$\tilde{\mathbf{s}}_n$ 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

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

$V(\mathbf{R})$ 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

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

$V(\mathbf{R})$ 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)

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

giving for the cross section, from (6.1.2.1),

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

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

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

For periodic magnetic structures,

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

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

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

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

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

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

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

is

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

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

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

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

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

$\mathbf{R}_j$ 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

$$|\mathbf{Q}(\mathbf{k})|^2 = 1 - (\hat{\mathbf{m}}\cdot\hat{\mathbf{k}})^2|m(\mathbf{k})|^2 = \sin^2\alpha|m(\mathbf{k})|^2 = q^2|m(\mathbf{k})|^2, \quad (6.1.2.12)$$

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.

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

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

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

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 $\mathbf{k}$.

references