4.1 The differential cross-section in the dipole approximation

A neutron-scattering experiment is performed by allowing a collimated beam of monochromatic (monoenergetic) neutrons to impinge upon a sample, and then measuring the energy distribution of neutrons scattered in different directions. As illustrated in Fig. 4.1, a uniform ensemble of neutrons in the initial state $|\mathbf{k}\mathbf{s}_n>$ is created, typically by utilizing Bragg-reflection in a large single-crystal monochromator, plus suitable shielding by collimators. We may write the state vector for this initial plane-wave state

$$|\mathbf{k}\mathbf{s}_n> = V^{-1/2}\exp(i\mathbf{k}\cdot\mathbf{r}_n)\,|\mathbf{s}_n>\,,$$

representing free neutrons with an energy $(\hbar k)^2/2M$ and a flux $\mathbf{j}(\mathbf{k}\mathbf{s}_n) = V^{-1}\hbar\mathbf{k}/M$. When passing through the target, the probability per unit time that a neutron makes a transition from its initial state to the state $|\mathbf{k}'\mathbf{s}'_n>$ is determined by *Fermi's Golden Rule*:

$$W(\mathbf{k}\mathbf{s}_n, \mathbf{k}'\mathbf{s}'_n) = \frac{2\pi}{\hbar}\sum_{if} P_i\,|<\mathbf{k}\mathbf{s}_n; i\,|\,\mathcal{H}_{\rm int}\,|\mathbf{k}'\mathbf{s}'_n; f>|^2\,\delta(\hbar\omega + E_i - E_f). \tag{4.1.1}$$

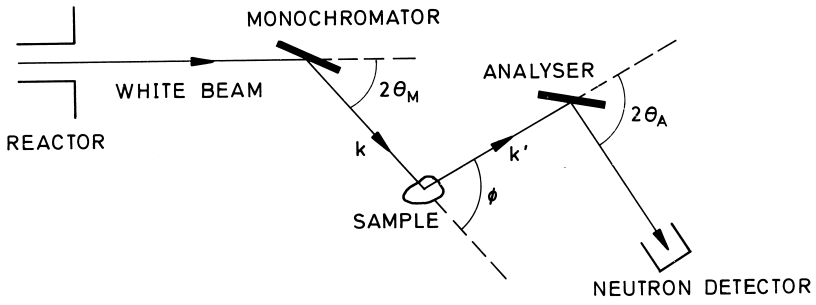

Fig. 4.1. The principle of a neutron-scattering experiment, carried out on a *triple-axis spectrometer*. An incident beam of neutrons, with well-defined momenta, is selected from the continuous reactor spectrum by the monochromator crystal, and scattered from the sample. The intensity of the scattered beam of neutrons, with generally different momenta defined by the analyser crystal, is measured by the detector. The scattered intensity, proportional to the scattering cross-section, is thus determined as a function of the energy transfer $\hbar\omega$ and the momentum transfer $\hbar\boldsymbol{\kappa}$ to the sample, whose orientation relative to $\boldsymbol{\kappa}$ can be varied by rotating the sample table.

$\mathcal{H}_{\rm int}$ is the Hamiltonian describing the interaction between the neutrons and the sample, and the sum extends over all possible scattering processes. It comprises a summation over all possible final states $|f>$ of the sample, and an average over all initial states $|i>$, which occur with the probability P_i. Energy conservation requires that the energy difference between the final and initial states of the sample, $E_f - E_i$, must be equal to the energy transferred from the neutron to it:

$$\hbar\omega = \frac{(\hbar k)^2}{2M} - \frac{(\hbar k')^2}{2M}. \tag{4.1.2}$$

The linear momentum transferred to the sample is $\hbar\boldsymbol{\kappa} = \hbar\mathbf{k} - \hbar\mathbf{k}'$, where $\boldsymbol{\kappa}$ is the *scattering vector*,

$$\boldsymbol{\kappa} = \mathbf{k} - \mathbf{k}'. \tag{4.1.3}$$

The information about the sample is obtained by measuring the scattered intensity as a function of the natural variables of the experiment, the *energy transfer* $\hbar\omega$ and the *momentum transfer* $\hbar\boldsymbol{\kappa}$.

The scattered neutrons with momenta lying in a narrow range around $\hbar\mathbf{k}'$ are counted by placing a detector in a direction along $\mathbf{k}'$, subtending a small element of solid angle $d\Omega$. The value of k', or the final

neutron energy, is determined by again making use of Bragg-reflection in a single-crystal analyser, so that only neutrons with energies in a small interval dE around $(\hbar k')^2/2M$ strike the counter. The number of neutrons in this range, corresponding to a state vector $|\mathbf{k}'\mathbf{s}'_n>$ for the scattered neutrons, is

$$\delta N = V(2\pi)^{-3}(k')^2 dk' d\Omega = V(2\pi)^{-3}(Mk'/\hbar^2) dE d\Omega.$$

The number of neutrons arriving at the counter per unit time and per incident neutron is proportional to the scattering area $d\sigma = |\mathbf{j}(\mathbf{k}\mathbf{s}_n)|^{-1} \times W(\mathbf{k}\mathbf{s}_n, \mathbf{k}'\mathbf{s}'_n)\delta N$, or to the *differential scattering cross-section*

$$\frac{d^2\sigma}{dEd\Omega} = \frac{k'}{k}\left(\frac{M}{2\pi\hbar^2}\right)^2 \sum_{if} P_i \,|<\mathbf{s}_n; i\,|\,\mathcal{H}_{\rm int}(\boldsymbol{\kappa})\,|\,\mathbf{s}'_n; f>|^2\, \delta(\hbar\omega + E_i - E_f), \tag{4.1.4a}$$

where

$$\mathcal{H}_{\rm int}(\boldsymbol{\kappa}) = \int \mathcal{H}_{\rm int}\, e^{-i\boldsymbol{\kappa}\cdot\mathbf{r}_n} d\mathbf{r}_n. \tag{4.1.4b}$$

This result of time-dependent perturbation theory, in the first Born approximation, is accurate because of the very weak interaction between the neutrons and the constituents of the sample.

In order to proceed further, it is necessary to specify the interaction Hamiltonian $\mathcal{H}_{\rm int}$. The magnetic moment of the neutron is

$$\boldsymbol{\mu}_n = -g_n \mu_N \mathbf{s}_n \qquad ; \quad g_n = 3.827 \qquad ; \quad \mu_N = \frac{m}{M}\mu_B = \frac{e\hbar}{2Mc},$$

with $s_n = \frac{1}{2}$. In this chapter, in the interest of conformity with the rest of the literature, we do not reverse the signs of the electronic angular-momentum vectors, which are therefore antiparallel to the corresponding magnetic moments, as is also the case for the neutron.

This magnetic dipole moment at $\mathbf{r}_n$ gives rise to a vector potential, at the position $\mathbf{r}_e$,

$$\mathbf{A}_n(\mathbf{r}_e, \mathbf{r}_n) = \mathbf{A}_n(\mathbf{r} = \mathbf{r}_e - \mathbf{r}_n) = \boldsymbol{\mu}_n \times \mathbf{r}/r^3,$$

with $r = |\mathbf{r}|$. The magnetic-interaction Hamiltonian for a neutron at $\mathbf{r}_n$ with a single electron of charge $-e$, with coordinate $\mathbf{r}_e$, momentum $\mathbf{p}$, and spin $\mathbf{s}$ is

$$\begin{aligned}\mathcal{H}_{\rm int}(\mathbf{r}_e, \mathbf{r}_n) &= \frac{1}{2m}\Big(\mathbf{p} + \frac{e}{c}(\mathbf{A}_n + \mathbf{A}_e)\Big)^2 - \frac{1}{2m}\Big(\mathbf{p} + \frac{e}{c}\mathbf{A}_e\Big)^2 + 2\mu_B \mathbf{s}\cdot\mathbf{B}_n \\ &= 2\mu_B\Big(\frac{1}{\hbar}\mathbf{A}_n \cdot \mathbf{p}' + \mathbf{s}\cdot(\nabla \times \mathbf{A}_n)\Big),\end{aligned} \tag{4.1.5}$$

neglecting the diamagnetic term of second order in μ_N. $\mathbf{A}_e$ denotes the additional contribution to the total vector potential from the surrounding electrons, or an external magnetic field. The prime on $\mathbf{p}$ only plays a role if $\mathbf{A}_e$ is non-zero, in which case $\mathbf{p}' = \mathbf{p} + \frac{e}{c}\mathbf{A}_e$. We note that $\mathbf{A}_n$ commutes with $\mathbf{p}'$, because $\nabla_e \cdot \mathbf{A}_n = \nabla \cdot \mathbf{A}_n$ and

$$\nabla \cdot \mathbf{A}_n(\mathbf{r}) = \nabla \cdot \{-\boldsymbol{\mu}_n \times \nabla(\tfrac{1}{r})\} = \boldsymbol{\mu}_n \cdot \nabla \times \nabla(\tfrac{1}{r}) = 0,$$

recalling that $\mathbf{r}/r^3 = -\nabla(\frac{1}{r})$.

The Fourier transform of $\mathbf{A}_n$ with respect to the neutron coordinate, defining $\mathbf{x} = \mathbf{r}_n - \mathbf{r}_e$, is

$$\begin{aligned}\int \mathbf{A}_n(\mathbf{r}_e - \mathbf{r}_n)\, e^{-i\boldsymbol{\kappa}\cdot\mathbf{r}_n} d\mathbf{r}_n &= e^{-i\boldsymbol{\kappa}\cdot\mathbf{r}_e} \int \mathbf{A}_n(-\mathbf{x})\, e^{-i\boldsymbol{\kappa}\cdot\mathbf{x}} d\mathbf{x} \\ &= -e^{-i\boldsymbol{\kappa}\cdot\mathbf{r}_e} \int (\boldsymbol{\mu}_n \times \mathbf{x})\, x^{-3} e^{-i\boldsymbol{\kappa}\cdot\mathbf{x}} d\mathbf{x} = -e^{-i\boldsymbol{\kappa}\cdot\mathbf{r}_e}\, \frac{4\pi}{i\kappa}\, \boldsymbol{\mu}_n \times \hat{\boldsymbol{\kappa}},\end{aligned}$$

where $\hat{\boldsymbol{\kappa}}$ is a unit vector along $\boldsymbol{\kappa}$ (the integration is performed straightforwardly in spherical coordinates). Applying Green's theorem and assuming V to be a sphere of radius r,

$$\int \nabla \times \left(e^{-i\boldsymbol{\kappa}\cdot\mathbf{x}} \mathbf{A}_n(\mathbf{x})\right) d\mathbf{x} \;\propto\; (\kappa r)^{-1} \to 0 \quad \text{for} \quad r \to \infty,$$

from which we deduce

$$\begin{aligned}\int \left(\nabla \times \mathbf{A}_n(\mathbf{x})\right) e^{-i\boldsymbol{\kappa}\cdot\mathbf{x}} d\mathbf{x} &= -\int \left(\nabla\, e^{-i\boldsymbol{\kappa}\cdot\mathbf{x}}\right) \times \mathbf{A}_n(\mathbf{x}) d\mathbf{x} \\ &= i\boldsymbol{\kappa} \times \int e^{-i\boldsymbol{\kappa}\cdot\mathbf{x}} \mathbf{A}_n(\mathbf{x}) d\mathbf{x} = 4\pi \hat{\boldsymbol{\kappa}} \times \boldsymbol{\mu}_n \times \hat{\boldsymbol{\kappa}}\end{aligned}$$

(we note that $\nabla \times \mathbf{A}_n(\mathbf{r}) = \nabla_{(\mathbf{x})} \times \mathbf{A}_n(\mathbf{x})$). From these results, we obtain

$$\begin{aligned}\mathcal{H}_{\text{int}}(\boldsymbol{\kappa}) &= \int \mathcal{H}_{\text{int}}(\mathbf{r}_e, \mathbf{r}_n) e^{-i\boldsymbol{\kappa}\cdot\mathbf{r}_n} d\mathbf{r}_n \\ &= 2\mu_B\, e^{-i\boldsymbol{\kappa}\cdot\mathbf{r}_e}\, 4\pi \left(\frac{i}{\hbar\kappa} \boldsymbol{\mu}_n \times \hat{\boldsymbol{\kappa}} \cdot \mathbf{p}' + \mathbf{s} \cdot (\hat{\boldsymbol{\kappa}} \times \boldsymbol{\mu}_n \times \hat{\boldsymbol{\kappa}})\right),\end{aligned}$$

or

$$\mathcal{H}_{\text{int}}(\boldsymbol{\kappa}) = 8\pi\mu_B\, \boldsymbol{\mu}_n \cdot \left(\frac{i}{\hbar\kappa} \hat{\boldsymbol{\kappa}} \times \mathbf{p}' + \hat{\boldsymbol{\kappa}} \times \mathbf{s} \times \hat{\boldsymbol{\kappa}}\right) e^{-i\boldsymbol{\kappa}\cdot\mathbf{r}_e}. \tag{4.1.6}$$

$\hat{\boldsymbol{\kappa}} \times \mathbf{p}'$ commutes with $\boldsymbol{\kappa} \cdot \mathbf{r}_e$ and therefore also with $\exp(-i\boldsymbol{\kappa} \cdot \mathbf{r}_e)$, and we have made use of the identity $\hat{\boldsymbol{\kappa}} \times \mathbf{a} \times \hat{\boldsymbol{\kappa}} = \mathbf{a} - (\hat{\boldsymbol{\kappa}} \cdot \mathbf{a})\hat{\boldsymbol{\kappa}}$.

For discussing the rare earths, we may restrict ourselves to the case of electrons localized around the lattice sites in a crystal. Further, we define $\mathbf{r}_e = \widetilde{\mathbf{R}}_j + \mathbf{r}$, with $\mathbf{r}$ now being the relative position of the electron belonging to the jth atom at the position $\widetilde{\mathbf{R}}_j$. Equation (4.1.6) may then be written

$$\mathcal{H}_{\rm int}(\boldsymbol{\kappa}) = 8\pi\mu_B\,\boldsymbol{\mu}_n \cdot (\mathbf{Q}_p + \mathbf{Q}_s)\, e^{-i\boldsymbol{\kappa}\cdot\widetilde{\mathbf{R}}_j}, \tag{4.1.7a}$$

introducing

$$\mathbf{Q}_p = \frac{i}{\hbar\kappa}\,\hat{\boldsymbol{\kappa}} \times \mathbf{p}'\, e^{-i\boldsymbol{\kappa}\cdot\mathbf{r}} \qquad ; \qquad \mathbf{Q}_s = \hat{\boldsymbol{\kappa}} \times \mathbf{s} \times \hat{\boldsymbol{\kappa}}\, e^{-i\boldsymbol{\kappa}\cdot\mathbf{r}}. \tag{4.1.7b}$$

In order to calculate the matrix element $< i\,|\,\mathbf{Q}_{p,s}\,|\,f >$, the factor $\exp(-i\boldsymbol{\kappa}\cdot\mathbf{r})$ is expanded in spherical Bessel functions $j_n(\rho)$, and with $\rho = \kappa r$ and $\cos\theta = \boldsymbol{\kappa}\cdot\mathbf{r}/\rho$,

$$\begin{aligned} e^{-i\boldsymbol{\kappa}\cdot\mathbf{r}} &= \sum_{n=0}^{\infty}(2n+1)\,(-i)^n\, j_n(\rho) P_n(\cos\theta) \\ &\simeq j_0(\rho) - 3i\, j_1(\rho)\cos\theta = j_0(\rho) - i\boldsymbol{\kappa}\cdot\mathbf{r}\{j_0(\rho) + j_2(\rho)\}, \end{aligned} \tag{4.1.8}$$

using $j_n(\rho) = \rho\{j_{n-1}(\rho) + j_{n+1}(\rho)\}/(2n+1)$. The truncation of the series is valid for small values of ρ, where

$$j_n(\rho) = (\rho^n/(2n+1)!!)\{1 - \rho^2/(4n+6) + \cdots\}.$$

We note that, although $\boldsymbol{\kappa}\times\mathbf{p}'$ commutes with $\exp(-i\boldsymbol{\kappa}\cdot\mathbf{r})$, it does not commute with the individual terms in (4.1.8). Introducing this expansion in the expression for $\mathbf{Q}_p$, we find

$$\mathbf{Q}_p = \hat{\boldsymbol{\kappa}} \times \Big(\frac{i}{\hbar\kappa} j_0(\rho)\mathbf{p}' + \frac{1}{\hbar}\{j_0(\rho) + j_2(\rho)\}(\hat{\boldsymbol{\kappa}}\cdot\mathbf{r})\mathbf{p}' + \cdots\Big),$$

which can be rearranged to read

$$\mathbf{Q}_p = \tfrac{1}{2}\{j_0(\rho) + j_2(\rho)\}\,\hat{\boldsymbol{\kappa}} \times \mathbf{l}' \times \hat{\boldsymbol{\kappa}} + \mathbf{Q}'_p. \tag{4.1.9a}$$

We have defined

$$\mathbf{Q}'_p = \hat{\boldsymbol{\kappa}} \times \Big(\frac{i}{\hbar\kappa} j_0(\rho)\mathbf{p}' + \frac{1}{2\hbar}\{j_0(\rho) + j_2(\rho)\}\{(\hat{\boldsymbol{\kappa}}\cdot\mathbf{r})\mathbf{p}' + (\hat{\boldsymbol{\kappa}}\cdot\mathbf{p}')\mathbf{r}\} + \cdots\Big), \tag{4.1.9b}$$

where the orbital momentum $\hbar\mathbf{l} = \mathbf{r}\times\mathbf{p}$ and $\hbar\mathbf{l}' = \hbar\mathbf{l} + \frac{e}{c}\,\mathbf{r}\times\mathbf{A}_e$, and used

$$\hat{\boldsymbol{\kappa}} \times \hbar\mathbf{l}' \times \hat{\boldsymbol{\kappa}} = -\hat{\boldsymbol{\kappa}} \times \{\hat{\boldsymbol{\kappa}} \times (\mathbf{r}\times\mathbf{p}')\} = \hat{\boldsymbol{\kappa}} \times \{(\hat{\boldsymbol{\kappa}}\cdot\mathbf{r})\mathbf{p}' - (\hat{\boldsymbol{\kappa}}\cdot\mathbf{p}')\mathbf{r}\},$$

where $[\,\mathbf{l}'\,,\, j_n(\rho)\,] = \mathbf{0}$ and $[\,\hat{\boldsymbol{\kappa}}\times\mathbf{r}\,,\,\hat{\boldsymbol{\kappa}}\cdot\mathbf{p}'\,] = \mathbf{0}$.

If $\mathcal{H}$ is defined to be the Hamiltonian for the electron, then

$$\mathbf{p}' = \mathbf{p} + \frac{e}{c}\mathbf{A}_e = m\, d\mathbf{r}/dt = m\frac{i}{\hbar}[\mathcal{H}\,,\,\mathbf{r}\,],$$

and $\mathbf{Q}'_p$ may be written

$$\mathbf{Q}'_p = \frac{m}{\hbar^2\kappa}\,\hat{\boldsymbol{\kappa}} \times \Big(-j_0(\rho)\,[\,\mathcal{H}\,,\,\mathbf{r}\,] + \frac{i\kappa}{2}\{j_0(\rho) + j_2(\rho)\}\,[\,\mathcal{H}\,,\,(\hat{\boldsymbol{\kappa}}\cdot\mathbf{r})\mathbf{r}\,] + \cdots\Big). \tag{4.1.10}$$

Considering an arbitrary operator $\hat{A}$, we have

$$<i\,|\,[\,\mathcal{H}\,,\,\hat{A}\,]\,|\,f> = <i\,|\,\mathcal{H}\hat{A} - \hat{A}\mathcal{H}\,|\,f> = (E_i - E_f)\,<i\,|\,\hat{A}\,|\,f>,$$

which implies that $\mathbf{Q}'_p$ does not contribute to the cross-section (4.1.4) in the limit $\boldsymbol{\kappa} \to \mathbf{0}$. In this limit, $j_n(0) = \delta_{n0}$ and, utilizing the energy δ-function in (4.1.4), the contribution to the cross section due to $\mathbf{Q}'_p$ is seen to be proportional to

$$\left|\frac{m}{\hbar^2\kappa}\,\hbar\omega\,\hat{\boldsymbol{\kappa}} \times <i\,|\,\mathbf{r}\,|\,f>\right|^2 \to 0 \quad \text{for} \quad \kappa \to 0,$$

since $|\hbar\omega| \le (\hbar\kappa)^2/2M$. Introducing the vector operator $\mathbf{K}(\boldsymbol{\kappa})$, defined so that

$$<i\,|\,\hat{\boldsymbol{\kappa}} \times \mathbf{K} \times \hat{\boldsymbol{\kappa}}\,|\,f> = <i\,|\,\mathbf{Q}_p + \mathbf{Q}_s\,|\,f>, \tag{4.1.11}$$

we find, neglecting $\mathbf{Q}'_p$ in the limit $\kappa \to 0$,

$$2\mu_B\mathbf{K}(\mathbf{0}) = \mu_B\,\Big(\mathbf{l} + \frac{e}{\hbar c}\mathbf{r} \times \mathbf{A}_e + 2\mathbf{s}\Big) \equiv -\boldsymbol{\mu}_e, \tag{4.1.12a}$$

or

$$\mathcal{H}_{\text{int}}(\mathbf{0}) = -4\pi\,\boldsymbol{\mu}_n \cdot (\hat{\boldsymbol{\kappa}} \times \boldsymbol{\mu}_e \times \hat{\boldsymbol{\kappa}}), \tag{4.1.12b}$$

implying that the magnetic cross-section (4.1.4), in the limit where the scattering vector approaches zero, is determined by the magnetic dipole moment $\boldsymbol{\mu}_e$ of the electron. In the treatment given above, we have included the diamagnetic contribution to $\boldsymbol{\mu}_e$, induced by external fields $\propto \mathbf{A}_e$. This term may however normally be neglected, as we shall do from now on.

At non-zero κ, we cannot employ directly the above procedure for obtaining an upper bound on the $\mathbf{Q}'_p$ matrix-element, because $j_n(\rho)$ does not commute with $\mathcal{H}$. However, if we restrict ourselves to scattering processes in which the l quantum number is conserved, the matrix element of the first term in (4.1.10) vanishes identically, because $j_0(\rho)$ and $\mathcal{H}$

are both diagonal with respect to l, whereas $\mathbf{r}$ has no diagonal elements (cf. the electric-dipole selection rule $\Delta l = \pm 1$). In the second term of (4.1.10) we can, to leading order, replace $\mathcal{H}$ by the kinetic-energy operator and, if we also make the assumption $\Delta l = 0$, this term transforms like a second-rank tensor and so is quadrupolar. Symmetrizing $\mathbf{Q}'_p$ with respect to the expansion in spherical Bessel functions, and taking $(\hat{\boldsymbol{\kappa}}\cdot\hat{\mathbf{r}})\hat{\mathbf{r}}$ outside the commutator, which is allowed because $\Delta l = 0$, we can write the second term in (4.1.10) as

$$(\hat{\boldsymbol{\kappa}} \times \hat{\mathbf{r}})(\hat{\boldsymbol{\kappa}} \cdot \hat{\mathbf{r}})\, Q_r,$$

with $\hat{\mathbf{r}} = \mathbf{r}/r$ and

$$Q_r = Q_r^\dagger = -\frac{i}{8}\Big(\{j_0(\rho) + j_2(\rho)\}[\,\nabla^2\,,\, r^2\,] + [\,\nabla^2\,,\, r^2\,]\{j_0(\rho) + j_2(\rho)\}\Big).$$

Thus the second term is a product of an angular and a radial operator, which are both Hermitian. Our next assumption is that the radial part of the wavefunction, as specified by the principal quantum number $\tilde{n}$, and by l, is the same in the initial and the final state, i.e. that both $\tilde{n}$ and l are unchanged. In this case, $<i\,|\,Q_r\,|\,f> = <\tilde{n}l\,|\,Q_r\,|\,\tilde{n}l>$ vanishes identically, because Q_r is an imaginary Hermitian operator; $Q_r = Q_r^\dagger = -Q_r^*$. If the radial part of the wavefunction is changed in the scattering process, or if $\mathcal{H}$ is not diagonal in l, then the quadrupole moment leads to an imaginary contribution to $\mathbf{K}(\boldsymbol{\kappa})$, and gives a contribution to the cross-section proportional to κ^2. In most cases of interest, however, this term is very small.

The assumption that $|\,i>$ and $|\,f>$ are linear combinations of the states $|\,(\tilde{n}ls)m_l m_s>$, where $(\tilde{n}ls)$ is constant, implies that the two lowest-order terms in the expansion of Q'_p in (4.1.9*b*) or (4.1.10) can be neglected. Furthermore, the radial and angular dependences are then factorized, both in the expansion of the operators and in the wavefunctions, so that the radial part of the matrix elements may be calculated separately. Hence the orbital contribution $\mathbf{K}_p$ to $\mathbf{K}$ is approximately

$$\mathbf{K}_p(\boldsymbol{\kappa}) = \tfrac{1}{2}\,\{\langle j_0(\kappa)\rangle + \langle j_2(\kappa)\rangle\}\,\mathbf{l}, \qquad (4.1.13a)$$

with

$$\langle j_n(\kappa)\rangle = \int_0^\infty r^2 R^2(r) j_n(\kappa r)\,dr \qquad ; \qquad \int_0^\infty r^2 R^2(r)\,dr = 1, \quad (4.1.13b)$$

where $R(r)$ is the normalized radial wavefunction. The assumption that the final and initial states have the same parity implies that only the terms in the expansion (4.1.8) for which n is odd may contribute to $\mathbf{K}_p$. By the same argument, the spin part $\mathbf{K}_s$ of $\mathbf{K}$ only involves the terms

in (4.1.8) with n even. Neglecting the $(n = 2)$-term in $\mathbf{K}_s$, proportional to $\mathbf{s}$ times an orbital quadrupole moment, we have $\mathbf{K}_s(\boldsymbol{\kappa}) \simeq \langle j_0(\kappa)\rangle\, \mathbf{s}$, or

$$\mathbf{K}(\boldsymbol{\kappa}) = \mathbf{K}(\kappa) = \tfrac{1}{2}\langle j_0(\kappa)\rangle(\mathbf{l} + 2\mathbf{s}) + \tfrac{1}{2}\langle j_2(\kappa)\rangle\, \mathbf{l}. \tag{4.1.14}$$

This result for $\mathbf{K}(\boldsymbol{\kappa})$ is the basis of the dipole approximation for the scattering cross-section. Within this approximation, it is straightforwardly generalized to the case of more than one electron per atom, as the contributions are additive, in the sense that $\mathbf{l}$ and $\mathbf{s}$ are replaced by $\mathbf{L} = \sum \mathbf{l}$ and $\mathbf{S} = \sum \mathbf{s}$, and $R^2(r)$ by the normalized distribution for all unpaired electrons belonging to the atom at $\widetilde{\mathbf{R}}_j$.

The orbital contribution is important in the case of rare earth or actinide ions. In transition-metal ions, the orbital momentum is frequently quenched, and $\mathbf{K}_p$ may then be neglected to leading order. In the rare earths, the spin–orbit coupling is strong and only matrix elements within the ground-state multiplet of $\mathbf{J}^2 = (\mathbf{L}+\mathbf{S})^2$ contribute. In this case, as discussed in Section 1.2, $\mathbf{L} + 2\mathbf{S} = g\mathbf{J}$ and $\mathbf{L} = (2 - g)\mathbf{J}$, where g is the Landé factor, and we have

$$\mathbf{K}(\kappa) = \tfrac{1}{2}\langle j_0(\kappa)\rangle(\mathbf{L} + 2\mathbf{S}) + \tfrac{1}{2}\langle j_2(\kappa)\rangle\mathbf{L} = \tfrac{1}{2}gF(\kappa)\mathbf{J}, \tag{4.1.15a}$$

where $F(\kappa)$ is the *form factor*

$$F(\kappa) = \langle j_0(\kappa)\rangle + \frac{1}{g}(2 - g)\langle j_2(\kappa)\rangle, \tag{4.1.15b}$$

defined so that $F(0) = 1$. When the spin–orbit interaction is introduced, the $(n = 2)$-term in the expansion of $\mathbf{K}_s$ gives a contribution to the dipolar part of $\mathbf{K}(\kappa)$ proportional to $\langle j_2(\kappa)\rangle$, but this is an order of magnitude smaller than the orbital term in (4.1.14). A more systematic approach, making extensive use of Racah tensor-algebra, is required to calculate this term and to include the contributions of the higher-rank multipoles produced by the expansion of $\exp(-i\boldsymbol{\kappa}\cdot\mathbf{r})$. This analysis may be found in Marshall and Lovesey (1971), Stassis and Deckman (1975, 1976), and references therein. Within the present approximation, only tensors of *odd* rank give a contribution to $\mathbf{K}$, proportional to $\kappa^{\tau-1}$, where τ is the rank of the tensors (terms with $\tau = 3$ appear already in order κ^2). In contrast to the dipole contributions, the higher-rank tensor couplings give rise to an angular dependence of $\mathbf{K} = \mathbf{K}(\boldsymbol{\kappa})$. The smaller the scattering wavelength $\lambda = 2\pi/\kappa$, the more the neutron senses the details of the spin and current distributions within the atom, but as long as λ is larger than approximately the mean radius $\langle r\rangle$ of the unpaired electrons, only the dipolar scattering is important. For rare earth ions, $\langle r\rangle \approx 0.6\,\text{Å}$, indicating that (4.1.15) is a valid approximation as long as κ is smaller than about $6\,\text{Å}^{-1}$.

Experimental studies of the form factor and the associated moment densities have been reviewed by Sinha (1978). For an accurate interpretation of the data, it is generally necessary to proceed beyond the dipole approximation. In the heavy rare earths, the deduced $4f$ densities are in good agreement with atomic calculations, provided that relativistic effects are included, but the conduction-electron distributions are much less certain. In the light elements, crystal-field effects become important, as observed for example in Pr and Nd by Lebech *et al.* (1979). Of especial interest is Sm, where the opposition of spin and orbital moments leads to a form factor which has its maximum at a non-zero κ, and the conduction-electron polarization seems to be very strong (Koehler and Moon 1972).

Labelling quantities pertaining to the jth atom with the index j, and summing over all the atoms in the sample, we find that the total $\mathcal{H}_{\rm int}(\boldsymbol{\kappa})$ (4.1.7), in the dipole approximation, is given by

$$\mathcal{H}_{\rm int}(\boldsymbol{\kappa}) = 8\pi\mu_B \sum_j \{\tfrac{1}{2} g F(\kappa)\}_j \, e^{-i\boldsymbol{\kappa}\cdot\widetilde{\mathbf{R}}_j} \, \boldsymbol{\mu}_n \cdot (\hat{\boldsymbol{\kappa}} \times \mathbf{J}_j \times \hat{\boldsymbol{\kappa}}).$$

The squared matrix element in (4.1.4) may furthermore be written

$$< \mathbf{s}_n; i \,|\, \mathcal{H}_{\rm int}(\boldsymbol{\kappa}) \,|\, \mathbf{s}'_n; f >< \mathbf{s}'_n; f \,|\, \mathcal{H}_{\rm int}(-\boldsymbol{\kappa}) \,|\, \mathbf{s}_n; i > .$$

We shall only consider the cross-section for unpolarized neutrons, so that we sum over all the spin states $|\,\mathbf{s}'_n>$ of the scattered neutrons, and average over the spin-states $|\,\mathbf{s}_n>$, with the distribution P_s, of the incoming neutrons. With an equal distribution of up and down spins, $P_s = \frac{1}{2}$, and introducing $\mathbf{Q}_j = \hat{\boldsymbol{\kappa}} \times \mathbf{J}_j \times \hat{\boldsymbol{\kappa}}$, we find that the cross-section is proportional to

$$\begin{aligned}\sum_{\mathbf{s}_n \mathbf{s}'_n} P_s &< \mathbf{s}_n \,|\, \boldsymbol{\mu}_n \cdot \mathbf{Q}_j \,|\, \mathbf{s}'_n >< \mathbf{s}'_n \,|\, \boldsymbol{\mu}_n \cdot \mathbf{Q}_{j'} \,|\, \mathbf{s}_n > \\ &= \sum_{\mathbf{s}} P_s < \mathbf{s}_n \,|\, (\boldsymbol{\mu}_n \cdot \mathbf{Q}_j)\,(\boldsymbol{\mu}_n \cdot \mathbf{Q}_{j'}) \,|\, \mathbf{s}_n > = \left(\tfrac{1}{2} g_n \mu_N\right)^2 \, \mathbf{Q}_j \cdot \mathbf{Q}_{j'},\end{aligned}$$

as may readily be shown by using the Pauli-matrix representation, in which $\mathrm{Tr}\{\sigma_\alpha \sigma_\beta\} = 2\,\delta_{\alpha\beta}$. We have further that $\mathbf{Q}_j \cdot \mathbf{Q}_{j'}$ may be written

$$\begin{aligned}(\hat{\boldsymbol{\kappa}} \times \mathbf{J}_j \times \hat{\boldsymbol{\kappa}}) \cdot (\hat{\boldsymbol{\kappa}} \times \mathbf{J}_{j'} \times \hat{\boldsymbol{\kappa}}) &= (\mathbf{J}_j - \hat{\boldsymbol{\kappa}}(\mathbf{J}_j \cdot \hat{\boldsymbol{\kappa}})) \cdot (\mathbf{J}_{j'} - \hat{\boldsymbol{\kappa}}(\mathbf{J}_{j'} \cdot \hat{\boldsymbol{\kappa}})) \\ &= \mathbf{J}_j \cdot \mathbf{J}_{j'} - (\mathbf{J}_j \cdot \hat{\boldsymbol{\kappa}})\,(\mathbf{J}_{j'} \cdot \hat{\boldsymbol{\kappa}}) = \sum_{\alpha\beta} \left(\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta\right) \, J_{j\alpha} \, J_{j'\beta},\end{aligned}$$

in terms of the Cartesian components. Defining $(\mathbf{J}_\perp)_j$ to be the projection of $\mathbf{J}_j$ on the plane perpendicular to $\boldsymbol{\kappa}$, we have

$$\sum_{\alpha\beta} \left(\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta\right) \, J_{j\alpha} \, J_{j'\beta} = (\mathbf{J}_\perp)_j \cdot (\mathbf{J}_\perp)_{j'}.$$

The various factors in these expressions may be combined to give

$$\frac{k'}{k}\left(\frac{M}{2\pi\hbar^2}\,8\pi\mu_B\,\tfrac{1}{2}g_n\mu_N\right)^2=\frac{k'}{k}\left(\frac{\hbar\gamma e^2}{mc^2}\right)^2\qquad;\quad\gamma=\frac{1}{2\hbar}\,g_n.$$

γ is the gyromagnetic ratio of the neutron, and $e^2/mc^2 = 2.82$ fm is the classical electron radius. The differential cross-section, in the dipole approximation, for the scattering of unpolarized neutrons is then finally

$$\frac{d^2\sigma}{dEd\Omega}=\frac{k'}{k}\left(\frac{\hbar\gamma e^2}{mc^2}\right)^2\sum_{\alpha\beta}(\delta_{\alpha\beta}-\hat{\kappa}_\alpha\hat{\kappa}_\beta)\sum_{jj'}\{\tfrac{1}{2}gF(\kappa)\}_j\{\tfrac{1}{2}gF(\kappa)\}_{j'}$$
$$\times\sum_{if}P_i<i\,|\,J_{j\alpha}\,e^{-i\boldsymbol{\kappa}\cdot\widetilde{\mathbf{R}}_j}\,|\,f><f\,|\,J_{j'\beta}\,e^{i\boldsymbol{\kappa}\cdot\widetilde{\mathbf{R}}_{j'}}\,|\,i>\delta(\hbar\omega+E_i-E_f),\tag{4.1.16}$$

where the total magnetic cross-section is $4\pi(\hbar\gamma e^2/mc^2)^2 = 3.65$ barns.