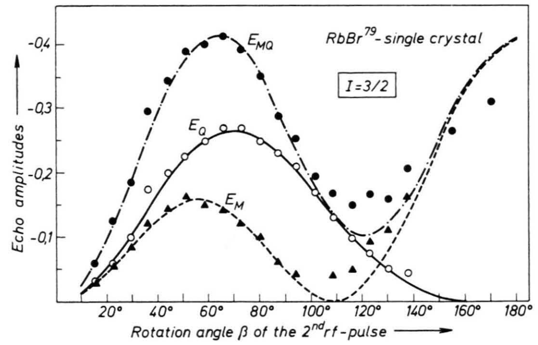


Fig. 7. Comparison of the calculated (see Fig. 1) and measured echo amplitudes in the case of spin $I=3/2$ as a function of β. The dots in the figure represent the experimental data, extrapolated to pulse distance $\tau=0$. The spin echo measurements were performed on a $RbBr^{79}$ single crystal.

The experimental values plotted in the figure were obtained by spin echo measurements on Br^{79} in a RbBr single crystal strongly deformed to generate a large mean quadrupole perturbation caused by the stress fields of dislocations (see [5]). In this case, the central and the satellite transition parts in the echo signal can easely be separated. For small values of the angle β the theoretical curves fit the measured values whereas there is a deviation between the experimental and theoretical data for $\beta < 100^\circ$ probably caused by an inhomogenity of the rf-field H_1. These measurements were done by means of a fast nmr pulse spectrometer in conjunction with a fast digital averaging technique as described by MEHRING and KANERT [8].

The normalized form $E_n(t)$ of the spin echo signal is represented by

$$E_n(t) = E(t)/E_{MQ} = A_M D(t) + \sum_{m=\frac{1}{2}}^{I-1} A_Q(m)\, D(t)\, Q((2m+1)\,t) = A_M D(t) + A_Q D(t)\, Q^+(t) \quad (29)$$

where $E_{MQ} = E_M + E_Q$ with $E_Q = \sum_m A_Q(m)$.

Here the amplitudes A are defined by

$$A_M = E_M/E_{MQ}, \quad A_Q(m) = E_Q(m)/E_{MQ}, \quad A_Q = \sum_m A_Q(m)$$

and the resulting quadrupole part $Q^+(t)$ is:

$$Q^+(t) = \sum_m (A_Q(m)/A_Q) \cdot Q((2m+1)\,t). \quad (30)$$

From Eqs. (27), (29) it follows

$$E_n(0) = D(0) = Q^+(0) = 1.$$

For the spins $I = 3/2$, $5/2$, $7/2$, $9/2$ the values of the amplitudes A at the optimum rotation angle β_{opt} are listed in Table 1.

Spin I	3/2	5/2	7/2	9/2
β_{opt}	64°	40°	30°	24°
$E_{MQ}(\beta_{opt})/E_{MQ}(\pi)$	1.03	1.425	1.80	2.20
$A_M(\beta_{opt})$	0.366	0.247	0.190	0.153
$E_Q(m)/E_Q$ for β_{opt}				
$m = 1/2$	1.0	0.622	0.446	0.359
$m = 3/2$	—	0.378	0.368	0.324
$m = 5/2$	—	—	0.186	0.243
$m = 7/2$	—	—	—	0.109
$A_Q(\beta_{opt})$	0.634	0.753	0.810	0.850
h_Q	0.683	0.623	0.595	0.578

Table 1. Spin Echo Signal Parameters.

II. Determination of Quadrupolar Perturbation by Means of Spin Echo Analysis

From Eq. (29) in conection with the data given in Table 1 one can calculate the spin echo shape $E_n(t)$ for a given dipolar function $D(t)$ [Eq. (25)] and quadrupolar function $Q((2m+1)\,t)$ [Eq. (26)] or vice versa. If the dipolar function $D(t)$ is known, from Eq. (29) in connection with the data given in Table 1 one can calculate the quadrupole function $Q((2m+1)\,t)$ from the measured spin echo signal $E_n(t)$. Since the dipolar function $D(t)$ can be written as a Gaussian function in a good approximation $D(t) = \exp(-0.693\, t^2/t_D{}^2)$ with the half width t_D, shown for example in Fig. 8 in the case of $RbBr^{79}$, $Q^+(t)$ can be calculated in a simple way if t_D is known. A Fourier transformation of $Q^+(t)$ yields the quadrupolar distribution function $p(a)$ as shown in ref. [5] in the case of dislocations and point defects respectively.

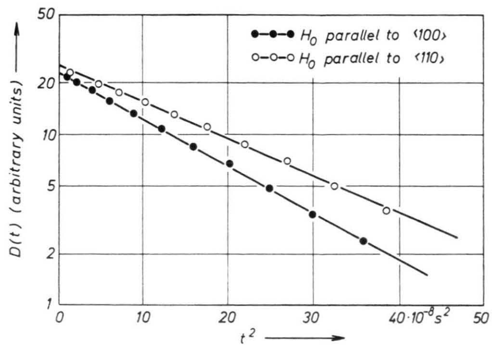


Fig. 8. Logarithmic plot of the dipolar echo shape $D(t)$ of Br^{79} in a RbBr single crystal versus time square t^2, obtained in a $\pi/2 - \tau - \pi$ echo experiment. The straight lines show the Gaussian behaviour of $D(t)$.

In many cases only the mean quadrupole perturbation is wanted. Thus one has to establish a relation between the width t_E of the measured echo $E_n(t)$ and the real half width t_Q of the quadrupolar function $Q(t) = \int p(a) \cos a t\, da$ [see Eq. (26)], which is correlated with the mean quadrupole perturbation $[\langle a^2 \rangle]^{1/2}$ of a Gaussian distribution function $p(a)$ by the relation $[\langle a^2 \rangle]^{1/2} = 1.18/t_Q$. Introducing in a first step the width t_{Q^+} of the quadrupole function Q^+ [Eq. (30)] one obtains according to Eq. (29)

$$E_n(t_{Q^+}) = D(t_{Q^+})\,(A_M + \tfrac{1}{2} A_Q) = D(t_{Q^+}) \cdot h_Q \quad (31)$$

where the parameter

$$h_Q = A_M + \tfrac{1}{2} A_Q \quad (32)$$

listed in Table 1 determines the experimental echo width t_E by the relation (see Fig. 9):

$$E_n(t_E) = h_Q. \quad (33)$$

[8] M. MEHRING and O. KANERT, Proc. XIVth Colloque Ampère, Ljubljana 1966, p. 988.

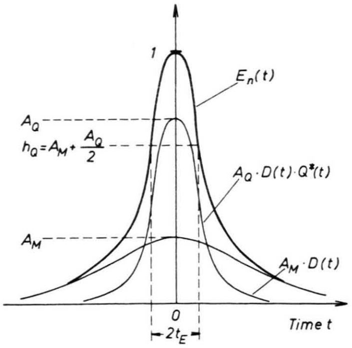


Fig. 9. Schematic diagram of the spin echo shape $E_n(t)$, resulting from the two contributions of the dipolar part $A_M\,D(t)$ and the satellite part $A_Q\,D(t)\;Q^+(t)$. The figure illustrates the experimental echo width t_E as defined in the text.

If the mean quadrupole distortion is large compared to the mean magnetic dipole interaction i. e. $t_{Q^+} \ll t_D$, it follows

$$D(t_{Q^+}) \approx 1 \quad \text{and} \quad E_n(t_{Q^+}) = h_Q = E_n(t_E)$$

or $t_E = t_{Q^+}$. If in contrast the quadrupolar width t_{Q^+} is of the same order of magnitude as the dipolar width t_D an iteration method has to be applied in general in order to compute the width t_{Q^+} from the measured echo width t_E. Assuming special analytical functions for the parts $D(t)$ and $Q^+(t)$ the calculation can be done without iteration. Starting from Eq. (29) and supposing a Gaussian function for the dipolar part $D(t)$ a straight forward calculation yields the relation

$$Q^+(\varkappa) = \frac{E_M}{E_Q}\left[\exp(0.693\,\varepsilon^2) - 1\right] + \tfrac{1}{2}\exp(0.693\,\varepsilon^2) \tag{34}$$

where the parameters $\varkappa$ and ε are defined by

$$\varkappa = t_{Q^+}/t_E \quad \text{and} \quad \varepsilon = t_E/t_D \tag{35}$$

the coefficient $\varkappa$ represents the correlation between the measured width t_E and the quadrupolar width t_{Q^+}.

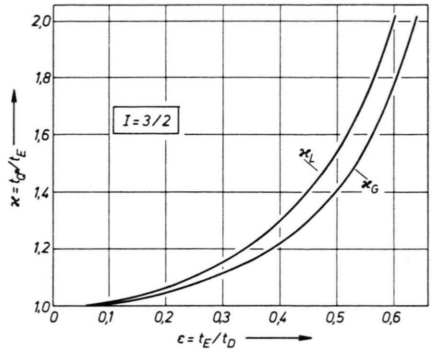
Choosing a Gaussian function for the quadrupole function $Q^+(t)$, Eq. (34) yields for the correction factor

$$\varkappa_G = \{-0.693/\ln[(A_M/A_Q + 0.5)\exp(0.693\,\varepsilon^2) - A_M/A_Q]\}^{1/2} \tag{36}$$

whereas in the case of a Lorentzian function for $Q^+(t)$ one gets

$$\varkappa_L = \left\{\frac{(A_M/A_Q+0.5)\,\exp(0.693\,\varepsilon^2) - A_M/A_Q}{A_M/A_Q+1-(A_M/A_Q+0.5)\,\exp(0.693\,\varepsilon^2)}\right\}^{1/2}. \tag{37}$$

Since the coefficient A_M/A_Q depends on the nuclear spin I, the values of the parameter $\varkappa$ subjects to the spin I as well. In Fig. 10 a, b the parameters $\varkappa_G$ and $\varkappa_L$ for the optimum rotation angle β_{opt} are plotted as a function of the normalized echo width ε for the two spins $I=3/2$ and $5/2$. The figures show, that the deviation of the correction factors $\varkappa_G$ and $\varkappa_L$ increases with increasing ε, i. e. with decreasing quadrupole distortion in the sample. In the region $\varepsilon \cdot \varkappa \approx 1$, i. e. $t_{Q^+} \approx t_D$ this deviation grows so large, that in calculating t_{Q^+} one has to make use of the iteration method mentioned above.



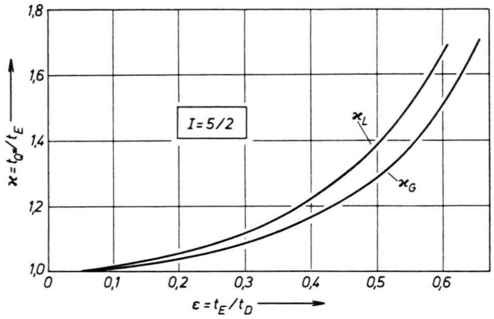


Fig. 10 a, b. Plot of the correction factors $\varkappa_G$ [Eq. (36)] and $\varkappa_L$ [Eq. (37)] as a function of the normalized measured echo width $\varepsilon = t_E/t_D$ for the spin $I=3/2$ (Fig. 10 a) and the spin $I=5/2$ (Fig. 10 b).

Finally one has to calculate the relationship between the width t_{Q^+} and the real half time t_Q of the quadrupole function $Q(t)$, which can be expressed by a coefficient λ given by the relation

$$t_Q = \lambda \cdot t_{Q^+}. \tag{38}$$

In order to compute the factor λ according to Eq. (30) one has to pay attention to the contributions of the different satellite transitions to the resulting quadrupole part $Q^+(t)$. With the data represented in Table 1 the result can be written for the different spins I:

spin I:

$$\begin{aligned}
3/2:&\quad Q^+(t) = Q(2\,t),\\
5/2:&\quad Q^+(t) = 0.622\,Q(2\,t) + 0.378\,Q(4\,t),\\
7/2:&\quad Q^+(t) = 0.446\,Q(2\,t) + 0.368\,Q(4\,t)\\
&\qquad + 0.186\,Q(6\,t), \qquad (39)\\
9/2:&\quad Q^+(t) = 0.359\,Q(2\,t) + 0.324\,Q(4\,t)\\
&\qquad + 0.243\,Q(6\,t) + 0.109\,Q(8\,t).
\end{aligned}$$

From this it follows for $I = 3/2$, that $\lambda = 2$ is independent of the line shape of the quadrupole function $Q(t)$. In all other cases an assumption must be done about line shapes of $Q(t)$ to determine the coefficient λ. Supposing for $Q(t)$ a Gaussian and a Lorentzian shape respectively, values for the resulting coefficients λ_G and λ_L are given in Table 2 for the different spins I.

Spins I:	3/2	5/2	7/2	9/2
λ_G	2.00	2.66	3.31	3.84
λ_L	2.00	2.58	3.16	3.58

Table 2. Correction coefficients λ.

Summing up the relations between the measured echo width t_E and the wanted quadrupole width t_Q the following equation is obtained

$$t_Q = \lambda \cdot \varkappa \cdot t_E \qquad (40)$$

where the coefficient $\varkappa$ and λ depend on the spin I, the strength of the quadrupole perturbation compared to the mean dipole interaction and the line functions of the dipolar and the quadrupolar parts respectively. According to Eq. (40), the half width t_Q of the quadrupole function $Q(t)$ can be determined from the measured echo width t_E. On the other hand the width t_Q is related to the width $[\langle a \rangle^2]^{1/2}$ of the quadrupolar distribution function $p(a)$, i. e. to the mean quadrupole distortion. Since the width $[\langle a^2 \rangle]^{1/2}$ depends on the defects in the sample, one gets information about these defects by means of spin echo measurements as done by the authors in the case of point defects and dislocations (see ref. [5]).

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