Historically, the first flippers used were radio-frequency coils set in a homogeneous magnetic field. These devices are wavelength dependent, but may be rendered wavelength independent by replacing the homogeneous magnetic field with a gradient field (Egorov, Lobashov, Nazarento, Porsev & Serebrov, 1974).

In some devices, the flipping action can be combined with another selection function. The wavelength-dependent magnetic wiggler flipper proposed by Agamalyan, Drabkin & Sbitnev (1988) in combination with a polarizer can be used as a polarizing monochromator (Majkrzak & Shirane, 1982). Badurek & Rauch (1978) have used flippers as choppers to pulse a polarized beam.

In neutron resonance spin echo (NRSE) (Gähler & Golub, 1987), the precession coil of the conventional spin-echo configuration is replaced by two resonance spin flippers separated by a large zero-field region. The radio-frequency field of amplitude B_1 is arranged orthogonal to the DC field, B_0, with a frequency $\omega = \omega_L$, and an amplitude defined by the relation $\omega_1 \tau = \pi$, where τ is the flight time in the flipper coil and $\omega_1 = \gamma B_1$. In this configuration, the neutron spin precesses through an angle π about the resonance field in each coil and leaves the coil with a phase angle φ. The total phase angle after passing through both coils, $\varphi = 2\omega L/v$, depends on the velocity v of the neutron and the separation L between the two coils. Thus, compared with conventional NSE, where the phase angle comes from the precession of the neutron spin in a strong magnetic field compared with a static flipper field, in NRSE the neutron spin does not precess, but the flipper field rotates. Effectively, the NRSE phase angle φ is a factor of two larger than the NSE phase angle for the same DC field B_0. Furthermore, the resolution is determined by the precision of the RF frequencies and the zero-field flight path L rather than the homogeneity of the line integral of the field in the NSE precession coil.

4.4.2.8. *Mechanical choppers and selectors*

Thermal neutrons have relatively low velocities (a 4 Å neutron has a reciprocal velocity of approximately 1000 μs m^{-1}), so that mechanical selection devices and simple flight-time measurements can be used to make accurate neutron energy determinations.

Disc choppers rotating at speeds up to 20 000 revolutions per minute about an axis that is parallel to the neutron beam are used to produce a well defined pulse of neutrons. The discs are made from absorbing material (at least where the beam passes) and comprise one or more neutron-transparent apertures or slits. For polarized neutrons, these transparent slits should not be metallic, as the eddy currents in the metal moving in even a weak guide field will strongly depolarize the beam. The pulse frequency is determined by the number of apertures and the rotation frequency, while the duty cycle is given by the ratio of open time to closed time in one rotation. Two such choppers rotating in phase can be used to monochromate and pulse a beam simultaneously (Egelstaff, Cocking & Alexander, 1961). In practice, more than two choppers are generally used to avoid frame overlap of the incident and scattered beams. The time resolution of disc choppers (and hence the energy resolution of the instrument) is determined by the beam size, the aperture size and the rotation speed. For a realistic beam size, the rotation speed limits the resolution. Therefore, in modern instruments, it is normal to replace a single chopper with two counter-rotating choppers (Hautecler *et al.*, 1985; Copley, 1991). The low duty cycle of a simple disc chopper can be improved by replacing the single slit with a series of slits either in a regular sequence (Fourier chopper) (Colwell, Miller & Whittemore, 1968; Hiismäki, 1997) or a pseudostatistical sequence (pseudostatistical chopper) (Hossfeld, Amadori & Scherm, 1970), with duty cycles of 50 and 30%, respectively.

The Fermi chopper is an alternative form of neutron chopper that simultaneously pulses and monochromates the incoming beam. It consists of a slit package, essentially a collimator, rotating about an axis that is perpendicular to the beam direction (Turchin, 1965). For optimum transmission at the required wavelength, the slits are usually curved to provide a straight collimator in the neutron frame of reference. The curvature also eliminates the 'reverse burst', *i.e.* a pulse of neutrons that passes when the chopper has rotated by 180°.

A Fermi chopper with straight slits in combination with a monochromator assembly of wide horizontal divergence can be used to time focus a polychromatic beam, thus maintaining the energy resolution while improving the intensity (Blanc, 1983).

Velocity selectors are used when a continuous beam is required with coarse energy resolution. They exist in either multiple disc configurations or helical channels rotating about an axis parallel to the beam direction (Dash & Sommers, 1953). Modern helical channel selectors are made up of lightweight absorbing blades slotted into helical grooves on the rotation axis (Wagner, Friedrich & Wille, 1992). At higher energies where no suitable absorbing material is available, highly scattering polymers [poly(methyl methacrylate)] can be used for the blades, although in this case adequate shielding must be provided. The neutron wavelength is determined by the rotation speed, and resolutions, $\Delta\lambda/\lambda$, ranging from 5% to practically 100% ($\lambda/2$ filter) can be achieved. The resolution is fixed by the geometry of the device, but can be slightly improved by tilting the rotation axis or relaxed by rotating in the reverse direction for shorter wavelengths. Transmissions of up to 94% are typical.

4.4.3. Resolution functions (By R. Pynn and J. M. Rowe)

In a *Gedanken* neutron scattering experiment, neutrons of wavevector $\mathbf{k}_I$ impinge on a sample and the wavevector, $\mathbf{k}_F$, of the scattered neutrons is determined. A number of different types of spectrometer are used to achieve this goal (*cf.* Pynn, 1984). In each case, finite instrumental resolution is a result of uncertainties in the definition of $\mathbf{k}_I$ and $\mathbf{k}_F$. Propagation directions for neutrons are generally defined by Soller collimators for which the transmission as a function of divergence angle generally has a triangular shape. Neutron monochromatization may be achieved either by Bragg reflection from a (usually) mosaic crystal or by a time-of-flight method. In the former case, the mosaic leads to a spread of $|k_I|$ while, in the latter, pulse length and uncertainty in the lengths of flight paths (including sample size and detector thickness) produce a similar effect. Calculations of instrumental resolution are generally lengthy and lack of space prohibits their detailed presentation here. In the following paragraphs, the concepts involved are indicated and references to original articles are provided.

In resolution calculations for neutron spectrometers, it is usually assumed that the uncertainty of the neutron wavevector does not vary spatially across the neutron beam, although this reasoning may not apply to the case of small samples and compact spectrometers. To calculate the resolution of the spectrometer in the large-beam approximation, one writes the measured intensity I as

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

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