

THE EMPLOYMENT OF FITTING PROGRAMS FOR DEUTERON POLARIZATION CALCULATION IN A NUCLEAR POLARIZED TARGET

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We have developed the fitting program used for deuteron polarization calculation. The simulation has been done for the deuterated 1,2-propanediol-D8 as a target material. Analyses of the uncertainties sources have been performed. The polarization calculated was $P=+34.0\%$ and $P=-36.6\%$ for above-mentioned target material.

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The accuracy of target polarization measurement for the polarized deuteron in situ is important for realization of physics experiments. In the best way the polarization of a target is determined by calibration of the enhanced signal against the signal of the spin system in thermal equilibrium (TE) with the lattice. But for deuterons the precision calibration is very difficult under conditions of thermal equilibrium since the TE signal has very low intensity. Therefore, the development of the nuclear magnetic resonance (NMR) line-shape analysis for a calculation of the deuteron polarization is the problem of current interest. The measurements procedure consists in recording the absorption spectrum of the nuclear magnetic resonance from the Q-meter for computing with subsequent determining the polarization value [1]. The multiple accumulation of these signals is executed for the purpose of raising the accuracy.

The typical materials for the polarized target are the deuterated alcohols. The C-D and O-D bonds leads to broadening Zeeman levels. The energy levels of such a spin system can be written as [2,3]

$$E_m = \nu_d m + \nu_q \{3 \cos^2(\theta) - 1 + \eta \sin^2(\theta) \cos(2\phi)\} \times \\ \times (3m^2 - 2),$$

where θ is the polar angle between the C-D and O-D bonds and the magnetic field direction;

$m = -1, 0, 1$ is the spin magnetic quantum number;

$\nu_q = eqeQ/8$ is the energy of the quadrupole interaction;

eq is the magnitude of the electric field gradient along the bound direction;

eQ is the electric quadrupole moment of deuteron,

ϕ is the azimuth angle;

η is the parameter of asymmetry of a quadrupole deuteron moment.

For ease let us use the normalized frequencies

$$x = 2(\nu - \nu_d) / \nu_d,$$

which can be written as

$$x = -(2m - 1)\lambda(\theta, \phi) \nu_Q / \nu_Q,$$

where $\lambda(\theta, \phi) = (3 \cos^2 \theta - 1 + \eta \sin^2 \theta \cos 2\phi) / 2$.

In this variables the full spectrum has the $F(x)$ and $F(-x)$ components, which are symmetrical relatively $x=0$.

The $F(x)$ and $F(-x)$ components are related to two Zeeman transitions $m \leftrightarrow m-1$. In normalized frequencies $F(x)$ is written as [4]:

$$F(x) = \frac{1}{p\pi} \int_0^r f[x - \psi_1(t)] K[k_1(t)] dt + \\ + \frac{1}{q\pi} \int_0^r f[x - \psi_2(t)] K[k_2(t)] dt,$$

where

$$p = \sqrt{2\eta},$$

$$r = \sqrt{3 + \eta},$$

$$\psi_1(t) = 1 - t^2/2,$$

$$\psi_2(t) = (t^2 - 1 - \eta) / 2,$$

$$k_1(t) = \psi_3(t) q / p,$$

$$k_2(t) = \psi_3(t) p / q,$$

$$\psi_3(t) = \sqrt{(r^2/t^2) - 1}.$$

$f(x)$ is the Gauss or Lorentz function, where σ is the dispersion. $K(x)$ is the elliptic integral of first kind. The contribution of the second type of the quadrupole bond is taken into account similarly, replacing

$$\psi^*(t) = \rho \cdot \psi_i(t), (i=1,2)$$

and $\rho = \nu_{Q2} / \nu_{Q1}$,

where ν_{Q2} and ν_{Q1} are given above.

In assumption of the equal spin temperature in the deuteron system, the relative population of the magnetic levels $R = \exp(-h\nu_d/kT_s)$, where ν_d and T_s are the central NMR frequency and the spin temperature, respectively. Therefore, the full spectrum with taking into account the C-D and O-D bonds is

$$S(x) = 2[2 \sum_{i=1} C_i \{RF_i(x) + F_i(-x)\}] / (1 + R),$$

where C_i is the relative deuteron number in the bond.

This spectrum is defined by 6 parameters:

$$R, \eta_1, \eta_2, \rho, \sigma \text{ and } C \text{ (as } C_1 + C_2 = 1),$$

which are defined by comparison of the model with the experimental NMR-absorption signal and characterize the substance under study. Thus, the η_1 and η_2 define the asymmetry of the quadrupole moment of C-D and O-D

bonds, R-parameter is used to calculate deuteron polarization:

$$P = (1 - R^2) / (1 + R + R^2).$$

We have developed the program complex to calculate deuteron polarization by analyzing the deuteron NMR line-shape in frozen alcohols, using above algorithm.

The program consists of two parts. In the first part we have to process the data file (DMR-line) received from Data Acquisition System to remove the apparatus distortions. These are the following.

1) Frequency sweeping has no linear dependence on digital step size. And we have to recalculate this frequency sweep to make dependence as linear one.

2) The measured DMR-line is real line plus some additional baseline. And the baseline usually is a polynomial-like line, which has to be simulated and removed.

3) The DMR-line size usually is narrower (and therefore has additional not needed parts) and not in the window center of Analog-to-Digital Converter. Then we have to recalculate DMR-line to make it of right size and put at right place.

This part of program has been designated as having the interactive and graphical windows. In the interactive window one is prompted the questions what one wants to do with DMR-line and the graphical window shows what is happening. If the DMR-line transforms are accepted then the new DMR-line is written into a new file and the interactive session is closed.

The frequency is extrapolated for each channel by the polynomial of the third degree. With the help of splines and with the regard for the frequency dependence the signal is formed from the primary DMR-signal. It has the linear frequency dependence of the sweep. The results are written down in the separate massive.

It is not in general possible to choose the optimal values of the resonance frequency and the deviation width for the Q-meter system. As result the measured signal is not found in the center of the sweep and has a different frequency width in the channel. It makes the fitting process difficult and increases the error of parameter definition. It has become necessary to correct these effects. After the frequency linearization program displaces the signal in the sweep center, remove the channels, not having signal information and do further signal extension over the whole channel range. The area of the obtained signal normalized per unity and result is recorded into the certain file. The result of the correction after these operations is shown in Fig. 1 and in Fig. 2.

On the second stage the model spectrum is fitted to the corrected spectrum. The program minimizes the functional describing the deviation of the theory function from the experimental data. In our case the functional

$$\chi^2(a) = \sum_{i=1}^n \frac{f(x_i, a) - e_i}{\sigma_{\text{exp}}}^2$$

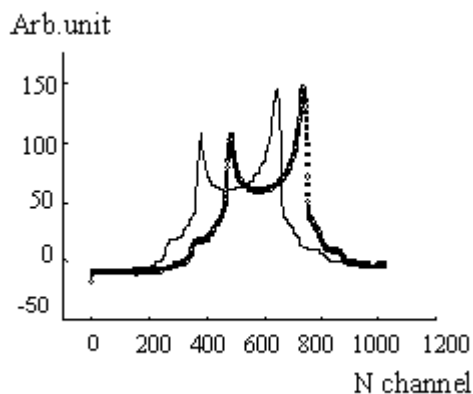


Fig. 1. Deuteron magnetic resonance signal. Correction of the frequency dependence. The solid line is the real Q-meter signal. The circles are the signal after correction

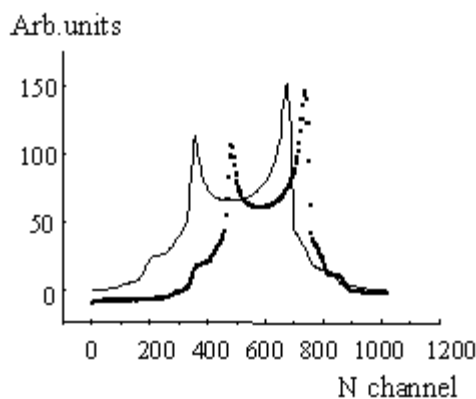


Fig. 2. Deuteron magnetic resonance signal. Correction of the boundaries, the base line and the extension over the whole channel range. The circles are signal before correction. The solid line is signal obtained after full correction.

was minimized, where e_i is the measurement result, a is the vector of parameters, σ_{exp} is the uncertainties in the individual e_i measurements.

The calculations were performed using the MINUIT package from CERN program library. This package enables to find the best parameter values for multi-parameter functions. It is possible to perform a fitting for parameters with user's restricted limits. Two files are prepared for this task. Two files are prepared for this task. The first file consists of the DMR-signal to be corrected. The second one contains command script to be executed by MINUIT at run-time. The script includes the work title, the parameter namelist, the initial values, the boundaries, the list of command describing the calling sequence of MINUIT fitters.

To find the correct full set initial parameters defining the DMR-line shape it is needed a long run time and we use SCAN algorithm because of it. After it is done the parameters of the measured DMR-signal are only

slightly changing. And the parameter, related to the polarization has to be fitted only. To do this the MIGRAD algorithm is used, which is more carefully and makes fitting more correctly.

We have made a number of program tests to estimate the errors introduced by the MINUIT program into the polarization value.

The source of errors is determined by the fact that the χ^2 -functional has a lot of the local extremes, which lead to the multivalued fitting parameters. This gives the dispersion deuteron polarization value. We have determined the area of parameter values, obtained after fitting, depending on the change of their initial values. For this we have generated a DMR-signal with the known parameters. Further these parameters were taken as initial ones and the fitting program determined the parameters of DMR-signal. During the next stage the changes (20–40%) were put into the values of initial parameters and DMR-signal parameters were determined again. Besides, we added Gaussian noise of different intensity into the DMR-signal and calculate the parameters again. We have got the following result of such simulation with the absence of changing in the initial parameter values.

The yielded parameters were absolutely aligned with initial ones. With 40% changing of the R- parameter the value of polarization being determined was changing not more than 0.3%. With simultaneous variation of all initial parameters up to 40% the changing of polarization value did not exceed 4%. In the absence of changing in initial parameter values the addition of Gaussian noise with intensity of 10% leads to the change of the polarization value not more than by 1%.

Under conditions of a real physical experiment with the calculation of a polarization value the initial parameter values of DMR-signal are unknown. So it is necessary to make some calculation to know the parameters of DMR-spectrum and every time it is necessary to take the parameters of the previous calculation as an initial but with insignificant changes. When stability of results is reached one can take the average value as a polarization value.

The result is shown in Figs. 3, 4. The fitting was made using the DMR-signal for 1,2 propanediol-D8 with the positive and negative deuteron polarization.

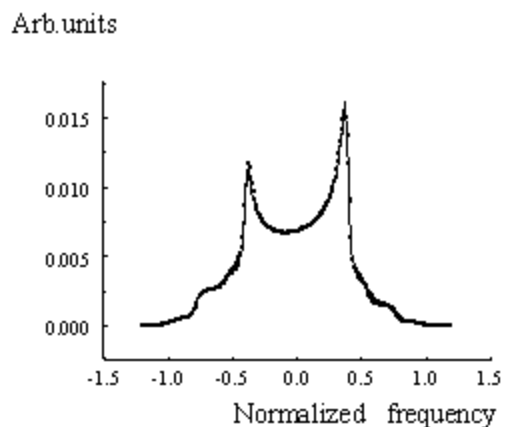


Fig. 3. The result of the fitting procedure by MINUIT program, applied to $P_D = -36.6 \pm 1.6\%$. The

circles are the DMR signal after full correction. The solid line is the fitted DMR signal.

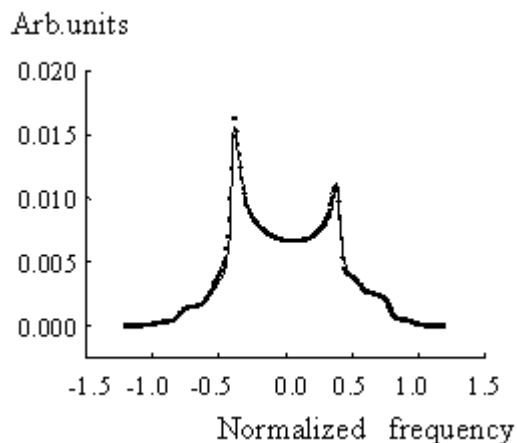


Fig. 4. The same as Fig. 3 for positive deuteron polarization $P_D = 34.0 \pm 1.4\%$.

The experimental signal from Q-meter consisted of 1000 enhanced polarization sweeps. All frequency range was sampled on 1024 channels. Only 256 channels were used to fit the theoretical absorption function to the experimental DMR-signal. The following value of the parameters for 1,2 propanediol-D8 were obtained: $\eta_1=0.18$; $\eta_2=0.017$; $\rho_0=0.78$; $\sigma=0.019$.

From this figures one can see that the program gives a good fitting and can be used for finding the deuteron polarization. At the conditions the equilibrium (thermal) the DMR-signal cannot be measured correctly enough and the method of calculation of deuteron polarization by analyzing DMR-line shape is an excellence alternative possibility.

REFERENCES

1. A.A. Belyaev et al. *The measurement of the deuteron polarization in the polarized target*. Preprint KIPT 87-27. M.: CNIIatominform, 1987. 9 p. (in Russian).
2. A. Abragam. *Nuclear magnetism*. M. IL, 1963. 551 p. (in Russian).
3. M.H. Cohen. and F. Reif. Nuclear quadrupole effects in solids // *Solid State Physics*. 1957, v. 5, p. 321.
4. O. Hamada. at all. Analysis of deuteron NMR spectrum in propanediol for polarization measurement // *Nucl. Instr. Meth.* 1981, v. 189, p. 561-568.