III.A.2. Choose Auxiliary Energy Grid

We wish to evaluate integrals of the form

$$f\left(E_i\right)=\int_{E_{\min}}^{E_{\max}} \overline{f}\left(E'\right)B\left(E_i,E'\right)dE' \quad , \tag{III A2.1}$$

where $\overline{f}(E')$ represents the unbroadened theoretical cross section (or transmission) and $f\left(E_i\right)$ the broadened. B represents the appropriate broadening function as described in Section III.B or III.C. The set of points E_i are the original grid, for which data are available and at which theoretical values are required.

Standard practice for evaluating integrals such as those in Eq (III A2.1) is to choose a set of points E'_j and associated weights W_j in such a way that

$$\int_a^b \overline{f}\left(E'\right)B\left(E_i,E'\right)dE' \cong \sum_j \overline{f}\left(E'_j\right)B\left(E_i,E'_j\right)W_j \quad , \tag{III A2.2}$$

where the approximation is exact if the product $\overline{f}\left(E'_j\right)B\left(E_i,E'_j\right)$ is a polynomial of some specified degree, say n. Use of these points and weights to evaluate the integral over a non-polynomial function [such as $\overline{f}\left(E'\right)B\left(E_i,E'\right)$ in Eq. (III A2.1)] will give a result that is accurate to the extent that the function can be approximated by a polynomial of degree n. In practice, if one divides the integration region [E_{min}, E_{max}] into sufficiently small subregions [a, b], the polynomial approximation will be quite accurate within each subregion.

The choice of points $\left\{E'_j\right\}$ is, to some extent, arbitrary. (Once $\left\{E'_j\right\}$ is fixed, weights $\left\{W_j\right\}$ are determined from Eq. (III A2.2).) Because it is necessary to integrate Eq. (III A2.1) many times (i.e., once for each E_i), it is expedient to have the set $\left\{E'_j\right\}$ be the same for each E_i in order to minimize the total number of evaluations of $\overline{f}\left(E'_j\right)$. These points $\left\{E'_j\right\}$ will hereafter be designated collectively as the "auxiliary grid," and the points $\left\{E_i\right\}$ for which data are given will be designated as the "original grid."

Several types of points contribute to the auxiliary grid:

a. All points in the original grid are included in the auxiliary grid.

b. "Extra" points are added between each point in the original grid. The number "NXTRA" of such points is specified by the user in the INPut file (see card set 2 of Table VIA.1). (See Section III.A.1 for a discussion of why this may be necessary.)

c. Points are added at the extremities of the data region, to be used in broadening the cross sections at the end points. The relative spacing of these points is similar to that of points inside the energy region being analyzed. The grid is chosen in one of two ways:

   1. Points from the data set, but outside the energy region being analyzed, are added to the auxiliary grid.

   2. If (1) is not possible because the data set contains no such points, then the spacing Δ between data points E_1 and E_2 is used to locate other points equally spaced at $E_1-\Delta$, $E_1-2\Delta$, $E_1-3\Delta$, ... ; a sufficient number of points are chosen to cover the integration region for E_1.

d. Equation (III A2.2) is a good approximation only if the integrand closely resembles a low-order polynomial. Therefore, it may be necessary to add points over the width of narrow resonances so that the structure of the integrand will be properly represented. Also, the auxiliary grid must vary smoothly to avoid numerical difficulties in evaluating the integrals. This problem can be broken into several pieces:

   1. Decide which resonances require additional points. IPTDOP is the number of points required across a resonance; the default value for IPTDOP is 9, but the user may increase this as desired (see Table VI A.1, card set 2). If there are fewer than IPTDOP points between (E_λ - D) and (E_λ + D), where D is the sum of the absolute values of the gamma and particle widths, then more points must be added near this resonance.

   2. For each narrow resonance, add auxiliary points at E_λ and at positions $E_\lambda \pm 2D_j/(\text{IPTDOP}-1)$, where j ranges from 1 to IPTDOP.

   3. Add points at $E_\lambda \pm 1.5D$ and $E_\lambda \pm 2D$.

   4. If IPTWID is positive (but smaller than 7), add additional points at positions $E_\lambda \pm 3D$, $E_\lambda \pm 4D$, and $E_\lambda \pm D(\text{IPTWID}+1)$, where the input quantity IPTWID is specified in Table VI A.1, card set 2.

   5. If IPTWID is negative, add points as in #4, and also at $E_\lambda \pm 10D$ and at $E_\lambda \pm 20D$.

   6. Test the resulting auxiliary grid to see that no two neighboring points are either very close together (relative to neighboring spacing) or very far apart. Drop or add points as needed.

Caveat: If the original (MULTI-style) Doppler broadening is used, and energy points in the auxiliary grid fall at negative energy, SAMMY will issue a warning and abort execution. For subsequent runs, the analyst has several options: either choose a higher E_{min}, specify "NO LOW-ENERGY BROADEning is to be used" in the INPut file (see Tables VI A.1 and VI A.2 for details), specify "USE LEAL,HWANG DOPPLer broadening" for the low-energy region (see Section III.B.2), or specify "USE FREE GAS MODEL Of doppler broadening." The final option (i.e., the free-gas model) is the default and is the author's recommendation for most calculations; see Section III.B.1.