scattering[15] at the lower strains; such scattering has been ignored in deriving (11).

CONCLUSIONS

The preliminary results presented here show quite clearly that the matrix element for "across the zone face" scattering in silicon is quite small and is consistent with the results of Long.[1] Both Long's results and the present ones assume a temperature-independent effective mass; if, as suggested,[16] the effective mass increases with temperature, the effect would be to make this scattering rate even less.

As an ancillary result, a value of 8.3 ± 0.3 eV has been obtained for Ξ_u, the shear deformation potential of the conduction band of silicon.

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Polarization Effects in the Magnetic Elastic Scattering of Slow Neutrons*

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The theory of the elastic scattering of polarized neutrons by magnetic crystals with ordered spins is developed. Several terms which were omitted by Halpern and Johnson in their original treatment of the subject are discussed. These terms vanish in the case of scattering from simple ferromagnetic or antiferromagnetic structures, but they give rise to some interesting effects in more complex structures. Among these is a polarization effect which occurs in antiferromagnetic spirals, proposed recently by Overhauser, Nagamiya, and Izyumov, and an effect which allows the determination of the imaginary part of the form factor in noncentrosymmetric systems. General formulas for the cross section and for the polarization of the scattered beam are given for arbitrary spin orderings.

INTRODUCTION

POLARIZED neutron scattering has, in the past few years, proved a most useful technique for the study of the magnetic properties of solids. The theory of the scattering of polarized beams was developed by Halpern and Johnson[1] in their now classic paper on the magnetic scattering of slow neutrons, and the expressions which they derived have been verified experimentally.[2,3] In their derivations they restricted their attention to the cases of ferromagnets and simple antiferromagnets. As a result of this restriction they omitted several terms which should appear in the cross section for scattering of a polarized beam and in the expression for the polarization of the scattered beam. These terms are of interest in view of the complicated and unusual spin arrangements found in the last few years. Two of these terms give rise to an interesting polarization effect in the case of scattering by spiral spin structures, as proposed recently by Overhauser,[4] Nagamiya, and Izyumov[5] while another is of interest in connection with the imaginary part of the magnetic form factor.

In this paper complete expressions for the elastic scattering cross section of a system of ordered spins are derived, along with relations for the polarization of the scattered beam. Several examples are presented to illustrate the occurrence of the terms omitted by Halpern and Johnson. In order to derive the formulas we make use of the density matrix description of the polarized beam. This was first used by Tolhoek and de Groot[6] and Wolfenstein[7] in the case of nuclear scattering, and was applied to the diffraction problem by Marshall.[8] Particularly clear descriptions of this useful concept are given by Fano and by ter Haar.[9]

The principal expressions derived are Eq. (15) for the cross section for elastic scattering of a polarized beam by ordered spins and Eq. (19) for the final polarization of a beam elastically scattered by ordered spins. Equations (8) and (17) are more general and may be

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used for calculating polarization effects in inelastic processes. These are not considered in detail in this paper, and reference in this regard may be made to work of Sáenz.[10]

CROSS SECTION FOR SCATTERING OF A POLARIZED BEAM

The cross section in Born approximation for scattering of a polarized beam is[1,8,11]

$$\frac{d^2\sigma}{d\Omega' d\epsilon'}=\frac{k'}{k}\left(\frac{m_0}{2\pi\hbar^2}\right)^2\sum_{qq'} p_q\,\mathrm{tr}[\mathcal{V}_{qq'}{}^\dagger(\mathbf{K})\mathcal{V}_{q'q}(\mathbf{K})\rho]\times\delta\left(\frac{\hbar^2}{2m_0}(k'^2-k^2)+E_{q'}-E_q\right). \quad (1)$$

Here $\mathcal{V}(\mathbf{K})$ is the Fourier transform of the interaction between the neutron and the scatterer. The quantum numbers q and q' label the initial and final states of the scatterer. They may refer to such properties of the solid as its state of magnetization, its distribution of phonons, etc. The factor p_q represents the probability that the scatterer is in the initial state labeled by q. Usually p_q is given by the Boltzmann factor $e^{-E_q/kT}(\sum_{q'} e^{-E_{q'}/kT})^{-1}$. The initial and final wave vectors of the neutron are denoted by $\mathbf{k}$ and $\mathbf{k}'$, respectively, and $\mathbf{K}=\mathbf{k}-\mathbf{k}'$. The density matrix ρ is given by

$$\rho=\tfrac{1}{2}\mathbf{1}+\mathbf{P}\cdot\mathbf{s}, \quad (2)$$

where $\mathbf{1}$ is the two-by-two unit matrix, and $\mathbf{s}$ is the neutron spin operator. The trace in Eq. (1) is understood to be taken only with respect to the neutron spin coordinates. The meaning of the vector $\mathbf{P}$ in (2) can be seen by using the relation

$$\langle\mathcal{A}\rangle=\mathrm{tr}(\rho\mathcal{A}), \quad (3)$$

where $\mathcal{A}$ is a quantum mechanical operator and $\langle\mathcal{A}\rangle$ denotes the average value of this quantity. We consider $\langle\mathbf{s}\rangle$, where $\mathbf{s}$ is the neutron spin operator. We have

$$\langle s^\alpha\rangle=\mathrm{tr}(\tfrac{1}{2}s^\alpha+s^\alpha s^\beta P^\beta), \quad (4)$$

where $\alpha=x, y, z$, and the summation convention has been introduced. The trace of an individual spin operator is zero, while $\mathrm{tr}(s^\alpha s^\beta)=\frac{1}{2}\delta^{\alpha\beta}$. Hence,

$$\langle s^\alpha\rangle=\tfrac{1}{2}\delta^{\alpha\beta}P^\beta=\tfrac{1}{2}P^\alpha. \quad (5)$$

The vector $\mathbf{P}$, therefore, represents the polarization of the incident neutron beam.[9] The magnitude of $\mathbf{P}$ is unity for a completely polarized beam, and is zero for an unpolarized beam.

When explicit forms for the Fourier transform of the potential are substituted in (1), we may immediately perform the traces indicated, and we have an expression for the cross section which contains the polarization $\mathbf{P}$ of the incident neutron beam. These explicit forms have been given by Halpern and Johnson. Following them we can write $\mathcal{V}(\mathbf{K})=\mathcal{V}_n(\mathbf{K})+\mathcal{V}_m(\mathbf{K})$, where

$$\mathcal{V}_n(\mathbf{K})=\frac{2\pi\hbar^2}{m_0}\left\{\sum_{\mathbf{n}j}\exp[i\mathbf{K}\cdot(\mathbf{n}+\mathbf{d}_j)]\frac{a_{\mathbf{n}j}{}^+(I_{\mathbf{n}j}+1)+a_{\mathbf{n}j}{}^-I_{\mathbf{n}j}}{2I_{\mathbf{n}j}+1}+2\sum_{\mathbf{n}j}\exp[i\mathbf{K}\cdot(\mathbf{n}+\mathbf{d}_j)]\frac{a_{\mathbf{n}j}{}^+-a_{\mathbf{n}j}{}^-}{2I_{\mathbf{n}j}+1}\mathbf{I}_{\mathbf{n}j}\cdot\mathbf{s}\right\},$$
$$=\frac{2\pi\hbar^2}{m_0}(T_0+\mathbf{T}_1\cdot\mathbf{s}),$$

and (6)

$$\mathcal{V}_m(\mathbf{K})=\frac{2\pi\hbar^2}{m_0}\frac{2\gamma e^2}{mc^2}\sum_i e^{i\mathbf{K}\cdot\mathbf{r}_i}\left[\hat{K}\times(\mathbf{s}_i\times\hat{K})-\frac{i}{K}(\hat{K}\times\mathbf{p}_i)\right]\cdot\mathbf{s},$$
$$=\frac{2\pi\hbar^2}{m_0}\frac{2\gamma e^2}{mc^2}\mathbf{s}\cdot\mathbf{Q}.$$

$\mathcal{V}_n$ represents the interaction with the nuclei of the scatterer, while $\mathcal{V}_m$ represents the magnetic interaction with the spin and orbital moments of the electrons. Here $\mathbf{n}+\mathbf{d}_j$ is the position of a nucleus, $\mathbf{n}$ being the vector from the origin to the origin of the unit cell in which the nucleus is located, while $\mathbf{d}_j$ is the position vector of the nucleus within the unit cell. The position, spin, momentum and mass of the ith electron are $\mathbf{r}_i$, $\mathbf{s}_i$, $\mathbf{p}_i$, and m, respectively, while the spin, gyromagnetic ratio, and mass of the neutron are, respectively, $\mathbf{s}$, $\gamma=-1.91$, and m_0. $\mathbf{I}_{\mathbf{n}j}$ is the spin operator for the nucleus at $\mathbf{n}+\mathbf{d}_j$, $I_{\mathbf{n}j}$ is the magnitude of the spin of this nucleus, and $a_{\mathbf{n}j}{}^+$ and $a_{\mathbf{n}j}{}^-$ are, respectively, the scattering lengths for neutron spin parallel and antiparallel to nuclear spin. To find the cross sections for a polarized beam we need only substitute (6) in (1) and perform the indicated traces. The evaluation of the traces is made easy by using the following formulas[8]:

$$\begin{aligned}&\mathrm{tr}\mathbf{1}=2,\\&\mathrm{tr}\,s^\alpha=0,\\&\mathrm{tr}\,s^\alpha s^\beta=\tfrac{1}{2}\delta^{\alpha\beta},\\&\mathrm{tr}\,s^\alpha s^\beta s^\gamma=\tfrac{1}{4}i\epsilon^{\alpha\beta\gamma},\\&\mathrm{tr}\,s^\alpha s^\beta s^\gamma s^\zeta=\tfrac{1}{8}(\delta^{\alpha\beta}\delta^{\gamma\zeta}-\delta^{\alpha\gamma}\delta^{\beta\zeta}+\delta^{\alpha\zeta}\delta^{\beta\gamma}).\end{aligned} \quad (7)$$

Here α, β, γ, ζ run over x, y, z, and $\epsilon^{\alpha\beta\gamma}$ is the unit

[10] A. W. Sáenz, Phys. Rev. **119**, 1542 (1960).
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antisymmetric tensor of third rank. These formulas follow from the properties of the Pauli spin matrices. Substituting (6) in (1) and using (7), we obtain

$$d^2\sigma/d\Omega' d\epsilon' = \frac{k'}{k}\sum_{qq'} p_q\Bigg[\langle q|T_0^\dagger|q'\rangle\langle q'|T_0|q\rangle + \tfrac{1}{4}\langle q|\mathbf{T}_1^\dagger|q'\rangle\cdot\langle q'|\mathbf{T}_1|q\rangle + \left(\frac{\gamma e^2}{mc^2}\right)\langle q|T_0^\dagger|q'\rangle\langle q'|\mathbf{P}\cdot\mathbf{Q}|q\rangle$$
$$+\left(\frac{\gamma e^2}{mc^2}\right)\langle q|\mathbf{P}\cdot\mathbf{Q}^\dagger|q'\rangle\langle q'|T_0|q\rangle + \left(\frac{\gamma e^2}{mc^2}\right)^2\langle q|\mathbf{Q}^\dagger|q'\rangle\cdot\langle q'|\mathbf{Q}|q\rangle + i\left(\frac{\gamma e^2}{mc^2}\right)^2\mathbf{P}\cdot(\langle q|\mathbf{Q}^\dagger|q'\rangle\times\langle q'|\mathbf{Q}|q\rangle)\Bigg]$$
$$\times\delta\left(\frac{\hbar^2}{2m_0}(k'^2-k^2)+E_{q'}-E_q\right). \quad (8)$$

In deriving (8) we have used the relation

$$(\mathbf{A}\times\mathbf{B})^\alpha = \sum_{\beta\gamma}\epsilon^{\alpha\beta\gamma}A^\beta B^\gamma$$

for the components of the vector product of two vectors **A** and **B**. We have also omitted terms which are linear in the nuclear spins. This is because we must average over nuclear spin orientations to obtain the final cross sections, and we assume that the nuclear spins are randomly oriented. This corresponds to the experimental situation in the vast majority of cases of interest.

Equation (8) is, except for the above restriction, quite general, and gives an expression for the cross section for elastic or inelastic scattering of a polarized beam. Before specializing to elastic scattering, it is worth noting that the last term in (8), a polarization-dependent purely magnetic contribution to the cross section, was not considered by Halpern and Johnson. The only polarization-dependent term discussed by them was the nuclear-magnetic interference term, also included in (8). That a purely magnetic polarization dependent term should occur may be seen by considering the scattering of polarized neutrons by a spin $\frac{1}{2}$ ion in a magnetic field. If the ion is in the ground state with $m_s=+\frac{1}{2}$, then a neutron polarized along the negative z axis can excite the ion to the $m_s=-\frac{1}{2}$ state, so that angular momentum can be conserved if the neutron's spin is flipped. The neutron's final energy will be less than its initial energy by an amount equal to the excitation energy of the $m_s=-\frac{1}{2}$ state of the ion. On the other hand, an ion in the $m_s=+\frac{1}{2}$ state cannot be excited to the $m_s=-\frac{1}{2}$ state by a neutron polarized along the positive z axis, since there is no way in which angular momentum can be conserved. Hence, in this case, the magnetic inelastic scattering cross section depends on the neutron polarization. This type of phenomenon is described mathematically by the last term of (8). As will be seen, this term can also be of interest in elastic scattering from certain complicated spin structures.

CROSS SECTIONS FOR ELASTIC SCATTERING

We wish now to limit our considerations to elastic scattering from magnetic substances in which the individual spins are all rigidly aligned, e.g., ferromagnetics, antiferromagnetics, etc., at low temperatures. For elastic scattering, we take $|q'\rangle=|q\rangle$. We assume that the nuclei are rigidly fixed, so that lattice vibrations are ignored. This simply amounts to dropping Debye-Waller temperature factors in the final result. We also assume a Heitler-London model for the magnetic structure, so that the ionic spins are taken to be localized. If, in addition, the orbital momentum is quenched, we may take over Halpern and Johnson's result that[12]

$$\langle q|\mathbf{Q}|q\rangle = \sum_{\mathbf{n}j}\exp[i\mathbf{K}\cdot(\mathbf{n}+\mathbf{d}_j)]f_{\mathbf{n}j}(\mathbf{K}) \times\langle q|\hat{K}\times(\mathbf{S}_{\mathbf{n}j}\times\hat{K})|q\rangle. \quad (9)$$

Here, $\mathbf{S}_{\mathbf{n}j}$ is the spin operator for the ion at site $(\mathbf{n},j)$, while $f_{\mathbf{n}j}(\mathbf{K})$ is the form factor for that ion, i.e., the Fourier transform of the ion's spin density.

To derive the elastic scattering cross section, we substitute (9) in (8). At very low temperatures only the ground state of the spin system will be occupied with appreciable probability, and for this state the matrix element in (9) is easily evaluated. We have

$$\langle q|\mathbf{S}_{\mathbf{n}j}|q\rangle = S_{\mathbf{n}j}\boldsymbol{\eta}_{\mathbf{n}j}, \quad (10)$$

where $S_{\mathbf{n}j}$ is the magnitude of the spin at lattice site $(\mathbf{n},j)$, and $\boldsymbol{\eta}_{\mathbf{n}j}$ is a unit vector in the direction of this spin. Defining

$$\mathbf{q}_{\mathbf{n}j} = \hat{K}\times(\boldsymbol{\eta}_{\mathbf{n}j}\times\hat{K}), \quad (11)$$

the elastic scattering cross section becomes

$$\frac{d\sigma}{d\Omega'} = \sum_{\mathbf{n}j,\mathbf{n}'j'}\exp[i\mathbf{K}\cdot(\mathbf{R}_{\mathbf{n}j}-\mathbf{R}_{\mathbf{n}'j'})]\{a_{\mathbf{n}j}\}\{a_{\mathbf{n}'j'}\} + \sum_{\mathbf{n}j}(\{a_{\mathbf{n}}{}^2{}_j\}-\{a_{\mathbf{n}j}\}^2) + \left(\frac{\gamma e^2}{mc^2}\right)\sum_{\mathbf{n}j,\mathbf{n}'j'}\exp[i\mathbf{K}\cdot(\mathbf{R}_{\mathbf{n}j}-\mathbf{R}_{\mathbf{n}'j'})]$$
$$\times\left(\{a_{\mathbf{n}'j'}\}f_{\mathbf{n}j}(\mathbf{K})S_{\mathbf{n}j}\mathbf{P}\cdot\mathbf{q}_{\mathbf{n}j} + \{a_{\mathbf{n}j}\}f_{\mathbf{n}'j'}{}^*(\mathbf{K})S_{\mathbf{n}'j'}\mathbf{P}\cdot\mathbf{q}_{\mathbf{n}'j'}\right) + \left(\frac{\gamma e^2}{mc^2}\right)^2\sum_{\mathbf{n}j,\mathbf{n}'j'}\exp[i\mathbf{K}\cdot(\mathbf{R}_{\mathbf{n}j}-\mathbf{R}_{\mathbf{n}'j'})]$$
$$\times S_{\mathbf{n}'j'}S_{\mathbf{n}j}f_{\mathbf{n}'j}{}^*(\mathbf{K})f_{\mathbf{n}j}(\mathbf{K})\left(\mathbf{q}_{\mathbf{n}'j'}\cdot\mathbf{q}_{\mathbf{n}j} + i\mathbf{P}\cdot(\mathbf{q}_{\mathbf{n}'j'}\times\mathbf{q}_{\mathbf{n}j})\right), \quad (12)$$

$\mathbf{R}_{\mathbf{n}j}=\mathbf{n}+\mathbf{d}_j$.

[12] Equation (9) can still be used if the orbital angular momentum is unquenched, as in rare-earth ions. In this event, the form factor $f(\mathbf{K})$ must be reinterpreted as

$$f(\mathbf{K}) = (\mathbf{L}\cdot\mathbf{J}f_L(K)+2\mathbf{S}\cdot\mathbf{J}f_s(K))/(\mathbf{L}\cdot\mathbf{J}+2\mathbf{S}\cdot\mathbf{J}),$$

An average over nuclear spin orientations has been performed in deriving this expression. The quantities $\{a_{nj}^2\}$ and $\{a_{nj}\}$, the averaged nuclear scattering lengths, are defined by

$$\{a_{nj}\}=\frac{(I_{nj}+1)a_{nj}^{+}+I_{nj}a_{nj}^{-}}{2I_{nj}+1},$$
$$\{a_{nj}^2\}=\frac{(I_{nj}+1)(a_{nj}^{+})^2+I_{nj}(a_{nj}^{-})^2}{2I_{nj}+1}. \tag{13}$$

Here I_{nj} is the magnitude of the spin of the nucleus at site $(\mathbf{n},j)$, while a_{nj}^{+} and a_{nj}^{-} are, as above, the scattering lengths of this nucleus for neutron spin parallel and antiparallel, respectively, to nuclear spin.

Equation (12) must be averaged over isotope distribution before it can be applied generally. Also, for scattering by disordered alloys, it must be averaged over the positions of the components of the alloys. We do not treat the latter case in this paper.

The first line of the equation gives the pure nuclear scattering, both coherent and incoherent. The second line represents the nuclear-magnetic interference term derived by Halpern and Johnson. It is present only for a polarized neutron beam. The last line gives the pure magnetic scattering. The term in this proportional to $\mathbf{P}$ gives the effects mentioned above for spiral spin structures.

We perform the isotopic averaging by defining

$$\langle\{a\}\rangle=\sum_\alpha C_\alpha\{a_\alpha\},$$

where C_α is the concentration of the αth isotope and $\{a_\alpha\}$ is the scattering length for this isotope, averaged over nuclear spins, as above. Since the isotopes are randomly distributed, we have

$$\langle\{a_{nj}\}\{a_{n'j'}\}\rangle=\langle\{a_j\}\rangle\langle\{a_{j'}\}\rangle \quad \text{for} \quad \mathbf{n}\neq\mathbf{n}' \quad \text{or} \quad j\neq j',$$
$$=\langle\{a_j\}^2\rangle \quad \text{for} \quad \mathbf{n}=\mathbf{n}' \quad \text{and} \quad j=j'.$$

These two results may be combined to give

$$\langle\{a_{nj}\}\{a_{n'j'}\}\rangle=\langle\{a_j\}\rangle\langle\{a_{j'}\}\rangle+(\langle\{a_j\}^2\rangle-\langle\{a_j\}\rangle^2)\delta_{nn'}\delta_{jj'}. \tag{14}$$

On averaging (12) over isotopic distributions and using (14), we obtain finally

$$\frac{d\sigma}{d\Omega'}=|\textstyle\sum_n e^{i\mathbf{K}\cdot\mathbf{n}}|^2|F_N(\mathbf{K})|^2+N\sum_j\Big(\langle\{a_j^2\}\rangle-\langle\{a_j\}\rangle^2\Big)+\left(\frac{\gamma e^2}{mc^2}\right)\sum_{nj,n'j'}\exp[i\mathbf{K}\cdot(\mathbf{R}_{nj}-\mathbf{R}_{n'j'})]\Big(\langle\{a_{j'}\}\rangle f_{nj}(\mathbf{K})S_{nj}\mathbf{P}\cdot\mathbf{q}_{nj}$$
$$+\langle\{a_j\}\rangle f_{n'j'}^*(\mathbf{K})S_{n'j'}\mathbf{P}\cdot\mathbf{q}_{n'j'}\Big)+\left(\frac{\gamma e^2}{mc^2}\right)^2\sum_{nj,n'j'}\exp[i\mathbf{K}\cdot(\mathbf{R}_{nj}-\mathbf{R}_{n'j'})]S_{n'j'}S_{nj}f_{n'j'}^*(\mathbf{K})f_{nj}(\mathbf{K})$$
$$\times\Big(\mathbf{q}_{n'j'}\cdot\mathbf{q}_{nj}+i\mathbf{P}\cdot(\mathbf{q}_{n'j'}\times\mathbf{q}_{nj})\Big). \tag{15}$$

Here $F_N(\mathbf{K})=\sum_j\exp[i\mathbf{K}\cdot\mathbf{d}_j]\langle\{a_j\}\rangle$ is the nuclear structure factor. This equation gives the elastic scattering from a set of ordered spins. Most aspects of it are quite familiar and have been discussed by many authors in the past. In a later section we illustrate the newer features as well as some of the well-known ones, by examples.

POLARIZATION OF THE SCATTERED BEAM

The formulas derived in the preceding sections assume an experimental arrangement in which each neutron of the scattered beam is counted, regardless of its polarization. In some experiments the polarization of the final beam is analyzed, and this data can yield valuable information not otherwise obtainable. In this section we derive general formulas for the final polarization of an initially polarized beam elastically scattered from a substance with fixed spins.

The final polarization $\mathbf{P}_f$ of a scattered beam is given in Born approximation by [1,8,11]

$$\tfrac{1}{2}\mathbf{P}_f\frac{d^2\sigma}{d\Omega'd\epsilon'}=\frac{k'}{k}\left(\frac{m_0}{2\pi\hbar^2}\right)^2\sum_{qq'}p_q\,\mathrm{tr}[\mathcal{V}_{qq'}^{\dagger}(\mathbf{K})\mathbf{s}\mathcal{V}_{q'q}(\mathbf{K})\rho]\delta\left(\frac{\hbar^2}{2m_0}(k'^2-k^2)+F_{q'}-E_q\right). \tag{16}$$

The notation used is the same as that for Eqs. (1) and (6). Allowance for the initial polarization $\mathbf{P}$ of the beam is contained in the density matrix ρ, given by Eq. (2). To obtain an expression analogous to (8) we substitute (6)

where $f_L(K)$ and $f_s(K)$ are the spherical parts of the orbital and spin form factors, respectively, and $\mathbf{J}$ is the total angular momentum. Also $\mathbf{S}_{nj}$ in (9) should be replaced by the total angular momentum $\mathbf{J}_{nj}$ of the ion at site $(\mathbf{n}j)$. This is a good approximation for small momentum transfer $\mathbf{K}$. See, e.g., G. T. Trammell, Phys. Rev. **92**, 1387 (1953); M. Blume, A. J. Freeman, and R. E. Watson, J. Chem. Phys. **37**, 1245 (1962).

in (16) and use the relations (7). We find

$$\tfrac{1}{2}\mathbf{P}_f\frac{d^2\sigma}{d\Omega' d\epsilon'}=\frac{k'}{k}\sum_{qq'}p_q\Big\{\tfrac{1}{2}\mathbf{P}\langle q|T_0^\dagger|q'\rangle\langle q'|T_0|q\rangle+\tfrac{1}{8}\langle q|\mathbf{T}_1^\dagger|q'\rangle\langle q'|\mathbf{P}\cdot\mathbf{T}_1|q\rangle+\tfrac{1}{8}\langle q|\mathbf{P}\cdot\mathbf{T}_1^\dagger|q'\rangle\langle q'|\mathbf{T}_1|q\rangle$$
$$-\tfrac{1}{8}\mathbf{P}(\langle q|\mathbf{T}_1^\dagger|q'\rangle\cdot\langle q'|\mathbf{T}_1|q\rangle)+\frac{1}{2}\left(\frac{\gamma e^2}{mc^2}\right)\langle q|T_0^\dagger|q'\rangle\langle q'|\mathbf{Q}|q\rangle+\frac{1}{2}\left(\frac{\gamma e^2}{mc^2}\right)\langle q|\mathbf{Q}^\dagger|q'\rangle\langle q'|T_0|q\rangle$$
$$+\tfrac{1}{2}i\left(\frac{\gamma e^2}{mc^2}\right)\langle q|\mathbf{P}\times\mathbf{Q}^\dagger|q'\rangle\langle q'|T_0|q\rangle-\tfrac{1}{2}i\left(\frac{\gamma e^2}{mc^2}\right)\langle q|T_0^\dagger|q'\rangle\langle q'|\mathbf{P}\times\mathbf{Q}|q\rangle-\tfrac{1}{2}i\left(\frac{\gamma e^2}{mc^2}\right)^2(\langle q|\mathbf{Q}^\dagger|q'\rangle\times\langle q'|\mathbf{Q}|q\rangle)$$
$$+\frac{1}{2}\left(\frac{\gamma e^2}{mc^2}\right)^2\langle q|\mathbf{Q}^\dagger|q'\rangle\langle q'|\mathbf{P}\cdot\mathbf{Q}|q\rangle+\frac{1}{2}\left(\frac{\gamma e^2}{mc^2}\right)^2\langle q|\mathbf{P}\cdot\mathbf{Q}^\dagger|q'\rangle\langle q'|\mathbf{Q}|q\rangle-\frac{1}{2}\left(\frac{\gamma e^2}{mc^2}\right)^2\mathbf{P}(\langle q|\mathbf{Q}^\dagger|q'\rangle\cdot\langle q'|\mathbf{Q}|q\rangle)\Big\}$$
$$\times\delta\left(\frac{\hbar^2}{2m_0}(k'^2-k^2)+E_{q'}-E_q\right).\quad(17)$$

In deriving this expression we have omitted, as in (6), terms which vanish on averaging over randomly oriented nuclear spins. Equation (17) is, except for this restriction, general, and yields the polarization of the scattered beam for elastic or inelastic scattering. There are several terms in (17) which did not appear in Halpern and Johnson's treatment. These are more clearly seen when the equation is simplified by restriction to elastic scattering. To do this we take $|q'\rangle=|q\rangle$ and we make the assumptions indicated in Eqs. (9), (10), and (11). On substituting these in (17) we find for the polarization of an elastically scattered beam

$$\tfrac{1}{2}\mathbf{P}_f\frac{d\sigma}{d\Omega'}=\tfrac{1}{2}\mathbf{P}\sum_{\mathrm{n}j,\mathrm{n}'j'}\exp[i\mathbf{K}\cdot(\mathbf{R}_{\mathrm{n}j}-\mathbf{R}_{\mathrm{n}'j'})]\{a_{\mathrm{n}j}\}\{a_{\mathrm{n}'j'}\}-\tfrac{1}{6}\mathbf{P}\sum_{\mathrm{n}j}(\{a_{\mathrm{n}j}^2\}-\{a_{\mathrm{n}j}\}^2)+\frac{1}{2}\left(\frac{\gamma e^2}{mc^2}\right)\sum_{\mathrm{n}j,\mathrm{n}'j'}\exp[i\mathbf{K}\cdot(\mathbf{R}_{\mathrm{n}j}-\mathbf{R}_{\mathrm{n}'j'})]$$
$$\times\Big(\{a_{\mathrm{n}'j'}\}S_{\mathrm{n}j}f_{\mathrm{n}j}(\mathbf{K})\mathbf{q}_{\mathrm{n}j}+\{a_{\mathrm{n}j}\}S_{\mathrm{n}'j'}f_{\mathrm{n}'j'}^*(\mathbf{K})\mathbf{q}_{\mathrm{n}'j'}-i\{a_{\mathrm{n}'j'}\}S_{\mathrm{n}j}f_{\mathrm{n}j}(\mathbf{K})(\mathbf{P}\times\mathbf{q}_{\mathrm{n}j})+i\{a_{\mathrm{n}j}\}S_{\mathrm{n}'j'}f_{\mathrm{n}'j'}^*(\mathbf{K})(\mathbf{P}\times\mathbf{q}_{\mathrm{n}'j'})\Big)$$
$$+\frac{1}{2}\left(\frac{\gamma e^2}{mc^2}\right)^2\sum_{\mathrm{n}j,\mathrm{n}'j'}\exp[i\mathbf{K}\cdot(\mathbf{R}_{\mathrm{n}j}-\mathbf{R}_{\mathrm{n}'j'})]S_{\mathrm{n}'j'}S_{\mathrm{n}j}f_{\mathrm{n}'j'}^*(\mathbf{K})f_{\mathrm{n}j}(\mathbf{K})\Big(-i(\mathbf{q}_{\mathrm{n}'j'}\times\mathbf{q}_{\mathrm{n}j})+\mathbf{q}_{\mathrm{n}'j'}(\mathbf{P}\cdot\mathbf{q}_{\mathrm{n}j})$$
$$+(\mathbf{P}\cdot\mathbf{q}_{\mathrm{n}'j'})\mathbf{q}_{\mathrm{n}j}-\mathbf{P}(\mathbf{q}_{\mathrm{n}'j'}\cdot\mathbf{q}_{\mathrm{n}j})\Big).\quad(18)$$

The average over isotope distribution is performed exactly as before. Using the same definitions for isotopic and spin averages on the scattering length, we have

$$\tfrac{1}{2}\mathbf{P}_f\frac{d\sigma}{d\Omega'}=\tfrac{1}{2}\mathbf{P}|\sum_n e^{i\mathbf{K}\cdot\mathbf{n}}|^2|F_N(\mathbf{K})|^2-\tfrac{1}{2}\mathbf{P}N\sum_j(\tfrac{1}{3}\langle\{a_j^2\}\rangle-\tfrac{4}{3}\langle\{a_j\}^2\rangle+\langle\{a_j\}\rangle^2)+\frac{1}{2}\left(\frac{\gamma e^2}{mc^2}\right)\sum_{\mathrm{n}j,\mathrm{n}'j'}\exp[i\mathbf{K}\cdot(\mathbf{R}_{\mathrm{n}j}-\mathbf{R}_{\mathrm{n}'j'})]$$
$$\times\Big(\langle\{a_{j'}\}\rangle S_{\mathrm{n}j}f_{\mathrm{n}j}(\mathbf{K})\mathbf{q}_{\mathrm{n}j}+\langle\{a_j\}\rangle S_{\mathrm{n}'j'}f_{\mathrm{n}'j'}^*(\mathbf{K})\mathbf{q}_{\mathrm{n}'j'}-i\langle\{a_{j'}\}\rangle S_{\mathrm{n}j}f_{\mathrm{n}j}(\mathbf{K})(\mathbf{P}\times\mathbf{q}_{\mathrm{n}j})$$
$$+i\langle\{a_j\}\rangle S_{\mathrm{n}'j'}f_{\mathrm{n}'j'}^*(\mathbf{K})(\mathbf{P}\times\mathbf{q}_{\mathrm{n}'j'})\Big)+\frac{1}{2}\left(\frac{\gamma e^2}{mc^2}\right)^2\sum_{\mathrm{n}j,\mathrm{n}'j'}\exp[i\mathbf{K}\cdot(\mathbf{R}_{\mathrm{n}j}-\mathbf{R}_{\mathrm{n}'j'})]S_{\mathrm{n}'j'}S_{\mathrm{n}j}f_{\mathrm{n}'j'}^*(\mathbf{K})f_{\mathrm{n}j}(\mathbf{K})$$
$$\times\Big(-i(\mathbf{q}_{\mathrm{n}'j'}\times\mathbf{q}_{\mathrm{n}j})+\mathbf{q}_{\mathrm{n}'j'}(\mathbf{P}\cdot\mathbf{q}_{\mathrm{n}j})+(\mathbf{P}\cdot\mathbf{q}_{\mathrm{n}'j'})\mathbf{q}_{\mathrm{n}j}-\mathbf{P}(\mathbf{q}_{\mathrm{n}'j'}\cdot\mathbf{q}_{\mathrm{n}j})\Big).\quad(19)$$

The notation is as in (15). To find the polarization of the final beam we divide this expression by the expression (15) for the cross section. The terms appearing here which are not present in Halpern and Johnson's analysis are just those which have a factor i. Two of these are present in the nuclear-magnetic interference term; these give rise to a rotation of the plane of polarization in systems for which the form factors are complex, and they present the possibility of determining the imaginary part of the form factor directly. The other term appears in the pure magnetic scattering, and it gives rise to a polarization of the scattered beam even though the incident beam is unpolarized. This term corresponds to the extra term in the cross section (15) discussed above, and it vanishes for a simple ferromagnet. All other terms in (19) have been discussed previously.

EXAMPLES

To illustrate the occurrence of the various terms in (19) and (15) we will consider more specific spin arrangements. Several well-known results are re-derived in order to contrast them with the effects of the additional terms derived here.

(a) We consider first the familiar expressions for pure nuclear scattering. The coherent elastic cross section is given by the first term of (15),

$$d\sigma/d\Omega' = |\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2 |F_N(\mathbf{K})|^2. \tag{20}$$

This is independent of the polarization of the incident beam. The factor $|\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2$ is well known as the diffraction interference function, which vanishes unless $\mathbf{K}$ is 2π times a reciprocal lattice vector. It describes the coherent nature of the scattering, which occurs only in Bragg peaks. The polarization of the final beam which has been scattered in a coherent nuclear elastic process is found, on dividing the first term of (19) by (20), to be the same as the initial polarization, $\mathbf{P}_f = \mathbf{P}$. This is well known, and is anticipated on physical grounds. The final polarization of the nuclear incoherent scattering is somewhat more complicated. The cross section in this case is given by the second term of (15),

$$d\sigma/d\Omega' = N \sum_j (\langle\{a_j^2\}\rangle - \langle\{a_j\}\rangle^2), \tag{21}$$

and the final polarization, obtained by dividing the second term of (19) by the above, is

$$\mathbf{P}_f = -\tfrac{1}{3}\mathbf{P}\frac{\sum_j (\langle\{a_j^2\}\rangle - 4\langle\{a_j\}^2\rangle + 3\langle\{a_j\}\rangle^2)}{\sum_j (\langle\{a_j^2\}\rangle - \langle\{a_j\}\rangle^2)}. \tag{22}$$

The complication of this expression is due to the fact that the incoherent scattering arises from disorder in the nuclear spin system as well as from the disordered arrangement of isotopes. The latter type of scattering does not lead to any change of polarization, but the nuclear spin disorder scattering does give rise to such a change. The final polarization is then an average over the isotopic and nuclear spin disorder scattering results. In the special case of pure spin disorder scattering (all constituents of the sample mono-isotopic) Eq. (22) can be simplified, since in this case we can ignore the angular brackets in the isotopic averaging of the scattering lengths. We have $\langle\{a_j\}\rangle^2 = \langle\{a_j\}^2\rangle$, and $\mathbf{P}_f = -\frac{1}{3}\mathbf{P}$. On the other hand, if all isotopes present have zero spin (pure isotopic disorder scattering) we can ignore the spin averaging of the scattering lengths, so that $\langle\{a_j^2\}\rangle = \langle\{a_j\}^2\rangle$, and $\mathbf{P}_f = \mathbf{P}$. In the general case[13] the final polarization is between $-\frac{1}{3}\mathbf{P}$ and $\mathbf{P}$.

(b) The occurrence of one of the extra terms in the expression for the polarization of the final beam can be illustrated by considering a uniaxial antiferromagnet without a center of symmetry (e.g., Cr_2O_3). In such a system the spins are either parallel or antiparallel to a unit vector $\boldsymbol{\eta}$, and $\mathbf{q}_{\mathbf{n}j} = \pm\mathbf{q}$, where $\mathbf{q} = \hat{K}\times(\boldsymbol{\eta}\times\hat{K})$ is independent of $\mathbf{n}$ and j. The cross section becomes

$$\frac{d\sigma}{d\Omega'} = |\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2 \bigg\{ |F_N(\mathbf{K})|^2 + \left(\frac{2\gamma e^2}{mc^2}\right) S \times \mathrm{Re}[F_N^*(\mathbf{K}) F_M(\mathbf{K}) f(\mathbf{K})]\mathbf{P}\cdot\mathbf{q} + \left(\frac{\gamma e^2}{mc^2}\right)^2 S^2 |F_M(\mathbf{K}) f(\mathbf{K})|^2 q^2 \bigg\}. \tag{23}$$

The purely nuclear incoherent scattering has been omitted here, since all other terms give rise to scattering in Bragg peaks. If one of the peaks is observed experimentally the incoherent contribution to the scattering will be much smaller than the coherent. $F_m(\mathbf{K}) = \sum_j (\pm)_j \exp(i\mathbf{K}\cdot\mathbf{d}_j)$ is the magnetic structure factor for the unit cell. The plus or minus sign is taken if the spin on the jth ion in the unit cell is parallel or antiparallel, respectively, to $\boldsymbol{\eta}$. All other terms have been defined previously. This expression was given by Halpern and Johnson. It should be noted that if the magnetic ions are not in a center of symmetry we should expect the form factor $f(\mathbf{K})$ to have an imaginary part. This follows from the definition of the form factor as the Fourier transform of the spin density:

$$f(\mathbf{K}) = \int e^{i\mathbf{K}\cdot\mathbf{r}} \rho(\mathbf{r}) d\mathbf{r} = \int \cos\mathbf{K}\cdot\mathbf{r}\rho(\mathbf{r}) d\mathbf{r} + i\int \sin\mathbf{K}\mathbf{r}\rho(\mathbf{r}) d\mathbf{r}. \tag{24}$$

If the ion is in a center of symmetry $\rho(\mathbf{r}) = \rho(-\mathbf{r})$, and the imaginary part of the form factor vanishes. If $\rho(\mathbf{r}) \neq \rho(-\mathbf{r})$ as for a noncentrosymmetric ion $\mathrm{Im}f(\mathbf{K}) \neq 0$. The cross section (23) for scattering by a polarized beam does not provide a simple method of determination of $\mathrm{Im}f(\mathbf{K})$. The extra terms in the expression for the polarization of the scattered beam do provide such a method, as will be seen.

From (19) we find for the polarization of the scattered beam

$$\tfrac{1}{2}\mathbf{P}_f \frac{d\sigma}{d\Omega'} = |\sum_{\mathbf{n}} e^{i\mathbf{K}\cdot\mathbf{n}}|^2 \bigg\{ \tfrac{1}{2}\mathbf{P}|F_N(\mathbf{K})|^2 + \left(\frac{\gamma e^2}{mc^2}\right) S\, \mathrm{Re}[F_N^*(\mathbf{K}) F_M(\mathbf{K}) f(\mathbf{K})]\mathbf{q} + \left(\frac{\gamma e^2}{mc^2}\right) S\, \mathrm{Im}[F_N^*(\mathbf{K}) F_M(\mathbf{K}) f(\mathbf{K})](\mathbf{P}\times\mathbf{q}) + \frac{1}{2}\left(\frac{\gamma e^2}{mc^2}\right)^2 S^2 |F_M(\mathbf{K}) f(\mathbf{K})|^2 \times [2\mathbf{q}(\mathbf{P}\cdot\mathbf{q}) - q^2\mathbf{P}] \bigg\}, \tag{25}$$

[13] D. J. Hughes, *Pile Neutron Research* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1953), p. 262.

where we have again omitted the purely nuclear incoherent scattering. The first, second, and fourth terms in this equation have been derived previously. The first simply states that the nuclear coherent scattering leaves the initial polarization unaffected. The second term is independent of the polarization of the incident beam, and it describes the manner in which a polarized beam may be produced by interference between nuclear and magnetic scattering. The last term describes the rotation of the direction of polarization produced by purely magnetic scattering from a magnetized sample. It has been discussed in detail recently by Izyumov and Maleev.[14]

The third term is one which was omitted by Halpern and Johnson. It vanishes for simple antiferromagnets in which each atom is at a center of symmetry, for then each of the structure factors and the form factor can be taken to be purely real. The term may be isolated in a relatively straightforward manner, for if $\mathbf{P}$ and $\mathbf{q}$ are arranged to be perpendicular to one another this term gives a component of polarization perpendicular to both $\mathbf{P}$ and $\mathbf{q}$, whereas all other terms give rise to components along either $\mathbf{P}$ or $\mathbf{q}$. Separate determination of this quantity would be of use in form factor studies. It should be emphasized that the above expression is for a single domain antiferromagnet, and it should in general be averaged over all directions $\boldsymbol{\eta}$ of magnetization.

(c) Scattering from a spiral spin[4,5] arrangement illustrates the occurrence of the other additional terms in (15) and (19). We consider an antiferromagnetic sinusoidal spiral in which the spins all lie in a plane perpendicular to the direction of propagation of the spiral. For simplicity we consider a single atom per unit cell. We take a system of axes described by three mutually perpendicular unit vectors $\hat{u}_1$, $\hat{u}_2$, $\hat{u}_3$ such that $\hat{u}_1$ and $\hat{u}_2$ lie in the plane of the spins and $\hat{u}_3$ lies along the direction of propagation. The unit vectors $\boldsymbol{\eta}_\mathbf{n}$ giving the direction of the spin in the unit cell $\mathbf{n}$ are then expressible as[15]

$$\begin{aligned}\boldsymbol{\eta}_\mathbf{n}&=\hat{u}_1\cos\boldsymbol{\varepsilon}\cdot\mathbf{n}+\hat{u}_2\sin\boldsymbol{\varepsilon}\cdot\mathbf{n},\\&=\tfrac{1}{2}(\mathbf{u}_-\exp(i\boldsymbol{\varepsilon}\cdot\mathbf{n})+\mathbf{u}_+\exp(-i\boldsymbol{\varepsilon}\cdot\mathbf{n})),\end{aligned}\tag{26}$$

where $\mathbf{u}_\pm=\hat{u}_1\pm i\hat{u}_2$ and $\boldsymbol{\varepsilon}=(2\pi/\lambda_s)\hat{u}_3$, where λ_s is the wavelength of the spiral.[15] In this case the magnetic Bragg peaks are split into satellite peaks so that the magnetic and nuclear peaks occur in different places. There is accordingly no interference between the nuclear and the magnetic scattering, and we will write down the magnetic cross section alone. On substituting (26) in (15) we find that the last term, proportional to $\mathbf{P}\cdot(\mathbf{q}_{\mathbf{n}'}\times\mathbf{q}_\mathbf{n})$ does not vanish in this case, as it did for the antiferromagnet. This term together with the ordinary magnetic cross section gives the total magnetic scattering from a spiral:

$$\begin{aligned}d\sigma/d\Omega'=&\tfrac{1}{4}(\gamma e^2/mc^2)^2S^2|f(\mathbf{K})|^2\\&\times\{[1+(\hat{K}\cdot\hat{u}_3)^2+2(\mathbf{P}\cdot\hat{K})(\hat{K}\cdot\hat{u}_3)]\\&\times|\textstyle\sum_n\exp[i(\mathbf{K}+\boldsymbol{\varepsilon})\cdot\mathbf{n}]|^2+[1+(\hat{K}\cdot\hat{u}_3)^2\\&-2(\mathbf{P}\cdot\hat{K})(\hat{K}\cdot\hat{u}_3)]|\textstyle\sum_n\exp[i(\mathbf{K}-\boldsymbol{\varepsilon})\cdot\mathbf{n}]|^2\}.\end{aligned}\tag{27}$$

This shows the splitting into two peaks such that $\mathbf{K}+\boldsymbol{\varepsilon}=\boldsymbol{\tau}$ and $\mathbf{K}-\boldsymbol{\varepsilon}=\boldsymbol{\tau}$, where $\boldsymbol{\tau}$ is 2π times a reciprocal lattice vector. The polarization dependence arose from the above mentioned term in (15). If the scattering vector $\mathbf{K}$ is parallel to the axis $\hat{u}_3$ of the spiral and if the incident beam is polarized parallel to $\hat{u}_3$ as well, the peak for which $\mathbf{K}-\boldsymbol{\varepsilon}=\boldsymbol{\tau}$ vanishes, while that for which $\mathbf{K}+\boldsymbol{\varepsilon}=\boldsymbol{\tau}$ increases to twice its intensity for the case of an unpolarized incident beam. If the direction of initial polarization is made antiparallel to the axis $\hat{u}_3$ of the spiral we have the opposite occurring, with the $\mathbf{K}+\boldsymbol{\varepsilon}=\boldsymbol{\tau}$ peak vanishing and the $\mathbf{K}-\boldsymbol{\varepsilon}=\boldsymbol{\tau}$ peak increasing its intensity. Experimental detection of this effect requires the preparation of a crystal in which some bias is found in the size of domains with spiral axes parallel and antiparallel to $\hat{u}_3$. The polarization of the scattered beam will be written down only for the case of an unpolarized incident beam. We obtain, on substituting (26) in (19) and setting $\mathbf{P}=0$,

$$\begin{aligned}\tfrac{1}{2}\mathbf{P}_f\frac{d\sigma}{d\Omega'}=&\frac{1}{4}\left(\frac{\gamma e^2}{mc^2}\right)^2S^2|f(\mathbf{K})|^2\hat{K}(\hat{K}\cdot\hat{u}_3)\\&\times\{-|\sum_\mathbf{n}\exp[i(\mathbf{K}+\boldsymbol{\varepsilon})\cdot\mathbf{n}]|^2\\&+|\sum_\mathbf{n}\exp[i(\mathbf{K}-\boldsymbol{\varepsilon})\cdot\mathbf{n}]|^2\}.\end{aligned}$$

Hence, the final polarization is parallel to $\mathbf{K}$ for the $\mathbf{K}-\boldsymbol{\varepsilon}=\boldsymbol{\tau}$ reflection and antiparallel to $\mathbf{K}$ for the $\mathbf{K}+\boldsymbol{\varepsilon}=\boldsymbol{\tau}$ reflection. The effect was first pointed out in this form by Overhauser.[4]

These two examples illustrate the importance of the omitted terms for experiments that are easily performed with present techniques. All formulas for scattering of polarized beams by other arrangements of ordered spins may be derived in the same way from (15) and (19).

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[14] Yu. A. Izyumov and S. V. Maleev, Zh. Eksperim. i Teor. Fiz. 41, 1644 (1961) [translation: Soviet Phys.—JETP 14, 1168 (1962)].

[15] W. C. Koehler, Acta Cryst. 14, 535 (1961).