III.A.3. Perform Numerical Integration

The numerical integration scheme used in SAMMY to evaluate the integrals shown in Eqs. (III A2.1) and (III A2.2) is borrowed from MULTI [GA74] and is based on the four-point progressive interpolation method of Mintz and Jordan [MM64]. For the value of an integral from x_2 to x_3 of some function $y(x)$, where the value of y is known only at the four values of x ($x = x_1, x_2, x_3,$ or x_4), this method uses the approximation

$$\int_{x_2}^{x_3} y(x)\,dx \cong \sum_{i=1}^{4} y(x_i)\,w_i \quad , \tag{III A3.1}$$

in which the weights w_i are given by

$$\begin{aligned}
w_1 &= \frac{(x_2 - x_3)^3}{12(x_1 - x_2)(x_1 - x_3)} \quad , \\
w_2 &= \frac{(x_2 - x_3)}{12}\left[\frac{(x_1 - x_3)}{(x_2 - x_1)} + \frac{(x_4 - x_3)}{(x_2 - x_4)} - 4\right] \quad , \\
w_3 &= \frac{(x_3 - x_2)}{12}\left[4 - \frac{(x_1 - x_2)}{(x_3 - x_1)} - \frac{(x_4 - x_2)}{(x_3 - x_4)}\right] \quad , \\
w_4 &= \frac{(x_2 - x_3)^3}{12(x_4 - x_2)(x_4 - x_3)} \quad .
\end{aligned} \tag{III A3.2}$$

These equations give the exact result if $y(x)$ is a polynomial of degree 2 or less [i.e., if $y(x)$ is a quadratic, linear, or constant function of x].

What is required for the broadening integrals is, however, a function of the form

$$\int_{E_{min}}^{E_{max}} y(E')\,dE' \cong \sum_{j=j_{min}}^{j_{max}-1} \int_{E'_j}^{E'_{j+1}} y(E')\,dE' \quad , \tag{III A3.3}$$

in which j_{min} and j_{max} are chosen such that $E'_{j_{min}} \le E_{min} \le E'_{j_{min}+1}$ and $E'_{j_{max}-1} \le E_{max} \le E'_{j_{max}}$. Each integral on the right-hand side of Eq. (III A3.3) may be evaluated using Eq. (III A3.1), with

$$x_1 = E_{j-1}, \quad x_2 = E_j, \quad x_3 = E_{j+1}, \text{ and } x_4 = E_{j+2} \quad . \tag{III A3.4}$$

Define w_{ij} as "w_i from Eq. (III A3.2) with the x_i given by Eq. (III A3.4)," or more precisely,

$$x_{ij} = E'_{j+i-2} \quad . \tag{III A3.5}$$

Equation (III A3.3) can then be put into the form

$$\int_{E_{min}}^{E_{max}} y(E')\, dE' \;\cong\; \sum_{j=j_{min}}^{j_{max}} \sum_{i=1}^{4} w_{ij}\, y\left(E'_{j+i-2}\right) \quad . \tag{III A3.6}$$

Performing the summation over i gives

$$\int_{E_{min}}^{E_{max}} y(E')\, dE' \;\cong\; \sum_{j=j_{min}}^{j_{max}} W_j\; y\left(E'_j\right) \quad , \tag{III A3.7}$$

where the weight W_j is given by

$$W_j = \sum_{i=1}^{4} w_{i\,(j+2-i)} \quad . \tag{III A3.8}$$

The summation in Eq. (III A3.8) may be evaluated explicitly using Eq. (III A3.1) with Eq. (III A3.4), yielding

$$\begin{aligned} W_j = {} & \left(E'_{j+1} - E'_{j-1}\right)/3 + \left(E'_{j+2} - E'_{j-2}\right)/12 \\ & + \frac{1}{12}\left[\frac{\left(E'_j - E'_{j-1}\right)^2 - \left(E'_{j+2} - E'_{j+1}\right)^2}{\left(E'_{j+1} - E'_j\right)} + \frac{\left(E'_{j+1} - E'_j\right)^2 - \left(E'_{j-1} - E'_{j-2}\right)^2}{\left(E'_j - E'_{j-1}\right)}\right] \quad . \end{aligned} \tag{III A3.9}$$

SAMMY uses the values given by Eq. (III A3.9) even for $j = j_{min}$ and $j = j_{max}$, even though they implicitly require the use of $E'_{j_{min}-1}$ and $E'_{j_{max}+1}$, which technically are outside the range of integration $\left(E_{min} \text{ to } E_{max}\right)$; this is legitimate because the range of integration is chosen so that the integrand $y(E')$ is effectively zero outside that range. Thus, the values of $y\left(E'_{j_{min}-1}\right)$ and $y\left(E'_{j_{max}+1}\right)$ are zero and are implicitly included in the above formulation. In contrast, the code MULTI performed extra calculations to end exactly at $\left(E'_{j_{min}} \text{ to } E'_{j_{max}}\right)$; our studies have found this an unneeded complication.

The scheme described above is used in SAMMY only if there are more than twelve points between $E'_{j_{min}}$ and $E'_{j_{max}}$, inclusive. If there are fewer than twelve but more than five points, Simpson's rule is used. For five or fewer points, it is assumed that the broadened value is equal to the unbroadened value, and no integration is performed.

It should be noted that there are situations in which it is imperative to end the integration precisely at the specified limits. At least two examples occur in the SAMMY code: (1) Multiple-scattering corrections for capture or fission experiments (Section III.D) involve integration over the scattering angle, from 0 to 180 degrees. When “integration over angle” is converted to “integration over energy of the scattered neutron,” one might be tempted to extend the energy integral to the nearest grid point. However, to obtain accurate results, the integration clearly must not extend beyond the energies corresponding to back-angle scattering or forward-angle scattering. (2) Absolute limits are also required for the calculation of average cross sections (Section V.C).

In situations in which the integrand does not smoothly approach zero outside the limits of the integration, Eq. (III A3.9) is modified to give the appropriate weights to define an absolute integration limit.