Algorithm for Calculation of Longitudinal Target Polarization

Yu Kiselev\textsuperscript{a}, N Doshita\textsuperscript{b}, K Kondo\textsuperscript{b}, T Iwata\textsuperscript{b}, G Nukazuka\textsuperscript{b}

\textsuperscript{a}JINR, VBLPHE, 141980 Dubna, Moscow Reg. Russia, E-mail: yury.kiselev@cern.ch
\textsuperscript{b}Department of Physics, Faculty of Science, Yamagata University, 990-8560, Yamagata, Japan

Abstract. We suggest using the Lagrange polynomial interpolation to calculate the longitudinal polarization of the large COMPASS target with a length of 2x55 cm. The algorithm does not change the polarizations measured by the NMR sensors. In addition, it allows taking into account the influence of the microwave field on the nuclear polarization at the resonator boundaries. As a result, measurements of polarization at several points of a long target and knowledge of the cavity design allow one to obtain a more explicit analytical expression for the target polarization. The work is performed in the COMPASS collaboration at CERN.

1. Introduction

Polarization of long targets produced by the method of dynamic nuclear polarization (DNP) depends on the inhomogeneity of the bias field, temperature of the material, and parameters of the microwave (MW) field. In these targets, the polarization is measured by several NMR probes. To reduce the inductive coupling between the probes, their number is limited, and the axial angles between the NMR coils are rotated by $\pi/2$. It is clear that between probes the polarization should be calculated by interpolation of local measurements. Here we consider the Lagrange interpolation that not only allows calculating polarization and its errors at any place along the target but also helps estimate the efficiency of the target design.

2. Lagrange interpolation of the long target polarization

In its canonical form, the Lagrange interpolation formula [1] of the $n$-th order approximates the functions $p_k(x_k)$ by the polynomial of the $n$-th degree $P(x)$. Here $p_k=(p_0, p_1, \ldots, p_n)$ are polarization values at $n + 1$ probe locations $x_k = (x_0, x_1, \ldots, x_n)$ and the function $P(x)$ has the form:

\[
P(x) = \frac{(x - x_1)(x - x_2)\ldots(x - x_n)}{(x_0 - x_1)(x_0 - x_2)\ldots(x_0 - x_n)} p_0 + \frac{(x - x_0)(x - x_2)\ldots(x - x_n)}{(x_1 - x_0)(x_1 - x_2)\ldots(x_1 - x_n)} p_1 + \ldots + \frac{(x - x_0)(x - x_1)\ldots(x - x_{n-1})}{(x_n - x_0)(x_n - x_1)\ldots(x_n - x_{n-1})} p_n. \tag{1}
\]
Let the coordinate of a probe be \( x=x_i \), then \( P(x_i) = p_i \) in (1), because the fraction at \( p_2 \) equals to one and all other terms of the sum are zeroed. Thus, at \( x=x_i \) and similarly for all other coordinates of the probes, the polarizations exactly coincides with the measured values. Hence, the Lagrange algorithm does not distort the measured polarizations. Apart from the data of the direct NMR measurements, the indirect data following from the Maxwell equations can be additionally used in (1). For example, since the polarizing effect is produced by the radial magnetic components of the MW field (TM-modes), which have the maximum at the ends of the cavity walls, the polarization produced over there must be no lower than those measured by the nearest NMR probe. Of course, this condition is fulfilled when inhomogeneity of the bias field falls within the allowable limits and the stopper-insulator effectively suppresses MW power penetration. Let us consider the helpful example.

Figure 1 shows coordinates of probes in the upstream and downstream COMPASS cells. The targets are located in the center of the cylindrical MW cavities (not shown in the figure) along the bias field. The MW stopper-isolator installed between the cells allows independent polarization of each target. Ten NMR coils of the NMR probes \( p_1, p_2, p_3, p_4, p_5 \) and \( p_6, p_7, p_8, p_9, p_{10} \) (Fig. 1) are connected by coaxial cables to ten measuring units (Q-meters) kept at room temperature. Following the above logic, for the upstream cell one can assume \( p_{up0} \equiv p_1 \) and \( p_{up5} \equiv p_5 \), where \( p_{up0} \) and \( p_{up5} \) are the nuclear polarizations at \( x=x_0 \) and \( x=\pm x_0 \), respectively (Fig. 1). Similarly, for the downstream cell we can put \( p_{down6} \equiv p_6 \) and \( p_{down10} \equiv p_{10} \) (Fig. 1).

**Fig. 1.** The two targets are built into the dilution chamber of the \(^3\)He/\(^4\)He refrigerator. The MW stopper isolates the MW field allowing independent DNP in targets. The circles show location of NMR probes; their numerical positions and polarizations.

Now, formula (1) for the upstream target takes the form:

\[
P_{up}(x) = P_0 + P_1 + P_2 + P_3 + P_4 + P_5 + P_{end}
\]

where each summand describes the contribution of the probe polarizations at the point \( x \).

\[
P_0 = (x-x_1)(x-x_2)(x-x_3)(x-x_4)(x-x_5)(x-x_{end}) \cdot p_0/C_0,
\]

\[
P_1 = (x-x_0)(x-x_2)(x-x_3)(x-x_4)(x-x_5)(x-x_{end}) \cdot p_1/C_1,
\]

\[
P_2 = (x-x_0)(x-x_1)(x-x_3)(x-x_4)(x-x_5)(x-x_{end}) \cdot p_2/C_2,
\]

\[
P_3 = (x-x_0)(x-x_1)(x-x_2)(x-x_4)(x-x_5)(x-x_{end}) \cdot p_3/C_3
\]

\[
P_4 = (x-x_0)(x-x_1)(x-x_2)(x-x_3)(x-x_5)(x-x_{end}) \cdot p_4/C_4,
\]

\[
P_5 = (x-x_0)(x-x_1)(x-x_2)(x-x_3)(x-x_4)(x-x_{end}) \cdot p_5/C_5,
\]

\[
P_{end} = (x-x_0)(x-x_1)(x-x_2)(x-x_3)(x-x_4)(x-x_5) \cdot p_{end}/C_{end}.
\]

As follows from (1), the constants \( C_0...C_{end} \) are

\[
C_0 = (x_0-x_1)(x_0-x_2)(x_0-x_3)(x_0-x_4)(x_0-x_5)(x_0-x_{end}),
\]

\[
C_1 = (x_0-x_1)(x_0-x_2)(x_0-x_3)(x_0-x_4)(x_0-x_5)(x_0-x_{end})/C,
\]

\[
C_2 = (x_0-x_1)(x_0-x_2)(x_0-x_3)(x_0-x_4)(x_0-x_5)(x_0-x_{end})/C^2,
\]

\[
C_3 = (x_0-x_1)(x_0-x_2)(x_0-x_3)(x_0-x_4)(x_0-x_5)(x_0-x_{end})/C^3,
\]

\[
C_4 = (x_0-x_1)(x_0-x_2)(x_0-x_3)(x_0-x_4)(x_0-x_5)(x_0-x_{end})/C^4,
\]

\[
C_5 = (x_0-x_1)(x_0-x_2)(x_0-x_3)(x_0-x_4)(x_0-x_5)(x_0-x_{end})/C^5,
\]

\[
C_{end} = (x_0-x_1)(x_0-x_2)(x_0-x_3)(x_0-x_4)(x_0-x_5)(x_0-x_{end})/C_{end}.
\]
In the RUN_2015, the upstream sensors had the following local coordinates (Fig. 1): $x_0=0.1$, $x_1=2.5$, $x_2=13.5$, $x_3=27.5$, $x_4=41.0$, $x_5=52.0$, and $x_{end}=55.2 \text{ cm}$. Substitution into (4) yields

$$C_0 = 1.03064 \times 10^8,$$

It is convenient to present probe coordinates together with measured polarizations as a list \{x_0,p_0\}, \{x_1,p_1\},...,\{x_{end},p_{end}\}. In this notation, the upstream list in Units \{cm,\%\} is

\{
{0.1,84.1},{2.5,84.1},{13.5,79.0},{27.5,82.1},{41.0,81.4},{52.0,86.8},{55.2,86.8}\}. \hspace{1cm} (6)

A similar the downstream list was obtained as

\{
{75.0,-72.7}, {78.0,-72.7}, {88.5,-71.1}, {103.0,-81.3}, {116.5,-82.5}, {127.5,-81.2}, {132.0,-81.2}\}. \hspace{1cm} (7)

The interpolation functions of both upstream (6) and downstream (7) are shown in Fig. 2.

![Polarization graphs](image)

Fig. 2. Upstream (left) and downstream (right) cell polarizations shown along their length X in \{cm\}. The stopper place is located at the coordinates 55.2 < X < 75.0 cm.

In the simplest application, the Lagrange algorithm allows a set of digital polarization data (6) and (7) to be replaced by a convenient graphical interface, which facilitates visualization of the DNP regime and allows refining the calculation of the polarization in long targets.

### 3. Results

Figure 2 shows that the targets were polarized oppositely, therefore MW penetration through the stopper could affect their inhomogeneity. We study this effect using calculations of average polarizations with their standard deviations in the form

$$\langle P \rangle_{up} = \frac{1}{N} \sum_{i=1}^{N} P_{up}(x_i) \pm \langle \sigma \rangle_{up}, \quad \text{where} \quad \langle \sigma \rangle_{up} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (P_{up}(x_i) - \langle P \rangle_{up})^2},$$

The same formulas for the downstream are denoted by the symbol «down». If $x_i$ is scanned within coordinate lists (6) and (7) i.e. $N=7$ we obtained

$$\langle P \rangle_{up} = \frac{1}{7} \sum_{i=1}^{7} P_{up}(x_i) = +83.5\% \pm 2.9\%, \quad \langle P \rangle_{down} = \frac{1}{7} \sum_{i=1}^{7} P_{down}(x_i) = -77.5\% \pm 5.1\%.$$


The refined values obtained with the Lagrange functions are,
\[
\langle P \rangle_{\text{up}} = \frac{1}{55} \sum_{i=0.1}^{55.1} P_{\text{up}}(x_i) = +82.1\% \pm 2.2\% , \quad 0.1 < X < 55.1 \text{ cm (N=55)}, \quad (10)
\]
\[
\langle P \rangle_{\text{down}} = \frac{1}{57} \sum_{i=75}^{132} P_{\text{down}}(x_i) = -78.0\% \pm 4.8\% , \quad 75 < X < 132 \text{ cm (N=57)}. \quad (11)
\]
Here the calculations are retained in the discrete form, and the coordinate is stepped at 1 cm. For comparison, in the interval 75 < X < 100 cm (Fig. 2), we have
\[
\langle P \rangle_{\text{down}} = \frac{1}{25} \sum_{i=75}^{100} P_{\text{down}}(x_i) = -73.2\% \pm 2.5\% , \quad 75 < X < 100 \text{ cm (N=25)}. \quad (12)
\]
While for 100 ≤ x_i ≤ 132 cm, where MW leakage is suppressed by absorption in the initial part of the downstream target, the absolute value of polarization becomes almost 9% higher
\[
\langle P \rangle_{\text{down}} = \frac{1}{32} \sum_{i=100}^{132} P_{\text{down}}(x_i) = -81.9\% \pm 1.1\% , \quad 100 < X < 132 \text{ cm (N=25)}. \quad (13)
\]
It can be seen that the average upstream polarization (10) almost exactly equals to the polarization at the end of the downstream target (13), which indicate the absence of significant temperature gradients in a long dilution chamber and a high enough homogeneous microwave field. It becomes clear that the heterogeneity (12) is closely related to a microwave penetration (leakage) through MW stopper.

4. Conclusion
The Lagrange algorithm allows a set of digital polarization data to replace by a convenient graphical interface, which facilitates visualization of the DNP regime and allows refining the calculation of the polarization in long targets. The use of the Lagrange algorithm makes it possible to more accurately estimate the efficiency of microwave irradiation and the cryogenic equipment of targets using the averaged magnitude and the structure of the polarization.

5. References
[1] G Korn and T Korn 1961 Mathematical Handbook for Scientists and Engineers. Ch. 20.5-2 (New York Toronto London)