Determination of NMR-spectrum moments of F^{19} in CaF_2 from the line shape parameters.

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Received April 28, 2000
Accepted May 17, 2000

Magnetic Resonance in Solids
Electronic Journal

Volume 4
No. 1, 2000

Abstract

Results of calculation of NMR line moments of F^{19} in CaF_2 compared with experimental data are presented.

PACS : 76.60.-k;75.20.Ck

Keywords : nuclear magnetic resonance, line shape, moments

For determination of suitability degree of applied line shape function in NMR experiments, it is convenient to compare the experimental line moments with those calculated. We carried out such a comparison for the free induction decay (FID) signal of F^{19} in CaF_2. In this compound fluorine has a simple cubic lattice, high Debye temperature and spin S=1/2, so we can neglect temperature contributions to line moments and exclude quadrupolar interactions.

Previously [1] we suggested to treat the FID signal as a convolution of two functions. The firat function

$$g_i = I_\nu(bt)/(bt)^\nu \tag{1}$$

is a solution of equation of motion of damped harmonic oscillator, and the second one

$$g_r = exp\{-\alpha^2\tau_c^2(\sqrt{1+t^2/\tau_c^2}-1)\} \tag{2}$$

determines a summation law for spin-system non-correlated responses on disturbing action of hf-impulse. Here b is the local field value determined by the first two zeros of FID oscillation; I_ν is the Bessel function of the first kind; τ_c is the correlation time of z-component of local fields; α^2 is the the second moment of $g_r(\omega)$.

Accoprding to the model [2], g_i describes a signal from the spins going into a zone of correlated dipole - dipole (d-d) interaction, and g_r - from all the rest. Here the correlation is meant to be full phase coherence of superposition of local fields from environmental nuclei on chosen nucleus.

In this publication on the basis of experimental data of precise FID measurements of F^{19} in CaF_2 made by Engelsberg and Lowe [3], we present results of calculation of line moments (up to 14^{th}) with the help of line form function as

$$G(t) = g_i * g_r \tag{3}$$

where g_i and g_r are determined by the expressions (1) and (2), and b, ν, α and τ_c have been determined from the data [3] according to procedure [1].

It is known that an arbitrary even moment of NMR symmetric line may be described by means of line shape function [4]:

$$M_{2n}(G(\omega)) = \mid \frac{d^{2n}G(t)}{dt^{2n}} \mid_{t=0} = G^{(2n)}(0). \tag{4}$$

An arbitrary full moment of $G(t)$ function, as a product of functions g_i and g_r, is easily defined according to Leibniz's formula [5]:

$$M_{2n} = G^{(2n)}(t)_{t=0} = \sum_{k=0}^{2n} C_{2n}^k g_i^{(k)}(0) g_r^{(2n-k)}(0) = \sum C_{2n}^k M_k^i M_{2n-k}^r \tag{5}$$

where $C_{2n}^k = \frac{2n!}{k!(2n-k)!}$. Thus, knowing a derivative of functions g_i and g_r, we learn, according to (4), their corresponding moments and consequently n^{th} full moment of relaxation function $G(\omega)$, too. Taking into account that for symmetric line odd moments are equal zero, we determine all even moments $G(\omega)$ up to 14^{th} one with the formula (5).

The n^{th} derivative of $g_r(t)$ is defined from recurrent formula [3]

$$\begin{aligned} & g_r^{(2n)}(0) = (-\alpha^2)[(2n-1)g_r^{(2n-2)}(0) + \\ & \sum_{k=1}^{n-1} \frac{(2n-2k-1)!!(2k-1)(2n-2k)!(-1)^{n-k}}{(2n-2k)!!\tau_c^{2n-2k}} C_{2n-2k}^{2n-1} g_r^{(2k-2)}(0)]. \end{aligned} \tag{6}$$

From equation (6), the following expression have been obtained for 12^{th} and 14^{th} derivatives $g_r(t)$

$$g_r^{(12)}(0) = 10395(945\frac{\alpha^2}{\tau_c^{10}} + 945\frac{\alpha^4}{\tau_c^8} + 420\frac{\alpha^6}{\tau_c^6} + 105\frac{\alpha^8}{\tau_c^4} + 15\frac{\alpha^{10}}{\tau_c^2} + \alpha^{12}) \tag{7}$$

$$g_r^{(14)}(0) = -135135(10395\frac{\alpha^2}{\tau_c^12} + 10395\frac{\alpha^4}{\tau_c^{10}} + 4725\frac{\alpha^6}{\tau_c^8} + 1260\frac{\alpha^8}{\tau_c^6} + 210\frac{\alpha^10}{\tau_c^4} + 21\frac{\alpha^{12}}{\tau_c^2} + \alpha^{14}). \tag{8}$$

The expressions for derivatives of $g_r(t)$ from 2^{th} to 10^{th} are presented in [3]. In [1] the simple expression is given for arbitrary even moment of a signal from the cell

$$M_{2n}^i = \frac{(2n-1)b^{2n}}{2n\prod_{k=1}^n(\nu+k)}. \tag{9}$$

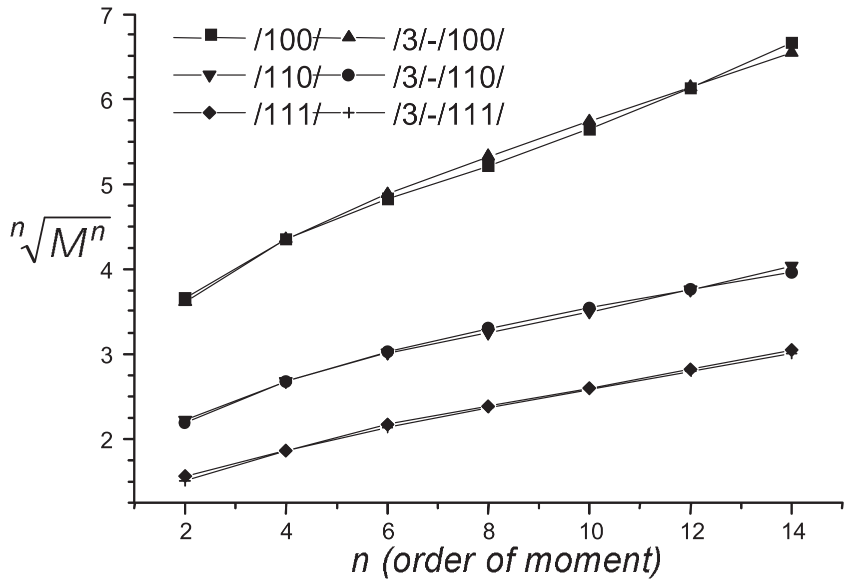

Figure 1: Calculated and experimental [3] values of square roots from FID signal moments of F^{19} in CaF_2 for magnetic field directions along the basic crystallographic axes.

Proceeding with calculations we supposed that

$$C_0^k = M_0^i = M_0^r = C_k^k \equiv 1$$

.

In Table 1 (see Appendix) we present the comparative data of moment values for NMR spectra of F^{19} in CaF_2 obtained by means of analysis of experimental data [3], and theoretical values from works [6, 7] calculated on the basis of parameters of the line form function suggested in [1]. The figure 1 illustrates the table data.

Thus it has been shown that analytical equation for a signal shape in crystalline diamagnetics not only describes the real spectrum but makes possible to determine the highest moments without labour-consuming procedures [6, 7]. The suggested approach permits to describe NMR signal in the case of quadrupole nuclei too. In this case it is sufficient to set correctly a distribution function of quadrupolar frequencies [8].

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Appendix
Table 1.

FID form parameters								
B_0	[1]				n	$(M_n)^{1/n} gauss$		
direct	b gauss	ν	$\tau_c (\mu sec)$	α gauss	Order of moment	Experiment [3]	Theory [6, 7]	Calculation (this work)
[100]	6.037	0.585	68.55	1.379	2	$3,614 \pm 0,036$	3,603	3.661
					4	$4,352 \pm 0,046$	4,349	4.352
					6	$4,882 \pm 0,055$	4,85	4.830
					8	$5,326 \pm 0,068$	5,37	5.212
					10	$5,736 \pm 0,078$		5.646
					12	$6,141 \pm 0,090$		6.134
					14	$6,55 \pm 0,11$		6.664
[111]	2.713	0.93	132.44	0.722	2	$1,508 \pm 0,019$	1,493	1.558
					4	$1,865 \pm 0,025$	1,854	1.865
					6	$2,134 \pm 0,028$	2,11	2.174
					8	$2,367 \pm 0,033$	2,36	2.384
					10	$2,585 \pm 0,041$		2.597
					12	$2,797 \pm 0,045$		2.819
					14	$3,004 \pm 0,049$		3.050
[110]	4.084	1.025	155.84	0.9	2	$2,191 \pm 0,029$	2,218	2.220
					4	$2,679 \pm 0,039$	2,715	2.679
					6	$3,026 \pm 0,052$	3,07	3.011
					8	$3,304 \pm 0,068$	3,42	3.248
					10	$3,544 \pm 0,078$		3.494
					12	$3,762 \pm 0,083$		3.757
					14	$3,967 \pm 0,090$		4.037