International Tables for Crystallography (2006). Vol. C, Section 6.1.2, pp. 590–593.

$$\exp(-V/2) = \coth k_s - \frac{1}{k_s} = \frac{I_{3/2}(k_s)}{I_{1/2}(k_s)}, \qquad (6.1.1.88)$$

the small V approximation being

$$V \simeq 2/k_s. \qquad (6.1.1.89)$$

Equations (6.1.1.86) and (6.1.1.87) are generalized to place the mode of the density at (r, θ', φ') by replacing $\cos\theta$ by $\cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\varphi - \varphi')$ and by replacing $P_n(\cos\theta)$ by

$$P(\cos\theta)P_n(\cos\theta') + 2\sum_{m=1}^{n}\frac{(n-m)!}{(n-m)!} \times P_n^m(\cos\theta)P_n^m(\cos\theta')\cos m(\varphi - \varphi').$$

The three-dimensional Fourier transform of the generalized form of (6.1.1.86) in terms of $\mathbf{S}$ in spherical coordinates (S, θ_S, φ_S) is

$$T(\mathbf{S}) = \sum_{q=0}^{\infty} i^q \frac{(2q+1)}{r^2}\exp[-q(q+1)V] \times \sum_{s=0}^{\infty}\frac{4}{2p+1}Y_{qs+}(\theta', \varphi')Y_{qs+}(\theta_S, \varphi_S)j_q(Sr), \qquad (6.1.1.90)$$

where r is the radius of the sphere, and j_n is the nth-order spherical Bessel function of the first kind. The real spherical harmonics Y_{lmp} are normalized as in (6.1.1.22).

The Fourier transform of the generalized form of (6.1.1.87) is identical to (6.1.1.90) except that the term $\exp[-q(q+1)V]$ in (6.1.1.90) is replaced by $I_{q+1/2}(k_s)/I_{1/2}(k_s)$.

The foregoing equations describe isotropic distributions on a sphere. The p.d.f. for general anisotropic Brownian diffusion (or rotation) on a sphere is not available in a convenient form. However, some of the results of Perrin (1934) and Favro (1960) on rotational Brownian motion are applicable to thermal motion. For example, the centre of mass of a p.d.f. resulting from anisotropic diffusion on a sphere is given by equation (6.8) of Favro (1960). The following equation valid in Cartesian coordinates is obtained if the diffusion tensor $\mathbf{D}$ of Favro's equation is replaced by the substitution $\mathbf{L} = 2\mathbf{D}$

$$\langle\mathbf{x}\rangle = \exp[-\tfrac{1}{2}(\mathrm{tr}(\mathbf{L})\mathbf{I} - \mathbf{L})]\mathbf{r} = \mathbf{r} - \tfrac{1}{2}[\mathrm{tr}(\mathbf{L})\mathbf{I} - \mathbf{L}]\mathbf{r} + \tfrac{1}{8}[\mathrm{tr}(\mathbf{L})\mathbf{I} - \mathbf{L}]^2\mathbf{r} - \ldots, \qquad (6.1.1.91)$$

where $\mathbf{r}$ is the vector from the centre of the sphere to the mode of the p.d.f. on the sphere and $\langle\mathbf{x}\rangle$ is the vector to the centre of mass. This equation, which is valid for all amplitudes of libration $\mathbf{L}$, can be used to describe the apparent shrinkage effect in molecules undergoing librational motion.

6.1.1.6.6. *The quasi-Gaussian approximation for curvilinear motion*

The p.d.f.'s defined by (6.1.1.77), (6.1.1.78), (6.1.1.86) and (6.1.1.87), and their Fourier transforms given in §6.1.1.6.5 may be considered 'inverted series' since zero-order terms describe uniform distributions. The inverted series converge slowly if the density is concentrated near the mode. If σ^2 in (6.1.1.76) is sufficiently small, the cyclic overlap on the circle becomes unimportant and the summation for $n \neq 0$ can be neglected. In this limiting case, the p.d.f. assumes the same form as a one-dimensional rectilinear Gaussian density function except that the variable is the angle φ. A similar relation must exist between the p.d.f. on the sphere and the two-dimensional Gaussian function. This 'quasi-Gaussian' approximation is the basis for a number of structure-factor equations for atoms with relatively small amplitude components of curvilinear motion (Dawson, 1970; Kay & Behrendt, 1963; Kendall & Stuart, 1963; Maslen, 1968; Pawley & Willis, 1970).

6.1.1.7. *Structure factor*

The amplitude of coherent scattering from the contents of one unit cell in a crystalline material is the structure factor

$$F(\mathbf{S}) = \int \rho(\mathbf{r})\exp(i\mathbf{S}\cdot\mathbf{r})\,\mathrm{d}r, \qquad (6.1.1.92)$$

where the integration extends over the unit cell. If there are N atoms in the cell, this may be expressed as

$$F(\mathbf{S}) = \sum_{j=1}^{N} f_j T_j \exp(i\mathbf{S}\cdot\mathbf{r}_j), \qquad (6.1.1.93)$$

where $\mathbf{r}_j$ is the mean position and T_j is the temperature factor of the jth atom. In an ideal model of the scattering process in which (6.1.1.93) is exact, f_j is the atomic scattering factor derived from (6.1.1.7). In practice, there are wavelength-dependent changes to the amplitude and phase of the atom's scattering due to dispersion or resonance. To correct for this, each scattering factor may be written

$$f = f^0 + f' + if'', \qquad (6.1.1.94)$$

where f^0 is the kinematic scattering factor and f' and f'' are real and imaginary corrections for dispersion.

6.1.1.8. *Reflecting power of a crystal*

The reflecting power of a small crystal of volume ΔV, rotated at angular velocity ω through a Bragg reflection, defined as the ratio of ω times the reflected energy to the incident-beam intensity, is

$$r_e^2\left(\frac{1+\cos^2 2\theta}{2\sin 2\theta}\right)\lambda^3\frac{F(\mathbf{S})^2}{V_C^2}\Delta V, \qquad (6.1.1.95)$$

where V_c is the unit-cell volume. This expression, which assumes negligible absorption, shows that the integrated intensity is proportional to the crystal volume. The maximum intensity is proportional to $(\Delta V)^2$, but the angular width of the reflecting region varies inversely as ΔV.

In the kinematic theory of diffraction, it is assumed that the crystal is comprised of small domains of perfect crystals for which the intensities are additive. In that case, (6.1.1.95) applies also to finite crystals.

6.1.2. Magnetic scattering of neutrons (By P. J. Brown)

6.1.2.1. *Glossary of symbols*

m_n	Neutron mass
m_e	Electron mass
γ	Neutron magnetic moment in nuclear magnetons (−1.91)
μ_B	Bohr magneton
μ_N	Nuclear magneton
r_e	Classical electron radius $\mu_B e^2/4\pi m_e$
$\mathbf{P}_i$	Electron momentum operator
$\mathbf{S}_e$	Electron spin operator
$\mathbf{S}_n$	Neutron spin operator
$\mathbf{M}(r)$	Magnetization density operator
$\mathbf{k}$	Scattering vector $(H/2\pi)$
$\hat{\mathbf{k}}$	A unit vector parallel to $\mathbf{k}$
$\mathbf{r}_n$	A lattice vector
$\mathbf{g}$	A reciprocal-lattice vector $(h/2\pi)$
$\boldsymbol{\tau}$	Propagation vector for a magnetic structure

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$\tilde{\mathbf{s}}_n$	A unit vector parallel to the neutron spin direction
q, q'	Initial and final states of the scatterer
σ, σ'	Initial and final states of the neutron
E_q	Energy of the state q.

6.1.2.2. *General formulae for the magnetic cross section*

The cross section for elastic magnetic scattering of neutrons is given in the Born approximation by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{m_n}{2\pi\hbar}\right)^2 \left|\left\langle q'\sigma' \middle| \int V(\mathbf{R}) \exp(i\mathbf{k}\cdot\mathbf{R})\,\mathrm{d}\mathbf{R}^3 \middle| q\sigma \right\rangle\right|^2 \times \delta(E_q - E_{q'}). \qquad (6.1.2.1)$$

$V(\mathbf{R})$ is the potential of a neutron at $\mathbf{R}$ in the field of the scatterer. If the field is due to N electrons whose positions are given by $\mathbf{r}_i$, $i = 1, N$, then

$$V(\mathbf{R}) = 4\gamma\mu_B\mu_N \left\{ \sum_{i=1}^{N} \frac{(\mathbf{R}-\mathbf{R}_i)\mathbf{P}_i}{|\mathbf{R}-\mathbf{r}_i|^3} \frac{\mathbf{S}_i}{|\mathbf{R}-\mathbf{r}_i|^3} + \frac{3\mathbf{S}_i\cdot(\mathbf{R}-\mathbf{r}_i)}{|\mathbf{R}-\mathbf{r}_i|^5} + 8\pi\mathbf{S}_i\delta(\mathbf{R}-\mathbf{r}_i) \right\} \cdot \mathbf{S}_n. \qquad (6.1.2.2)$$

$V(\mathbf{R})$ is more simply written in terms of a *magnetization density* operator $\mathbf{M}(\mathbf{r})$, which gives the magnetic moment per unit volume at r due to both the electron's spin and orbital motions. The potential of (6.1.2.2) can then be written (Trammell, 1953)

$$V(\mathbf{R}) = \frac{2\gamma\mu_N\mathbf{S}_n}{\pi^2} \cdot \left\{ \int_0^\infty \int_0^\infty [\hat{\mathbf{k}} \times \mathbf{M}(\mathbf{r}) \times \hat{\mathbf{k}}] \times \exp[i\mathbf{k}\cdot(\mathbf{R}-\mathbf{r})]\,\mathrm{d}\mathbf{k}^3\,\mathrm{d}\mathbf{r}^3 \right\}, \qquad (6.1.2.3)$$

giving for the cross section, from (6.1.2.1),

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = (\gamma r_e)^2 \left| \left\langle q\sigma' \middle| \mathbf{S}_n \cdot \int [\hat{\mathbf{k}} \times \mathbf{M}(\mathbf{r}) \times \hat{\mathbf{k}}] \times \exp(i\mathbf{k}\cdot\mathbf{r})\,\mathrm{d}\mathbf{r}^3 \middle| q\sigma \right\rangle \right|^2. \qquad (6.1.2.4)$$

The *unit-cell magnetic structure factor* $M(\mathbf{k})$ is defined as

$$M(\mathbf{k}) = \left\langle q \int_{\text{unit cell}} \mathbf{M}(r) \exp(i\mathbf{k}\cdot\mathbf{r})\,\mathrm{d}\mathbf{r}^3 \middle| q \right\rangle. \qquad (6.1.2.5)$$

For periodic magnetic structures,

$$\mathbf{M}(\mathbf{r}) = \sum_{\text{lattice vectors}} \mathbf{P}(\mathbf{r}_n\cdot\boldsymbol{\tau}) \cdot \mathbf{M}_u(\mathbf{r}-\mathbf{r}_n),$$

where $\mathbf{P}$ is a periodic function with a period of unity, which describes how the magnitude and direction of the magnetization density, defined within one chemical unit cell by $\mathbf{M}_u(\mathbf{r})$, propagates through the lattice. The magnetic structure factor $\mathbf{m}(\mathbf{k})$ is then given by

$$\mathbf{m}(\mathbf{k}) = (g - j\boldsymbol{\tau})\mathbf{A}(j) \cdot \mathbf{M}(\mathbf{k}), \qquad (6.1.2.6)$$

where $\mathbf{A}(j)$ is the jth term in the Fourier expansion of $\mathbf{P}$ defined by

$$\mathbf{P}(\mathbf{r}\cdot\boldsymbol{\tau}) = \sum_{j=-\infty}^{\infty} \mathbf{A}(j) \exp\{i(j\boldsymbol{\tau}\cdot\mathbf{r})\} \qquad (6.1.2.7)$$

and the scattering cross section given in terms of the magnetic interaction vector $Q(\mathbf{k})$,

$$Q(\mathbf{k}) = \hat{\mathbf{k}} \times \mathbf{m}(\mathbf{k}) \times \hat{\mathbf{k}}, \qquad (6.1.2.8)$$

is

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = (\gamma r_e)^2 |\langle\sigma'|\mathbf{S}_n \cdot \mathbf{Q}(\mathbf{k})|\sigma\rangle|^2. \qquad (6.1.2.9)$$

Equation (6.1.2.9) leads to two independent scattering cross sections: one for scattering of the neutron with no change in spin state ($\sigma' = \sigma$) proportional to $|\mathbf{S}_n \cdot \mathbf{Q}(\mathbf{k})|^2$, and the other to scattering with a change of neutron spin ('spin flip scattering') proportional to $|\mathbf{S}_n \times \mathbf{Q}(\mathbf{k})|^2$. The sum over all final spin states gives

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = (\gamma r_e)^2 |\mathbf{Q}(\mathbf{k})|^2. \qquad (6.1.2.10)$$

6.1.2.3. *Calculation of magnetic structure factors and cross sections*

If the magnetization within the unit cell can be assigned to independent atoms so that each has a total moment μ_i aligned in the direction of the axial unit vector $\hat{\mathbf{m}}_i$, then the unit-cell structure factor can be written

$$\mathbf{M}(\mathbf{k}) = \sum_j \sum_i \mathbf{T}_j\mathbf{R}_j \cdot \hat{\mathbf{m}}_i \mu_i f_i(k) \exp[i\mathbf{k}\cdot(\mathbf{R}_j\mathbf{r}_i + \mathbf{t}_j)]. \qquad (6.1.2.11)$$

$\mathbf{R}_j$ and $\mathbf{t}_j$ are the rotations and translations associated with the jth element of the space group and $\mathbf{T}_j$ is an operator that reverses all the components of moment whenever the element j includes time reversal in the magnetic space group. $f_i(k)$ is the magnetic form factor of the ith atom (see Subsection 6.1.2.3).

The vector part of the magnetic structure factor can be factored out so that

$$\mathbf{m}(\mathbf{k}) \quad \text{becomes} \quad \hat{\mathbf{m}}[m(\mathbf{k})],$$

where $m(\mathbf{k})$ is now a scalar. For collinear structures, all the atomic moments are either parallel or antiparallel to $\hat{\mathbf{m}}$, which in this case is independent of $\mathbf{k}$. The intensity of a magnetic Bragg reflection is proportional to $|\mathbf{Q}(\mathbf{k})|^2$ and

$$\begin{aligned} |\mathbf{Q}(\mathbf{k})|^2 &= 1 - (\hat{\mathbf{m}}\cdot\hat{\mathbf{k}})^2 |m(\mathbf{k})|^2 \\ &= \sin^2\alpha |m(\mathbf{k})|^2 \\ &= q^2 |m(\mathbf{k})|^2, \end{aligned} \qquad (6.1.2.12)$$

where α is the angle between the moment direction $\hat{\mathbf{m}}$ and the scattering vector $\mathbf{k}$. The factor $1 - (\hat{\mathbf{m}}\cdot\hat{\mathbf{k}})^2$, often referred to as q^2, is the means by which the moment direction in a magnetic structure can be determined from intensity measurements. If the intensities are obtained from measurements on polycrystalline samples then the average of q^2 over all the different $\mathbf{k}$ contributing to the powder line must be taken.

$$\overline{q^2} = 1 - \frac{1}{n_g} \sum_j (\mathbf{R}_j\hat{\mathbf{k}} \cdot \hat{\mathbf{m}})^2, \qquad (6.1.2.13)$$

the sum being over all n_g rotations $\mathbf{R}_j$ of the point group. $\overline{q^2}$ is given for different crystal symmetries by Shirane (1959). For uniaxial groups, the result is

$$\overline{q^2} = 1 - \tfrac{1}{2}(\sin^2\Psi \sin^2\varphi - \cos^2\Psi \cos^2\varphi), \qquad (6.1.2.14)$$

where Ψ and φ are the angles between the unique axis and the scattering vector and moment direction, respectively. For cubic groups $\overline{q^2} = 2/3$ independent of the moment direction and of the direction of $\mathbf{k}$.

6.1.2.4. *The magnetic form factor*

The magnetic form factor introduced in (6.1.2.11) is determined by the distribution of magnetization within a single atom. It can be defined by

$$f(\mathbf{k}) = \frac{\langle q | \int \mathbf{M}(\mathbf{r}) \exp(i\mathbf{k}\cdot\mathbf{r})\,\mathrm{d}r^3 | q\rangle}{\langle q | \int \mathbf{M}(\mathbf{r})\,\mathrm{d}r^3 | q\rangle}, \qquad (6.1.2.15)$$

where q now represents a state of an individual atom.

In the majority of cases, the magnetization of an atom or ion is due to a single open atomic shell: the d shell for transition metals, the $4f$ shell for rare earths, and the $5f$ shell for actinides. Magnetic form factors are calculated from the radial wavefunctions of the electrons in the open shells. The integrals from which the form factors are obtained are

$$\langle j_l(k)\rangle = \int_0^\infty U^2(r) j_l(kr) 4\pi r^2\,\mathrm{d}r, \qquad (6.1.2.16)$$

where $U(r)$ is the radial wavefunction for the atom and $j_l(kr)$ is the lth-order spherical Bessel function. Within the dipole approximation (spherical symmetry), the magnetic form factor is given by

$$f(k) = \langle j_0(k)\rangle + (1 - 2/g)\langle j_2(k)\rangle, \qquad (6.1.2.17)$$

where g is the Landé splitting factor (Lovesey, 1984). Higher approximations are needed if the orbital contribution is large and to describe departures from spherical symmetry. They involve terms in $\langle j_4\rangle\langle j_6\rangle$ *etc*. Fig. 6.1.2.1 shows the integrals $\langle j_0\rangle$, $\langle j_2\rangle$, and $\langle j_4\rangle$ for Fe^{2+} and in Fig. 6.1.2.2 the spherical spin-only form factors $\langle j_0\rangle$ for $3d$, $4d$, $4f$, and $5f$ electrons are compared. Tables of magnetic form factors are given in Section 4.4.5.

6.1.2.5. *The scattering cross section for polarized neutrons*

The cross section for scattering of neutrons with an arbitrary spin direction is obtained from (6.1.2.9) but adding also nuclear scattering given by the nuclear structure factor $F(\mathbf{k})$, which is assumed to be spin independent. In this case,

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \langle\sigma|(\gamma r_e)\mathbf{S}_n\cdot\mathbf{Q}(\mathbf{k}) + F(\mathbf{k})|\sigma\rangle^2, \qquad (6.1.2.18)$$

the scattering without change of spin direction is

$$I^{++} \propto |F'(\boldsymbol{\kappa})|^2 + |\hat{\mathbf{s}}_n\cdot\mathbf{Q}(\mathbf{k})|^2 + \hat{\mathbf{s}}_n\cdot[\mathbf{Q}^*(\mathbf{k})F'(\mathbf{k}) + \mathbf{Q}(\mathbf{k})F'^*(\mathbf{k})], \qquad (6.1.2.19)$$

and, for the spin flip scattering,

$$I^{+-} \propto [\hat{\mathbf{s}}_n\times\mathbf{Q}(\mathbf{k})]\cdot[\hat{\mathbf{s}}_n\cdot\mathbf{Q}^*(\mathbf{k})] + \hat{\mathbf{s}}_n\cdot[\mathbf{Q}(\mathbf{k})\times\mathbf{Q}^*(\mathbf{k})] \qquad (6.1.2.20)$$

with $F'(\mathbf{k}) = F(\mathbf{k})/(\gamma r_e)$.

The cross section I^{++} implies interference between the nuclear and the magnetic scattering when both occur for the same $\mathbf{k}$. This interference is exploited for the production of polarized neutrons, and for the determination of magnetic structure factors using polarized neutrons.

In the classical method for determining magnetic structure factors with polarized neutrons (Nathans, Shull, Shirane & Andresen, 1959), the 'flipping ratio' R, which is the ratio between the cross sections for oppositely polarized neutrons, is measured:

$$R = \frac{|F'(\mathbf{k})|^2 + 2P\hat{\mathbf{s}}_n\cdot[\mathbf{Q}(\mathbf{k})F'^*(\mathbf{k}) + \mathbf{Q}^*(\mathbf{k})F'(\mathbf{k})] + |\mathbf{Q}(\mathbf{k})|^2}{|F'(\mathbf{k})|^2 - 2Pe\hat{\mathbf{s}}_n\cdot[\mathbf{Q}(\mathbf{k})F'^*(\mathbf{k}) + \mathbf{Q}^*(\mathbf{k})F'(\mathbf{k})] + |\mathbf{Q}(\mathbf{k})|^2}. \qquad (6.1.2.21)$$

In this equation, $\hat{\mathbf{s}}_n$ is a unit vector parallel to the polarization direction. P is the neutron polarization defined as

$$P = (\langle S^+\rangle - \langle S^-\rangle)/(\langle S^+\rangle + \langle S^-\rangle),$$

where $\langle S^+\rangle$ and $\langle S^-\rangle$ are the expectation values of the neutron spin parallel and antiparallel to $\hat{\mathbf{s}}_n$ averaged over all the neutrons in the beam. e is the 'flipping efficiency' defined as $e = (2f - 1)$, where f is the fraction of the neutron spins that are reversed by the flipping process. Equation (6.1.2.21) is considerably simplified when both $F(\mathbf{k})$ and $\mathbf{Q}(\mathbf{k})$ are real and the polarization direction is parallel to the magnetization direction, as in a sample

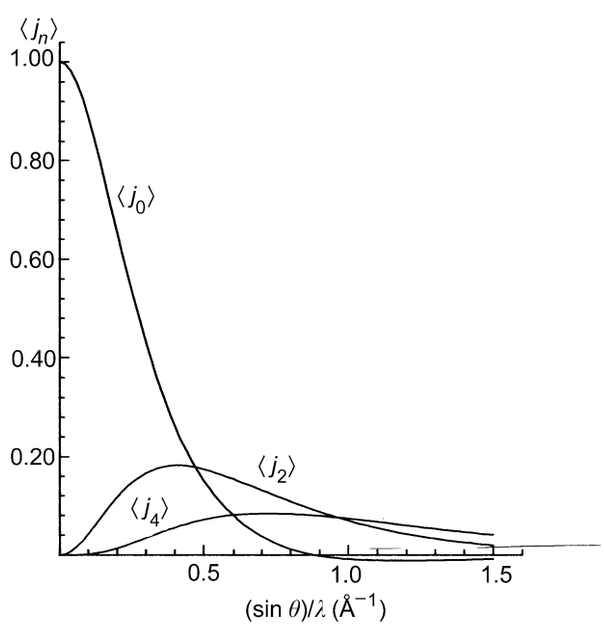

Fig. 6.1.2.1. The integrals $\langle j_0\rangle$, $\langle j_2\rangle$, and $\langle j_4\rangle$ for the Fe^{2+} ion plotted against $(\sin\theta)/\lambda$. The integrals have been calculated from wavefunctions given by Clementi & Roetti (1974).

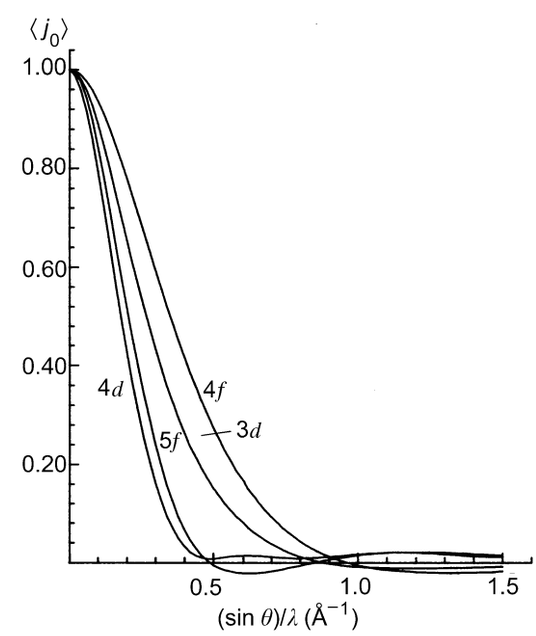

Fig. 6.1.2.2. Comparison of $3d$, $4d$, $4f$, and $5f$ form factors. The $3d$ form factor is for Co, and the $4d$ for Rh, both calculated from wavefunctions given by Clementi & Roetti (1974). The $4f$ form factor is for Gd^{3+} calculated by Freeman & Desclaux (1972) and the $5f$ is that for U^{3+} given by Desclaux & Freeman (1978).

magnetized by an external field. The 'flipping ratio' then becomes

$$R = \frac{1 + 2Py\sin^2\rho + y^2\sin^2\rho}{1 - 2Pey\sin^2\rho + y^2\sin^2\rho}, \qquad (6.1.2.22)$$

with $y = (\gamma r_e)M(\mathbf{k})/F(\mathbf{k})$, ρ being the angle between the magnetization direction and the scattering vector. The solution to this equation is

$$y = \{P\sin\rho(Re+1) \pm [P^2\sin^2\rho(Re+1)^2 - (R-1)^2]^{1/2}\} \times [(R-1)\sin\rho]^{-1}; \qquad (6.1.2.23)$$

the relative signs of $F(\mathbf{k})$ and $M(\mathbf{k})$ are determined by whether R is greater or less than unity. The uncertainty in the sign of the square root in (6.1.2.23) corresponds to not knowing whether $F(\mathbf{k}) > M(\mathbf{k})$ or *vice versa*.

6.1.2.6. *Rotation of the polarization of the scattered neutrons*

Whenever the neutron spin direction is not parallel to the magnetic interaction vector $\mathbf{Q}(\mathbf{k})$, the direction of polarization is changed in the scattering process. The general formulae for the scattered polarization are given by Blume (1963). The result for most cases of interest can be inferred by calculating the components of the scattered neutron's spin in the x, y, and z directions for a neutron whose spin is initially parallel to z. For simplicity, y is taken parallel to $\mathbf{k}$; x and z define a plane that contains $\mathbf{Q}(\mathbf{k})$. From (6.1.2.18),

$$\begin{aligned}
S_x &= \tfrac{1}{2}\{[Q_z(\mathbf{k}) + F'(\mathbf{k})]Q_x^*(\mathbf{k}) \\
&\quad + [Q_z^*(\mathbf{k}) + F'^*(\mathbf{k})]Q_x(\mathbf{k})\}/N \\
S_y &= \frac{1}{2i}\{[Q_z(\mathbf{k}) + F'(\mathbf{k})]Q_x^*(\mathbf{k}) \\
&\quad - [Q_z^*(\mathbf{k}) + F'^*(\mathbf{k})]Q_x(\mathbf{k})\}/N \\
S_z &= \tfrac{1}{2}\{[Q_z(\mathbf{k}) + F'(\mathbf{k})][Q_z^*(\mathbf{k}) + F'^*(\mathbf{k})]\}/N \\
N &= |Q_z(\mathbf{k}) + F'(\mathbf{k})|^2 + |Q_x(\mathbf{k})|^2.
\end{aligned} \qquad (6.1.2.24)$$

It is clear from this set of equations that S_x and S_y are zero if $Q_x(\mathbf{k}) = 0$. Three simple cases may be taken as examples of the use of (6.1.2.24):

(*a*) A magnetic reflection from a simple antiferromagnet for which $\mathbf{Q}(\mathbf{k})$ is real, $F(k) = 0$; under these conditions,

$$\begin{aligned}
S_x &= Q_x(\mathbf{k})[Q_z(\mathbf{k})]/|\mathbf{Q}(\mathbf{k})|^2 \\
S_y &= 0 \\
S_z &= \tfrac{1}{2}[Q_z(\mathbf{k})^2 - Q_x(\mathbf{k})^2]/|\mathbf{Q}(\mathbf{k})|^2,
\end{aligned}$$

showing that the direction of polarization is turned through an angle 2φ in the xy plane where φ is the angle between $\mathbf{Q}(\mathbf{k})$ and the initial polarization direction.

(*b*) A satellite reflection from a magnetic structure described by a *circular helix* for which $Q_x(\mathbf{k}) = iQ_z(\mathbf{k})$, $F'(\mathbf{k}) = 0$; in this case,

$$\begin{aligned}
S_x &= 0 \\
S_y &= Q_z^2(\mathbf{k})/|\mathbf{Q}(\mathbf{k})|^2 = \tfrac{1}{2} \\
S_z &= 0
\end{aligned}$$

and the scattered polarization is parallel to the scattering vector independent of its initial direction.

(*c*) A mixed magnetic and nuclear reflection from a Cr_2O_3-type antiferromagnet for which $\mathbf{Q}(\mathbf{k})$ is imaginary, $\mathbf{Q}(\mathbf{k}) = -\mathbf{Q}^*(\mathbf{k})$, $F(\mathbf{k})$ is real. Then,

$$\begin{aligned}
S_x &= Q_x(\mathbf{k})Q_z(\mathbf{k})/[F'(\mathbf{k})^2 + |\mathbf{Q}(\mathbf{k})|^2] \\
S_y &= iF(\mathbf{k})Q_x(\mathbf{k})/[F'(\mathbf{k})^2 + |\mathbf{Q}(\mathbf{k})|^2] \\
S_z &= \tfrac{1}{2}[|Q_z(\mathbf{k}) + F'(\mathbf{k})|^2 - |Q_x(\mathbf{k})|^2] \\
&\quad \times [F'(\mathbf{k})^2 + |\mathbf{Q}(\mathbf{k})|^2]^{-1}
\end{aligned}$$

so that in this case the final polarization has components along all three directions.

6.1.3. Nuclear scattering of neutrons (By B. T. M. Willis)

6.1.3.1. *Glossary of symbols*

b	Bound nuclear scattering length
$b_{\rm free}$	Free nuclear scattering length
b_0	Potential scattering length
b', b''	Real and imaginary parts of resonant scattering length
$b_{\rm coh}$	Coherent scattering length
$F(\mathbf{h})$	Structure factor for nuclear Bragg scattering
$2\pi\mathbf{h}$	Reciprocal-lattice vector
$\mathbf{H}$	Scattering vector ($= \mathbf{k} - \mathbf{k}_0$)
I	Nuclear spin
$\mathbf{k}$	Wavevector of scattered neutron
$\mathbf{k}_0$	Wavevector of incident neutron
M	Nuclear mass
m_n	Neutron mass
N	Number of unit cells in crystal
V	Volume of unit cell
W_j	Exponent of temperature factor $\exp(-W_j)$ of jth atom
w_+	Weight of spin state $I + \frac{1}{2}$
w_-	Weight of spin state $I - \frac{1}{2}$
$\sigma_{\rm coh}$	Coherent scattering cross section
$\sigma_{\rm inc}$	Incoherent scattering cross section
$\sigma_{\rm tot}$	Total scattering cross section ($= \sigma_{\rm coh} + \sigma_{\rm inc}$)
$\left(\frac{d\sigma}{d\Omega}\right)_{\rm coh,el}$	Differential coherent elastic scattering cross section
$\left(\frac{d\sigma}{d\Omega}\right)_{\rm inc,el}$	Differential incoherent elastic scattering cross section

The nucleus is the fundamental unit involved in the scattering of neutrons by atoms. For magnetic materials, electronic scattering takes place as well (see Section 6.1.2). Apart from these two main interactions, there are a number of subsidiary ones (Shull, 1967) that are extremely weak and can be ignored in nearly all diffraction studies.

In this section, we discuss the neutron–nucleus interaction only, starting from scattering by a single nucleus, then scattering by an atom, and finally scattering by a single crystal. For a more detailed account, see Bacon (1975).

6.1.3.2. *Scattering by a single nucleus*

The nuclear forces giving rise to the scattering of neutrons have a range of 10^{-14} to 10^{-15} m. This is much smaller than the wavelength of thermal neutrons, and so (from elementary diffraction theory) the neutron wave scattered by the nucleus is spherically symmetrical. Unlike magnetic scattering, there is no 'form-factor' dependence of nuclear scattering on the scattering angle.

The incident neutron beam can be represented by the plane wave

$$\psi_0 = \exp(i\mathbf{k}_0 \cdot \mathbf{r}),$$

references