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be increased accordingly.

6. Instrumental Configurations and Efficiencies

In this section we will describe the corrections which must be made for imperfect polarizer and flipper efficiencies in extracting spin-dependent cross sections from measured intensities. For the purpose of illustration, we will consider a conventional triple-axis spectrometer configuration with polarized beam incident on the sample and with one-dimensional polarization analysis of the scattered beam where only the final neutron spin eigenstate is determined. The same fundamental principles apply to time-of-flight instruments.

A schematic of a triple-axis spectrometer is shown in Figure 6-1 with monochromator, analyser, polarizers, and flippers such that, in the most general case, spin-dependent elastic or inelastic scattering cross sections can be obtained. We will make the explicit stipulation that any beam depolarization which occurs within the guide field be included as part of the effective polarization efficiency of the appropriate polarizing element, depending upon where the depolarization occurs, i.e., prior to or following the sample. We also take the flippers to be perfectly transparent and attribute any transmission losses (in the wire windings of a flat coil flipper, for example) to be incorporated in the effective reflection efficiencies of the monochromator-polarizer or analyzer-polarizer devices. We can then represent our spectrometer by the somewhat simpler schematic shown in Figure 6-2.

Our goal, again, is to obtain four spin-dependent cross sections, namely σ_{++}, σ_{--}, σ_{+-} and σ_{-+}, from four measured intensities, $I^{\text{off off}}$, $I^{\text{on on}}$, $I^{\text{off on}}$, and $I^{\text{on off}}$ where the superscripts "off" and "on" signify whether the front or rear flipper is off (no spin flip) or on (π spin turn), respectively. If only a single superscript appears, it refers specifically to the front flipper and the status of the rear flipper is automatically assumed to be either off or irrelevant. X

The first question we need to ask is what are the intensities of + and - neutrons incident on the sample with the front flipper either off or on. Identifying the intensities incident on the sample by the subscript "o", we can write

$$I_o^{\text{off}} = I_{o+}^{\text{off}} + I_{o-}^{\text{off}}$$

and

$$I_o^{on} = I_{o+}^{on} + I_{o-}^{on} \tag{6-1}$$

where

$$I_o^{off} = I_o^{on} \equiv I_o$$

and where the subscripts "+" and "-" signify the + and - neutron spin eigenstates. Of course, if the efficiencies of the front polarizer and flipper were perfect and no instrumental depolarization occurred, then

$$I_o^{off} = I_{o+}^{off} \ (\text{or } I_{o-}^{off}) \text{ and } I_o^{on} = I_{o-}^{on} \ (\text{or } I_{o+}^{on}).$$

If we define the quantity ϕ to represent a fraction of the beam intensity, then we can write

$$\frac{I_{o+}^{off}}{I_o} + \frac{I_{o-}^{off}}{I_o} \equiv \phi_{o+}^{off} + \phi_{o-}^{off} = 1 \tag{6-2}$$

so that the polarization of the beam incident on the sample with the front flipper off, P_o^{off}, is given by

$$P_o^{off} = \phi_{o+}^{off} - \phi_{o-}^{off} \tag{6-3}$$

Analogously, when the front flipper is on,

$$\frac{I_{o+}^{on}}{I_o} + \frac{I_{o-}^{on}}{I_o} \equiv \phi_{o+}^{on} + \phi_{o-}^{on} = 1 \tag{6-4}$$

so that

$$P_o^{on} = \phi_{o+}^{on} - \phi_{o-}^{on} \tag{6-5}$$

Now the ϕ's defined in equations (6-2) and (6-4) are related through the flipping efficiency of the front flipper which we shall define as f ($0 \le f \le 1$):

$$\phi_{o+}^{on} = f\,\phi_{o-}^{off} + (1 - f)\,\phi_{o+}^{off}$$

and (6-6)

$$\phi_{o-}^{on} = f\,\phi_{o+}^{off} + (1 - f)\,\phi_{o-}^{off}$$

so that

$$P_o^{on} = P_o^{off}\,(1-2f) \tag{6-7}$$

If we now take P_o^{off} to be the efficiency of the front polarizer and call it F, then the intensities incident on the sample are given by

$$
\begin{aligned}
I_{o+}^{off} &= \frac{I_o}{2}(1+F) \\
I_{o-}^{off} &= \frac{I_o}{2}(1-F) \\
I_{o+}^{on} &= \frac{I_o}{2}[1+F(1-2f)] \\
I_{o-}^{on} &= \frac{I_o}{2}[1-F(1-2f)]
\end{aligned}
\tag{6-8}
$$

Next, the intensities scattered by the sample, I_s, are, in general, given by

$$
\begin{aligned}
I_{s+}^{off} &= \sigma_{++}\, I_{o+}^{off} + \sigma_{-+}\, I_{o-}^{off} \\
I_{s-}^{off} &= \underline{\sigma_{--}}\, I_{o-}^{off} + \sigma_{+-}\, I_{o+}^{off} \\
I_{s+}^{on} &= \sigma_{++}\, I_{o+}^{on} + \sigma_{-+}\, I_{o-}^{on} \\
I_{s-}^{on} &= \underline{\sigma_{--}}\, I_{o-}^{on} + \sigma_{+-}\, I_{o+}^{on}
\end{aligned}
\tag{6-9}
$$

where $0 \leq \sigma\text{'s} \leq 1$.

Finally, we need to determine the intensities I_D measured in the detector with the rear flipper either off or on. Consider first the case with the rear flipper off. Let the rear polarizer have a polarizing efficiency R ($0 \leq R \leq 1$). The reflectivity of the rear polarizer is then proportional to $(1 + R)$ for + neutrons and to $(1 - R)$ for - neutrons. Consequently, the intensities I_D which can be measured in the detector with the rear flipper off are

$$I_D^{\mathrm{off\,off}} = C\,[\,I_{s+}^{\mathrm{off}}\,(1 + R) + I_{s-}^{\mathrm{off}}\,(1 - R)]$$

and (6-10)

$$I_D^{\mathrm{on\,off}} = C\,[\,I_{s+}^{\mathrm{on}}\,(1 + R) + I_{s-}^{\mathrm{on}}\,(1 - R)]$$

where C is a normalization constant to be derived below.

Now if the rear flipper is on and we designate its efficiency to be r ($0 \le r \le 1$), then the intensities scattered by the sample after traversing the rear flipper are

$$\begin{aligned} I_{s+}^{\mathrm{off\,on}} &= r\,I_{s-}^{\mathrm{off}} + (1 - r)\,I_{s+}^{\mathrm{off}} \\ I_{s-}^{\mathrm{off\,on}} &= r\,I_{s+}^{\mathrm{off}} + (1 - r)\,I_{s-}^{\mathrm{off}} \\ I_{s+}^{\mathrm{on\,on}} &= r\,I_{s-}^{\mathrm{on}} + (1 - r)\,I_{s+}^{\mathrm{on}} \\ I_{s-}^{\mathrm{on\,on}} &= r\,I_{s+}^{\mathrm{on}} + (1 - r)\,I_{s-}^{\mathrm{on}} \end{aligned} \qquad (6\text{-}11)$$

The remaining intensities I_D which can be measured in the detector with the rear flipper on are then

$$\begin{aligned} I_D^{\mathrm{off\,on}} &= C\,[\,I_{s+}^{\mathrm{off\,on}}\,(1 + R) + I_{s-}^{\mathrm{off\,on}}\,(1 - R)] \\ I_D^{\mathrm{on\,on}} &= C\,[\,I_{s+}^{\mathrm{on\,on}}\,(1 + R) + I_{s-}^{\mathrm{on\,on}}\,(1 - R)] \end{aligned} \qquad (6\text{-}12)$$

If we now go back and substitute into equations (6-9) the expressions for the I_o's given by equations (6-8), then equations (6-10), (6-11) , and (6-12) can in turn be simplified and written in terms of I_o, F, R, f, r and C. The I_D's are then given by (defining $I_o\,C/2 \equiv \beta$)

$$\begin{aligned} I_D^{\mathrm{off\,off}}/\beta = {} & \sigma_{++}\,(1+F)\,(1+R) \\ & + \sigma_{-+}\,(1-F)\,(1+R) \\ & + \sigma_{--}\,(1-F)\,(1-R) \\ & + \sigma_{+-}\,(1+F)\,(1-R) \end{aligned} \qquad (6\text{-}13)$$

$$\begin{aligned} I_D^{\mathrm{on\,off}}/\beta = {} & \sigma_{++}\,(1+R)\,[\,1 + F(1-2f)] \\ & + \sigma_{-+}\,(1+R)\,[\,1 - F(1-2f)] \\ & + \sigma_{--}\,(1-R)\,[\,1 - F(1-2f)] \\ & + \sigma_{+-}\,(1-R)\,[\,1 + F(1-2f)] \end{aligned} \qquad (6\text{-}14)$$

8 β bc invert these
4 equations & σ_{++} σ_{-+} σ_{+-} & σ_{--}
solve for
which are corrected intensity.

$$
\begin{aligned}
I_D^{off\,on}/\beta = {} & \sigma_{++}\,(1+F)\,[\,1 + R(1-2r)] \\
& + \sigma_{-+}\,(1-F)\,[\,1 + R(1-2r)] \\
& + \sigma_{--}\,(1-F)\,[\,1 - R(1-2r)] \\
& + \sigma_{+-}\,(1+F)\,[\,1 - R(1-2r)]
\end{aligned}
\tag{6-15}
$$

and

$$
\begin{aligned}
I_D^{on\,on}/\beta = {} & \sigma_{++}\,[\,1 + F\,(1-2f)\,]\,[\,1 + R\,(1-2r)] \\
& + \sigma_{-+}\,[\,1 - F\,(1-2f)\,]\,[\,1 + R\,(1-2r)] \\
& + \sigma_{--}\,[\,1 - F\,(1-2f)]\,[\,1 - R\,(1-2r)] \\
& + \sigma_{+-}\,[\,1 + F\,(1-2f)]\,[\,1 - R\,(1-2r)]
\end{aligned}
\tag{6-16}
$$

Equations (6-13, 14, 15, 16) are of general utility. Given the instrumental polarizing and flipping efficiencies F, R, f, and r, and the normalization parameter β, this set of equations can be solved for σ_{++}, σ_{--}, σ_{+-}, and σ_{-+} in terms of the measured intensities $I_D^{off\,off}$, $I_D^{on\,on}$, $I_D^{off\,on}$, and $I_D^{on\,off}$.

We need, however, to address the problem of determining the instrumental parameters F, R, f, r, and β. Suppose that intensities I_{NS} are measured with no sample ("NS") in the beam. Then $\sigma_{++} = \sigma_{--} = 1$ and $\sigma_{+-} = \sigma_{-+} = 0$ and equations (6-13, 14, 15, 16) reduce to

$$
\begin{aligned}
I_{NS}^{off\,off} &= 2\beta\,[\,1 + FR\,] \\
I_{NS}^{on\,off} &= 2\beta\,[\,1 + (1-2f)\,FR\,] \\
I_{NS}^{off\,on} &= 2\beta\,[\,1 + (1-2r)\,FR\,] \\
I_{NS}^{on\,on} &= 2\beta\,[\,1 + (1-2f)\,(1-2r)\,FR\,]
\end{aligned}
\tag{6-17}
$$

From the above equations (6-17) we obtain

Formula for β

$$
2\beta = \frac{I_{NS}^{onon}\;I_{NS}^{offoff} - I_{NS}^{onoff}\;I_{NS}^{offon}}{I_{NS}^{onon} + I_{NS}^{offoff} - I_{NS}^{onoff} - I_{NS}^{offon}}
\tag{6-18}
$$

$$FR = (I_{NS}^{off\,off}/2\beta) - 1 \tag{6-19}$$

Formula for pf*pr (i.e. F*R)

$$x{:}\ (1-2f) = [(I_{NS}^{on\,off}/2\beta) - 1\,]/FR \tag{6-20}$$

Formula for x

Formular for γ (i.e. r)

and

$$\gamma = (1\text{-}2r) = [(I_{NS}^{off\,on}/2\beta) - 1\,]/FR \tag{6-21}$$

Thus all the parameters except the separate values of F and R are determined by measuring intensities without a sample. In order to obtain F and R individually, we need to make one more set of measurements, this time with a sample for which $\sigma_{+-} = \sigma_{-+} = 0$ but σ_{++} and σ_{--} are different, the bigger the difference, the better. In fact, the actual values of σ_{++} and σ_{--} need not be known at all (except that they are sufficiently different!). If we measure a set of intensities I_{RS} for such a reference sample ("RS"), we can sequentially eliminate σ_{++} and σ_{--} from equations (6-13, 14, 15, 16) (having set $\sigma_{+-} = \sigma_{-+} = 0$) and solve for F in terms of the intensities I_{RS} and the other parameters FR, (1-2f), and (1-2r), which we have already determined from equations (6-18, 19, 20, 21). The result of these computations is the following expression for F:

Formular for ρ^f (+ ρ^r)

$$F = \frac{-B \pm \sqrt{B^2 - 4AC}}{2A} \tag{6-22}$$

where

$$A = (1\text{-}2f)\,(I_{RS}^{off\,on} - I_{RS}^{off\,off}) + I_{RS}^{on\,off} - I_{RS}^{on\,on}$$

$$\begin{aligned} B = {} & I_{RS}^{off\,on}\,[\,1 - FR\,(1\text{-}2f)] \\ & - I_{RS}^{off\,off}\,[\,1 - FR\,(1\text{-}2f)\,(1\text{-}2r)] \\ & + I_{RS}^{on\,off}\,[\,1 - FR\,(1\text{-}2r)] \\ & - I_{RS}^{on\,on}\,[\,1 - FR\,] \end{aligned}$$

and

$$C = FR \cdot [\,I_{RS}^{on\,on} - I_{RS}^{off\,on} + (1\text{-}2r)\,(I_{RS}^{off\,off} - I_{RS}^{on\,off})].$$

Once F is so determined, R = FR/F and all instrumental parameters are known.

In order to illustrate the application of the instrumental corrections described here, consider the following example. The reflectivity of an Fe-Cr multilayer was measured on the polarized neutron reflectometer at NIST (Ankner et al., 1992) which was determined to have efficiencies F = 0.986, R = 0.924, f = 0.999, and r = 0.985 (using an Fe-Si multilayer sample as the calibration standard and following the procedure outlined above). The raw, uncorrected specular

Scale factors on slit scan

$$\beta(kA, kB, kC, kD) = \frac{1}{2}\frac{kA\,kD - kB\,kC}{kA + kD - kB - kC}$$

$$= \frac{1}{2}\frac{k^2 AD - k^2 BC}{k(A+D-B-C)}$$

$$= \frac{k}{2}\frac{AD-BC}{A+D-B-C}$$

$$= k\beta(A,B,C,D)$$

$$FR(kA, k\beta) = \frac{kA}{2k\beta} - 1 = \frac{A}{2\beta} - 1 = FR(A,\beta)$$

$$x(kB, k\beta, FR) = \left(\frac{kB}{2k\beta} - 1\right)/FR = \left(\frac{B}{2\beta} - 1\right)/FR = x(B, \beta, FR)$$

$$y(kC, k\beta, FR) = \left(\frac{kC}{2k\beta} - 1\right)/FR = \left(\frac{C}{2\beta} - 1\right)/FR = y(C, \beta, FR)$$

flip F, flip R depends on x, y, which are unchanged after scaling.

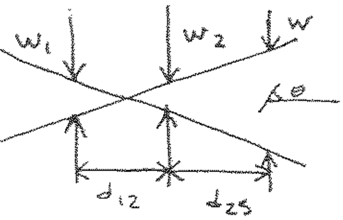
pol F, pol R depends on FR, FRratio, which are unchanged after scaling.

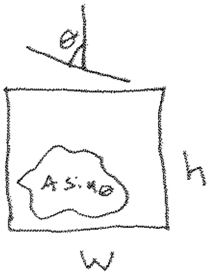
For the actual correction, the system we are solving,

$Hz = b$ for H depending on F, R, x, y and

$$b = \begin{pmatrix} \frac{kA}{k\beta} \\ \frac{kB}{k\beta} \\ \frac{kC}{k\beta} \\ \frac{kD}{k\beta} \end{pmatrix} = \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix}$$

is independent of monitor.





$$w = \frac{w_1 d_{2s} + w_2(d_{12}+d_{2s})}{d_{12}}$$

$$I_D = r I A \sin(\theta - \theta_0)$$

$$I_S = I h w$$

$$r = \frac{I_D}{I A \sin(\theta-\theta_0)} = \frac{I_D}{I_S}\left(\frac{I_S}{I A \sin(\theta-\theta_0)}\right) = \frac{I_D}{I_S}\left(\frac{I h w}{I A \sin(\theta-\theta_0)}\right)$$

$$r = \frac{I_D}{I_S}\frac{hw}{A\sin(\theta-\theta_0)}$$

$$\theta < \theta_c \Rightarrow r = 1 \Rightarrow \frac{A}{h}\sin(\theta-\theta_0) = \frac{I_D}{I_S} w$$

Figprep: compute $\left(\frac{I_D}{I_S}\right) w$. Fit: determine $\frac{A}{h}$, $-\frac{A}{h}\theta_0$
from data.f, or data.s

Figcor2: compute $\left(\frac{I_D}{I_S}\right)\frac{w}{\frac{A}{h}\sin(\theta-\theta_0)} = r$

from data.f or data.s

$$w_1 = s_{10} + s_{11}\cdot(2\theta)$$

$$w_2 = s_{20} + s_{21}\cdot(2\theta)$$