Appendix A

The cross section

The double differential cross section of a typical neutron scattering process can be obtained from the single differential cross section, which is associated to the elastic scattering events, i.e., those in which the neutron does not transfer energy to the sample. If the flux of incident neutrons is \( \Phi_0 \) (neutrons crossing the unit area per unit time) and the sample has \( N \) atoms in the beam, then the number of scattered neutrons into the solid angle \( d\Omega \) is given by

\[
W_{k\rightarrow k'} = N\Phi_0 \frac{d\sigma}{d\Omega}, \quad (A.1)
\]

where \( d\sigma/d\Omega \) is the differential cross section which is a constant for a given process. Hence, the differential cross section becomes

\[
\frac{d\sigma}{d\Omega} = \frac{1}{N\Phi_0 d\Omega} W_{k\rightarrow k'}, \quad (A.2)
\]

If the wave functions corresponding to the neutron beam before and after the scattering event are taken to be plane waves normalized to 1 in the volume \( V \)

\[
\psi_k = \frac{1}{\sqrt{V}} e^{ik \cdot r}, \quad \psi_{k'} = \frac{1}{\sqrt{V}} e^{i k' \cdot r}, \quad (A.3)
\]

then the flux of incident neutrons becomes

\[
\Phi_0 = \frac{1}{2mi} \left[ \psi_k^* \nabla \psi_k - \psi_k \nabla \psi_k^* \right] = \frac{k}{mV}, \quad (A.4)
\]

Due to the unit normalization of the flux, the number of scattered particles per unit time \( W_{k\rightarrow k'} \) can be identified with the transition probability per unit time. Consider a
process in which neutrons change from state $|\mathbf{k}, \sigma\rangle$ to $|\mathbf{k'}, \sigma'\rangle$, ($\sigma$ and $\sigma'$ being the third component of the spin) and the system changes from state $|\lambda\rangle$ to $|\lambda'\rangle$, then Fermi’s Golden Rule allows to write

$$W_{k,\sigma,\lambda \rightarrow k',\sigma',\lambda'} = 2\pi \langle \mathbf{k'}, \sigma', \lambda' | \mathcal{V} | \mathbf{k}, \sigma, \lambda \rangle^2 \rho_{k',\sigma'}(E')$$  \hspace{1cm} (A.5)$$

where $\mathcal{V}$ is the interaction potential between the neutron and the nuclei in the sample, and $\rho_{k',\sigma'}(E')$ is the density of final states per unit energy interval where the neutron can go after the scattering (consistent with the final momentum $\mathbf{k'}$ and spin $\sigma'$). As neutrons are described by plane waves, the last quantity reads

$$\rho_{k',\sigma'}(E')dE' = \frac{V}{(2\pi)^3} \frac{d\mathbf{k'}}{dE'}dE' = \frac{V}{(2\pi)^3} mk'd\Omega dE'$$  \hspace{1cm} (A.6)$$

where use has been made of the relation $dE' = k'dk'/m$. Substituting eqs. (A.4) and (A.6) in (A.2), the differential cross section results in

$$\frac{d\sigma}{d\Omega} = \frac{V^2 k'}{N k} \left( \frac{m}{2\pi} \right)^2 \langle \mathbf{k'}, \sigma', \lambda' | \mathcal{V} | \mathbf{k}, \sigma, \lambda \rangle^2$$  \hspace{1cm} (A.7)$$

The double differential cross section can be readily obtained from the last result. First, the energy conservation constrain

$$\omega = E\lambda - E\lambda'$$  \hspace{1cm} (A.8)$$

is introduced in the form of a Dirac’s delta

$$\frac{d\sigma}{d\Omega d\omega} = \frac{V^2 k'}{N k} \left( \frac{m}{2\pi} \right)^2 \langle \mathbf{k'}, \sigma', \lambda' | \mathcal{V} | \mathbf{k}, \sigma, \lambda \rangle^2 \delta (\omega - E\lambda' + E\lambda) .$$  \hspace{1cm} (A.9)$$

Second, expression (A.9) must be summed over all final states of the sample $\lambda'$ and neutron polarizations $\sigma'$, and averaged over all the initial states of the sample (which occur with probability $p_{\lambda}$) and initial polarizations of the neutron (which occur with probability $p_{\sigma}$). With this

$$\frac{d\sigma}{d\Omega d\omega} = \frac{V^2 k'}{N k} \left( \frac{m}{2\pi} \right)^2 \sum_{\lambda,\sigma} p_{\lambda} p_{\sigma} \sum_{\lambda',\sigma'} \langle \mathbf{k'}, \sigma', \lambda' | \mathcal{V} | \mathbf{k}, \sigma, \lambda \rangle^2 \delta (\omega - E\lambda' + E\lambda) .$$  \hspace{1cm} (A.10)$$

In the particular case of scattering on condensed matter systems, the momenta of interest is of the order of several inverse Angstroms. Its inverse (the wavelength of the neutrons) is therefore three or four orders of magnitude larger than the characteristic range of the nuclear forces. In this case, the interaction potential between the nucleus
The cross section

\[ \mathcal{V}(R) = \frac{2\pi}{m} \sum_j b_j \delta(\mathbf{R} - \mathbf{r}_j) \]  

(A.11)

where \( b_j \) is the scattering length of the neutron–nucleus interaction, which in general depend on the spin state of the neutron–nucleus system, and \( \mathbf{R} \) and \( \mathbf{r}_j \) are the instantaneous position of the neutron and the atoms in the sample.

The form of the Fermi pseudopotential allows for the evaluation of the matrix element between the momentum states of the neutron

\[ \langle k' \mid V \mid k \rangle = \frac{2\pi}{m} \sum_j b_j \frac{1}{V} \int d\mathbf{r}_j e^{-\mathbf{k}' \cdot \mathbf{R}} \delta(\mathbf{R} - \mathbf{r}_j) e^{i\mathbf{k} \cdot \mathbf{R}} \]  

(A.12)

leading to

\[ \frac{d\sigma}{d\Omega d\omega} = \frac{1}{N} \frac{k'}{k} \sum_{\lambda, \sigma} \sum_{\lambda', \sigma'} p_{\lambda, \sigma} \left| \sum_j \left\langle \sigma, \lambda' \mid b_j e^{i\mathbf{q} \cdot \mathbf{r}_j} e^{iHt} e^{-i\mathbf{q} \cdot \mathbf{r}_j} e^{-iHt} \mid \sigma, \lambda \right\rangle \right|^2 \]  

(A.14)

When the beam used in the scattering is unpolarized, equal population of spin up and spin down neutrons fall into the sample and the \( \sigma, \sigma' \) dependence of (A.14) disappears. Besides, the energy conserving delta can be written as an integral over exponentiated energies

\[ \delta(\omega - E_\lambda + E_{\lambda'}) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{-i(\omega - E_\lambda + E_{\lambda'})t} \]  

(A.15)

and the sum over \( \lambda' \) eliminated, leaving

\[ \frac{d\sigma}{d\Omega d\omega} = \frac{1}{2\pi N} \frac{k'}{k} \sum_{\lambda, \sigma} p_{\lambda, \sigma} \int_{-\infty}^{\infty} dt \sum_{j, j'} \left\langle \lambda \mid b_j^* b_{j'} e^{i\mathbf{q} \cdot \mathbf{r}_j} e^{iHt} e^{-i\mathbf{q} \cdot \mathbf{r}_{j'}} e^{-iHt} \mid \lambda \right\rangle e^{-i\omega t} \]  

(A.16)

The nuclear spins are usually uncorrelated, so the scattering lengths \( b_j \) may be substituted by an average \( b \) over random nuclear spin orientations. However, labels \( j \) and \( j' \) may correspond to the same or to different particles, and the average of \( b_j^* b_{j'} \) becomes \( \overline{b^2} \) if \( j \neq j' \) or \( |\overline{b}|^2 \) of \( j = j' \). This means than one can write

\[ \overline{b_j^* b_{j'}} = |\overline{b}|^2 + \delta_{j, j'} (|\overline{b}|^2 - |\overline{b}|^2) \]  

(A.17)

Upon substitution of (A.17) in eq. (A.16), the scattering cross-section becomes the sum of two terms

\[ \frac{d^2\sigma}{d\Omega d\omega} = \frac{1}{N} \frac{k'}{k} |\overline{b}|^2 \sum_{j, j'} S_{j, j'} + \frac{1}{N} \frac{k'}{k} \left( |\overline{b}|^2 - |\overline{b}|^2 \right) \sum_j S_{j, j} \]  

(A.18)
where
\[ S_{j,j'}(q, \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left\langle e^{-i\mathbf{q}_j(0)} e^{i\mathbf{q}_j'(t)} \right\rangle e^{-i\omega t} dt \] (A.19)
valid for both \( j \neq j' \) and \( j = j' \). Notice that here the brackets \( \langle \cdots \rangle \) denote the average over the states \( |\lambda\rangle \) with probabilities \( p_\lambda \). In the particular case of \( T = 0 \), the one considered here, this average reduces to a groundstate expectation value.

Equations (A.18) and (A.19) are usually expressed in terms of the coherent and incoherent total cross sections \( \sigma_c = 4\pi |\bar{b}|^2 \) \& \( \sigma_i = 4\pi \left( |\bar{b}|^2 - |\bar{b}'|^2 \right) \), and the incoherent and coherent scattering functions as follows
\[ \frac{d^2\sigma}{d\Omega d\omega} = \frac{\sigma_c}{4\pi} k' \frac{k}{k} S_{\text{coh}}(q, \omega) + \frac{\sigma_i}{4\pi} k' \frac{k}{k} S_{\text{inc}}(q, \omega) , \] (A.20)
where
\[ S_{\text{inc}}(q, \omega) = \frac{1}{2\pi N} \sum_j \int_{-\infty}^{\infty} \left\langle e^{-i\mathbf{q}_j(0)} e^{i\mathbf{q}_j(0)} \right\rangle e^{-i\omega t} \] (A.21)
\[ S_{\text{coh}}(q, \omega) = \frac{1}{2\pi N} \sum_{j,j'} \int_{-\infty}^{\infty} \left\langle e^{-i\mathbf{q}_j(0)} e^{i\mathbf{q}_j'(0)} \right\rangle e^{-i\omega t} \]
\[ = \frac{1}{N} \sum_{\{\lambda\}} |\langle 0 | \rho^\dagger_q | \lambda \rangle|^2 \delta (E_{\lambda'} - E_0 - \omega) , \] (A.22)
\( \rho^\dagger_q \) being the operator \( \sum_{j=1}^{N} e^{i\mathbf{q}_j} \). Unfortunately, the definition of coherent and incoherent scattering functions is not unique and may lead to confusion. As defined in eq. (A.22), \( S_{\text{coh}}(q, \omega) \) coincides with the definition of the dynamic structure function \( S(q, \omega) \), which is the main quantity studied in this work.

Notice that in pure \(^4\text{He}\) the incoherent cross section is zero [Lov84], and thus the differential cross section becomes directly proportional to the dynamic structure function
\[ \frac{d^2\sigma}{d\Omega dE} = \frac{\sigma_c}{4\pi} k' \frac{k}{k} S(q, \omega) . \] (A.23)