Polarized Neutron Scattering

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Polarized neutron Scattering is a crucial spectroscopic technique that divulges the polarization of the neutrons to uncover valuable information regarding the sample environment that otherwise remains hidden. The polarized neutrons interact with the sample via strong nuclear forces and magnetic forces. This paper reviews the theory behind the production of polarized neutrons and the basic working of this spectroscopic technique.

I. INTRODUCTION

The magnetic structure was first determined on a MnO sample by Shull and Smart in the year 1949 [1]. The neutron powder diffraction data at room temperature, i.e., in the sample's paramagnetic state, showed no magnetic peak intensities. But, below the antiferromagnetic ordering temperature, the observed Bragg reflections were actually a sum of nuclear and magnetic intensities. The comparison between these two types of measurements paved the way for magnetic structure determination, and to date, hundreds of magnetic structures have potentially been solved [2].

The next big step, which came in 1959, was the use of polarized neutrons in the scattering experiments [3]. In these experiments, the incoming neutron beam is either polarized up or down. Thus we have two kinds of scattered neutron intensities to compare based on the neutron beam's initial polarization. Therefore, polarized neutrons seemingly impart increased information from a typical unpolarized neutron scattering experiment.

Speaking of the neutron, the properties that make it unique in scattering experiments and condensed matter research are hidden in its spin and magnetic moment. A typical neutron-matter interaction has two aspects, firstly, the strength of the nuclear interaction of the neutron and the nucleus depends on the parallel or antiparallel alignment of their spins, and secondly, when magnetic scattering is at play, the magnetic moment of the neutron interacts with the unfilled electron shells of the atoms involved in the scattering. The scattering process will also affect the neutron spin; thus, we can have a situation where controlling the neutron's spin will provide us with more flexibility and information in our experiment.

This project report revolves around the working of the polarized neutron scattering technique and its polarization analysis. This powerful technique has helped separate scattering terms in experimental results based on their magnetic and structural origins and presented detailed contributions from factors that remained hidden in our trivial unpolarized scattering experiments.

II. POLARIZED NEUTRONS: WHAT DOES IT MEAN?

When one says polarized neutron, one implies a polarized neutron beam. Each neutron carries a spin $\mathbf{S}$, which is an intrinsic angular momentum with a quantum number 1/2. The eigenvalue of the projection of $\mathbf{S}$ along z-axis (i.e., the eigenvalue of the S_z operator) is given by $m_S = \pm 1/2\hbar$. A polarized neutron beam has all the neutrons in one of these two eigenstates ($\uparrow$ or $\downarrow$).
$\mathbf{s}$ has three components S_x, S_y, S_z, and these operators can be expressed in terms of the three known Pauli matrices for the spin 1/2 particle. Let's define the operator $\boldsymbol{\sigma} = 2\mathbf{S}/\hbar$. Thus, one can now write:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1}$$

For a neutron j which is a part of the beam, the polarization $\mathbf{p_j}$ is a vector with 3 components and is given by the equation (2) below:

$$\mathbf{p_j} = \langle \boldsymbol{\sigma} \rangle = \begin{pmatrix} \langle \sigma_x \rangle \\ \langle \sigma_y \rangle \\ \langle \sigma_z \rangle \end{pmatrix} \tag{2}$$

Thus, the neutron beam's polarization is written as an average over all the individual neutron polarization. This is given by equation (3).

$$\mathbf{P} = \frac{1}{N} \sum_j \mathbf{p_j} \tag{3}$$

We see that the polarization vector $\mathbf{P}$ is a 3 component vector which can be measured. If we consider any particular direction α, the component of P_α is given as:

$$P_\alpha = \frac{n^+ - n^-}{n^+ + n^-} \tag{4}$$

Here, n^+ is the number of neutrons in the $\uparrow$ state, and n^- is the number of neutrons in the $\downarrow$ state [4]. Clearly,

$$0 \leq |\mathbf{P}| \leq 1 \tag{5}$$

Because it has spin, the neutron also carries a magnetic moment.The relation between the spin and the magnetic moment is given by:

$$\mu_n = g_n S \mu_N \simeq \mp 1.913 \mu_N = \pm \gamma_n \mu_N \tag{6}$$

where $\gamma_n = -g_n S$ is the gyromagnetic factor of the neutron, and the neutron g -factor, $g_n = -3.8260837(18)$, in units of the nuclear magneton $\mu_N = \frac{e\hbar}{2m_p}$.
For neutron, a feature different from electron and proton, the magnetic moment is aligned opposite to the spin [5].

A. Interaction with Magnetic field

An exciting result is the effect of an applied magnetic field on the neutron path. What the field does is that it exerts a torque on the neutron magnetic moment. This torque is given by :

$$\Gamma = \mu \times B = \gamma_L S \times B \tag{7}$$

where, the gyromagnetic ratio $\gamma_L = (2/\hbar)\gamma_n \mu_N$ (not to be confused with the gyromagnetic factor in equation 6).
Because of this torque, the neutron magnetic moment, and as a direct consequence, the polarization vector precesses around the field. Therefore, we can see that magnetic fields are excellent tools to control the polarization of the neutron beam. If the magnetic field is constant, the neutrons will rotate around the field with a frequency (Larmor frequency):

$$\omega_L = \gamma_L H \tag{8}$$

This motion is popularly known as the Larmor precession (see Figure 1). Another seemingly important question is what happens to the neutrons when the field varies along the neutron path. Here, the two extreme cases are of importance. Firstly, if the field is varied slowly compared to the ω_L, the neutron faces many turns before settling with the final field direction. Thus, during this process, the neutron doesn't feel the change, and it slowly follows the field during the rotation. This process is called **slow adiabatic field variation** (see Figure 2). Secondly, if the field changes abruptly w.r.t ω_L, the neutron has no time to react to the field change. Such a process is known as the **sudden field** reversal, and it used to reverse the polarization of the neutron beam w.r.t the guiding field(i.e., create a flip in the polarization) (see Figure 3).

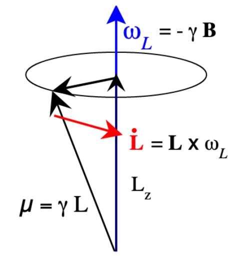

FIG. 1. Showing the Larmor Precession of the neutron in presence of a constant magnetic field [5]

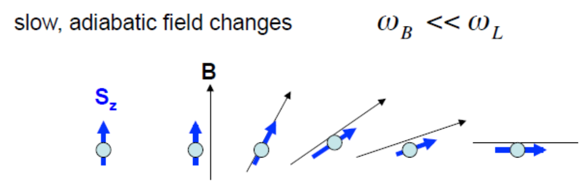

FIG. 2. Neutron Polarization in case of a slowly varying magnetic field. [5]

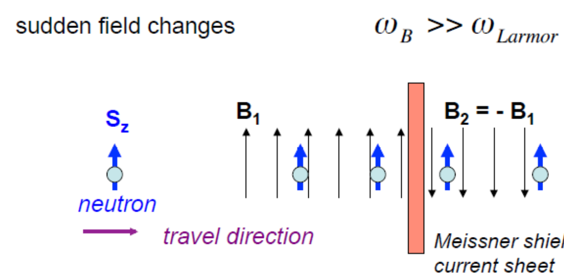

FIG. 3. Neutron Polarization in case of a suddenly varying magnetic field. [5]

III. EXPERIMENTAL DEVICE: POLARIZATION SPECTROMETER

A typical experimental setup for the polarization measurements is shown in Figure 4. This is known as the polarization spectrometer. It has a polarizer, a magnetic crystal used to monochromatize and polarize the incident neutron beam using Bragg reflection. The other end of the spectrometer has an analyzer that is a similar crystal used to measure the spin state and the scattered neutron beam's energy. Along the neutron path, a guide field preserves the neutron beam's spin state. This field is present both along the incident and scattered path of the beam.

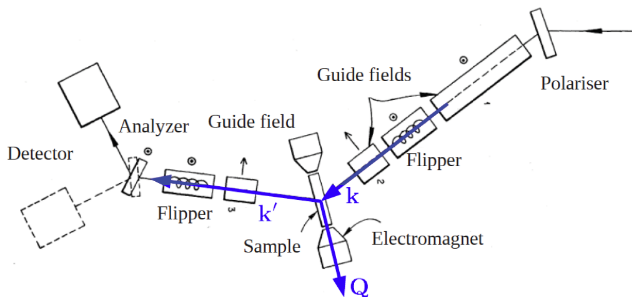

FIG. 4. Schematic diagram of a polarization spectrometer used by *Moon* et al., (1969) at the Oak Ridge National Laboratory. [5, 6]

A device known as the flipper sits between the polarizer and the sample. This flipper works to produce a radio-frequency field perpendicular to the guide field. When this flipper is on, it changes the spin state of the neutrons. A second flipper is also present between the scattering sample and the analyzer. When made to work together, both of these flippers give us the different combinations possible for the initial and final spin state of the neutron beam. For example, if both the flippers are off, we get the scattering cross-section for the spin-state transition from ↑ to ↑ state; and with the first flipper off and second flipper on, we get the scattering cross-section for the ↑ to ↓ transition.
The sample sits between the poles of an electromagnet. The magnetic field of this electromagnet dictates the polarization. In this entire setup, the electromagnet, along with the guide fields can rotate, so that the polarization axis can be easily made either parallel or perpendicular to the scattering vector $\mathbf{Q} = \mathbf{k_i} - \mathbf{k_f}$.

IV. SCATTERING AND POLARIZATION

A. Interaction of neutrons with matter

The unpolarized neutron scattering experiments consider the transition of the neutron from one momentum state to the other. However, when we consider polarized neutron scattering, we consider the change from one spin-momentum state of the neutron to another.
Most samples that we find in nature contain magnetic moments, either from the nuclei of the individual atoms present in the sample or the electrons. Therefore, the scattered polarization of the neutrons and the scattering cross-section of the process depends on the relative orientation between the sample's magnetic moments and the neutron beam's polarization. When we analyze this scattered beam, we are awarded more information about the system. Figure 5 shows the two processes involved in our experiment. In most cases, the scattered polarization is measured along the direction of the incident polarization; this is known as longitudinal polarization analysis [7].

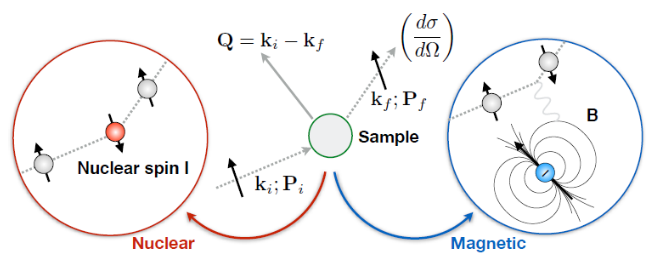

FIG. 5. A schematic showing the two processes involved in polarized neutron scattering experiments.[8]

The amplitude of neutron scattering $\mathbf{F_Q}$ for a given scattering potential $\mathbf{V_Q}$ is given by:

$$F_{\mathbf{Q}} = \langle \mathbf{k_f S_f} \,| V_{\mathbf{Q}} |\, \mathbf{k_i S_i} \rangle \tag{9}$$

This gives a scattering cross section that in general depends on the scattering vector $\mathbf{Q} = \mathbf{k_i} - \mathbf{k_f}$ and some known constants. The expression for the scattering cross section is given (by equation 10) below:

$$\frac{d\sigma}{d\Omega} = \left(\frac{m_n}{2\pi\hbar^2}\right)^2 |\mathbf{F}_Q|^2 \tag{10}$$

B. Applications

If we consider the **nuclear interaction**, the operator describing this potential is given by:

$$\hat{V} = \left(2\pi\hbar^2/m_n\right)\hat{b} \tag{11}$$

The scattering length vector $\hat{b}$ is a scalar for a nuclei with zero spin, and hence the interaction is spin independent. For the interaction to be spin dependent the involved nuclei has to have a non-zero spin $\mathbf{I}$. In this scenario, $\hat{b}$ is given by:

$$\hat{\mathbf{b}} = A + B\hat{\boldsymbol{\sigma}} \cdot \hat{\mathbf{I}} \tag{12}$$

where A = the coherent part, and $B\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{I}}$ is the fluctuating spin-dependent part. Both A and B are well defined constants.
If we define the z axis as our neutron polarization axis, $\mathbf{P} = 2\langle\hat{\mathbf{S}}\rangle = \langle\hat{\boldsymbol{\sigma}}\rangle$ with the eigen states given by $|\uparrow\rangle = |+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|\downarrow\rangle = |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. The transition matrix elements are given by equation 13, for the two spin-flip and two non-spin-flip scattering amplitudes respectively.

$$\begin{aligned} \langle +|\hat{\sigma}\cdot\hat{\mathbf{I}}|+\rangle &= I_z \\ \langle -|\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{I}}|+\rangle &= I_x + \mathrm{i}I_y \\ \langle +|\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{I}}|-\rangle &= I_x - \mathrm{i}I_y \\ \langle -|\hat{\sigma}\cdot\hat{\mathbf{I}}|-\rangle &= -I_z \end{aligned} \tag{13}$$

From the above results, it can be noted that $2/3^{\mathbf{rd}}$ of the spin-incoherent scattering is spin flipped, and $\mathbf{P_f} = -1/3$.
To summarize, there are three contributions to the nuclear scattering; the average of the **coherent scattering**, the isotopic i.e. the spin independent part of the incoherent scattering (**isotopic-incoherent scattering**), and the spin dependent part of the incoherent scattering (**spin-incoherent scattering**), and when magnetic scattering is absent, the sum of the coherent and isotopic-incoherent scattering can be separated from the spin-incoherent scattering by measuring the spin-flip and non-spin-flip scattering.

$$\begin{aligned} \frac{d\sigma^N}{d\Omega_{\mathbf{Q},coh}} + \frac{d\sigma^N}{d\Omega_{isotop-inc}} &= \frac{d\sigma^{NSF}}{d\Omega} - \frac{1}{2}\frac{d\sigma^{SF}}{d\Omega} \\ \frac{d\sigma}{d\Omega_{spin-inc}} &= \frac{3}{2}\frac{d\sigma^{SF}}{d\Omega} \end{aligned} \tag{14}$$

It should be noted that whatever we got here is independent of the direction of $\mathbf{P}$ or $\mathbf{Q}$ (see Figure 6 for an example of nuclear scattering).

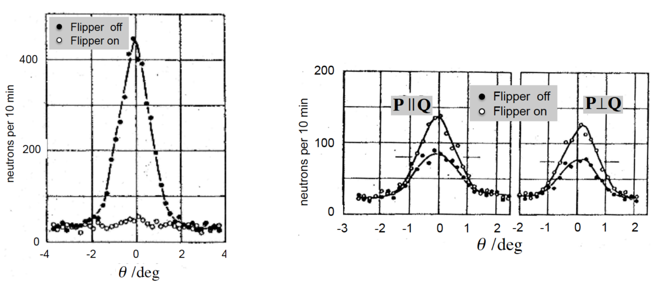

FIG. 6.
Left: Nuclear isotopic-incoherent scattering from a Nickel. Right: Showing the independence of the nuclear scattering (from Vanadium)from the relative direction between $\mathbf{P}$ and $\mathbf{Q}$ [5, 6].

Similar to nuclear scattering potential, the **magnetic interaction** potential is given by:

$$V_m = -\left(\gamma_n r_0/2\right)\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{M}}^{\perp}_{\mathbf{Q}} \tag{15}$$

Here $\hat{\mathbf{M}}^{\perp}_{\mathrm{Q}}$ is the operator of the magnetic interaction vector, and

$$\mathbf{M}^{\perp}_{\mathbf{Q}} = \mathbf{e_Q}\times\mathbf{M_Q}\times\mathbf{e_Q} \tag{16}$$

$\mathbf{M_Q}$ is the Fourier transform of the total magnetization density present in the sample. The only part of $\mathbf{M_Q}$ which contributes to the interaction is the one perpendicular to $\mathbf{Q}$. This happens because of the dipolar interaction between the neutron spin and the sample's magnetic moments. The components of magnetic moment parallel to $\mathbf{Q}$ tend to interfere destructively and cancel out. Therefore, magnetic scattering has a directional dependence on Q. Similar to what was discussed for nuclear scattering, the transition matrix elements in this case are given by:

$$\begin{aligned} \left\langle + \left| \hat{\sigma}\cdot\hat{\mathrm{M}}^{\perp}_{\mathrm{Q}} \right| + \right\rangle &= \mathrm{M}^{\perp}_{z,\mathrm{Q}} \\ \left\langle - \left| \hat{\sigma}\cdot\hat{\mathrm{M}}^{\perp}_{\mathrm{Q}} \right| + \right\rangle &= \mathrm{i}\mathrm{M}^{\perp}_{y,\mathrm{Q}} \\ \left\langle + \left| \hat{\sigma}\cdot\hat{\mathrm{M}}^{\perp}_{\mathrm{Q}} \right| - \right\rangle &= -\mathrm{i}\mathrm{M}^{\perp}_{y,\mathrm{Q}} \\ \left\langle - \left| \hat{\sigma}\cdot\hat{\mathrm{M}}^{\perp}_{\mathrm{Q}} \right| - \right\rangle &= -\mathrm{M}^{\perp}_{z,\mathrm{Q}} \end{aligned} \tag{17}$$

Here, we have chosen z as the polarization axis, and $\mathbf{Q}\|x$, $\mathbf{M}^{\perp}_{x,\mathrm{Q}} = 0$. It can be seen that the component of $\mathbf{P}$ parallel to $\mathbf{M}^{\perp}_{\mathbf{Q}}$ remains unchanged, whereas the perpendicular component reverses its sign.
In sum, we can say that if $\mathbf{P}$ is parallel to $\mathbf{Q}$, the magnetic scattering is represented by spin-flip scattering. Thus, if we demonstrate our experiment, such that $\mathbf{P}\|\mathbf{Q}$, the spin-flip scattering will correspond to magnetic scattering and the non-spin-flip scattering corresponds to nuclear scattering (see Figure 7 for reference).

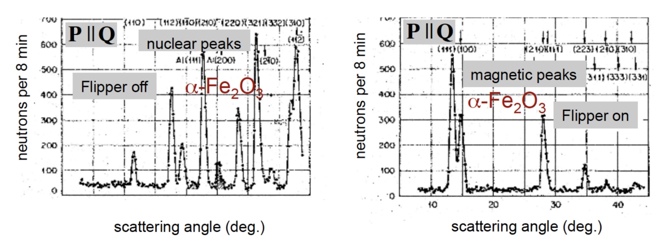

FIG. 7.
This figure shows the separation of magnetic and nuclear Bragg peaks, for an Iron Oxide sample, by doing spin-flip and non-spin-flip scattering when $\mathbf{P}\|\mathbf{Q}$ [5, 6].

V. ACKNOWLEDGEMENTS

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