$$I \propto \int \mathrm{d}^3k_i \int \mathrm{d}^3k_f P_i(\mathbf{k}_i) S(\mathbf{k}_i \rightarrow \mathbf{k}_f) P_f(\mathbf{k}_f), \qquad (4.4.3.1)$$

where $P_i(\mathbf{k}_i)$ is the probability that a neutron of wavevector $\mathbf{k}_i$ is incident on the sample, $P_f(\mathbf{k}_f)$ is the probability that a neutron of wavevector $\mathbf{k}_f$ is transmitted by the analyser system and $S(\mathbf{k}_i \rightarrow \mathbf{k}_f)$ is the probability that the sample scatters a neutron from $\mathbf{k}_i$ to $\mathbf{k}_f$. The fluctuation spectrum of the sample, $S(\mathbf{k}_i \rightarrow \mathbf{k}_f)$, does not depend separately on $\mathbf{k}_i$ and $\mathbf{k}_f$ but rather on the scattering vector $\mathbf{Q}$ and energy transfer $\hbar\omega$ defined by the conservation equations

$$\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f; \quad \hbar\omega = \frac{\hbar^2}{2m}(k_i^2 - k_f^2), \qquad (4.4.3.2)$$

where m is the neutron mass.

A number of methods of calculating the distribution functions $P_i(\mathbf{k}_i)$ and $P_f(\mathbf{k}_f)$ have been proposed. The method of independent distributions was used implicitly by Stedman (1968) and in more detail by Bjerrum Møller & Nielson (MN) (Nielsen & Bjerrum Møller, 1969; Bjerrum Møller & Nielsen, 1970) for three-axis spectrometers. Subsequently, the method has been extended to perfect-crystal monochromators (Pynn, Fujii & Shirane, 1983) and to time-of-flight spectrometers (Steinsvoll, 1973; Robinson, Pynn & Eckert, 1985). The method involves separating P_i and P_f into a product of independent distribution functions each of which can be convolved separately with the fluctuation spectrum $S(\mathbf{Q}, \omega)$ [*cf.* equation (4.4.3.1)]. Extremely simple results are obtained for the widths of scans through a phonon dispersion surface for spectrometers where the energy of scattered neutrons is analysed (Nielson & Bjerrum Møller, 1969). For diffractometers, the width of a scan through a Bragg peak may also be obtained (Pynn *et al.*, 1983), yielding a result equivalent to that given by Caglioti, Paoletti & Ricci (1960). In this case, however, the singular nature of the Bragg scattering process introduces a correlation between the distribution functions that contribute to P_i and P_f and the calculation is less transparent than it is for phonons.

A somewhat different approach, which does not explicitly separate the various contributions to the resolution, was proposed by Cooper & Nathans (CN) (Cooper & Nathans, 1967, 1968; Cooper, 1968). Minor errors were corrected by several authors (Werner & Pynn, 1971; Chesser & Axe, 1973). The CN method calculates the instrumental resolution function $R(\mathbf{Q} - \mathbf{Q}_0, \omega - \omega_0)$ as

$$R(\Delta\mathbf{Q}, \Delta\omega) = R_0 \exp -\tfrac{1}{2} \sum_{\alpha,\beta} M_{\alpha\beta} X_\alpha X_\beta, \qquad (4.4.3.3)$$

where X_1, X_2, and X_3 are the three components of $\Delta\mathbf{Q}$, $X_4 = \Delta\omega$, and $\mathbf{Q}_0$ and ω_0 are obtained from (4.4.3.2) by replacing $\mathbf{k}_i$ and $\mathbf{k}_f$ by $\mathbf{k}_I$ and $\mathbf{k}_F$, respectively. The matrix $\boldsymbol{M}$ is given in explicit form by several authors (Cooper & Nathans, 1967, 1968; Cooper, 1968; Werner & Pynn, 1971; Chesser & Axe, 1973) and the normalization R_0 has been discussed in detail by Dorner (1972). [A refutation (Tindle, 1984) of Dorner's work is incorrect.] Equation (4.4.3.3) implies that contours of constant transmission for the spectrometer [$R(\Delta\mathbf{Q}, \Delta\omega) = \text{constant}$] are ellipsoids in the four-dimensional $\mathbf{Q}$–ω space. Optimum resolution (focusing) is achieved by a scan that causes the resolution function to intersect the feature of interest in $S(\mathbf{Q}, \omega)$ (*e.g.* Bragg peak or phonon dispersion surface) for the minimum scan interval. The optimization of scans for a diffractometer has been considered by Werner (1971).

The MN and CN methods are equivalent. Using the MN formalism, it can be shown that

$$\boldsymbol{M} = (\boldsymbol{A})^{-1} \quad \text{with} \quad A_{\alpha\beta} = \sum_j \chi_{j\alpha}\chi_{j\beta}, \qquad (4.4.3.4)$$

where the $\chi_{j\alpha}$ are the components of the standard deviations of independent distributions (labelled by index j) defined by Bjerrum Møller & Nielsen (1970). In the limit $Q \rightarrow 0$, the matrices $\boldsymbol{M}$ and $\boldsymbol{A}$ are of rank three and other methods must be used to calculate the resolution ellipsoid (Mitchell, Cowley & Higgins, 1984). Nevertheless, the MN method may be used even in this case to calculate widths of scans.

To obtain the resolution function of a diffractometer (in which there is no analysis of scattered neutron energy) from the CN form for $\boldsymbol{M}$, it is sufficient to set to zero those contributions that arise from the mosaic of the analyser crystal. For elastic Bragg scattering, the problem is further simplified because X_4 [*cf.* equation (4.4.3.3)] is zero. The spectrometer resolution function is then an ellipsoid in $\mathbf{Q}$ space.

For the measurement of integrated intensities (of Bragg peaks for example), the normalization R_0 in (4.4.3.3) is required in order to obtain the Lorentz factor. The latter has been calculated for an arbitrary scan of a three-axis spectrometer (Pynn, 1975) and the results may be modified for a diffractometer as described in the preceding paragraph.

4.4.4. Scattering lengths for neutrons (By V. F. Sears)

The use of neutron diffraction for crystal-structure determinations requires a knowledge of the scattering lengths and the corresponding scattering and absorption cross sections of the elements and, in some cases, of individual isotopes. This information is needed to calculate unit-cell structure factors and to correct for effects such as absorption, self-shielding, extinction, thermal diffuse scattering, and detector efficiency (Bacon, 1975; Sears, 1989). Table 4.4.4.1 lists the best values of the neutron scattering lengths and cross sections that are available at the time of writing (January 1995). We begin by summarizing the basic relationships between the scattering lengths and cross sections of the elements and their isotopes that have been used in the compilation of this table. More background information can be found in, for example, the book by Sears (1989).

4.4.4.1. *Scattering lengths*

The scattering of a neutron by a single bound nucleus is described within the Born approximation by the Fermi pseudopotential,

$$V(\mathbf{r}) = \left(\frac{2\pi\hbar^2}{m}\right) b\delta(\mathbf{r}), \qquad (4.4.4.1)$$

in which $\mathbf{r}$ is the position of the neutron relative to the nucleus, m the neutrons mass, and b the bound scattering length. The neutron has spin $\mathbf{s}$ and the nucleus spin $\mathbf{I}$ so that, if $I \neq 0$, the Fermi pseudopotential and, hence, the bound scattering length will be spin dependent. Since $s = 1/2$, the most general rotationally invariant expression for b is

$$b = b_c + \frac{2b_i}{\sqrt{I(I+1)}}\,\mathbf{s}\cdot\mathbf{I}, \qquad (4.4.4.2)$$

in which the coefficients b_c and b_i are called the bound coherent and incoherent scattering lengths. If $I = 0$, then $b_i = 0$ by convention.

references