into account. For an unpolarized incident beam, the usual case in neutron powder diffraction, it is a useful consequence of the triple vector product that the magnetic scattering depends on the sine of the angle that the scattering vector makes with the magnetic moment on the scattering atom (see Section 2.3.4 and Chapter 7 in Kisi & Howard, 2008). The extent of the unpaired electron distribution (usually outer electrons) implies that the scattering diminishes as a function of Q, an effect that can be described by a magnetic form factor. For a well defined direction for the magnetic moment $\mathbf{M}$, and with a distribution of moment that can be described by a normalized scalar $m(\mathbf{r})$, the form factor as a function of the scattering vector $\mathbf{h}$ [defined in equation (1.1.17) in Chapter 1.1][6] is the Fourier transform of $m(\mathbf{r})$,

$$f(\mathbf{h}) = \int m(\mathbf{r}) \exp(2\pi i \mathbf{h} \cdot \mathbf{r})\, \mathrm{d}\mathbf{r},$$

where $m(\mathbf{r})$ can comprise both spin and orbital contributions [Section 6.1.2 of Volume C (Brown, 2006*a*)]. The tabulated form factors are based on the assumption that the electron distributions are spherically symmetric, so that $m(\mathbf{r}) = m(r) = U^2(r)$, where $U(r)$ is the radial part of the wave function for the unpaired electron. In the expansion of the plane-wave function $\exp(2\pi i \mathbf{h} \cdot \mathbf{r})$ in terms of spherical Bessel functions, we find that the leading term is just the zeroth-order spherical Bessel function $j_0(2\pi hr)$ with a Fourier transform

$$\langle j_0(h) \rangle = 4\pi \int_0^\infty U^2(r) j_0(2\pi hr) r^2 \,\mathrm{d}r.$$

This quantity is inherently normalized to unity at $h = 0$, and may suffice to describe the form factor for spherical spin-only cases. In other cases it may be necessary to include additional terms in the expansion, and these have Fourier transforms of the form

$$\langle j_l(h) \rangle = 4\pi \int_0^\infty U^2(r) j_l(2\pi hr) r^2 \,\mathrm{d}r$$

with l even; these terms are zero at $h = 0$ (Brown, 2006*a*). In practice these quantities are evaluated using theoretical calculations of the radial distribution functions for the unpaired electrons [Section 4.4.5 of Volume C (Brown, 2006*b*)].

Form factors can be obtained from data tabulated in Section 4.4.5 of Volume C (Brown, 2006*b*). Data are available for elements and ions in the 3*d*- and 4*d*-block transition series, for rare-earth ions and for actinide ions. These data are provided by way of the coefficients of analytical approximations to $\langle j_l(h) \rangle$, the analytical approximations being

$$\langle j_0(s) \rangle = A \exp(-as^2) + B \exp(-bs^2) + C \exp(-cs^2) + D$$

and for $l \neq 0$

$$\langle j_l(s) \rangle = s^2 \left[A \exp(-as^2) + B \exp(-bs^2) + C \exp(-cs^2) + D\right],$$

where $s = h/2$ in Å^{-1}. These approximations, with the appropriate coefficients, are expected to be coded in to any computer program purporting to analyse magnetic structures. Although the tabulated form factors are based on theoretical wave functions, it is worth noting that the incoherent scattering from an ideally disordered (*i.e.*, paramagnetic) magnetic system will display the magnetic form factor directly.

It is often convenient to define a (Q-dependent) magnetic scattering length

$$p = \left(\frac{e^2 \gamma}{2 m_e c^2}\right) g J f,$$

where m_e and e are the mass and charge of the electron, γ (= μ_n) is the magnetic moment of the neutron, c is the speed of light, J is the total angular momentum quantum number, and g is the Landé splitting factor given in terms of the spin S, orbital angular momentum L, and total angular momentum quantum numbers by

$$g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}.$$

For the spin-only case, $L = 0$, $J = S$, so $g = 2$. The differential magnetic scattering cross section per atom is then given by $q^2 p^2$ where $|q| = \sin\alpha$, α being the angle between the scattering vector and the direction of the magnetic moment. This geometrical factor is very important, since it can help in the determination of the orientation of the moment of interest; there is no signal, for example, when the moment is parallel to the scattering vector. Further discussion appears in Chapters 2 (Section 2.3.4) and 7 in Kisi & Howard (2008).

2.3.2.6. *Structure factors*

The locations of the Bragg peaks for neutrons are calculated as they are for X-rays[7] (Section 1.1.2), and the intensities of these peaks are determined by a structure factor, which in the nuclear case is [*cf*. Chapter 1.1, equation (1.1.56)]

$$F_{hkl}^{\rm nuc} = \sum_{i=1}^{m} b_i T_i \exp(2\pi i \mathbf{h} \cdot \mathbf{u}_i), \qquad (2.3.7)$$

where b_i here denotes the coherent scattering length, T_i has been introduced to represent the effect of atomic displacements (thermal or otherwise, see Section 2.4.1 in Kisi & Howard, 2008), $\mathbf{h}$ is the scattering vector for the *hkl* reflection, and the vectors $\mathbf{u}_i$ represent the positions of the m atoms in the unit cell.

For coherent magnetic scattering, the structure factor reads

$$F_{hkl}^{\rm mag} = \sum_{i=1}^{m} p_i \mathbf{q}_i T_i \exp(2\pi i \mathbf{h} \cdot \mathbf{u}_i), \qquad (2.3.8)$$

where p_i is the magnetic scattering length. The vector $\mathbf{q}_i$ is the 'magnetic interaction vector' and is defined by a triple vector product (Section 2.3.4 in Kisi & Howard, 2008), and has modulus $\sin\alpha$ as already mentioned. In this case the sum needs to be taken over the magnetic atoms only.

As expected by analogy with the X-ray case, the intensity of purely nuclear scattering is proportional to the square of the modulus of the structure factor $|F_{hkl}^{\rm nuc}|^2$. In the simplest case of a collinear magnetic structure and an unpolarized incident neutron beam, the intensity contributed by the magnetic scattering is proportional to $|F_{hkl}^{\rm mag}|^2$, and the nuclear and magnetic contributions are additive.

2.3.3. Neutron sources

2.3.3.1. *The earliest neutron sources*

The earliest neutron source appears to have been beryllium irradiated with α-particles (helium nuclei), as emitted for example by polonium or radon. First described as 'beryllium radiation', the radiation from a Po/Be source was identified by

[6] To reiterate, $\mathbf{h} = \mathbf{s} - \mathbf{s}_0$, where $\mathbf{s}_0$ and $\mathbf{s}$ are vectors, each of magnitude $1/\lambda$, defining the incident and scattered beams. Note that $\mathbf{Q} = 2\pi\mathbf{h}$.

[7] The nuclear unit cell is expected to coincide with the X-ray unit cell, but the magnetic unit cell may be larger. So, although the methods of calculation are the same, the larger magnetic cell may give rise to additional (magnetic) Bragg peaks.