## III.C.1.a. Resolution broadening: Gaussian

1. *Square distribution in flight-path length*

Broadening in $L$ is due to the "spread" or "distribution of locations" at which the flight path begins or ends (for details, see ref. [DL84]). This distribution may include contributions from both the source and the detector, and may be described by a square function in length $L$; that is,

$$dE''\rho_L\left(E',E''\right)=\begin{cases}\dfrac{d\,L''}{\Delta L} & \text{for } L'-\Delta L/2 \;\le\; L'' \;\le\; L'+\Delta L/2\\[2ex] 0 & \text{otherwise} \quad .\end{cases} \tag{III C1 a.1}$$

Note that $\Delta L$ is equal to $\sqrt{12}$ times the standard deviation of an "equivalent" Gaussian distribution in length. Note also that the input quantity $\Delta L$ may be expressed either as a constant (see variable DELTAL in card set 5 of the INPut file, Table VI A.1, or card set 4 of the PARameter file, Table VI B.2), or as an energy-dependent function of the form

$$\Delta L = E\,\Delta L_1 + \Delta L_0 \quad . \tag{III C1 a.2}$$

(See card set 11, line number 2, of the PARameter file, Table VI B.2).

For convenience in later calculations, this square function in length will be converted to a Gaussian function in energy; that is,

$$dE''\rho_L\left(E',E''\right)\cong\frac{dE''}{\Delta_L\sqrt{\pi}}\exp\left\{-\left|\frac{E''-\bar{E}}{\Delta_L}\right|^2\right\} \quad , \tag{III C1 a.3}$$

where $\bar{E}$ and $\Delta_L$ are found by equating means and variances of the two expressions in Eqs. (III C1 a.1) and (III C1 a.3).

The mean energy for the distribution described in Eq. (III C1 a.1) is given by

$$\begin{aligned}\int_{L'-\Delta L/2}^{L'+\Delta L/2} E''\frac{dL''}{\Delta L} &= \frac{m}{2t^2}\frac{1}{\Delta L}\int_{L'-\Delta L/2}^{L'+\Delta L/2}\left(L''\right)^2 dL'' \\ &= \frac{m}{2t^2}\frac{1}{\Delta L}\left(L'^2\,\Delta L+\left(\Delta L\right)^3/12\right) = E'\left[1+\frac{\Delta^2 L}{12\;L'^2}\right] \quad .\end{aligned} \tag{III C1 a.4}$$

Similarly, the second moment of that distribution is given to first order in $\left(\Delta L/L'\right)^2$ by

$$\int_{L'-\Delta L/2}^{L'+\Delta L/2} E''^2\,\frac{d\,L''}{\Delta L} \cong E'^2\left[1+\frac{\Delta^2 L}{2L'^2}\right] \tag{III C1 a.5}$$

so that the variance of the square distribution is given by

$$E'^2\left[1+\left(\Delta L/L'\right)^2/2\right]-E'^2\left[1+\left(\Delta L/L'\right)^2/12\right]^2 \cong E'^2\left[1+\left(\Delta L/L'\right)^2/3\right] \quad .\text{(III C1 a.6)}$$

Since the mean of the Gaussian distribution in Eq. (III C1 a.3) is $\bar{E}$ and the variance is $\Delta_L^2/2$, the parameters of the Gaussian are given (to lowest order) by

$$\bar{E}=E' \qquad \text{(III C1 a.7)}$$

and

$$\Delta_L=\sqrt{2/3}\,E'\left(\Delta L/L'\right) \quad . \qquad \text{(III C1 a.8)}$$

2. *Square distribution in time*

Finite channel width is one contributor to broadening in time (for details, see [DL84]). The channel width is represented by a square function in time with width $\Delta t_c$ as

$$dE'\rho_c\left(E,E'\right)=\begin{cases}\dfrac{dt'}{\Delta t_c} & \text{for } t-\Delta t_c/2\le t'\le t+\Delta t_c/2\\ 0 & \text{otherwise} \quad .\end{cases} \qquad \text{(III C1 a.9)}$$

Generally the channel width is constant for a certain energy range, but changes from one range to the next. SAMMY input accommodates this characteristic: values for $\Delta t_c$ are given as a constant DELTAB times a "crunch factor" CF$_i$ for energies between Bc$_{i-1}$ and Bc$_i$. Details are given in Table VI A.1, card set 6.

This component of the resolution function also will be converted to an equivalent Gaussian function in the energy variable. Arguments similar to those given above for Eqs. (III C1 a.3) through (III C1 a.8) show that this Gaussian has the form

$$dE'\rho_c\left(E,E'\right)=\frac{dE'}{W_c\sqrt{\pi}}\exp\left\{-\frac{\left(E'-E\right)^2}{W_c^2}\right\} \qquad \text{(III C1 a.10)}$$

where

$$W_c=\sqrt{2/3}\;E\,\Delta t_c/t \quad . \qquad \text{(III C1 a.11)}$$

3. *Gaussian distribution in time*

Neutron burst width is another contributor to the resolution broadening. This effect may be approximated by a Gaussian (or convolution of Gaussian plus exponential; see Sections III.C.1.b and III C1.c) with full width at half max $\Delta t_G$. (See variable DELTAG in Table VIA.1, card set 5, or Table VI B.2, card set 4.) That is, the Gaussian distribution function in time is given by

$$dE'\rho_G\left(E,E'\right)=\frac{dt'}{w_G\sqrt{\pi}}\exp\left\{-\frac{\left(t-t'\right)^2}{w_G^2}\right\} \quad , \tag{III C1 a.12}$$

which translates into

$$dE'\rho_G\left(E,E'\right)=\frac{dE'}{W_G\sqrt{\pi}}\exp\left\{-\frac{\left(E-E'\right)^2}{W_G^2}\right\} \quad , \tag{III C1 a.13}$$

in which the quantities $w_G$ and $W_G$ are defined in terms of the full width at half max via

$$w_G=\Delta t_G/\sqrt{\ln 2} \tag{III C1 a.14}$$

and

$$W_G=\sqrt{\frac{E^3}{\left(m/2\right)\ln 2}}\left(\frac{\Delta t_G}{L}\right) \quad . \tag{III C1 a.15}$$

[The derivation of Eq. (III C1 a.13) requires the approximation that $\sqrt{E'}\approx\sqrt{E}$ to zeroth order.]

4. *Gaussian distribution in energy*

For some applications the resolution is best described by a Gaussian function of energy rather than time or length. For example, neutrons produced by (p,Li7) or (p,t) using protons from Van de Graaff accelerators have relatively small energy spreads determined by beam energy spread, target thickness, etc. The Gaussian widths of such neutron distributions are often approximately constant in energy. The distribution has the form

$$dE'\rho_C\left(E,E'\right)=\frac{dE'}{\Delta_C\sqrt{\pi}}\exp\left\{-\frac{\left(E-E'\right)^2}{\Delta_C^2}\right\} \quad , \tag{III C1 a.16}$$

in which the width $\Delta_C$ is given by

$$\Delta_C=\Delta_{C1}+\Delta_{C2}E \quad . \tag{III C1 a.17}$$

Parameters $\Delta_{C1}$ and $\Delta_{C2}$ are input as DELTC1 and DELTC2 in Table VI B.2, card set 4.

5. *Convolution of the pieces*

The resolution-broadened cross section (or other function) is expressed as the convolution of the resolution function(s) with the unbroadened cross section, as

$$
\begin{aligned}
f_{all}\left(E\right) \;=\; & \frac{1}{W_c\sqrt{\pi}}\int_{-\infty}^{+\infty} dE_1 \exp\left\{-\frac{\left(E_1-E\right)^2}{W_c^2}\right\} \\
& \times \frac{1}{\Delta_L\sqrt{\pi}}\int_{-\infty}^{+\infty} dE_2 \exp\left\{-\frac{\left(E_2-E_1\right)^2}{\Delta_L^2}\right\} \\
& \times \frac{1}{W_G\sqrt{\pi}}\int_{-\infty}^{+\infty} dE_3 \exp\left\{-\frac{\left(E_3-E_2\right)^2}{W_G^2}\right\} \\
& \times \frac{1}{\Delta_C\sqrt{\pi}}\int_{-\infty}^{+\infty} dE_4 \exp\left\{-\frac{\left(E_4-E_3\right)^2}{\Delta_C^2}\right\} f\left(E_4\right) \quad ,
\end{aligned}
\qquad \text{(III C1 a.18)}
$$

in which we have combined Eqs. (III C1 a.3), (III C1 a.10), (III C1 a.13), and (III C1 a.16). This formula can be written in the form

$$
f_{all}\left(E\right) \;=\; \frac{1}{\Delta_{all}\sqrt{\pi}}\int_{-\infty}^{+\infty} dE' \exp\left\{-\frac{\left(E'-E\right)^2}{\Delta_{all}^2}\right\} f\left(E'\right) \quad , \qquad \text{(III C1 a.19)}
$$

in which the combined resolution function is found from

$$
\begin{aligned}
& \frac{1}{\Delta_{all}\sqrt{\pi}} \exp\left\{-\frac{\left(E'-E\right)^2}{\Delta_{all}^2}\right\} \;=\; \\
& \quad \frac{1}{W_c\sqrt{\pi}}\int_{-\infty}^{+\infty} dE_1 \exp\left\{-\frac{\left(E_1-E\right)^2}{W_c^2}\right\} \times \frac{1}{\Delta_L\sqrt{\pi}}\int_{-\infty}^{+\infty} dE_2 \exp\left\{-\frac{\left(E_2-E_1\right)^2}{\Delta_L^2}\right\} \\
& \quad \times \frac{1}{W_G\sqrt{\pi}}\int_{-\infty}^{+\infty} dE_3 \exp\left\{-\frac{\left(E_3-E_2\right)^2}{W_G^2}\right\} \times \frac{1}{\Delta_C\sqrt{\pi}}\left\{-\frac{\left(E'-E_3\right)^2}{\Delta_C^2}\right\} \quad .
\end{aligned}
\qquad \text{(III C1 a.20)}
$$

It is well-known that the convolution of two or more Gaussians is also a Gaussian, with the variance given by the sum of the variances of the components. This could also be demonstrated by direct integration of Eq. (III C1 a.20).

[In our situation, this is strictly true only if the width $\Delta_L$ of the second Gaussian is independent of the variable of integration $E_1$ of the first Gaussian. Nevertheless, we may approximate $E'$ and $L'$ in our expression for $\Delta_L$, Eq. (III C1 a.8), by $E$ and $L$ since the integrand of Eq. (III C1 a.20) is large only near $E' \cong E$ (i.e., $L' \cong L$).]

The variance for the combined resolution function of Eq. (III C1 a.20) may therefore be written as

$$\Delta_{all}^2 = \frac{2}{3} E^2 \left[ \left( \frac{\Delta t_c}{t} \right)^2 + \left( \frac{\Delta L}{L} \right)^2 \right] + \frac{E^3}{\frac{m}{2} \ln 2} \left( \frac{\Delta t_G}{L} \right)^2 + \Delta_C^2 \quad . \qquad \text{(III C1 a.21)}$$

Replacing $t$ in Eq. (III C1 a.21) by its equivalent in terms of $E$ and $L$ and rearranging give

$$\Delta_{all}^2 = \frac{2}{3} E^2 \left( \frac{\Delta L}{L} \right)^2 + \frac{2}{m} E^3 \frac{2}{3} \left( \frac{\Delta t_c}{L} \right)^2 + \frac{2}{m} E^3 \frac{1}{\ln 2} \left( \frac{\Delta t_G}{L} \right)^2 + \frac{2}{3} E^2 \left( \frac{\Delta L}{L} \right)^2 + \Delta_C^2 \quad , \qquad \text{(III C1 a.22)}$$

which may be rewritten in the form

$$\Delta_{all}^2 = aE^3 + bE^2 + cE^2 + \Delta_C^2 \quad , \qquad \text{(III C1 a.23)}$$

with

$$a = \frac{2}{3} \left( \frac{\Delta L}{L} \right)^2 \quad , \quad b = \frac{2}{m} \frac{2}{3} \left( \frac{\Delta t_c}{L} \right)^2 \quad \text{, and} \quad c = \frac{2}{m} \frac{1}{\ln 2} \left( \frac{\Delta t_G}{L} \right)^2 \quad . \qquad \text{(III C1 a.24)}$$

If $E$ is in units of eV, $\Delta t_G$ in μsec, and $L$ in meters, then neutron mass $m$ may be expressed as

$$m \cong 2 (72.3)^2 \quad . \qquad \text{(III C1 a.25)}$$

This follows directly from $m = 1.67482 \times 10^{-24} g$ and $1 \text{ erg} = g \text{ cm}^2/\text{s}^2 = 6.2418 \times 10^{11} \text{eV}$. With this value for the mass, the parameters in Eq. (III C1 a.23) become

$$a = \left( \sqrt{\frac{2}{3}} \frac{\Delta L}{L} \right)^2 \cong \left( 0.81650 \, \Delta L / L \right)^2 \quad ,$$

$$b = \left( \left( \frac{2}{3} \frac{2}{m} \right)^{1/2} \frac{\Delta t_c}{L} \right)^2 \cong \left( 0.011293 \frac{\Delta t_c}{L} \right)^2 \quad , \qquad \text{(III C1 a.26)}$$

$$c = \left( \left( \frac{2}{m \ln 2} \right)^{1/2} \frac{\Delta t_G}{L} \right)^2 \cong \left( 0.01661 \frac{\Delta t_G}{L} \right)^2 \quad .$$

It should be noted that more accurate values than these are used in the SAMMY code, as discussed in Section IX.A.

**Partial derivatives**

From Eqs. (III C1 a.19) and (III C1 a.22), the partial derivative of cross section (or transmission) $f_{all}$ with respect to the component widths may be found using the chain rule as

$$\frac{\partial f_{all}}{\partial x} = \frac{\partial \Delta_{all}}{\partial x} \frac{\partial f_{all}}{\partial \Delta_{all}} \quad . \tag{III C1 a.27}$$

Partial derivatives of $\Delta_{all}$ are, using Eq. (III C1 a.22) through (III C1 a.24),

$$\frac{\partial \Delta_{all}}{\partial \Delta L} = \frac{E^2 a}{\Delta_{all} \, \Delta L} \quad , \tag{III C1 a.28}$$

$$\frac{\partial \Delta_{all}}{\partial \Delta t_c} = \frac{E^3 b}{\Delta_{all} \, \Delta t_c} \quad , \tag{III C1 a.29}$$

$$\frac{\partial \Delta_{all}}{\partial t_G} = \frac{E^3 c}{\Delta_{all} \, \Delta t_G} \quad , \tag{III C1 a.30}$$

$$\frac{\partial \Delta_{all}}{\partial \Delta_{C1}} = \frac{\Delta_C}{\Delta_{all}} \quad , \tag{III C1 a.31}$$

and

$$\frac{\partial \Delta_{all}}{\partial \Delta_{C2}} = \frac{E \Delta_C}{\Delta_{all}} \quad . \tag{III C1 a.32}$$

The partial derivative with respect to $\Delta_{all}$ is found numerically via

$$\frac{\partial f_{all}}{\partial \Delta_{all}} \cong \frac{f_{all}\left(\Delta_{all} + d\right) - f_{all}\left(\Delta_{all} - d\right)}{2d} \quad , \tag{III C1 a.33}$$

where *d* is set equal to $\Delta_{all}\, q$ with $q = 0.02$ .