Estimation of Non-Linearity in NMR Polarization Measurement

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Abstract

The non-linearity of the proton NMR signal of the SMC target during the 1993 run is considered here. It is estimated that the highest negative (positive) polarizations were systematically overestimated (underestimated) by about 5% when the total scan width used was 400 KHz, and by about 3% when the total scan width was 600 KHz.

1. Introduction

The polarization measurement of the NA47 (SMC) experiment at CERN [1], which measures the spin dependent structure functions of the proton and neutron, is done by the continuous wave Nuclear Magnetic Resonance (NMR) [2, 3] method. There are two target halves which are polarized in opposite directions in order to reduce the systematic errors in the NA47 experiment. The polarization of the protons is measured by 10 coils embedded in the target material and read by 10 series Q-meters.

The absolute polarization is proportional to the integral of the absorption part of the susceptibility [4]:

$$P = \frac{2}{\pi\hbar\gamma^2 NI}\int_0^\infty \chi''(\omega)\,d\omega \tag{1}$$

where γ is the nuclear gyromagnetic ratio, I the spin of the species in question and N the spin density of the material. The complex susceptibility is $\chi(\omega) = \chi'(\omega) - \imath\chi''(\omega)$ in the SI units that are used throughout this text. $\chi'(\omega)$ is the dispersion and $\chi''(\omega)$ the absorption part of the susceptibility. The enhanced proton polarization signal is compared to the proton NMR integral at a thermal equilibrium (TE) with the lattice temperature at about $1\,K$:

$$P = \frac{\int_0^\infty S(\omega)\,d\omega}{\int_0^\infty S_{TE}(\omega)\,d\omega} P_{TE}, \tag{2}$$

where $S(\omega) = V_{out}(\chi(\omega)) - V_{out}(\chi(\omega) \equiv 0)$ and V_{out} is the series Q-meter signal.

For Eq. (2) to hold true the Q-meter circuit must respond linearly in a wide range since the ratio of the largest signal to the TE signal is more than 400.

There are more works [5, 6] on computer based analysis of the NMR Q-meters but here we will show explicitly why to first order the non-linearity cancels and how to find the remaining error and correct for it. A more complete version of this work can be found in [7].

2. Circuit Analysis

The equivalent circuit [8, 9] used for NMR is shown in Fig. 1. The real and imaginary parts of the voltage output are [9]:

$$\begin{aligned} Re(V_{out}) &= \frac{GV_0}{R_0}\frac{Re(Z) + X[Re^2(Z) + Im^2(Z)]}{[(1+XRe(Z))^2 + X^2 Im^2(Z)]} \\ Im(V_{out}) &= \frac{GV_0}{R_0}\frac{Im(Z)}{[(1+XRe(Z))^2 + X^2 Im^2(Z)]} \end{aligned} \tag{3}$$

where $X = \frac{1}{R_i} + \frac{1}{R_0}$, with R_i the amplifier input impedance, R_0 the current limiting resistor, G the amplifier gain, and V_0 the synthesizer voltage output.

The impedance of the coil in the target material is

$$Z_L = R_L + \imath\omega L(1 + \phi(\omega)) \tag{4}$$

where R_L is the coil resistance, L the coil inductance and $\phi(\omega) = \phi'(\omega) - \imath\phi''(\omega) = \eta(\chi'(\omega) - \imath\chi''(\omega))$ with η the coil filling factor. The proton polarization can be detected by integrating the change of the coil RF impedance when scanning over the proton Larmor frequency. In practice it is the $Re(V_{out})$ that is integrated. Unfortunately, there is always a need for a cable that transports the signal to the detector and tuning system, which distorts it somewhat. The total impedance $Z(\omega)$ including the cable and the tuning electronics is then

$$Z(\omega) = R + \frac{1}{\imath\omega C} + Z'_L \tag{5}$$

with

$$Z'_L = Z_c \frac{Z_L + Z_c \tanh \gamma_c \ell_c}{Z_c + Z_L \tanh \gamma_c \ell_c} \tag{6}$$

where Z'_L is the image impedance of the coil impedance which is also responsible for introducing the non-linearity in the final signal, C the value of the tuning capacitor, and R the damping resistance. Z_c is the cable impedance and is equal to [9]:

$$Z_c \approx Z_0 \sqrt{1 + \frac{R_c}{\imath\omega L_c}} \approx Z_0\{1 + \frac{1}{\imath 2Q_c}\} \tag{7}$$

with $Z_0 = (L_c/C_c)^{1/2}$ the cable characteristic impedance (equal to 50Ω for the cables used in our case). R_c, L_c, C_c are the cable resistance, inductance and capacitance per unit length respectively. $Q_c = \omega L_c/R_c$ is the cable "quality" factor, and ℓ_c the cable length. The propagation constant γ_c can be approximated to

$$\gamma_c = \sqrt{(R_c + \imath\omega L_c)\imath\omega C_c} \approx \frac{\omega\sqrt{L_c C_c}}{2Q_c} + \imath\omega\sqrt{L_c C_c} \tag{8}$$

which can be identified with the expression

$$\gamma_c = \alpha + \imath\beta \tag{9}$$

where α is the attenuation constant and β the phase constant of the cable ($\beta = D\omega$, and D is the propagation delay).

The cable length is chosen so that on resonance (the Larmor frequency) $\tanh(\gamma_c \ell_c)$ is purely real, i.e.

$$\ell_c = \frac{n\pi}{\omega_c\sqrt{L_c C_c}} \tag{10}$$

where ω_c is the cable resonance angular frequency, which here we will assume is the same as the Larmor angular frequency ω_0, and n is the number of half wavelengths of the Larmor frequency in the cable. Then

$$\gamma_c \ell_c = \imath n\pi \frac{\omega}{\omega_0}\sqrt{1 + \frac{1}{\imath Q_c}} \approx \imath n\pi \frac{\omega}{\omega_0}(1 + \frac{1}{\imath 2Q_c}). \tag{11}$$

At $\omega = \omega_0$, $\tanh(\gamma_c \ell_c) = \tanh \frac{n\pi}{2Q_c}$ and the length of the cable is $\ell_c = n\lambda/2$ with λ the wavelength of the ω_0 in the cable.

In principle, the circuit is analyzed and once knowing the various parameters one can reproduce the observed Q-curves and NMR signals. In practice, only some of the parameters are measured with very high accuracy, and therefore we will fit the Q-curves in order to obtain more precise values of them.

It is clear that the voltage output of the Q-meter is highly non-linear in view of the Eqs. (3,6,11), and it is the size of the signal itself that determines the amount of error made when applying Eq. (2). In other words the non-linear contributions depend on the relative height (or else the modulation depth M) which is the ratio of the absolute height of the signal divided by the minimum value of the RF-level:

$$M = \frac{S(\omega_0)}{V_{out}^{min}(\chi(\omega) \equiv 0)} \tag{12}$$

3. Kramers-Kronig Relations

With the help of the *Mathematica* [10] software package we developed the real part of the V_{out} of Eq. (3) (we give it here in units of volts after setting the term $GV_0/R_0 \approx 0.1A$):

$$\begin{aligned} Re(V_{out}) \;=\;& 3.5 - 17.0\Delta + 1200\Delta^2 \\ & + (3.0 + 110\Delta - 550\Delta^2)\phi'' \\ & + (0.3 + 58\Delta + 2900\Delta^2)\phi' \\ & + (1.5 + 70\Delta + 1900\Delta^2)(\phi'^2 - \phi''^2) \\ & - (0.5 + 5.0\Delta + 4900\Delta^2)\phi'\phi'' \end{aligned} \tag{13}$$

with $\Delta = (\omega - \omega_0)/\omega_0$, from where we can see that the coefficient of the non-linear term is only 50% less than that of the linear term and is potentially very damaging. Of course the non-linear term would be negligible if ϕ was very small but we have observed modulations (M) as much as 65% for the negative and 40% for the positive polarization and therefore this is not the case here.

Fortunately the non-linear terms ϕ'^2 and ϕ''^2 enter in Eq. (13) with the same coefficient and opposite sign so that their contributions are in competition with each other. It turns out that because the dispersion and absorption parts of the susceptibility are related through the Kramers-Kronig relations [11]:

$$\begin{aligned} \phi'(\omega_0) &= \frac{2}{\pi} P \int_0^\infty \frac{\omega\phi''(\omega)}{\omega^2 - \omega_0^2}\, d\omega \\ \phi''(\omega_0) &= -\frac{2\omega_0}{\pi} P \int_0^\infty \frac{\phi'(\omega)}{\omega^2 - \omega_0^2}\, d\omega \end{aligned} \tag{14}$$

(where P denotes the principal value of the integral), the following is also true [12]:

$$\int_0^\infty \phi'^2(\omega)\, d\omega = \int_0^\infty \phi''^2(\omega)\, d\omega. \tag{15}$$

Even though the two integrals are the same, the frequency dependence of $\phi'^2(\omega)$ and $\phi''^2(\omega)$ is very different and the two do not quite cancel when integrating the NMR signal in a finite frequency range. The remnant $\int_{\omega_0-\omega_B}^{\omega_0+\omega_B}(\phi'^2 - \phi''^2)\, d\omega$ depends on the ratio of the signal (ϕ'') width over the total scan width ($2\omega_B$). Therefore the signal width is a very important parameter in this analysis and special care should be taken to determine it. The term $\phi'\phi''$ is antisymmetric and does not contribute to the signal integral.

The shape of the absorption part of the susceptibility is calculated using the modified Lorentzian function[1]

$$\phi''(\omega) = \frac{1}{1 + |\frac{\Delta}{\Delta_H}|^{2.5}} \tag{16}$$

where Δ_H is half the Full Width at Half Maximum (FWHM). The FWHM is taken from the experimental TE signals, where the contribution of $\phi'(\omega)$ to the line width can be neglected. The higher order contributions to the width of the TE signals are totally negligible. Fig. 2 shows the function

$$F(\Delta) = -\frac{\int_0^\Delta(\phi'^2 - \phi''^2)\, d\omega}{\int_0^\Delta(\phi'^2 + \phi''^2)\, d\omega} \times 200 \tag{17}$$

versus Δ for FWHM $= 53.2$ KHz, which goes asymptotically to zero as the angular frequency goes to infinity. The non-cancelation of the integrals of ϕ'^2 and ϕ''^2 is 15% for 400 KHz scan and 10.5% for 600 KHz.

4. Q-Curve Fitting, Correction Formulas

In order to simulate the response function of the detector, the non-linearity, the signal shape change etc., there is a need to know the circuit parameters. Those we have obtained by a fit to the Q-curve and restricting their values to be around the measured ones. For the fit we used the *exact* formulas from Section 2, and the subroutine HFITH from the HBOOK which in turn is based on the Minuit package [13].

As is apparent from Eq. (3) the factor $\frac{GV_0}{R_0}$ would also be needed to fit the real data. In order to avoid this we have normalized the data and the fitting function by their minimum values, making the knowledge of that parameter unnecessary [14]. After we have obtained the rest of the parameters (5) from the fit, we used those to fit GV_0/R_0 to the original data, with the result given here for reference ($GV_0/R_0 = 0.10$ A).

The width of the TE NMR signals is $FWHM = 66$ KHz, i.e. 6.2×10^{-4} relative. This is more than 6 times than that which can be due to the magnet inhomogeneity. This width is assigned to be due to the dipolar broadening which becomes less important at high polarizations. Fig. 3 shows how a positive (dashed) and an inverted negative signal, using the same input signal with the above width, would look like at the output of the Q-meter circuit. The definite conclusion is that the positive signal

[1] The final result will not be different for a Gaussian, or Lorentzian Function.

Total Scan	a	b	c	d
400 KHz	6.5×10^{-2}	$-10. \times 10^{-2}$	-5.9×10^{-4}	-2.6×10^{-6}
600 KHz	4.5×10^{-3}	-6.3×10^{-2}	-3.7×10^{-4}	-1.6×10^{-6}

Table 1: Estimated parameters a, b, c, d for the different scan widths.

becomes wider, and the negative narrower, the reason being that the non-linearity contributes to the signal shape in different ways (see Eq. (13)). The width of the simulated negative signal becomes $FWHM = 51$ KHz (i.e. a reduction of 22%) and that of the positive $FWHM = 75$ KHz (i.e. an increase of 15%). Assuming about (20%) reduction in the dipolar broadening effect, at high polarizations, we would get a net slow reduction of the positive signal widths and a much faster reduction of the negative ones as the polarization increases, consistent with the experimental data. Taking this into account we have simulated the final signals with a $FWHM = 53.2$ KHz which is about 20% less than that of the TE signals. This 20% reduction in the signal width results in the reduction of the corrections by about 10% which we will treat as a source of error.

Another important feature of the non-linear terms is that the positive and negative (inverted) signals cross the zero line and become negative doing this at different points. Because the determination of the real zero point is in practice difficult, we take, after the baseline subtraction, the average of 20 points from the left end, and the same from the right end of the signals, and assume that those are the real zero points.

Using the simulated signals we show in Figs. 4a and 4b how much the relative polarization is overestimated (negative polarization) or underestimated (positive polarization) as a function of the signal output modulation, when using scan width of 400 and 600 KHz respectively. We have fitted the function

$$\frac{P_{real} - P_{meas}}{P_{meas}}[\%] = a + bM[\%] + c(M[\%])^2 + d(M[\%])^3, \tag{18}$$

and used the χ^2 minimization to determine the parameters. Figs. 4a and 4b show the corresponding estimations for 400 KHz and 600 KHz total scan width, and the parameters are given in Table 1. Even though the modulations of the positive and negative signals, for the same absolute polarization values, are very different, the non-linearity is roughly the same in magnitude for the same polarization.

The total error of about 20% is the total estimated error due to uncertainties in the circuit simplifications, the dipolar broadening change with polarization, and the fact that each coil is tuned slightly different from every other one (i.e. the circuit parameters are not the same for every coil).

6. Conclusions

The maximum experimentally observed modulation for the negative signals was 65% and that of the positive 40%. From Fig. 4a we then see that the polarizations were overestimated (underestimated) by a maximum of about 5% for the negative (positive) signals when 400 KHz total scan width was used. The same numbers go down to 3% when 600 KHz total scan width is used. These corrections have been already applied to the data [15], and it turns out that the positive and negative polarization values are much closer than before.

The impact of this result on the SMC experiment is small because the overestimation of the negative polarization and underestimation of the positive polarization are largely cancelled when the two target halves have the same absolute polarization and in the limit that the acceptance for both target halves is the same. This is so, because for the spin asymmetry analysis the difference between the two polarizations is relevant. However, experiments which only use a single target could benefit more from this analysis. This analysis helps the polarized target group to give more accurate absolute polarization values, since the non-linearity was the source of the highest single error in the polarization measurement.

Appendix

Various circuit and signal parameters are given here for reference. Some of the values are measured directly, and some are taken from the fit of the Q-curve (baseline).

$P_{TE} = 0.00255$	Proton TE polarization at 1 K and 2.5 Tesla.
$f_0 = 106.5$ MHz	Proton Larmor frequency at 2.5 Tesla.
$\omega_0 = 2\pi f_0$	Proton Larmor angular frequency at 2.5 Tesla.
$\Delta = \frac{\omega - \omega_0}{\omega_0}$	Fractional angular frequency. For a 600 KHz total scan $\Delta \approx 2.82 \times 10^{-3}$ at the right end of the scan.
$\Delta_H = 2.5 \times 10^{-4}$	Is the half width at half maximum of $\phi''(\omega)$ equal to 26.6 KHz which is used for the signal simulation.
$n = 5$	The length of the cables was $5\lambda/2$.
$C = 20\,pF$	Tuning capacitor.
$R = 34\Omega$	Damping resistor.
$L = 90nH$	Coil Inductance.
$R_L = 0.35\Omega$	Coil resistance.
$X = \frac{1}{R_i} + \frac{1}{R_0}$ $= 9.5 \times 10^{-3}\Omega^{-1}$	$R_i = 118\Omega$ is the sum of the amplifier input impedance of 50Ω and the external series resistor of 68Ω. $R_0 = 940\Omega$ is the current limiting resistor.
$Q = \frac{\omega L}{R} \approx 170$	Coil quality factor.
$Q_c = \frac{\omega L_c}{R_c} \approx 65$	Combined cable quality factor.
$Z_0 = 50\Omega$	Cable characteristic impedance.
$\alpha = 0.0242 Np/m$	Cable attenuation constant.
$\beta = D\omega \approx 3.16\,rad/m$	Phase constant of the cable.
$D = 4.72 \times 10^{-9} s/m$	Cable propagation delay.
$\beta = \omega\sqrt{\epsilon}/c$	$\epsilon \simeq 2.0$ is the dielectric constant of the cable, and c the speed of light in vacuum.

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[14] However, in the Q-meter circuit there is also a DC offset card whose functionality is to provide a better dynamic range for the readout system. It works by detecting the voltage of the left most data point (at the beginning of the baseline scan) with an A/D converter and then applying a DC voltage offset of the same value and opposite polarity with a D/A converter. Afterwards there is a card with software selectable nominal gains of 1, 227 and 315. During the SMC proton data run of 1993 the nominal gain of 1 was used throughout, which was determined by Dirk Krämer to be equal to 0.90, the value that was used in this paper.

[15] "Error Analysis for the NMR Polarization Measurement", SMC Polarized Target Group, SMC/94/7.

Figure captions

Figure 1. Series Q-meter NMR circuit.

Figure 2. Function $F(\Delta)$ versus Δ (see Eq. (17)) with $FWHM = 53.2$ KHz. The right end corresponds to $f - f_0 = 319.5$ KHz.

Figure 3. Simulated positive (dashed) and inverted negative signals at the output of the Q-meter. The FWHM for the input absorption function is 66 KHz. The output signals have FWHM of 75 KHz and 51 KHz for the positive and negative polarities respectively. The positive modulation is 0.34 and the negative 0.57.

Figure 4a. Non-linear contributions to the integrated series Q-meter signal for negative and positive polarizations, as a function of the output voltage modulation M. The total scan width is 400 KHz.

Figure 4b. Same as Figure 4a, but here the total scan width is 600 KHz.