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In a region of a vacuum in which a uniform magnetic field **B** is present, a neutron beam experiences a magnetic potential energy represented by the matrix

$$-\mu_n \boldsymbol{\sigma} \cdot \mathbf{B} = \begin{pmatrix} -\mu_n B & 0 \\ 0 & \mu_n B \end{pmatrix},$$

μ_n being the neutron magnetic moment, if the directions of **B** and of the spin-quantization axis coincide. Consequently, different indices of refraction $n = 1 \pm (\mu_n B/2E)$, where E is the neutron energy, should be associated with the spinor components c and d; this induces between these spinor components a phase difference which is a linear function of the time (or, equivalently, of the distance travelled by the neutrons), hence, according to (5.3.3.1), a rotation around the magnetic field of the component of the neutron polarization perpendicular to this magnetic field. The time frequency of this so-called Larmor precession is $2\mu_n B/h$, where h is Planck's constant.

A neutron beam may be partially polarized; such a beam is conveniently represented by a spin-density matrix ρ, which is the statistical average of the spin-density matrices associated to the polarized beams which are mixed incoherently, the density matrix associated to the spinor

$$|\varphi\rangle = \begin{pmatrix} c \\ d \end{pmatrix}$$

being

$$|\varphi\rangle\langle\varphi| = \begin{pmatrix} c \\ d \end{pmatrix} \begin{pmatrix} c^* & d^* \end{pmatrix} = \begin{pmatrix} cc^* & cd^* \\ c^*d & dd^* \end{pmatrix}.$$

The polarization vector **P** is then obtained as

$$\mathbf{P} = \mathrm{Tr}(\boldsymbol{\sigma}\rho). \qquad (5.3.3.2)$$

In the common case of a non-polarized beam, the spin-density matrix is

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

It is easily seen that all components of **P** are then equal to 0.

Equation (5.3.3.2) is therefore applicable to the general case (polarized, partially polarized or non-polarized beam). The inverse relation giving the density matrix ρ as function of **P** is

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{2}\mathbf{P} \cdot \boldsymbol{\sigma}. \qquad (5.3.3.3)$$

5.3.3.2. *Magnetic scattering by a single ion having unpaired electrons*

The spin and orbital motion of unpaired electrons in an atom or ion give rise to a surrounding magnetic field $\mathbf{B}(\mathbf{r})$ which acts on the neutron *via* the magnetic potential energy $-\boldsymbol{\mu}_n \cdot \mathbf{B}(\mathbf{r})$, where $\boldsymbol{\mu}_n$ is the neutron magnetic moment. Since this is a long-range interaction, in contrast to the nuclear interaction, the magnetic scattering length p, which is proportional to the Fourier transform of the magnetic potential energy distribution $-\boldsymbol{\mu}_n \cdot \mathbf{B}(\mathbf{r})$, depends on the angle of scattering.

The classical relation div $\mathbf{B}(\mathbf{r}) = 0$ shows clearly that the vector $\mathbf{B}(\mathbf{s})$, which is the Fourier transform of $\mathbf{B}(\mathbf{r})$, is perpendicular to the reciprocal-space vector **s**. If we consider the magnetic field $\mathbf{B}(\mathbf{r})$ as resulting from a point-like magnetic moment $\boldsymbol{\mu}$ at position $\mathbf{r} = 0$, we get

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi} \mathrm{curl} \frac{\boldsymbol{\mu} \times \mathbf{r}}{r^3},$$

where $\mu_0 = 4\pi \times 10^{-7}$ H m^{-1} is the permittivity of a vacuum and $\times$ denotes the cross product. $\mathbf{B}(\mathbf{r})$ can be Fourier-transformed into

$$\mathbf{B}(\mathbf{s}) = \mu_0 \mathbf{s} \times \frac{\boldsymbol{\mu} \times \mathbf{s}}{s^2} = \mu_0 \boldsymbol{\mu}_\perp(\mathbf{s}), \qquad (5.3.3.4)$$

where $\boldsymbol{\mu}_\perp(\mathbf{s})$ is the projection of $\boldsymbol{\mu}$ on the plane perpendicular to **s** (reflecting plane).

This result can be applied by volume integration to the more general case of a spatially extended magnetization distribution, which for a single magnetic ion corresponds to the atomic shell of the unpaired electrons. It is thus shown that the magnetic scattering length is proportional to $\boldsymbol{\mu}_n \cdot \boldsymbol{\mu}_{i\perp}$, where $\boldsymbol{\mu}_{i\perp}$ is the projection of the magnetic moment of the ion on the reflecting plane.

For a complete description of magnetic scattering, which involves the spin-polarization properties of the scattered beam, it is necessary to represent the neutron wavefunction in the form of a two-component spinor and the ion's magnetic moment as a spin operator which is a matrix expressed in terms of the Pauli matrices $\boldsymbol{\sigma}$ $(\sigma_x, \sigma_y, \sigma_z)$. The magnetic scattering length is therefore itself a (2×2) matrix:

$$(\mathrm{p}) = -(2\pi m/h^2)\mu_n \boldsymbol{\sigma} \cdot \mathbf{B}(\mathbf{s}) = -\mu_0(2\pi m/h^2)\mu_n \boldsymbol{\sigma} \cdot \boldsymbol{\mu}_{i\perp}(\mathbf{s}) f_i(\sin\theta/\lambda), \qquad (5.3.3.5)$$

where $f_i(\sin\theta/\lambda)$ is the dimensionless magnetic form factor of the ion considered and tends towards a maximum value of 1 when the scattering angle θ tends towards 0 (forward scattering). The value of $\mu_0(2\pi m/h^2)\mu_n\mu_i$ is $p_1 = 2.70 \times 10^{-15}$ m for $\mu_i = 1$ Bohr magneton.

According to (5.3.3.4) or (5.3.3.5), there is no magnetic scattering in directions such that the scattering vector **s** is in the same direction as the ion magnetic moment $\boldsymbol{\mu}_i$. Magnetic scattering effects are maximum when **s** and $\boldsymbol{\mu}_i$ are perpendicular.

The matrix (p) is diagonal if the direction of $\boldsymbol{\mu}_{i\perp}(\mathbf{s})$ is chosen as the spin-quantization axis. Therefore, there is no spin-flip scattering if the incident beam is polarized parallel or antiparallel to the direction of $\boldsymbol{\mu}_{i\perp}(\mathbf{s})$.

It is more usual to choose the spin-quantization axis (Oz) along $\boldsymbol{\mu}_i$. Let β be the angle between the vectors $\boldsymbol{\mu}_i$ and **s**; the (x, y, z) components of $\boldsymbol{\mu}_{i\perp}(\mathbf{s})$ are then $(-\mu_i \sin\beta\cos\beta, 0, \mu_i \sin^2\beta)$ if the y axis is chosen along $\boldsymbol{\mu}_i \times \mathbf{s}$. The total scattering length, which is the sum of the nuclear and the magnetic scattering lengths, is then represented by the matrix

$$(\mathrm{q}) = \begin{pmatrix} b + p\sin^2\beta & -p\sin\beta\cos\beta \\ -p\sin\beta\cos\beta & b - p\sin^2\beta \end{pmatrix}, \qquad (5.3.3.6)$$

where b is the nuclear scattering length and

$$p = -\mu_0 \frac{2\pi m}{h^2} \mu_n \mu_i f_i\left(\frac{\sin\theta}{\lambda}\right) = -p_1 \mu_i f_i\left(\frac{\sin\theta}{\lambda}\right),$$

with μ_i expressed in Bohr magnetons. The relations

$$(\mathrm{q})\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} b + p\sin^2\beta \\ -p\sin\beta\cos\beta \end{pmatrix} \quad \text{and}$$

$$(\mathrm{q})\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -p\sin\beta\cos\beta \\ b - p\sin^2\beta \end{pmatrix}$$

show clearly that the diagonal and the non-diagonal elements of the matrix (q) are, respectively, the spin-flip and the non-spin-flip scattering lengths. It is usual to consider the scattering cross sections, which are the measurable quantities. The cross sections for neutrons polarized parallel or antiparallel to the ion magnetic moment are

$$(\mathrm{d}\sigma/\mathrm{d}\Omega)_\pm = b^2 \pm 2bp\sin^2\beta + (p\sin\beta)^2. \qquad (5.3.3.7)$$

These expressions are the sum of the spin-flip and non-spin-flip cross sections, which are equal to $(b \pm p \sin^2 \beta)^2$ and $(p \sin \beta \cos \beta)^2$, respectively. In the case of non-polarized neutrons, the interference term $(\pm 2bp \sin^2 \beta)$ between the nuclear and the magnetic scattering disappears; the cross section is then

$$(\mathrm{d}\sigma/\mathrm{d}\Omega) = b^2 + (p \sin \beta)^2. \quad (5.3.3.8)$$

In the general case of a partially polarized beam we can use the density-matrix representation. Let $\rho_{\rm inc}$ be the density matrix of the incident beam; it can be shown that the density matrix of the diffracted beam is equal to the following product of matrices: $(\mathrm{q})\rho_{\rm inc}(\mathrm{q}^*)$. Using the relations between the density matrix and polarization vector presented in the preceding section, we can obtain a general description of the diffracted beam as a function of the polarization properties of the incident beam. Such a formalism is of interest for dealing with new experimental arrangements, in which a three-dimensional polarization analysis of the diffracted beam is possible, as shown by Tasset (1989).

5.3.3.3. *Dynamical theory in the case of perfect ferromagnetic or collinear ferrimagnetic crystals*

The most direct way to develop this dynamical theory in the two-beam case, which involves a single Bragg-diffracted beam of diffraction vector $\mathbf{h}$, is to consider spinor wavefunctions of the following form:

$$\varphi(\mathbf{r}) = \exp(i\mathbf{K_0}\cdot\mathbf{r})\begin{pmatrix} D_0 \\ E_0 \end{pmatrix} + \exp[i(\mathbf{K_0}+\mathbf{h})\mathbf{r}]\begin{pmatrix} D_h \\ E_h \end{pmatrix} \quad (5.3.3.9)$$

as approximate solutions of the wave equation inside the crystal,

$$\Delta\varphi(\mathbf{r}) + k^2\varphi(\mathbf{r}) = [u(\mathbf{r}) - \boldsymbol{\sigma}\cdot\mathbf{Q}(\mathbf{r})]\varphi(\mathbf{r}), \quad (5.3.3.10)$$

where $u(\mathbf{r})$ and $-\boldsymbol{\sigma}\cdot\mathbf{Q}(\mathbf{r})$ are, respectively, equal to the nuclear and the magnetic potential energies multiplied by $2m/\hbar^2$. In the calculation of $\varphi(\mathbf{r})$ in the two-beam case, we need only three terms in the expansions of the functions $u(\mathbf{r})$ and $\mathbf{Q}(\mathbf{r})$ into Fourier series:

$$\begin{aligned} u(\mathbf{r}) &= u_\mathbf{0} + u_\mathbf{h}\exp(i\mathbf{h}\cdot\mathbf{r}) + u_{-\mathbf{h}}\exp(-i\mathbf{h}\cdot\mathbf{r}) + \ldots, \\ \mathbf{Q}(\mathbf{r}) &= \mathbf{Q_0} + \mathbf{Q_h}\exp(i\mathbf{h}\cdot\mathbf{r}) + \mathbf{Q_{-h}}\exp(-i\mathbf{h}\cdot\mathbf{r}) + \ldots. \end{aligned}$$

We suppose that the crystal is magnetically saturated by an externally applied magnetic field $\mathbf{H}_a$. $\mathbf{Q_0}$ is then proportional to the macroscopic mean magnetic field $\mathbf{B} = \mu_0(\mathbf{M} + \mathbf{H}_a + \mathbf{H}_d)$, where $\mathbf{M}$ is the magnetization vector and $\mathbf{H}_d$ is the demagnetizing field. The results of Section 5.3.3.2 show that $\mathbf{Q_h}$ and $\mathbf{Q_{-h}}$ are proportional to the projection of $\mathbf{M}$ on the reflecting plane.

The four coefficients D_0, D_h, E_0 and E_h of (5.3.3.9) are found to satisfy a system of four homogeneous linear equations. The condition that the associated determinant has to be equal to 0 defines the dispersion surface, which is of order 4 and has four branches. An incident plane wave thus excites a system of four wavefields of the form of (5.3.3.9), generally polarized in various directions. A particular example of a dispersion surface, having an unusual shape, is shown in Fig. 5.3.3.1.

This is a much more complicated situation than in the case of non-magnetic crystals, in which one only needs to consider scalar wavefunctions which depend on two coefficients, such as D_0 and D_h, and which are related to hyperbolic dispersion surfaces of order 2, as fully described in Chapter 5.1 on X-ray diffraction.

In fact, all neutron experiments related to dynamical effects in diffraction by magnetic crystals have been performed under such conditions that the magnetization vector in the crystal is perpendicular to the diffraction vector $\mathbf{h}$. In this case, the vectors $\mathbf{Q_h}$ and $\mathbf{Q_{-h}}$ are parallel or antiparallel to the vector $\mathbf{Q_0}$ which is chosen as the spin-quantization axis. The matrices $\boldsymbol{\sigma}\cdot\mathbf{Q_0}$, $\boldsymbol{\sigma}\cdot\mathbf{Q_h}$ and $\boldsymbol{\sigma}\cdot\mathbf{Q_{-h}}$ are then all diagonal matrices, and we obtain for the two spin states (±) separate dynamical equations which are similar to the dynamical equations for the scalar case, but with different structure factors, which are either the sum or the difference of the nuclear structure factor F_N and of the magnetic structure factor F_M:

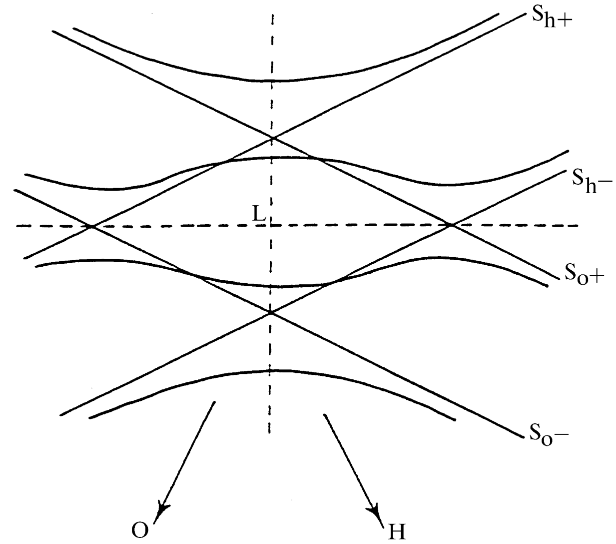

Fig. 5.3.3.1. Schematic plot of the two-beam dispersion surface in the case of a purely magnetic reflection such that $\mathbf{Q_h} = \mathbf{Q_{-h}} = \mathbf{Q_0}$ and that the angle between $\mathbf{Q_0}$ and $\mathbf{Q_h}$ is equal to $\pi/4$.

$$F_+ = F_N + F_M \text{ and } F_- = F_N - F_M. \quad (5.3.3.11)$$

F_N and F_M are related to the scattering lengths of the ions in the unit cell of volume V_c:

$$F_N = V_c u_\mathbf{h} = \sum_i b_i \exp(-i\mathbf{h}\cdot\mathbf{r}_i);$$

$$F_M = V_c|\mathbf{Q_h}| = -\frac{\mu_0 m}{2h^2}\mu_n\boldsymbol{\sigma}\cdot\sum_i \boldsymbol{\mu}_{i\perp}(\mathbf{h})f_i\left(\frac{\sin\theta}{\lambda}\right)\exp(-i\mathbf{h}\cdot\mathbf{r}_i).$$

The dispersion surface of order 4 degenerates into two hyperbolic dispersion surfaces, each of them corresponding to one of the polarization states (±). The asymptotes are different; this is related to different values of the refractive indices for neutron polarization parallel or antiparallel to $\mathbf{Q_0}$.

In some special cases the magnitudes of F_N and F_M happen to be equal. Only one polarization state is then reflected. Magnetic crystals with such a property (reflections 111 of the Heusler alloy Cu_2MnAl, or 200 of the alloy Co–8% Fe) are very useful as polarizing monochromators and as analysers of polarization.

If the scattering vector $\mathbf{h}$ is in the same direction as the magnetization, this reflection is a purely nuclear one (with no magnetic contribution), since F_M is then equal to 0. Purely magnetic reflections (without nuclear contribution) also exist if the magnetic structure involves several sublattices.

If $\mathbf{h}$ is neither perpendicular to the average magnetization nor in the same direction, the presence of non-diagonal matrices in the dynamical equations cannot be avoided. The dynamical theory of diffraction by perfect magnetic crystals then takes the complicated form already mentioned.

Theoretical discussions of this complicated case of dynamical diffraction have been given by Stassis & Oberteuffer (1974), Mendiratta & Blume (1976), Sivardière (1975), Belyakov & Bokun (1975, 1976), Schmidt *et al.* (1975), Bokun (1979), Guigay & Schlenker (1979*a*,*b*), and Schmidt (1983). However, to our knowledge, only limited experimental work has been carried out

references