Neutron depolarization in aligned holmium and tests of time-reversal invariance

E. I. Sharapov
Joint Institute for Nuclear Research, 141980 Dubna, Russia

C. M. Frankle
Los Alamos National Laboratory, Los Alamos, New Mexico 87545
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The general formalism of quantum mechanics for the depolarization of neutrons in a magnetically anisotropic media is reviewed. This formalism is applied to the analysis of recent results on holmium single crystals. Such crystals have been prepared for testing time-reversal invariance in resonance neutron transmission experiments.

I. INTRODUCTION

Recently, Haase *et al.*[1] found a large neutron spin depolarization upon transmission of a longitudinally polarized neutron beam through a holmium single crystal. The parity violation effect in the 0.734 eV p-wave resonance in ^{139}La was used as the polarization analyzer. The phenomena was confirmed at other energy points, in particular at 1.7 eV, by Alfimenkov *et al.*[2] It would at first seem that these results pose a fundamental difficulty for the time-reversal invariance test proposed by Haase *et al.*[3] using an aligned holmium target with transversely polarized resonance neutrons. The geometry for such an experiment is depicted in Fig. 1.

The holmium samples used were right circular cylinders 2.1 cm in diameter and 3 cm in length. They were magnetically aligned at a temperature of 4 K in cryostats without any applied magnetic field. The magnetic structure of holmium under such conditions is known to be a set of antiphase ferromagnetic domains with saturation field $|\mathbf{B}| = 0.66$ T aligned with the c axis of the crystal. The situation is analogous to the case of an antiferromagnet. For a perfect holmium single crystal the depolarization was not expected, as opposed to the case of a ferromagnetic holmium polycrystalline sample where such an effect was found many years ago.[4]

The vector of the neutron spin, $\mathbf{S}$, in the suggested experiment of Haase *et al.*,[3] should stay perpendicular to both the neutron momentum and the c axis of the crystal. In a recent depolarization experiment, Haase *et al.*[1] were not working in exactly the geometry proposed for the time-reversal experiment. They have used a neutron beam polarized along the neutron momentum $\mathbf{k}$ and have placed the crystal c axis initially in the same direction. Rotating the c axis of the crystal by an angle θ off the direction of beam polarization $\mathbf{p}_0$, they have found that the transmitted neutron beam was totally depolarized at $\theta = 90°$ and partially depolarized at $\theta = 0°$. Their experimental data are presented in Fig. 2. Though not anticipated quantitatively, these results were not a total surprise. The crystal was not perfect, and from early time-of-flight depolarization measurements with thermal neutrons,[5] it followed that the velocity-dependent depolarization of the $\mathbf{p}_0$ component perpendicular to $\mathbf{B}$ should persist in the resonance energy region for thick enough samples.

The foundation for all modern depolarization work was laid as early as 1941 by Halpern and Holstein[6] in their treatment of neutron depolarization classically as being due to the precession of neutron spin in magnetic domains. Haase *et al.*[1] introduced a specific model of the depolarization as being due to spin rotations in an array of highly correlated domains characterized by the param-

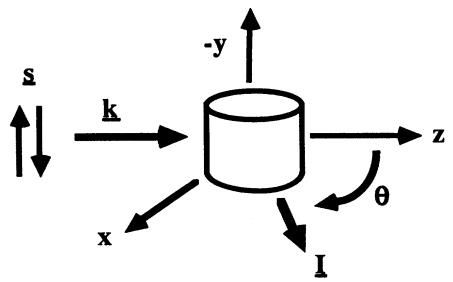

FIG. 1. Geometry of the proposed time-reversal invariance experiment.

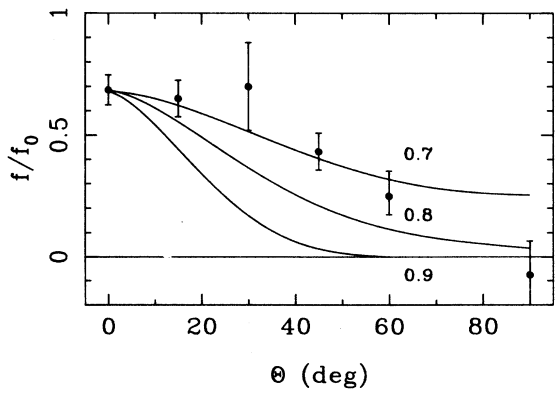

FIG. 2. Depolarization of 0.734 eV neutrons in holmium.

eters $\bar{B}$ and R, the last being the average domain size. Given a definite angle between the directions of $\mathbf{B}$ and $\mathbf{p_0}$, this model (and the general approach of Halpern and Holstein[6]) makes no distinction between cases having different orientations of $\mathbf{p_0}$ in space. The more elaborate approach of Rekveldt and van Schaik[7] is based on the introduction of a 3×3 matrix with the depolarization elements $D_{ij}(i,j=x,y,z)$ expressed in terms of numerous domain parameters. In relation to such a three-dimensional polarization analysis the work of Haase *et al.*[1] represents the measurement of only the D_{zz} element where the z axis is along the neutron momentum.

There exists a quite different quantum mechanical approach by Maleev and Ruban,[8] in which the depolarization is considered to be the result of small angle magnetic scattering within the angular spread of the passing beam. This phenomenon, namely, a depolarization anisotropy relative to the neutron momentum, is predicted with such an approach. For a magnetically isotropic sample, such an effect comes from the dependence of the magnetic scattering amplitude on the product $(\boldsymbol{\sigma}\cdot\mathbf{e})\,\mathbf{e}$, where $\boldsymbol{\sigma}$ is the Pauli matrix for the neutron spin and $\mathbf{e}$ is the unit vector of the momentum transfer. In the case of elastic scattering $\mathbf{e}$ is perpendicular to the neutron momenum $\mathbf{k}$. The existense of such a depolarization asymmetry was experimentally demonstrated by Drabkin, Okorokov, and Runov[9] for thermal neutrons. The goal of this work is to apply the Maleev-Ruban approach to the analysis of recent resonance neutron experiments with holmium single crystals.

II. DEPOLARIZATION IN THE QUANTUM DESCRIPTION

A quantum description was formulated by Maleev and Ruban for the case of thin samples and small domains. The former means that it is valid for samples of a thickness ΔL, satisfying the condition $\Delta L \ll l$, where l is the mean free path with respect to magnetic scattering. This condition is not fullfilled in many experiments. On the contrary, the condition of small domains is always satisfied for resonance neutrons. This means that the Born approximation is applicable to the calculation of scattering by domains and it is identical to the classical condition of having a small precession angle in each domain.

In the approach of Maleev and Ruban,[8] the entire depolarization $\Delta\mathbf{p}$ in the expression $\mathbf{p}=\mathbf{p_0}+\Delta\mathbf{p}$ is due to scattered neutrons. Recall that the transmitted beam consists of scattered neutrons with polarization $\mathbf{p_{sc}}$ as well as of those which have not experienced interaction and have preserved the polarization $\mathbf{p_0}$. The following general expressions have been obtained for the depolarization:

$$\Delta\mathbf{p}=2\Delta L N_0\sigma_0\int d\Omega(\mathbf{p_{sc}}-\mathbf{p_0})\frac{d\sigma}{d\Omega}, \tag{1}$$

$$\mathbf{p_{sc}}=2(\mathbf{n}_\perp\cdot\mathbf{p_0})\mathbf{n}_\perp-\mathbf{p_0}, \tag{2}$$

$$\frac{\mathbf{n}_\perp}{|n|}=\mathbf{m}-(\mathbf{e}\cdot\mathbf{m})\mathbf{e}. \tag{3}$$

Here N_0 is the density of magnetic atoms and $\mathbf{m}$ is the unit vector of the magnetization: $\mathbf{M}=g_e\mu_B N_0 S\mathbf{m}(\mathbf{r})$ where S is the effective atomic spin, and μ_B and g_e are the Bohr magneton and the electronic g factor, respectively. The angular polarization anisotropy is introduced through the vector $\mathbf{n}_\perp$ which is the transverse component of the magnetization lying in the plane perpendicular to the scattering vector $\mathbf{e}$. The differential magnetic scattering cross section $d\sigma/d\Omega$ and the total cross section σ_0 were calculated by Maleev and Ruban[8] for the case of a uniaxial ferromagnet model without net magnetization. With the assumption of homogeneity of the magnetization inside domains the model has five parameters $|\mathbf{B}|$, $R_\parallel$, $R_\perp$, x, and c_0. The second and third parameters represent the domain sizes in the directions parallel and perpendicular to the c axis. The parameter x describes the correlation between different domain orientations through the angle (θ_{mc}) between the directions of $\mathbf{m}$ and the c axis,

$$x=\frac{1}{2}(3\langle\cos^2\theta_{mc}\rangle-1). \tag{4}$$

This parameter reflects the depolarizing influence of the mean square fluctuations $\langle\Delta B_\parallel^2\rangle$, $\langle\Delta B_\perp^2\rangle$ of the domain field components parallel and perpendicular to the c axis. The last parameter c_0 describes the domain shape. For the simple case of a domain representing the ellipsoid of revolution with the axis c along the crystal c axis and the axis a perpendicular, it is expressed as

$$c_0=\frac{1-\frac{a}{c}}{1+\frac{a}{c}}. \tag{5}$$

The final results of the Maleev-Ruban calculations can be reduced to the following formulas for the five geometry situations ($\mathbf{k}$ is along the z axis in all cases; see Fig. 1):

$$\text{case 1}: \quad \frac{p}{p_0}=-(\gamma_\omega B)^2\frac{\Delta L}{v^2}\frac{R_\perp}{2}\left(1-\frac{x}{4}-c_0\right), \qquad \mathbf{p_0}\parallel y, c\parallel x; \tag{6}$$

$$\text{case 2}: \quad \frac{p}{p_0}=-(\gamma_\omega B)^2\frac{\Delta L}{v^2}\frac{R_\perp}{2}\left(1-\frac{3x}{4}-\frac{c_0}{3}(1-x)\right), \qquad \mathbf{p_0}\parallel x, c\parallel x; \tag{7}$$

$$\text{case 3}: \quad \frac{p}{p_0}=-(\gamma_\omega B)^2\frac{\Delta L}{v^2}\frac{R_\parallel}{3}(1-x), \qquad \mathbf{p_0}\parallel z, c\parallel z; \tag{8}$$

$$\text{case 4}: \quad \frac{p}{p_0}=-(\gamma_\omega B)^2\frac{\Delta L}{v^2}\frac{R_\perp}{3}\left(1+\frac{x}{2}-\frac{c_0}{2}x\right), \qquad \mathbf{p_0}\parallel z, c\parallel x; \tag{9}$$

$$\text{case 5}: \quad \frac{p}{p_0}=-(\gamma_\omega B)^2\frac{\Delta L}{v^2}\frac{R_\parallel}{2}(1+x), \qquad \mathbf{p_0}\parallel x, c\parallel z. \tag{10}$$

Here B, in tesla, is the value of the magnetic induction inside the domain, v is the velocity of the neutron, and $\gamma_\omega = 2\pi(2.9 \times 10^7)(\mathrm{T\,sec})^{-1}$. With the value of the parameter $x \simeq 1$ the maximum effect of depolarization is expected in the geometry of case 5, the minimum in case 3. Measurements of these two cases will allow one to extract the values of parameters x and $R_\parallel$ if the value of B is known. Other measurements, if performed, can give the values of the other parameters. In most experiments, as previously mentioned, the condition of having a thin sample is not always satisfied. It is trivial to obtain the following relation for a thick sample:

$$\frac{p}{p_0} = e^{-\alpha L}, \tag{11}$$

where α is any of the expressions (6)–(10) with ΔL term excluded. The problem is not trivial at all for the cases of intermediate (between 0° and 90°) values for the angle θ, which we have not considered. Complications arise from the fact that, as shown by Maleev and Ruban, with the beam initially polarized along z, for example, one has both polarizations p_z and p_x at some depth of a thick sample, that is, the polarization rotates in addition to being depolarized. The rotated polarization will be transmitted by the next layer of the sample in a different way. As a result, in the case of a thick sample with the initial polarization $\mathbf{p}_0$ along either $\mathbf{k}$ or the x axis, the angular dependence of the depolarization might have an oscillatory behavior and the depolarization itself might not follow the simple v^2 law.

III. APPLICATION TO THE CASE OF A HOLMIUM SINGLE CRYSTAL AT 4 K

The holmium depolarization measurements of Haase *et al.*[1] were made with longitudinally polarized neutrons in the geometry of cases 3 and 4. The four unknown parameters $R_\parallel$, $R_\perp$, x, and c_0 are present in Eqs. (8) and (9). Therefore, further simplifying assumptions are necessary. As with Haase *et al.*,[1] let us assume no distinction between the parameters $R_\parallel$ and $R_\perp$ and let us instead introduce a uniform domain size $R = R_\parallel = R_\perp$ (then $c_0 = 0$). The experimental data are shown in Fig. 2. The point at $\theta = 0°$ corresponds to Eq. (8) and gives the value of the product

$$R(1 - x) = 0.65 \pm 0.13\ \mu\mathrm{m}. \tag{12}$$

The error bar of the point at $\theta = 90°$, though large, can also be used if one takes into account the additional information on the expected range of the parameter x. The pattern of aligned magnetic domains in holmium at a temperature 4 K suggests that the value of the parameter x is close to 1. A value of $x = 0.9$, for example, corresponds to an average misalignment angle of antiphase domains $\theta_{mz_c} = 15°$, whereas the value $x = 1.0$ is the limiting case of total alignment. It is then seen from Eqs. (9) and (11) that the data point at $\theta = 90°$ sets the lower limit $R > 2.1\ \mu m$ independently of exact knowledge of value of the parameter x and that Eq. (12) gives the value of correlated pairs $(x; R)$, for example,

$$x = 0.7,\ R = 2.1\ \mu\mathrm{m}$$
$$x = 0.8,\ R = 3.15\ \mu\mathrm{m}$$
$$x = 0.9,\ R = 6.3\ \mu\mathrm{m}$$

and so on. The three curves in Fig. 2 correspond to these three pairs of parameters $(x; R)$. Taking into account only the data at $\theta = 0°$ and 90°, one is forced to conclude that the parameter values are $0.7 < x < 1$ and $2\ \mu\mathrm{m} < R < 60\ \mu\mathrm{m}$ (with an upper limit 60 μm taken, as by Haase *et al.*,[1] from the residual resistivity data). Considering all data points and curves in Fig. 2, one is tempted to make the strictest conclusion

$$x = 0.8 \pm 0.1,\quad R = (3^{+3}_{-1})\ \mu\mathrm{m}. \tag{13}$$

It should be emphasized, however, that the curves of Fig. 2 were calculated neglecting the possible influence of the aforesaid rotation of polarization $\mathbf{p}$ for the intermediate angles between 0° and 180°.

The second depolarization experiment[10] was performed in the geometry of case 1 using a much smaller holmium single crystal at neutron energies $E_n = 0.2$–5 eV. According to the preliminary results the neutron depolarization was small, as expected qualitatively from Eq. (6) when $x \simeq 1$. The third experiment with holmium was performed using the neutron energy $E_n = 1.7$ eV and for the angles $\theta = 0°$–180°.[2] The corresponding limiting cases 2 and 5 are described by Eqs. (7) and (10). The crystal was of the same size, and fabricated from the same material and by the same method as the crystal used in the work of Haase *et al.*[1] The original depolarization results revealed some "left-right" asymmetry between the data points in the regions $\theta = 0°$–90° and $\theta = 90°$–180°; however, the averaged left-right results will be presented here as given in Fig. 3 (triangles) for comparison with the data of Haase *et al.*[1] (circles). Two curves are calculated for $E_n = 0.75$ eV and $E_n = 1.7$ eV using the model and parameters of Haase *et al.*[1] It is seen that two sets of data being interpreted in the framework of the model of Haase *et al.*[1] do not confirm the expected energy dependence of the depolarization, implying a problem for suggested resonance neutron time-reversal invariance (TRI) exper-

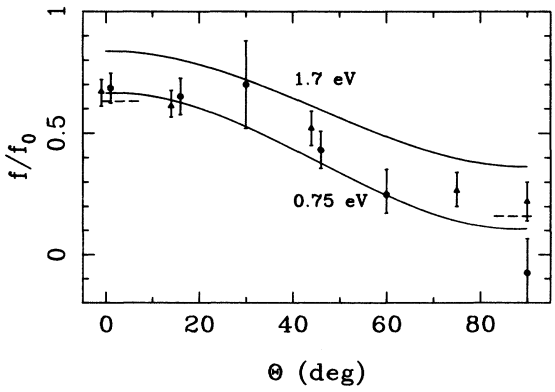

FIG. 3. Comparison of the depolarization at different neutron energies.

iments. The conclusion is just the opposite, however, if the data are interpreted in the framework of the model of Maleev and Ruban.[8] Here, with the parameter $x = 0.75$, the calculated values of the depolarization at the energy $E_n = 1.7$ eV (the dashed lines for $\theta = 0°$ and $90°$) are in agreement with the experiment. The apparent cancellation of the energy dependence is due to the influence of the different geometries discussed above. Therefore, trusting the $1/v^2$ dependence of the depolarization (at identical geometries), one can expect a very low value of the depolarization for resonance neutrons with energies above 20 eV, for which the experiments testing TRI were suggested recently.[11]

Of course, all experimental data, especially those obtained in different geometries but with the same crystal, should be analyzed together (when such data become available) to fix all parameters of the model.

IV. CONCLUSION

The quantum description of depolarization elaborated by Maleev and Ruban for thermal neutrons and thin targets works for the case of resonance neutrons and a thick sample. It emphasizes the role of the orientation of the polarization of the beam relative to neutron momentum in addition to the orientation relative to the magnetization axis. The approach is well suited to the analysis of neutron depolarization in the holmium single crystal investigated in several laboratories in view of its potential use in the proposed experiments to test time-reversal invariance in resonance neutron reactions. The analysis of the existing data is in favor of the expected strong energy dependence of the depolarization. In view of our analysis and the fact that the possible candidate resonances for the TRI experiment are located at relatively high energies, the neutron depolarization apparently presents no fundamental problem for the suggested TRI experiments.

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