III.C.1.c. Resolution broadening: convolution of Gaussian and exponential

Gaussian and exponential resolution broadening may be invoked simultaneously, giving the broadened cross section (or transmission) as

$$f_{GE}\left(E\right)=\frac{1}{\Delta_E\Delta_G\pi}\int_{E-\Delta E_S}^{\infty}dE''\exp\left\{-\frac{\left(E''-\left(E-\Delta E_S\right)\right)}{\Delta_E}\right\} \times\int_{-\infty}^{+\infty}dE'\exp\left\{-\frac{\left(E'-E''\right)^2}{\Delta_G^2}\right\}f\left(E'\right) \quad , \tag{III C1 c.1}$$

where the shift ΔE_S is introduced in order that the maximum of the broadening function be located at $E=E'$.

Rearrangement of the integrands in Eq. (III C1 c.1) and explicit integration over the E^0 variable yield

$$f_{GE}\left(E\right)=\frac{1}{2\Delta_E}\exp\left\{\frac{\Delta_G^2}{4\Delta_E^2}\right\}\int_{-\infty}^{+\infty}dE'\,f\left(E'\right)\exp\left\{-\frac{\left(E'-E+\Delta E_S\right)}{\Delta_E}\right\} \times\operatorname{erfc}\left(\frac{\Delta_G}{2\Delta_E}-\frac{\left(E'-E+\Delta E_S\right)}{\Delta_G}\right) \quad . \tag{III C1 c.2}$$

Historical Note: this is not the form which is given in the MULTI manual [GA74] but is the (correct) form that is used in both the MULTI and the SAMMY codes.

The energy shift ΔE_S is found by setting $g\left(E'\right)=\exp\left(.\right)\operatorname{erfc}\left(.\right)$ from the integrand of Eq. (III C1 c.2) and locating the value of $E'_{\max}$ for which $g\left(E'_{\max}\right)$ is a maximum by setting $dg/dE'=0$ at that value. This value $E'_{\max}$ is then set equal to *E*, and the resulting equation solved for ΔE_S. Newton's method is used to find the solution.

Alternatively, one can assume that the energy shift is zero. This requires the inclusion of a line in the INPut file reading

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DO NOT SHIFT ENERGY for exponential tail on resolution broadening
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The lower and upper integration limits in Eq. (III C1 c.2) are truncated to $E-5\Delta_G$ and $\max\left(E+6.25\Delta_E\,,\,E+5\Delta_G\right)$, respectively.

Partial derivatives

Derivatives of the broadened cross section (or transmission) f_{GE} with respect to Δt_G, ΔL, or Δt_E are found exactly as in the previous two subsections, with f_G and $f_{\exp}$ replaced by f_{GE}.