SCATTERING OF POLARIZED NEUTRONS BY FERROMAGNETS AND ANTIFERROMAGNETS

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We consider the change in polarization resulting from scattering of polarized neutrons by ferromagnets and antiferromagnets. We show how one can determine the magnetic scattering cross section from measurements of the scattering cross section in a given direction and the polarization of the scattered neutrons.

RECENTLY one of the present authors showed[1] that by studying the polarization resulting from the scattering of unpolarized neutrons by ferromagnets one can, in certain cases, separate out from the scattering in a given direction a part which is due to inelastic magnetic scattering and a part which is due to magneto-vibrational scattering. It is obvious that polarization cannot result from the scattering of unpolarized neutrons by antiferromagnets. This is related to the fact that the system as a whole (neutron + scatterer) is not characterized by any pseudovector along which the polarization of the scattered neutron might be directed. (The direction of magnetization of the sublattices does provide an axis for the system, but not a direction, since the sublattices are equivalent.) Nevertheless it is obvious that the polarization vector can be rotated upon scattering of polarized neutrons in an antiferromagnet. Similarly, in the scattering of polarized neutrons by a ferromagnet, in addition to a change in the magnitude of the polarization vector there may also be a rotation of its direction.

In this paper we show how, by studying the polarization after scattering, one can separate from the cross section for scattering in a given direction parts which are associated with inelastic magnetic scattering and with magneto-vibrational scattering. We start with the scattering by ferromagnets. It is well known that the neutron polarization vector after scattering is given by the formula

$$\mathbf{P} = \mathrm{Sp}\, f^{+}\sigma f \rho / \mathrm{Sp}\, f^{+} f \rho, \qquad (1)$$

where $\frac{1}{2}\sigma$ is the neutron spin and

$$\rho = \tfrac{1}{2}(1 + \sigma\mathbf{P}_0) \qquad (2)$$

is the spin density matrix of the incident neutrons, $\mathbf{P}_0$ is the polarization of the beam before the scattering, and f is the scattering amplitude which, according to Halpern and Johnson,[2] is given by the formula

$$f = \frac{1}{N}\sum_l e^{i\mathbf{qR}_l}\left[A_l + \frac{1}{2}B_l(\mathbf{I}_l\sigma)\right] - \frac{N_m}{N}\frac{1}{N_m}\sum_j e^{i\mathbf{qR}_j} \times \gamma r_0 F(q)\,(\sigma - (\mathbf{e}\sigma)\,\mathbf{e},\, \mathbf{S}_j). \qquad (3)$$

Here N is the total number of atoms in the system, $\mathbf{R}_l$ and $A_l + \frac{1}{2}B_l(\mathbf{I}_l\sigma)$ are the coordinate and the nuclear scattering amplitude of the l'th atom (where $\mathbf{I}_l$ is the spin of the nucleus of the l'th atom). The sum on l is extended over all atoms in the system (where N_m is the number of magnetic atoms), $\mathbf{R}_j$ and $\mathbf{S}_j$ are the coordinate and spin of the j'th magnetic atom (where the sum over j goes over all the magnetic atoms in the system)*, $\mathbf{q} = \mathbf{p} - \mathbf{p}'$ is the momentum transferred by the neutron to the scatterer, $\mathbf{e} = \mathbf{q}/q$, $F(q)$ is the magnetic form factor of the atom, γ is the absolute value of the neutron magnetic moment in nuclear magnetons, and $r_0 = e^2(mc^2)^{-1}$ is the classical radius of the electron.

For simplicity, we shall assume that the ferromagnet consists of atoms of one sort, i.e., $N_m = N$ and the sum over l coincides with the sum over j. Using (1) — (3), it is easy to calculate the polarization vector resulting from the nuclear scattering and the interference between nuclear and magnetic scattering (such interference being possible both for elastic scattering and for scattering with emission or absorption of phonons), and also the polarization vector resulting from magnetic inelastic scattering; in doing this we shall assume that the nuclei are unpolarized.

The polarization vector from incoherent nuclear scattering of neutrons has the form

*For simplicity, we assume that all the magnetic atoms in the system are identical.

$$\mathbf{P}_{\text{inc}} = \mathbf{P}_0 \frac{\overline{|A_l|^2} - |\overline{A}_l|^2 - \frac{1}{12}\overline{|B_l|^2 I_l(I_l+1)}}{\overline{|A_l|^2} - |\overline{A}_l|^2 + \frac{1}{4}\overline{|B_l|^2 I_l(I_l+1)}}. \quad (4)$$

The bar denotes an average over the distribution of isotopes in the lattice.

The polarization vector for neutrons which are scattered without a change in the magnetic state of the scatterer (i.e. without emission or absorption of spin waves) is given by the formula

$$\mathbf{P}_{nm} = \{\mathbf{P}_0|\overline{A}_l|^2 - 2\gamma r_0 F(q)\langle S_z\rangle(\mathrm{Re}\,\overline{A}_l\mathbf{M} + \mathrm{Im}\,\overline{A}_l[\mathbf{MP}_0]) + \gamma^2 r_0^2 F^2(q)\langle S_z^2\rangle[2\mathbf{M}(\mathbf{MP}_0) - \mathbf{P}_0 M^2]\}\{|\overline{A}_l|^2 - 2\gamma r_0 F(q)\langle S_z\rangle\,\mathrm{Re}\,\overline{A}_l(\mathbf{MP}_0) + \gamma^2 r_0^2 F^2(q)\langle S_z^2\rangle M^2\}^{-1}, \quad (5)^*$$

where the vector $\mathbf{M}$ is

$$\mathbf{M} = \mathbf{m} - (\mathbf{em})\,\mathbf{e} \quad (6)$$

($\mathbf{m}$ is a unit vector along the direction of magnetization of the scatterer), and $\langle S_z\rangle$ and $\langle S_z^2\rangle$ are the average values of the spin projection along the direction of magnetization and of its square; it is usually assumed that $\langle S_z\rangle^2 = \langle S_z^2\rangle$. In particular, expression (5) gives the polarization of neutrons which are scattered in the directions of the Bragg peaks, since along these directions we can neglect the contribution to the total intensity from incoherent nuclear scattering and from inelastic scattering.

The polarization vector $\mathbf{P}_m^+$ (or $\mathbf{P}_m^-$) which results from scattering with emission (or absorption) of one spin wave, or more precisely from a scattering process in which the total number of spin waves increases (or decreases) by unity, and in which phonons may be emitted or absorbed, has the form

$$\mathbf{P}_m^{\pm} = \frac{\mp 2\mathbf{e}(\mathbf{em}) + 2\mathbf{M}_x(\mathbf{M}_x\mathbf{P}_0) + 2\mathbf{M}_y(\mathbf{M}_y\mathbf{P}_0) - \mathbf{P}_0(M_x^2 + M_y^2)}{1 + (\mathbf{em})^2 \pm 2(\mathbf{P}_0\mathbf{e})(\mathbf{em})}. \quad (7)$$

The x and y coordinate axes are perpendicular to the direction of $\mathbf{m}$. The vectors $\mathbf{M}_{x,y} = \mathbf{n}_{x,y} - (\mathbf{e}\cdot\mathbf{n}_{x,y})\,\mathbf{e}$, while $\mathbf{n}_x$ and $\mathbf{n}_y$ are unit vectors in the directions of the x and y axes. It is easily seen that the expression (7) is independent of rotation around the direction of the vector $\mathbf{m}$. We shall show this when we discuss polarization from antiferromagnets (see below).

The average value of the polarization vector of the neutrons scattered in a given direction has the form†

$$\mathbf{P} = \frac{\mathbf{P}_{\text{inc}}\sigma_{\text{inc}}(\mathbf{n}) + \mathbf{P}_{nm}\sigma_{nm}(\mathbf{n},\mathbf{P}_0) + \mathbf{P}_m^+\sigma^+(\mathbf{n},\mathbf{P}_0) + \mathbf{P}_m^-\sigma^-(\mathbf{n},\mathbf{P}_0)}{\sigma_{\text{inc}}(\mathbf{n}) + \sigma_{nm}(\mathbf{n},\mathbf{P}_0) + \sigma_m^+(\mathbf{n},\mathbf{P}_0) + \sigma_m^-(\mathbf{n},\mathbf{P}_0)}. \quad (8)$$

Here $\mathbf{n}$ is the scattering direction, σ_{inc} is the cross section for incoherent scattering, and

$$\frac{\sigma_{nm}(\mathbf{n},\mathbf{P}_0)}{\sigma_n(\mathbf{n})} = 1 + \frac{-2\gamma r_0 F(q)\langle S_z\rangle\,\mathrm{Re}\,\overline{A}_l\mathbf{MP}_0 + \gamma^2 r_0^2 F^2(q)\langle S_z^2\rangle M^2}{|\overline{A}_l|^2}. \quad (9)$$

$$\frac{\sigma_m^{\pm}(\mathbf{n},\mathbf{P}_0)}{\sigma_m^{\pm}(\mathbf{n})} = \frac{1 + (\mathbf{em})^2 \pm 2(\mathbf{P}_0\mathbf{e})(\mathbf{em})}{1 + (\mathbf{em})^2}, \quad (10)$$

where $\sigma_n(\mathbf{n})$ is the cross section for nuclear scattering of unpolarized neutrons, and $\sigma_m^{\pm}(\mathbf{n})$ is the cross section for magnetic scattering of unpolarized neutrons in which the number of spin waves increases or decreases by unity.

The quantity $\sigma_{nm}(\mathbf{n},\mathbf{P}_0)$ is the cross section for coherent scattering of polarized neutrons (with no change in the magnetic state of the scatterer). It consists of the coherent nuclear scattering cross section, the cross section for magneto-vibrational scattering, and an interference term. The expression on the right of formula (9) includes all three of these terms; $\sigma_m^{\pm}(\mathbf{n},\mathbf{P}_0)$ is the cross section for magnetic scattering of polarized neutrons with increase or decrease of the number of spin waves by unity. Since neutrons which undergo scatterings of different types do not interfere, formula (8) is obtained by adding the vectors (4), (5), and (7) with weights corresponding to the relative intensities of the different scattering processes.

Formula (8) describes the polarization of neutrons scattered in a given direction. In writing it we have neglected the fact that the vector $\mathbf{e}$ depends on the energy of the scattered neutrons. We can do this because usually the intensity of neutrons from magnetic scattering is significantly different from zero only when $\mathbf{q}$ is approximately equal to $\boldsymbol{\tau}$ (where $\boldsymbol{\tau}$ is any vector of the reciprocal lattice), but then $\mathbf{e} = \mathbf{q}q^{-1} \approx \boldsymbol{\tau}/\tau$, so that it is independent of the energy. It is interesting to note the following. When $\sigma_{\text{inc}}(\mathbf{n}) = 0$ (which is the case for a lattice consisting of atoms of a single spinless isotope), the polarization vector of the neutrons scattered into a given direction is given by a linear combination of the three vectors $\mathbf{P}_{mn}$, $\mathbf{P}_m^+$ and $\mathbf{P}_m^-$, which in general are not coplanar. These vectors are defined by (5) and (7). From these equations, we see that we can calculate them beforehand if we know the nuclear scattering amplitude, the vector $\mathbf{e}$, $F(q)$, $\mathbf{P}_0$ and $\langle S_z\rangle$. Thus, having measured $\mathbf{P}$, we can determine the coefficients appearing in these three vectors. By measuring, in addition, the total cross section in the same direction,

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*$[\mathbf{MP}_0] = \mathbf{M}\times\mathbf{P}_0$; $(\mathbf{MP}_0) = \mathbf{M}\cdot\mathbf{P}_0$.

†In general there is also a polarization whose vector has the form $\mathbf{P}' = 2(\mathbf{P}\,\mathbf{M}_0)\mathbf{M}/M^2 - \mathbf{P}_0$, which is associated with the absorption or emission of an even number of spin waves. We shall neglect this polarization, since it can be shown that such processes are improbable; in any case it is easy to include it if necessary.

$$\sigma(\mathbf{n}, \mathbf{P}_0) = \sigma_{mn}(\mathbf{n}, \mathbf{P}_0) + \sigma_m^+(\mathbf{n}, \mathbf{P}_0) + \sigma_m^-(\mathbf{n}, \mathbf{P}_0),$$

we can obviously determine $\sigma_{mn}(\mathbf{n}, \mathbf{P}_0)$, $\sigma_m^+(\mathbf{n}, \mathbf{P}_0)$ and $\sigma_m^-(\mathbf{n}, \mathbf{P}_0)$ individually, and consequently find $\sigma_n(\mathbf{n})$ and $\sigma_m^{\pm}(\mathbf{n})$.

Now let us go on to the scattering from antiferromagnets. Since the chemical elementary cell of an antiferromagnet consists, as a rule, of atoms of different sorts, we cannot represent the incoherent nuclear scattering in the form (4). However, the essential point for us is that this polarization is proportional to the polarization vector of the incident beam, and can therefore be written in the form

$$\mathbf{P}_{\text{inc}} = \alpha \mathbf{P}_0, \qquad (11)$$

where the coefficient α has a quite complicated form which does not matter for our purposes. We give the expression only for the case of purely elastic scattering:

$$\alpha = \frac{\sum \left\{ \overline{(|A_i|^2} - |\overline{A}_i|^2) - \frac{1}{12} \overline{|B_i|^2 I_i (I_i+1)} \right\} e^{-2W_i}}{\sum \left\{ (\overline{|A_i|^2} - |\overline{A}_i|^2) + \frac{1}{4} \overline{|B_i|^2 I_i (I_i+1)} \right\} e^{-2W_i}}, \qquad (12)$$

where the summation over i extends over all atoms in the chemical unit cell, and W_i is the Debye-Waller factor for the i'th atom of the cell.

The polarization does not change in coherent nuclear scattering. The interference term between nuclear and magnetic scattering does not appear in the expression for the polarization. This is easily understood if we note that in the ferromagnetic case the interference term contained the spontaneous magnetization vector linearly. Since the spontaneous magnetization in an antiferromagnet is equal to zero and the sublattices are completely equivalent, it is obvious that the interference must go to zero.

The polarization vector resulting from scattering with no change in the magnetic state of the scatterer (or with a change in state for which the total number of spin waves changes by an even number) is easily calculated if we assume that the antiferromagnet consists of two sublattices. It has the form

$$\mathbf{P}_{m0} = 2(\mathbf{M}\mathbf{P}_0)\mathbf{M}/M^2 - \mathbf{P}_0, \qquad (13)$$

where $\mathbf{M} = \mathbf{m} - (\mathbf{e}\cdot\mathbf{m})\mathbf{e}$, and $\mathbf{m}$ is the direction of the magnetization vector of either sublattice.

In particular, this formula describes the polarization of neutrons scattered into those Bragg peaks of the magnetic scattering which do not coincide with nuclear Bragg peaks, since in these directions we can neglect all scattering processes other than magnetic elastic scattering. It is not hard to show that the vector $\mathbf{P}_{m0}$ is equal to $\mathbf{P}_0$ in absolute value. Resolving the vector $\mathbf{P}_0$ into two components, parallel and perpendicular to $\mathbf{M}$, and substituting in (13), we can easily show that $\mathbf{P}$ is obtained from $\mathbf{P}_0$ by a rotation about $\mathbf{M}$ through 180°.

Thus if $\mathbf{P}_0$ is parallel to $\mathbf{M}$, then the polarization is not changed by the magnetic reflection, and this result is obviously valid for any Bragg peak. But if $\mathbf{P}_0$ is perpendicular to $\mathbf{M}$, then for magnetic Bragg peaks which do not coincide with nuclear peaks the polarization changes sign, while for magnetic Bragg peaks which coincide with nuclear peaks the polarization is equal to

$$\mathbf{P} = \mathbf{P}_0(\sigma_{\text{nuc}} - \sigma_{\text{mag}})/(\sigma_{\text{nuc}} + \sigma_{\text{mag}}), \qquad (14)$$

where σ_{nuc} and σ_{mag} are the cross sections for nuclear and magnetic scattering in the direction of the Bragg peak. From here on the cross sections for nuclear and magnetic scattering are taken for the total number of atoms in the scatterer.

We still must find the formula for the polarization vector from scattering in which the number of spin waves changes by one. Noting that such scattering is associated with the components of the atomic spin vectors which are perpendicular to the magnetization of the sublattices, we can get the formula

$$\mathbf{P}_{m1} = 2\frac{\mathbf{M}_x(\mathbf{M}_x\mathbf{P}_0) + \mathbf{M}_y(\mathbf{M}_y\mathbf{P}_0)}{M_x^2 + M_y^2} - \mathbf{P}_0 \qquad (15)$$

(for more detail concerning inelastic scattering from antiferromagnets, cf. [4]). This expression can be written in invariant form:

$$\mathbf{P}_{m1} = 2\frac{\mathbf{P}_{0\perp} - \mathbf{e}_{\perp}(\mathbf{P}_0\mathbf{e}) + \mathbf{e}(\mathbf{em})(\mathbf{MP}_0)}{1 + (\mathbf{em})^2} - \mathbf{P}_0, \qquad (16)$$

where $\mathbf{P}_{0\perp}$ and $\mathbf{e}_{\perp}$ are the components of the vectors $\mathbf{P}_0$ and $\mathbf{e}$, perpendicular to the vector $\mathbf{m}$. Thus, for example, $\mathbf{P}_{0\perp} = \mathbf{P}_0 - (\mathbf{Pm})\mathbf{m}$. It is natural that the scattering in an antiferromagnet with absorption or with emission of spin waves is the same, since the operators for creation and annihilation of spin waves enter symmetrically in the scattering amplitude if we disregard factors which are unimportant in calculating the polarization (cf. [4]). Now using (11), (13) and (15), we can represent the average polarization of the neutrons scattered in a given direction in the form

$$\mathbf{P} = \frac{\alpha\sigma_{\text{inc}}(\mathbf{n})\mathbf{P}_0 + \sigma_{m0}(\mathbf{n})\mathbf{P}_{m0} + \sigma_{m1}(\mathbf{n})\mathbf{P}_{m1}}{\sigma_n(\mathbf{n}) + \sigma_{m0}(\mathbf{n}) + \sigma_{m1}(\mathbf{n})}. \qquad (17)$$

Here $\sigma_n(\mathbf{n})$ is the cross section for nuclear scattering in the direction of $\mathbf{n}$, $\sigma_{m0}(\mathbf{n})$ is the cross section for magnetic scattering in which the number of spin waves does not change or changes by an even number, and finally $\sigma_{m1}(\mathbf{n})$ is the cross section for scattering in which the number of spin waves changes by unity. With respect to the applicability of this formula, the same remark applies as was made concerning formula (8). Formula (17) obviously allows us to determine α, $\sigma_{m0}(\mathbf{n})$ and $\sigma_{m1}(\mathbf{n})$ if we know the polarization $\mathbf{P}_0$ and the total cross section for scattering in the given direction:

$$\sigma(\mathbf{n}) = \sigma_n(\mathbf{n}) + \sigma_{m0}(\mathbf{n}) + \sigma_{m1}(\mathbf{n}). \tag{18}$$

It should be mentioned that (17), like formula (8), is valid only close to Bragg peaks, so that $\mathbf{e} \approx \boldsymbol{\tau}/\tau$.

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[3] S. V. Maleev, JETP 34, 1518 (1958), Soviet Phys. JETP 7, 1048 (1958).

[4] V. G. Bar'yakhtar and S. V. Maleev, JETP 39, 1430 (1960), Soviet Phys. JETP 12, 995 (1961).

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