Appendix A1

A1.1 COHERENT SCATTERING AND THE STRUCTURE FACTOR $S(Q)$

Equation (2.36) gives the scattering cross section for an assembly of atoms. To obtain the cross section per atom, which is the way data are normally presented, it is necessary to divide (2.36) by the number of atoms present in the scatterer, N. Doing this and concentrating on the first (coherent scattering) term we can write:

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{coh}} = \frac{a_{\mathrm{coh}}^2}{N}\left\langle\left|\int \mathrm{d}^3 r\, \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}} \sum_i \delta^{(3)}(\boldsymbol{r}-\boldsymbol{R}_i)\right|^2\right\rangle \tag{A1.1}$$

where the brackets refer to an average over the distribution of the positions R_i of the scattering atoms. This is the form we would obtain if we refrained from evaluating the integral as we did in going from (2.28) to (2.29). We rewrite (A1.1) as

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{coh}} = \frac{a_{\mathrm{coh}}^2}{N}\left\langle\int \mathrm{d}^3 r \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}} \sum_i \delta^{(3)}(\boldsymbol{r}-\boldsymbol{R}_i)\int \mathrm{d}^3 r' \mathrm{e}^{-\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}'} \sum_j \delta^{(3)}(\boldsymbol{r}'-\boldsymbol{R}_j)\right\rangle \tag{A1.2}$$

which can be transformed into

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{coh}} = \frac{a_{\mathrm{coh}}^2}{N}\int \mathrm{d}^3 r_0\, \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}_0}\left\langle\sum_{i,j} \delta^{(3)}(\boldsymbol{r}_0+\boldsymbol{R}_j-\boldsymbol{R}_i)\right\rangle \tag{A1.3}$$

by substituting $\boldsymbol{r}-\boldsymbol{r}'=\boldsymbol{r}_0$. By separating the terms with $i=j$ from the double sum we obtain

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{coh}} = a_{\mathrm{coh}}^2\int \mathrm{d}^3 r_0\, \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}_0}\left(\delta^{(3)}(\boldsymbol{r}_0)+\frac{1}{N}\sum_{i\neq j}\left\langle\delta^{(3)}(\boldsymbol{r}_0+\boldsymbol{R}_j-\boldsymbol{R}_i)\right\rangle\right). \tag{A1.4}$$

We can understand the significance of the second term in (A1.4) by first considering that we keep j fixed and noting that the δ-function gives a contribution every time $r_0 = R_i - R_j$, that is every time there is a particle (i) displaced by r_0 from the jth particle. Since the jth particle is not special in any way the contribution from the sum over j will be simply N times the contribution of the jth particle. Hence the double sum of the δ-function will be $Ng(r_0)$ where $g(r_0)$ is the probability of finding a particle at a position r_0 relative to a given particle and (A1.4) can be rewritten as

$$\begin{aligned}\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{coh}} &= a_{\mathrm{coh}}^2 \int \mathrm{d}^3 r_0 \mathrm{e}^{\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{r}_0}\left[\delta^{(3)}\left(\boldsymbol{r}_0\right) + g\left(\boldsymbol{r}_0\right)\right] \\ &\equiv a_{\mathrm{coh}}^2 S\left(\boldsymbol{Q}\right). \end{aligned} \tag{A1.5}$$

The integral, called the structure factor $S(Q)$, is simply one plus the Fourier transform of $g(r_0)$. The structure factor, or its Fourier transform, represents all the information about the static distribution of atoms in the scattering system that can be determined by scattering. It can be measured by X-ray as well as neutron scattering.