International Tables for Crystallography (2006). Vol. C, Figure 6.1.2.1, p. 592.

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

$$\langle j_l(k)\rangle = \int\limits_0^\infty U^2(r) j_l(kr) 4\pi r^2\,\mathrm{d}r, \qquad (6.1.2.16)$$

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

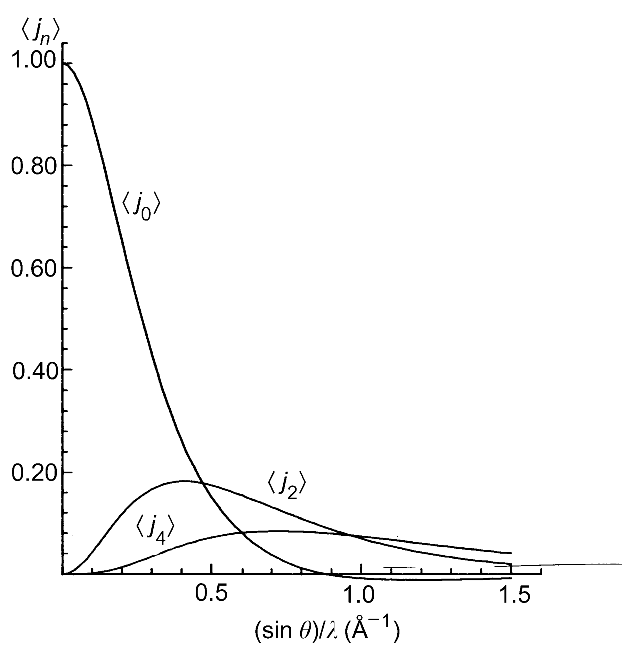

Fig. 6.1.2.1. The integrals $\langle j_0\rangle$, $\langle j_2\rangle$, and $\langle j_4\rangle$ for the Fe^{2+} ion plotted against $(\sin\theta)/\lambda$. The integrals have been calculated from wavefunctions given by Clementi & Roetti (1974).

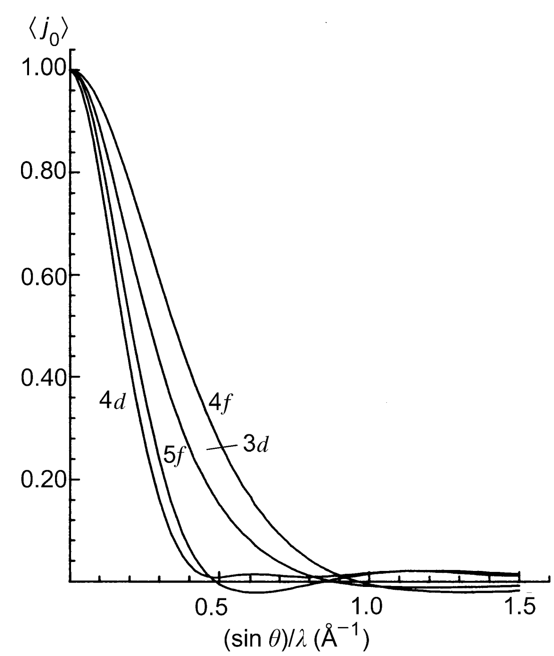

Fig. 6.1.2.2. Comparison of 3d, 4d, 4f, and 5f form factors. The 3d form factor is for Co, and the 4d for Rh, both calculated from wavefunctions given by Clementi & Roetti (1974). The 4f form factor is for Gd^{3+} calculated by Freeman & Desclaux (1972) and the 5f is that for U^{3+} given by Desclaux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

references