III.E.7. Corrections for Angular Distributions

Angular distribution measurements may require additional treatments for experimental conditions beyond those required by angle-integrated measurements. Two kinds of treatment are currently available in SAMMY; as experiments improve and the need arises for more sophisticated treatments, others will be added to the code.

Attenuation

One type of correction for finite sample size in angular distributions is handled in much the same manner as in the code RFUNC, which was developed by F. G. Perey [FP89a] for calculating elastic angular distributions using the R-function approximation for spin-zero samples. Two effects are included, which are denoted "incident neutron attenuation" and "scattered neutron attenuation," respectively.

Incident neutron attenuation is accomplished by multiplying the cross section by the factor

$$\exp\left\{-n_{in}\left(\theta\right)\sigma_{tot,D}\left(E\right)\right\} \quad , \tag{III E7.1}$$

where the "thickness" or attenuation $n_{in}\left(\theta\right)$ may be specified independently for each angle and may be treated as a search parameter. The cross section appearing in Eq. (III E7.1) is the Doppler-broadened total cross section.

The so-called "scattered neutron attenuation" is used to approximately describe three distinct effects: (1) Neutrons initially scattered in the direction of the detector may be re-scattered (or captured, or involved in some other reaction). (2) Neutrons not initially scattered toward the detector may, after two or more scatterings, ultimately reach the detector. (3) Both the sample and the detectors have large angular spreads.

To describe these effects, the cross section is multiplied by the attenuation factor

$$\exp\left\{-n_{out}\left(\theta\right)\sigma_{tot,x}\left(E'\right)\right\} \quad . \tag{III E7.2}$$

Here the attenuation $n_{out}\left(\theta\right)$ again may be different for each angle and may be treated as a search parameter. The cross section in this equation is evaluated at the scattered energy for the particular angle and has been broadened (using a triangular resolution function) to approximate the effects of the angular spread of the detector and sample.

See Table VI B.2, card set 11, line 4, for details of the input for these attenuation factors.

Angle Average

Another available correction for the finite sample size is a straight-line average over solid angle, of the form

$$\left\langle \frac{d\sigma}{d\Omega} \right\rangle = \int_{\cos(\theta+D\theta)}^{\cos(\theta-D\theta)} \frac{d\sigma}{d\Omega} d\mu \Bigg/ \int_{\cos(\theta+D\theta)}^{\cos(\theta-D\theta)} d\mu \quad , \qquad \text{(III E7.3)}$$

in which the differential elastic cross section is assumed to be a function of cos(θ) but a constant with respect to the azimuthal angle φ.

The actual calculation in SAMMY is carried out in a relatively crude approximation which implicitly assumes that the angular spread is not large. The cross section is calculated at three angles: $\theta + D\theta$, θ, and $\theta - D\theta$. Quadratic interpolation in cos(θ) is used so that the cross section at other angles is assumed to be given by

$$\sigma(\mu) = A \frac{(\mu-b)(\mu-c)}{(a-b)(a-c)} + B \frac{(\mu-a)(\mu-c)}{(b-a)(b-c)} + C \frac{(\mu-a)(\mu-b)}{(c-a)(c-b)} \quad , \qquad \text{(III E7.4)}$$

in which we have set

$$a = \cos(\theta + D\theta) \qquad b = \cos(\theta - D\theta) \qquad c = \cos(\theta) \qquad \text{(III E7.5)}$$

and

$$A = \frac{d\sigma(a)}{d\Omega} \qquad B = \frac{d\sigma(b)}{d\Omega} \qquad C = \frac{d\sigma(c)}{d\Omega} \quad . \qquad \text{(III E7.6)}$$

Substituting Eq. (III E7.4) into Eq. (III E7.3) and integrating gives the resulting average cross section

$$\left\langle \frac{d\sigma}{d\Omega} \right\rangle = \frac{1}{6} \left[A \frac{3c-b-2a}{c-a} + B \frac{-3c+2b+a}{b-a} + C \frac{(b-a)^2}{(c-a)(b-c)} \right] \quad . \qquad \text{(III E7.7)}$$

To invoke this option, include the phrase

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ANGLE-AVERAGE FOR DIfferential cross sections
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in the command section of the INPut file. The angles θ and angular spreads $D\theta$ are given in card set 8 of that file (see Table VI A.1).