III.E.3.a. Explicit normalization and/or background functions

A constant overall normalization and a variety of different analytical models for backgrounds may be applied to the theoretical values (cross sections, transmissions, etc.) generated within SAMMY. These corrections are applied to the theory, not to the data. Normalization is applied first, followed by background corrections, so that the backgrounds are not multiplied by the normalization.

Let T_u represent the uncorrected theoretical value (for cross section, transmission, etc.); then the corrected value is given by

$$T(E) = aT_u(E) + b(E) \quad , \qquad \text{(III E3 a.1)}$$

in which energy dependences have been explicitly displayed.

Input for the normalization a and four specific backgrounds is specified in card set 6 of the PARameter file. The four backgrounds are

$$\begin{aligned} b_1(E) &= B_a \quad , \\ b_2(E) &= B_b / \sqrt{E} \quad , \\ b_3(E) &= B_c \sqrt{E} \quad , \\ \text{and} \qquad b_4(E) &= B_d \exp\left\{-B_f / \sqrt{E}\right\} \quad . \end{aligned} \qquad \text{(III E3 a.2)}$$

With this format, the user provides one value (which may be zero) for each of the five background parameters B_a through B_f. It is not possible, however, to give more than one value for any of the backgrounds; hence, one cannot, with this format, specify two exponential decay rates for the background.

A second, more general, format for background functions is given in card set 13 of the PARameter file. Here there are nine different types of background functions; however, unlike those given above, any number of each type may be included, so that the actual background is the sum of all such functions. The functional forms for the first four of these backgrounds are, respectively, constant, exponential, power, and exponential of a logarithmic function. An energy range (*E*min to *E*max) may be specified for each of these functions. Explicitly, these functions are

$$\begin{aligned} b_1 &= A \quad , \\ b_2(E(t)) &= Ae^{-Bt} \quad , \\ b_3(E(t)) &= At^B \quad , \\ \text{and} \qquad b_4(E(t)) &= \exp\left\{A + Bt + C/\ln(t)\right\} \quad , \end{aligned} \qquad \text{(III E3 a.3)}$$

in which the flight time t is derived from the energy in the usual manner,

$$t = \sqrt{\frac{mL^2}{2E}} \quad , \qquad \text{(III E3 a.4)}$$

where L is the flight-path length. If the value for L is already given (e.g., for transmission data), that value can be used here. Otherwise, L can be specified along with the other parameters for these functions.

The fifth type of background function is a point-wise linear function in time. This function has the form

$$b_5\left(E\left(t\right)\right) = A_i \frac{t_{i+1} - t}{t_{i+1} - t_i} + A_{i+1} \frac{t - t_{i+1}}{t_{i+1} - t_i} \quad , \qquad \text{(III E3 a.5)}$$

in which the value of $b_5\left(E\left(t_i\right)\right) = A_i$ is specified at two or more particular times t_i. Equation (III E3 a.5) is valid for $t_i \le t \le t_{i+1}$. For time t outside the range of times given for this background type, the value of $b_5\left(E\left(t\right)\right)$ is set to zero. As with the other types of background function, the flight-path length L may be given with the input for this function if it is not already specified.

The sixth type of background is a point-wise linear function in energy. Specifically,

$$b_6\left(E\right) = A_i \frac{E_{i+1} - E}{E_{i+1} - E_i} + A_{i+1} \frac{E - E_{i+1}}{E_{i+1} - E_i} \quad , \qquad \text{(III E3 a.6)}$$

in which the value of $b_6\left(E_i\right) = A_i$ is specified at two or more particular energies E_i. Equation (III E3 a.6) is valid for $E_i \le E \le E_{i+1}$. For energy E outside the range of energies given for this background type, the value of $b_6\left(E\right)$ is set to zero.

The seventh type of background is again a point-wise linear function in time, with essentially the same form as type 5 except for a multiplicative factor B:

$$b_7\left(E\left(t\right)\right) = B\left[A_i \frac{t_{i+1} - t}{t_{i+1} - t_i} + A_{i+1} \frac{t - t_{i+1}}{t_{i+1} - t_i} \right] \quad . \qquad \text{(III E3 a.7)}$$

Likewise, the eighth type of background is a point-wise linear function in energy, with essentially the same form as type 6 except for a multiplicative factor B:

$$b_8\left(E\right) = B\left[A_i \frac{E_{i+1} - E}{E_{i+1} - E_i} + A_{i+1} \frac{E - E_{i+1}}{E_{i+1} - E_i} \right] \quad . \qquad \text{(III E3 a.8)}$$

For both type 7 and type 8, the point-wise values are listed in a separate file and cannot be varied. The multiplicative factor can, however, be varied. Details are given in Table VI B.2.

Because most of these parameters [excluding *E*min, *E*max, t_i, E_i, and L, and the A_i of Eqs. (III E3 a.7) and (III E3 a.8)] can be varied, partial derivatives of the theoretical values T are required. These derivatives are found directly from Eqs. (III E3 a.1) through (III E3 a.4) and are not listed explicitly here. Derivatives generated prior to these corrections (e.g., derivatives with respect to resonance parameters or broadening parameters) are also corrected by the normalization factor, as needed.

The ninth type of background is of the form

$$b_9(E) = AE^{-B} \quad , \qquad \text{(III E3 a.9)}$$

where both A and B may be varied.

For examples of the use of normalization and/or background functions, the reader is referred to the test cases that are distributed with the SAMMY code. Test cases tr032 and tr045 (among others) include normalization and constant background in card set 6 of the PARameter file. Test case tr056 specifically addresses the use of more general background functions (types 1 through 9) provided in card set 13 of the PARameter file.