APPENDIX D

Resonance Region Formulae

D.1. The resolved resonance region

The following resonance formalisms are given for a particular isotope in the laboratory system, without Doppler broadening.

D.1.1. Single-Level Breit-Wigner (SLBW): LRU=1, LRF=1

D.1.1.1. Elastic Scattering Cross Sections[1]

$$\sigma_{n,n}(E) = \sum_{l=0}^{NSL-1} \sigma_{n,n}^{l}(E) ,$$

where

$$\sigma_{n,n}^{l}(E) = (2l+1)\frac{4\pi}{k^2}\sin^2\phi_l + \frac{\pi}{k^2}\sum_J g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr}^2 - 2\Gamma_{nr}\Gamma\sin^2\phi_l + 2(E-E'_r)\Gamma_{nr}\sin 2\phi_l}{(E-E'_r)^2 + \frac{1}{4}\Gamma_r^2}$$

The hard-sphere phase shifts φ_l, the wave number k, the primed resonance energy E'_r, the neutron width Γ_{nr}, and through it the total width Γ_r, are all functions of energy, $\varphi_l(E)$, k(E), $E'_r(E)$, $\Gamma_{nr}(E)$, and $\Gamma_r(E)$, but this dependence is not shown explicitly. Also, each resonance parameter carries the implicit quantum numbers *l* and J, determined by the appropriate entries in the ENDF/B file. In case a given pair (*l*,J) is compatible with two different values of the channel spin, s, the width is a sum over the two partial channel spin widths. This allows one to omit an explicit sum over channel spin when defining the cross sections.

D.1.1.2. Radiative Capture Cross Section

$$\sigma_{n,\gamma}(E) = \sum_{l=0}^{NLS-1} \sigma_{n,\gamma}^{l}(E)$$

where

$$\sigma_{n,\gamma}^{l}(E) = \frac{\pi}{k^2}\sum_J g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr}\Gamma_{\gamma r}}{(E-E'_r) + \frac{1}{4}\Gamma_r^2}$$

and $\Gamma_{\gamma r}$, the radiative capture width, is constant in energy

[1] Processing codes should sum the cross section, as shown, from *l*=0 to *l*=NLS-1, including any "empty" or "non-resonant" channels, in order to get the potential-scattering contribution. If higher *l*-values contribute to the scattering in the resonance region, it is the responsibility of the evaluator to provide a suitable File 3 contribution. (See Sections 2.4.23 and 2.4.24.)

D.1.1.3. Fission Cross Section

$$\sigma_{n,f}(E) = \sum_{l=0}^{NLS-1} \sigma_{n,f}^{l}(E) \quad ,$$

where

$$\sigma_{n,f}^{l}(E) = \frac{\pi}{k^2} \sum_{J} g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr}\Gamma_{fr}}{\left(E - E'_r\right)^2 + \frac{1}{4}\Gamma_r^2}$$

and Γ_{fr}, the fission width, is constant in energy.

D.1.1.4. The Competitive Reaction Cross Section.

The competitive reaction cross section, $\sigma_{n,x}(E)$, is given in terms of analogous formulas involving Γ_{xr}, the competitive width. By convention, the cross section for the competitive reaction is given entirely in File 3, and is not to be computed from the resonance parameters. The reason for this is that the latter calculation can be done correctly only for a single competitive channel, since the file can define only one competitive width.

The statistical factor $g_J = (2J+1)/2(2I+1)$ is obtained from the target spin I and the resonance spin J given in File 2 as SPI and AJ, respectively.

The sum on *l* extends over all *l*-values for which resonance parameters are supplied. There will be NLS terms in the sum. NLS is given in File 2 for each isotope. In general, ENDF/B resonance files are limited to *l*=0, 1, and 2, so that the potential-scattering contribution will be represented by hard-sphere scattering up to the energy where f-wave (*l*=3) potential scattering starts. At that point, the evaluator may have to supply File 3 scattering to simulate the higher *l*-values. He may also require a File 3 contribution at lower energies to represent any differences between hard-sphere scattering and experiment.

The sum on J extends over all possible J-values for a particular *l*-value. NR_J is the number of resonances for a given pair of *l* and J values and may be zero. NRS is the total number of resonances for a given *l*-value and is given in File 2 for each *l*-value.

$$NRS = \sum_{J=JMIN}^{J=JMAX} NR_J \ ,$$

where

$$JMAX = l + I + \frac{1}{2}$$

and

$$JMIN = \left| l - I - \frac{1}{2} \right| \quad \text{if } l \geq I$$

$$= \left| I - l - \frac{1}{2} \right| \quad \text{if } I \geq l$$

$$= \left| |I - l| - \frac{1}{2} \right|$$

$\Gamma_{nr}(|E_r|) \equiv GN_r$ is the neutron width, for the r^{th} resonance for a particular value of *l* and J, evaluated at the resonance energy E_r. For bound levels, the absolute value $|E_r|$ is used.

$$\Gamma_{nr} = \frac{P_l(E)\,\Gamma_{nr}\left(|E_r|\right)}{P_l\left(|E_r|\right)}$$

$\Gamma_r = \Gamma_{nr}(E)+\Gamma_{\gamma r}+\Gamma_{fr}+\Gamma_{xr}$ is the total width, a function of energy through Γ_{nr} and Γ_{xr}, since $\Gamma_{\gamma r}$ and Γ_{fr} are constant with respect to energy. The "competitive" width, Γ_{xr} is not entered explicitly in File 2. It is calculated from the equation:

$$\Gamma_{xr} = \Gamma_r - \Gamma_{nr} - \Gamma_{\gamma r} - \Gamma_{fr} \quad \text{at} \quad E = E_r$$

The following quantities are given in File 2 for each resonance:

E_r = ER, the resonance energy
J = AJ, the angular momentum ("spin") of the resonance state
I = SPI, the angular momentum ("spin") of the target nucleus
g_J = statistical factor (2J+1)/2(2I+1)
$\Gamma_{nr}(|E_r|)$ = GN, the neutron width
$\Gamma_{\gamma r}$ = GG, the radiation width
Γ_{fr} = GF, the fission width and
$\Gamma_r(|E_r|)$ = GT, the total width evaluated at the resonance energy.

Since the competitive width Γ_{xr}, is not given, Γ_r should be obtained from File 2 directly, and ***not*** by summing partial widths.

For p-, d- and higher *l*-values, the primed resonance energy E'_r is energy-dependent:

$$E'_r = E_r + \frac{S_l\left(|E_r|\right) - S_l\left(E\right)}{2P_l\left(|E_r|\right)}\,\Gamma_{nr}\left(|E_r|\right).$$

The fact that the shift is zero at ***each*** E_r is an artifact of the SLBW formalism, and implies a different R-matrix boundary condition for each resonance.

The neutron wave number in the center-of-mass system is given as:

$$k = \frac{\sqrt{2m_n}}{\hbar}\,\frac{AWRI}{AWRI + 1.0}\,\sqrt{|E|}\,,$$

where

AWRI = ratio of the mass of a particular isotope to that of the neutron.
E = laboratory energy in eV.

The energy is written with absolute value signs so that the same formula can be used for positive incident neutron energies and for negative (bound state) resonance energies. (When inelastic scattering can occur, resonances below the level threshold are at "negative energy" in the inelastic channel.)

S_l is the shift factor,

$$S_0 = 0, \qquad S_2 = -\frac{18+3\rho^2}{9+3\rho^2+\rho^4},$$

$$S_1 = -\frac{1}{1+\rho^2}, \qquad S_3 = -\frac{675+90\rho^2+6\rho^4}{225+45\rho^2+6\rho^4+\rho^6}.$$

(the quantity ρ is defined below).

For higher *l*-values, S_l is defined by Equation (2.9) in Reference 1. In conventional R-matrix theory, the shift factors are defined differently for negative energies (Reference 1, Equations 2.11a-c). In ENDF, the positive-energy formulas are used, but the absolute value of E is used in SLBW and MLBW. For the Hybrid R-Function, Section 2.2.1.4, all shifts are set to zero, and this is also an option for the General R-matrix, Section D.1.5.2.

P_l is the penetration factor,

$$P_0 = \rho\,, \qquad P_2 = \frac{\rho^5}{9 + 3\rho^2 + \rho^4}\,,$$

$$P_1 = \frac{\rho^3}{1 + \rho^2}\,, \quad P_3 = \frac{\rho^7}{225 + 45\rho^2 + 6\rho^4 + \rho^6}\,.$$

For higher *l*-values, the P_l are defined by Equation (2.9) in Reference 1. In conventional R-matrix theory, the penetrabilities are zero for negative energies. The theory uses the "theoretical" definition of a reduced width, $\Gamma(E)=2P_l(E)\gamma^2$, where E is a channel energy (center-of-mass), and it suffices to say that $P_l(E) = 0$ if $E < 0$.

In ENDF, the "experimental" definition is used, $\Gamma(E)= \Gamma(|E_r|)P_l(E)/P_l(|E_r|)$, and it is necessary to make the convention that a penetrability for a negative ***resonance*** energy is evaluated at its absolute value. A negative kinetic energy can occur in an exit channel if the reaction is exothermic, and in this case $P_l(E < 0)$ is zero.

φ_l is the (negative of a) hard-sphere phase shift,

$$\phi_0 = \hat{\rho}\,,$$

$$\phi_1 = \hat{\rho} - \tan^{-1}\hat{\rho}\,,$$

$$\phi_2 = \hat{\rho} - \tan^{-1}\left\{\frac{3\hat{\rho}}{3 - \hat{\rho}^2}\right\},$$

$$\phi 3 = \hat{\rho} - \tan^{-1}\left\{\frac{\hat{\rho}\left(15 - \hat{\rho}\right)^2}{15 - 6\hat{\rho}^2}\right\}.$$

For higher *l*-values, the φ_l are defined by Equation 2.12 in Reference 1. It is not necessary to evaluate a phase shift at negative energies.

ρ and $\hat{\rho}$ are defined as $k \times$ RADIUS, where RADIUS is defined as follows:

Let a = channel radius in units of 10^{-12} cm
= $0.123\ \mathrm{AWRI}^{1/3} + 0.08$ [2] (D.0)

AP = energy-independent scattering radius, which determines the low-energy scattering cross section. It is given in File 2 following SPI.

AP(E) = energy-dependent scattering radius, given as a TAB1 card preceding the "SPI AP.... NLS..." card.

[2] The channel radius, strictly speaking, involves $A^{1/3}$ (the target mass in amu), and not $(\mathrm{AWRI})^{1/3}$, but as long as the mass of the incident particle is approximately unity, as it is for neutrons, the difference is not important. AWRI = A/m_n, where m_n is the neutron mass (see Appendix H).

If NRO = 0 (AP energy-independent)
NAPS = 0 $\rho = ka$; $\hat{\rho} = k\,AP$
NAPS = 1 $\rho = \hat{\rho} = k\,AP$

If NRO = 1 (AP energy-dependent)
NAPS = 0 $\rho = ka$; $\hat{\rho} = k\,AP(E)$
NAPS = 1 $\rho = \hat{\rho} = k\,AP(E)$
NAPS= 2 $\rho = k\,AP$; $\hat{\rho} = k\,AP(E)$

D.1.2. Multilevel Breit-Wigner (MLBW): LRU=1, LRF=2

The equations are the same as **SLBW**,[3] except that a resonance-resonance interference term is included in the equation for elastic scattering of l-wave neutrons, $\sigma_{n,n}^{l}(E)$:

$$\frac{\pi}{k^2}\sum_J g_J \sum_{r=2}^{NR_J}\sum_{s=1}^{r-1}\frac{2\Gamma_{nr}\Gamma_{ns}\left(\left(E-E_r'\right)\left(E-E_s'\right)+\frac{1}{4}\Gamma_r\Gamma_s\right)}{\left(\left(E-E_r'\right)^2+\left(\Gamma_r/2\right)^2\right)\left(\left(E-E_s'\right)^2+\left(\Gamma_s/2\right)^2\right)}. \tag{D.1}$$

This form, which has $\sim NR_J^2$ energy-dependent terms and can involve a great deal of computer time, may be written in the following form with only NR_J terms: (See Section 2.4.14)

$$\frac{\pi}{k^2}\sum_J g_J \sum_{r=1}^{NR_J}\frac{G_r\Gamma_r+2H_r\left(E-E_r'\right)}{\left(E-E_r'\right)^2+\left(\Gamma_r/2\right)^2} \tag{D.2}$$

where

$$G_r=\frac{1}{2}\sum_{\substack{s=1\\(s\neq r)}}^{NR_J}\frac{\Gamma_{nr}\Gamma_{ns}\left(\Gamma_r+\Gamma_s\right)}{\left(E_r'-E_s'\right)^2+\frac{1}{4}\left(\Gamma_r+\Gamma_s\right)^2}, \tag{D.3}$$

$$H_r=\sum_{\substack{s=1\\(s\neq r)}}^{NR_J}\frac{\Gamma_{nr}\Gamma_{ns}\left(E_r'-E_s'\right)}{\left(E_r'-E_s'\right)^2+\frac{1}{4}\left(\Gamma_r+\Gamma_s\right)^2} \tag{D.4}$$

For the user who does not require ψ- and χ-broadening, the following equations, which are mathematically identical to the MLBW equations, require less computing time: (See Section 2.4.19)

$$\sigma_{n,n}(E)=\sum_{l=0}^{NLS-1}\sigma_{n,n}^{l}(E) \tag{D.5}$$

$$\sigma_{n,n}^{l}(E)=\frac{\pi}{k^2}\sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}}\sum_{J=|l-s|}^{l+s}g_J\left|1-U_{nn}^{lsJ}(E)\right|^2 \tag{D.6}$$

$$U_{nn}^{lsJ}\left(E\right)=e^{-2i\phi_l}\left(1+\sum_{r=1}^{NR_{sJ}}\frac{i\,\Gamma_{nr}^{lsJ}}{E_r'-E-i\,\Gamma_r/2}\right) \tag{D.7}$$

[3] Including footnote on page D.1.

D.1.3 Reich-Moore (R-M): LRU = 1, LRF = 3

This description of the ENDF Reich-Moore formalism differs from previous versions by using notation in closer agreement with References 1 and 5. The dependence of all quantities on channel spin has been made explicit, to support a format extension which permits specifying the individual channel-spin components of the neutron width.

Partial cross sections may be obtained from a collision matrix U_{ab}, which connects entrance channels *a* with exit channels *b*. In ENDF, the formalism is applied to neutron reactions, *a* = *n*:

$$\sigma_{nb} = \frac{\pi}{k^2} g_n \left| \delta_{nb} - U_{nb} \right|^2 \tag{D.8}$$

These partial cross sections are not observable, but must be summed over the appropriate entrance and exit channels to yield observable cross sections. The statistical factor g_n is a result of prior averaging over channels with different magnetic sub-states, since the ENDF formulae apply to unpolarized particles.

In the Reich-Moore formalism, the only reactions requiring explicit channel definitions are elastic scattering and fission; capture is obtained by subtraction (although it is possible to obtain it directly from the collision matrix elements). Neutron channels are labeled by three quantum numbers, *l*, *s*, and *J*. In the ENDF format, *l* runs from zero to NLS-1, the highest *l*-value that contributes to the cross section in the energy range of interest. The channel spin *s* is the vector sum of the target spin *I* and the neutron spin *i* (1/2), and takes on the range of values $|I - 1/2|$ to $I + 1/2$. The total angular momentum *J* is the vector sum of *l* and *s*, and runs from $|l - s|$ to $l + s$. The fission channels do not correspond to individual two-body fission product breakup, but to Bohr-channels in deformation space, which is why two are adequate for describing many neutron-induced fission cross sections. It is not necessary to specify the quantum numbers associated with the two "ENDF-allowed" fission channels, and they can simply be labeled f1 and f2.

If one sums over all incident channels *n* and exit channels *b*, and invokes unitarity, the resulting total cross section can be expressed in terms of the diagonal matrix elements as

$$\sigma_T(E) = \frac{2\pi}{k^2} \sum_{l=0}^{NLS} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} g_J \, \mathrm{Re}\left(1 - U_{lsJ\,lsJ}\right) \tag{D.9}$$

The elastic cross section is obtained by summing the incident neutron channels over all possible *lsJ* values and the exit neutron channels over those quantities $l's'J'$ that have the same ranges as *lsJ*. Conservation of total angular momentum requires that $J' = J$; the ENDF format imposes additional "conservation rules" $l' = l$ and $s' = s$ which are actually just simplifying assumptions, with some basis in theory and experiment. The six-fold summation then reduces to the familiar form

$$\sigma_{nn}(E) = \frac{2\pi}{k^2} \sum_{l=0}^{NLS} \sum_{s=\left|I-1/2\right|}^{I+1/2} \sum_{J=|l-s|}^{l+s} g_J \left|1 - U_{lsJ\,lsJ}\right|^2 . \tag{D.10}$$

The absorption (non-elastic) cross section is obtained by subtraction:

$$\sigma_{abs}(E) = \sigma_T(E) - \sigma_{nn}(E) . \tag{D.11}$$

Fission is obtained from the collision matrix by summing Eq. (D.8) over all incident *lsJ* values and over the two exit fission channels, b = f1 and b = f2,

$$\sigma_f(E) = \frac{2\pi}{k^2} \sum_{l=0}^{NLS} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} g_J \left[\left| U_{nf1}^{lsJ} \right|^2 + \left| U_{nf2}^{lsJ} \right|^2 \right]. \tag{D.12}$$

The Reich-Moore formalism is described in Reference 2. Here we repeat the level-matrix form of the collision matrix as given in the earlier versions of this manual:

$$U_{nb}^{J} = e^{-i(\phi_n + \phi_b)} \left[2\left(\left(I - K \right)^{-1} \right)_{nb} - \delta_{nb} \right] \quad , \tag{D.13}$$

where

$$(I - K)_{nb} = \delta_{nb} - \frac{i}{2} \sum_r \frac{\Gamma_{nr}^{1/2} \Gamma_{br}^{1/2}}{E_r - E - i\Gamma_{\gamma r}/2}. \tag{D.14}$$

Here ϕ_b is zero for fission, $\phi_n = \phi_l$ (defined previously), and the summation is over those resonances r which have partial widths in both of the channels n and b; E_r is the resonance energy; $\Gamma_{\gamma r}$ is the "eliminated" radiation width; Γ_{nr} and Γ_{br} are the partial widths for the r^{th} resonance in channels n and b.

If we define a matrix ρ by the equation

$$\rho_{nb} = \delta_{nb} - \left((1 - K)^{-1} \right)_{nb} \tag{D.15}$$

then the various cross sections take the following forms:

Total:

$$\sigma_T(E) = \frac{2\pi}{k^2} \sum_{l\,s\,J} g_J \left[(1 - \cos 2\phi_l) + 2\mathrm{Re}(\rho_{nn} e^{-2i\phi_l}) \right]. \tag{D.16}$$

Elastic:

$$\sigma_{nn} = \frac{\pi}{k^2} \sum_{l\,s\,J} g_J \left[2 - 2\cos 2\phi_l + 4\mathrm{Re}(\rho_{nn} e^{-2i\phi_l}) - 4\mathrm{Re}(\rho_{nn}) + 4\left|\rho_{nn}\right|^2 \right]. \tag{D.17}$$

Absorption (fission plus capture):

$$\sigma_{n,abs}(E) = \frac{4\pi}{k^2} \sum_{lsJ} g_J \left[\mathrm{Re}(\rho_{nn}) - \left|\rho_{nn}\right|^2 \right] \tag{D.18}$$

Fission:

$$\sigma_{nf}(E) = \frac{4\pi}{k^2} \sum_{lsJ} g_J \left[\left|\rho_{nf_1}\right| + \left|\rho_{nf_2}\right|^2 \right] \tag{D.19}$$

The phase shifts and penetrabilities are evaluated in terms of a and AP as described earlier. The shift factor has been set equal to zero in the above equations ($E_r' \rightarrow E_r$); hence they are strictly correct only for s-wave resonances. Originally, the ENDF Reich-Moore format was used for low-energy resonances in fissile materials, which **are** s-waves. However, it is believed that the "no-shift" formulae can be safely applied to higher l-values also, since the difference in shape between a shifted resonance and one that is not shifted at the same energy has no practical significance.

Footnote 1 applies to the Reich-Moore formalism also. Until this revision, the format did not permit the specification of channel spin; therefore, if an evaluation includes $l > 0$ resonances for $I > 0$ nucleus, it was necessary for the processing codes to include the potential-scattering contributions from the "missing" channels. (It is adequate to arbitrarily assume that the supplied values are for the $s = I - 1/2$ channels, and to use the same potential-scattering radius in the missing $I + 1/2$ channels. See Sections 2.4.23 and 2.4.24.) Having the ability to specify which channel spin is intended does not solve this problem, unless the evaluator actually supplies resonances for both channels. In cases where the data can be fit with all the resonances in the same *s*-channel, the "other one" will still be absent from the ENDF file, since the format stipulates nothing about avoiding missing channels. This is why it is reasonable for the processing codes to run over the triple *lsJ* loop, inserting potential scattering in every channel, and resonances whenever they are supplied.

Note: When both positive and negative AJ values are given in the file, negative AJ implies $s = I - 1/2$ and positive AJ implies $s = I + 1/2$. When AJ = 0, one and only one of $I - 1/2$ or $I + 1/2$ is possible, so the possible ambiguity of ±0 does not arise. In this case $s = l$, parity conservation prevents the occurrence, for a given J, of two s-values differing by one unit.

D.1.4. Adler-Adler (AA): LRU=1, LRF=4

The formulae, taken from References 3 and 4, are given for the total, radiative capture, and fission cross sections. They have been slightly re-cast to make them conform to the definitions used earlier in this Appendix. Furthermore, only the $\boldsymbol{l}$=0 terms are given, consistent with current usage of this formalism. Procedures are discussed in Section 2.4.15. Since only s-waves are considered, higher $\boldsymbol{l}$-wave contributions to the potential scattering must be put into File 3 by the evaluator.

1. Total Cross Section:

$$\sigma_T(E) = \frac{4\pi}{k^2}\sin^2\phi_0 + \frac{\pi\sqrt{E}}{k^2}\left[\sum_{r=1}^{NRS}\frac{\nu_r\left(G_r^T\cos 2\phi_0 + H_r^T\sin 2\phi_0\right) + \left(\mu_r - E\right)\left(H_r^T\cos 2\phi_0 - G_r^T\sin 2\phi_0\right)}{\left(\mu_r - E\right)^2 + \nu_r^2}\right. \quad \text{(D.20)}$$
$$\left. + AT_1 + AT_2/E + AT_3/E^2 + AT_4/E^3 + BT_1E + BT_2E^2\right].$$

2. Radiative Capture Cross Section:

$$\sigma_{n,\gamma}(E) = \frac{\pi\sqrt{E}}{k^2}\left[\sum_{r=1}^{NRS}\frac{\nu_r G_r^{\gamma} + \left(\mu_r - E\right)H_r^{\gamma}}{\left(\mu_r - E\right)^2 + \nu_r^2}\right. \quad \text{(D.21)}$$
$$\left. + AC_1 + AC_2/E + AC_3/E^2 + AC_4/E^3 + BC_1E + BC_2E^2\right]$$

3. Fission Cross Section:

$$\sigma_{n,f}(E) = \frac{\pi\sqrt{E}}{k^2}\left[\sum_{r=1}^{NRS}\frac{\nu_r G_r^{f} + (\mu_r - E)H_r^{f}}{(\mu_r - E)^2 + \nu_r^2}\right. \quad \text{(D.22)}$$
$$\left. + AF_1 + AF_2/E + AF_3/E^2 + AF_4/E^3 + BF_1E + BF_2E^2\right]$$

Although the format uses different names for μ and ν for each reaction, they are equal:

$DET_r = DEF_r = DEC_r = \mu_r$

$DWT_r = DWF_r = DWG_r = \nu_r$

D.1.5. General R-Matrix (GRM): LRU = 1, LRF=5

D.1.5.1. Calculation of the R-matrix elements

The basic element in an R-matrix calculation is the contribution of a single resonance to the R-matrix,

$$R_{c,d,\lambda} = \frac{\gamma_{\lambda,c}\,\gamma_{\lambda,d}}{E_\lambda - E_{c.m.} - (i/2)\Gamma_{\gamma,\lambda}}$$

or in terms of the laboratory quantities defined in Section 2.2.1.4.2,

$$R_{c,d,\lambda} = \frac{AG_{\lambda,c}\,AG_{\lambda,d}}{ER_\lambda - E_{lab} - (i/2)\,GG_\lambda}$$

The matrix itself is obtained by summing over the appropriate λ-values and adding in the background R-matrix:

$$R_{c,d} = \Sigma_\lambda R_{c,d,\lambda} + RBK_{c,d}\,.$$

If there are altogether N channels, then the calculation will involve N(N + 1)/2 distinct R-matrix elements, $R_{c,d}$, since the matrix is symmetric. Those elements with different J and π in the two channels are zero, and the remaining ones can be rearranged in diagonal blocks labeled by J and π. The information needed to compute the elements of each block is contained in the spin-group list, together with the background R-matrix list, which specifies how the evaluation deals with distant-level effects.

Since the format gives the channel indices for each spin-group, i.e., each Jπ sub-matrix, explicitly in the spin-group list, the using code is relieved of the necessity of doing any angular momentum bookkeeping. The evaluator needs to be concerned with the details of the multiple sums over $\boldsymbol{l}, \boldsymbol{l'}$, s, s′, and J, but the user needs only to invert the sub-matrices specified by each spin-group, and then sum the partial cross sections according to the MT-list. Unlike the SLBW, MLBW, and Reich-Moore formalisms, here the burden of specifying ***all*** the necessary channels is on the evaluator, not the processing codes.

Following the usual procedure, the background R-matrix is assumed to be diagonal and non-zero only in the incident neutron channels, i.e., those for which PMT=SMT=2 in the spin-group list.

$$RBK_{c,d} = RBK_n \delta_{c,n} \delta_{c,d}\,,$$

where n stands for an incident neutron channel.

Three different representations are allowed for the background R-matrix:

a. a tabulated complex function of the energy,

b. the logarithmic parameterization used in SAMMY,

$$\begin{aligned} RBK_n \quad &= R0_n + R1_n\,E + R2_n\,E^2 - S1_n\,[EU_n - ED_n] \\ &\quad - [S0_n + S1_n\,E]\;\boldsymbol{ln}[\{EU_n - E\}/\{E - ED_n\}] \end{aligned}$$

c. a statistical parameterization using R_∞ (RIN), a strength function (SF), the energy interval (INT) over which the explicit resonances are given, the interval midpoint (EBAR) and an average gamma width (AVGG) over that interval (references 6 and 10):

$$\begin{aligned} RBK_n \;=\; & RIN_n + 2SF_n \Big[\operatorname{arctanh}[2\,(E - EBAR)/INT] \\ & + i\,[AVGG\;INT/\{(INT)^2 - 4(E - EBAR)^2\}] \Big] \end{aligned}$$

D.1.5.2. Calculation of the U-matrix elements

The collision, or U-matrix, is obtained by the usual inversion formula from the R-matrix:

$$U = \Omega\, P^{1/2}\, [1 - R\,(L - B)]^{-1}\, [1 - R(L^* - B)]\, P^{-1/2}\, \Omega$$

$$\Omega = exp\,(-i\theta)\,, \quad L = S + iP$$

It has the same diagonal block structure as the R-matrix, but its elements are complicated functions of all the R-matrix elements involved in the inversion. In addition to the R-matrix elements, this step in the calculation requires phase shifts, penetrabilities, shift factors, nuclear radii, and boundary-condition parameters. These are specified in the following lists, or are calculated by the using code, depending on the options specified by the evaluator.

As an option, the shift factor may be set to zero. In R-matrix theory, the shift factor occurs because the underlying complete set of nuclear states on which the theory is built do not coincide with the actual nuclear states, due to the artificial boundary condition imposed on the former. In practice, only the ***form*** of the theory is used, and not its basic theoretical content, so that for neutron cross section evaluation in ENDF, the shift is an irrelevant artifact and can be ignored. It is true that a shifted and a resonance that is not shifted fitted to the same experimental data will have slight shape differences, but these will have no technological significance. Eliminating the shift also removes one barrier to the use of R-matrix parameters in multigroup slowing-down and self-shielding codes, which naively assume that a resonance energy ER will be associated with a Lorentzian bump at that energy. Anti-resonances, and strange channel-interference patterns will still cause problems in such applications, but will at least occur in the expected locations.

For the same reason, it is recommended that the boundary-condition parameter be set to zero. With S = B = 0, the above formula reduces to

$$U = \Omega\, P^{1/2}\, [1 - iRP]^{-1}\, [1 + iRP]\, P^{-1/2}\, \Omega$$

which can often reproduce experimental data as well as the more general form above.

It is assumed that the phase shifts in

$$\Omega = exp\,(-i\theta)$$

are either hard-sphere values, or the ones defined in the phase-shift list. That is, hard-sphere values are assumed to be ***included*** in the tabulated values, and are not to be added by the user.

D.1.5.3. Calculation of the channel cross section

Each element of a U-sub-matrix, $U_{c,d}$, defines a channel-to-channel cross sections,

$$\sigma_{c,d} = \frac{\pi g_c}{k^2} \left| \delta_{c,d} - U_{c,d} \right|^2$$

These cross sections are not observable, but are the ingredients for ones that are. The statistical factor depends on *c* through *J*.

D.1.5.4. Calculation of the PMT-cross sections (Particular MT-values)

An observable PMT-cross section is obtained by summing the channel-to-channel cross section over all the incident channels, and over those exit channels belonging to a particular MT-value, PMT. Both of these summations are defined by the MT-list, which tells which channels are incident, SMT=PMT=2, and which channels belong to each PMT. The code used needs only to keep track of the indices, and is not required to book keep the angular momentum quantum numbers.

$$\sigma_{PMT} = \Sigma_{c \text{ in } n,\ d \text{ in } PMT}\ \sigma_{c,d}$$

D.1.5.5. Calculation of the SMT-cross sections (Summed MT-values)

The complete reaction cross sections, corresponding to the summed-MT's, are then obtained by summing over the appropriate PMT's. The MT-list specifies which PMT's belong to each SMT.

$$\sigma_{SMT} = \Sigma_{PMT\ in\ SMT}\, \sigma_{PMT}$$

The elastic cross section, SMT=2, is the same as its only component, σ(PMT=2). The same is true of the fission cross section, SMT=PMT=18.

D.1.5.6. Calculation of the total cross section

The total cross section is obtained from the diagonal elements corresponding to the incident channels. It cannot be obtained by summing partial cross sections because radiative capture is not calculated according to the above scheme, but is treated as an eliminated channel. Hence its cross section is not available for summing.

$$\sigma_{TOT} = \sum_{c\,\mathrm{in}\,n} \frac{2\pi g_c}{k^2}\left[\, 1 - \mathrm{Re}\, U_{c,c} \,\right]$$

The summation here is over all channels belonging to SMT=PMT=2.

D.1.5.7. Calculation of the capture cross section

This is obtained as the total cross section minus the sum of all the SMT-cross sections:

$$\sigma_{CAP} = \sigma_{TOT} - \Sigma_{SMT}\, \sigma_{SMT}$$

If the eliminated width were read in as the sum of the capture width and some other reaction width(s), the above difference cross section would correspond to the sum of those reactions. This fact is exploited in the Hybrid R-function formalism to simplify the treatment of competitive reactions, which often do not require the complication of a full R-matrix treatment.

D.1.5.8. Calculation of the absorption cross section

$$\sigma_{ABS} = \sigma_{TOT} - \sigma_{SMT=2}$$

If the inelastic cross section, $\sigma_{SMT=4}$, is not zero, it is necessary also to subtract it.

D.1.5.9. Calculation of the angular distributions

These may be found from the Blatt and Biedenharn formalism. However, the summations required do not lend themselves to expression in terms of channel indices, the way the integrated cross sections do. If the angular distributions are calculated directly from the scattering amplitudes, one has to deal with magnetic quantum numbers in addition to α, *l*, s, and J. If one eliminates the magnetic quantum numbers ala Blatt and Biedenharn, the sums over *l*, s, and J are each treated differently and do not stay together in neat channel packages. To utilize these formulas, it is necessary to pick apart the c's and d's and extract the quantum numbers. The format has not been optimized for that, although the information is contained in the MT- and spin-group-lists. To use the angular distribution formula, the code needs to perform the indicated 9-fold summation, and to locate a given U-matrix element from its seven arguments α_1, α_2, l_1, l_2, s_1, s_2, and J. To facilitate the summation, the limits are given explicitly in the following paragraph.

Using a normalization in which B_0 is also the angle-integrated cross section, the Blatt and Biedenharn formula is[4]

$$\frac{d\sigma_{\alpha,\alpha'}}{d\Omega} = \sum_L \frac{2L+1}{4\pi} B_L P_L(\mu)$$

$$B_L = \frac{\pi}{(2i+1)(2I+1)(2L+1)\,k^2} \sum \left\{ ss' l_1 l'_1 l_2 l'_2 J_1 J_2 \right\}$$
$$\times (-1)^{s-s'} \overline{Z}_{l_1 J_1 l_2 J_2; sL} \overline{Z}_{l'_1 J_1 l'_2 J_2; s'L}$$
$$\times \left[\delta_{\alpha l_1 s, \alpha' l'_1 s'} - U_{\alpha l_1 s J_1, \alpha' l'_1 s' J_1} \right]$$
$$\times \left[\delta_{\alpha l_2 s, \alpha' l'_2 s'} - U_{\alpha l_2 s J_2, \alpha' l'_2 s' J_2} \right]$$

where $P_L(\mu)$ is a Legendre polynomial in $\cos \theta_{\alpha\alpha'}$, and

$$Z_{l_1 J_1 l_2 J_2; sL} = \sqrt{(l_1+1)(2l_2+1)(2J_1+1)(J_2+1)} \times (l_1 l_2 00; L0\ )\, W(l_1 J_1 l_2 J_2; sL)$$

$(l_1 l_2 00; L0)$ and *W* are the Clebsch-Gordan and Racah coefficients.

From outside to inside, the sum limits are

1) $0 \le L \le 2*(NLSC-1)$, where NLSC-1 is a cutoff value chosen by the evaluator to converge the angular distributions. (See Sections 2.4.23 and 2.4.24).
2) $|I - i| \le s \le I + i$ (incident spins)
3) $|I' - i'| \le s' \le I' + i'$ (exit spins)
4) $0 \le l_1 \le NLSC-1$
5) $0 \le l'_1 \le NLSC-1$
6) $|L - l_1| \le l_2 \le \min\{NLSC-1, L+l_1\}$
7) $|L - l'_1| \le l'_2 \le \min\{NLSC-1, L+l'_1\}$
8) $\max\{|l_1 - s|, |l'_1 - s'|\} \le J_1 \le \min\{l_1 + s, l'_1 + s'\}$
9) $\max\{|l_2 - s|, |l'_2 - s'|, |L - J_1|\} \le J_2 \le \min\{l_2 + s, l'_2 + s', L + J_1\}$

D.1.6 Hybrid R-function (HRF): LRU=1, LRF=6

The formulae are from standard R-matrix theory, References 1, 5, and 6, augmented by the single-level Breit-Wigner formalism for the calculation of competitive reactions. The mixing of the two methods is indicated by the term "hybrid." As in the previous section, D.1.5, R, S, and U are center-of-mass quantities, written in terms of laboratory widths and energies.

[4] Sum variables in curly brackets. This formula is not applicable to either capture or fission. Both $d\sigma/d\Omega$ and B_L are center-of-mass quantities, in terms of laboratory widths and energies.

D.1.6.1. Elastic Scattering Cross Section

$$\sigma_{n,n}(E) = \sum_{l=0}^{NLS-1} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} \sigma_{n,n}^{lsJ}(E)$$

$$\sigma_{n,n}^{lsJ}(E) = \frac{\pi}{k^2} g_J \left|S_{lsJ}(E)\right|^2$$

where $S_{lsJ}(E) \equiv 1 - U_{lsJ}(E)$

$$U_{lsJ}(E) = \exp(-2i\delta_{lsJ}) \frac{1 + iP_{lsJ}(E) R_{lsJ}(E)}{1 - iP_{lsJ}(E) R_{lsJ}(E)}, \text{ and}$$

$$S_{lsJ}(E) = \frac{(1 - \exp(-2i\delta_{lsJ})) - iP_{lsJ}(E) R_{lsJ}(E)(1 + \exp(-2i\delta_{lsJ}))}{1 - iP_{lsJ}(E) R_{lsJ}(E)}$$

$$R_{lsJ}(E) = \sum_{r=1}^{NLSJ} \frac{\Gamma_{nr}(|E_r|)}{2P_{lsJ}(|E_r|)\left[E_r - E - i\Gamma_{er}(|E_r|)/2\right]} + R_{lsJ}^0(E)$$

The eliminated width, Γ_{er}, in the denominator of the R-function is a constant, evaluated at the resonance energy. It is the sum of the partial widths for capture and competitive reactions (see Section 2.2.1-4). Its omitted energy-dependence has a negligible effect on the shape of the elastic resonances. If the flag LPS is 0, the phase shift δ_{lsJ} will be calculated from the hard-sphere formulas. If LPS=1, tabulated phase shifts will be supplied in every channel. This permits parameterization of optical-model evaluations. Hard-sphere values depend on the channel- dependent radius AC. The formulas of section D.1.1 are used with $\rho = \hat{\rho} = k \times AC$ being dependent on *l*, s and J. Note that the above equations are all scalar. No matrix inversion is required. The background R-function $R_{lsJ}^0(E)$, if supplied, must be tabulated, although the analytic formulae of Section 2.2.1.4.3 may be used as a guide.

As in the footnote on page D.1, the processing codes must sum over all channels, whether they contain resonances or not. The evaluator must specify suitable values of NLS and NLSC to converge the cross-section and angular-distribution calculations.

D.1.6.2. Partial Reaction Cross Sections

The following formulas are the same as SLBW, except that an explicit sum on channel spin has been introduced, so that the same J-value can occur in two different channels, $l s_1 J$ and $l s_2 J$:

$$\sigma_{n,x}(E) = \sum_{l=0}^{NLS-1} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} \sigma_{n,x}^{lsJ}(E)$$

$$\sigma_{n,x}^{lsJ}(E) = \frac{\pi}{k^2} g_J \sum_{r=1}^{NLSJ} \frac{\Gamma_{nr}(E)\Gamma_{xr}(E)}{\left(E - E'_r\right)^2 + \frac{1}{4}\Gamma_r^2} \quad ,$$

x can represent any of four reaction types:

a) Radiative capture

$\Gamma_{xr}(E) = \Gamma_{\gamma r}$, a constant in energy

b) Fission

$\Gamma_{xr}(E) = \Gamma_{fr}$, a constant in energy. This convention is the same as that used in the SLBW and MLBW formalisms.

c) Inelastic scattering

$$\Gamma_{xr}(E) = \Gamma_{n'r} \frac{P_{l'}(E - E_p^*)}{P_{l'}(|E_r - E_p^*|)}.$$

E_p^* is the laboratory threshold energy for exciting the p[th] level in the target nucleus. It is determined from the Q-value in File 2 (QRE_n) by

$$E_p^* = -\frac{AWRI + 1}{AWRI} Q.$$

$P_{l'}$ is to be calculated using the AC values for the first channel in the file. The prime on the subscript l denotes the fact that an inelastically-scattered neutron may have a different l-value from the incident neutron. l' is the library quantity $ALRE_n$. AWRI is the same as for the incident neutron, because the reduced mass in an inelastic channel is (essentially) the same as in the incident channel. $P_{l'}$ is zero if its argument is a negative incident energy. If its argument is a negative resonance energy, $P_{l'}$ is evaluated at the absolute value of its argument.

d) Charged-particle scattering

The charged-particle penetrability will be supplied by the evaluator as a tabulated function of the incident neutron's laboratory energy. The conversion from the charged-particle channel energy to the neutron's energy is discussed in Section D.3.1(c). This choice of energy eliminates the need for the user to do any conversion, and the energy-dependent charged-particle exit width is simply

$$\Gamma_{xr}(E) = \Gamma_{cpr} \frac{P_{cpl's'J'}(E)}{P_{cpl's'J'}(|E_r|)}$$

The choice also eliminates the need to specify an exit mass ratio, AWRIC, an exit Q-value, or an exit channel radius, as these are incorporated by the evaluator into the tabulated penetrability.

D.1.6.3. Total Reaction Cross Section

This is calculated as the sum of the above partial reaction cross sections,

$$\sigma_R(E) = \sum_x \sigma_{n,x}(E).$$

In the important case that radiative capture is the only reaction specified (NFRE = NIRE = NCRE = 0), the total reaction cross section is also the radiative capture cross section, and is to be calculated from the R-function formula

$$\sigma_{n,\gamma}(E) = \sum_{l=0}^{NLS-1} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} \sigma_{n,\gamma}^{lsJ}(E) \quad ,$$

where

$$\sigma_{n,\gamma}^{lsJ}(E) = \frac{\pi}{k^2} g_J \left(1 - \left| U_{lsJ}(E) \right|^2\right) = \frac{\pi}{k^2} g_J \left[2 \operatorname{Re} S_{lsJ}(E) - \left| S_{lsJ}(E) \right|^2 \right].$$

This formula is applicable also in the "trivial" case of pure elastic scattering (NGRE = NFRE = NIRE = NCRE = 0). This formula, when applicable, eliminates all reference to the SLBW formalism, and reduces the hybrid R-function to a "pure" R-function.

D.1.6.4. Total Cross section

The total cross section is calculated as the sum of the elastic scattering and total reaction cross section defined above,

$$\sigma_T(E) = \sigma_{n,n}(E) + \sigma_R(E)$$

In the two special cases noted in D.1.6.3, the total cross section may also be calculated from the mathematically-equivalent form:

$$\sigma_T(E) = \sum_{l=0}^{NLS-1} \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{J=|l-s|}^{l+s} \sigma_T^{lsJ}(E), \text{ and}$$

$$\sigma_T^{lsJ}(E) = \frac{2\pi}{k^2} g_J \left(1 - \operatorname{Re} U_{lsJ}(E)\right) = \frac{\pi}{k^2} g_J \operatorname{Re} S_{lsJ}(E).$$

These special cases are standard R-function theory, as no use is made of the single-level Breit-Wigner formalism (see Section D.3.3.).

D.1.6.5. The Angular Distribution of Elastically-Scattered Particles

Scattering-matrix theory predicts an angular distribution which varies across a resonance. For some applications this variation might be worth calculating. The general formula of Blatt and Biedenharn, Reference 7, reduced to the present case of an R-function that is diagonal in *l*, s, and J is (center of mass):

$$\frac{d\sigma}{d\Omega} = \sum_{L}^{NLS-1} \frac{2L+1}{4\pi} B_L(E) P_L(\cos\theta) \quad \text{barns/steradian},$$

where

$$B_L(E) = \frac{\pi}{(2i+1)(2I+1)(2L+1)k^2} \sum_{s l_1 l_2 J_1 J_2} \overline{Z}^2(l_1 J_1 l_2 J_2; sL)\, S_{l_1 s J_1}(E)\, S^*_{l_2 s J_2}(E),$$

$$\overline{Z}(l_1 J_1 l_2 J_2; sL) = \sqrt{(2l_1+1)(2l_2+1)(2J_1+1)(2J_2+1)}\, (l_1 l_2 00; L0)\, W(l_1 J_1 l_2 J_2; sL),$$

and *i* is the neutron spin (1/2). Here $(l_1 l_2 00; L0)$ and $W(l_1 J_1 l_2 J_2 l; sL)$ are Clebsch-Gordan and Racah coefficients, respectively.

The limits on the summation variables are as follows, from outside to inside:

1) $0 \le L \le 2$ (NLSC-1), where NLSC-1 is the highest partial wave required to specify the angular distribution. It may be necessary to calculate U_{lsJ} for non-resonant channels which contribute just hard-sphere or optical-model scattering, $U_{lsJ} = \exp(-2i\delta_{lsJ})$.
2) $|I - ½| \le s \le I + ½$
3) $0 \le l_1 \le$ NLSC-1
4) $|L - l_1| \le l_2 \le \min\{\text{NLSC-1}, L + l_1\}$
5) $|l_1 - s| \le J_1 \le l_1 + s$
6) $\max\{|l_2 - s|, |J_1 - L|\} \le J_2 \le \min\{l_2 + s, J_1 + L\}$

D.2. THE UNRESOLVED RESONANCE REGION: LRU=2, LRF=1 or 2

Average resonance parameters are provided in File 2 for the unresolved region. Parameters are given for possible *l*- and J-values (up to d-wave, $l = 2$) and the following parameters may be energy dependent: $D_{l,J}, \overline{\Gamma}^{0}_{nlJ}, \overline{\Gamma}_{\gamma lJ}, \overline{\Gamma}_{flJ}$, and $\overline{\Gamma}_{xlJ}$. The parameters are for the single-level Breit-Wigner formalism. Each width is distributed according to a chi-squared distribution with a designated number of degrees of freedom. The number of degrees of freedom may be different for neutron and fission widths and for different (*l*,J) values. These formulae do not consider Doppler broadening.

D.2.1. Cross Sections in the Unresolved Region

Definitions and amplifying comments on the following are given in Section D.2.2.

a. Elastic Scattering Cross Section

$$\sigma_{n,n}(E) = \sum_{l=0}^{NLS-1} \sigma^{l}_{n,n}(E),$$

$$\sigma^{l}_{n,n}(E) = \frac{4\pi}{k^2}(2l+1)\sin^2\phi_l + \frac{2\pi^2}{k^2}\sum_{J}^{NJS}\left[\frac{g_J}{\overline{D}_{l,J}}\left\langle\frac{\Gamma_n\Gamma_n}{\Gamma}\right\rangle_{l,J} - 2\overline{\Gamma}_{nl,J}\sin^2\phi_l\right]$$

The asymmetric term in $E - E'_r$ is assumed to average to zero under the energy-averaging denoted by $\langle\ \rangle$.

b. Radiative Capture Cross Section

$$\sigma_{n,\gamma}(E) = \sum_{l=0}^{NLS-1} \sigma^{l}_{n,\gamma}(E),$$

$$\sigma^{l}_{n,\gamma}(E) = \frac{2\pi^2}{k^2}\sum_{J}^{NJS}\frac{g_J}{\overline{D}_{l,J}}\left\langle\frac{\Gamma_n\Gamma_\gamma}{\Gamma}\right\rangle_{l,J}$$

c. Fission Cross Section

$$\sigma_{n,f}(E) = \sum_{l=0}^{NLS-1} \sigma^{l}_{n,f}(E),$$

$$\sigma^{l}_{n,f}(E) = \frac{2\pi^2}{k^2}\sum_{J}^{NJS}\frac{g_J}{\overline{D}_{l,J}}\left\langle\frac{\Gamma_n\Gamma_f}{\Gamma}\right\rangle_{l,J}.$$

The sum over l in the above equations extends up to l = 2 or NLS-1 (the highest l-value for which data are given). For each value of l, the sum over J has NJS terms. The number of J-states for a particular l-state will depend on the value of l. NLS and NJS are given in File 2.

The averages are re-written as

$$\left\langle \frac{\Gamma_n \Gamma_n}{\Gamma} \right\rangle_{l,J} = \left(\frac{\overline{\Gamma}_{nl,J} \overline{\Gamma}_{nl,J}}{\overline{\Gamma}_{l,J}} \right) R_{n,l,J}$$

$$\left\langle \frac{\Gamma_n \Gamma_\gamma}{\Gamma} \right\rangle_{l,J} = \left(\frac{\overline{\Gamma}_{nl,J} \overline{\Gamma}_{\gamma l,J}}{\overline{\Gamma}_{l,J}} \right) R_{\gamma l,J} \text{ , and}$$

$$\left\langle \frac{\Gamma_n \Gamma_f}{\Gamma} \right\rangle_{l,J} = \left(\frac{\overline{\Gamma}_{nl,J} \overline{\Gamma}_{fl,J}}{\overline{\Gamma}_{l,J}} \right) R_{fl,J}$$

where $R_{\gamma l,J}$, $R_{fl,J}$ and $R_{nl,J}$ are width-fluctuation factors for capture, fission, and elastic scattering, respectively. Associated with each factor is the number of degrees of freedom for each of the average widths, and the integrals are to be evaluated using the MC^2-II method.

Data given in File 2 for each (l,J) state

$\mu_{nl,J}$ = AMUN, the number of degrees of freedom for neutron widths

$\mu_{fl,J}$ = AMUF, the number of degrees of freedom for fission widths

$\mu_{xl,J}$ = AMUX, the number of degrees of freedom for competitive widths

$\mu_{\gamma l,J}$ = AMUG, the number of degrees of freedom for radiation widths

$\overline{\Gamma}_{x,l,J}$ = GX, the average competitive reaction width

$\overline{\Gamma}^0_{n,l,J}$ = GN0, the average reduced neutron width

$\overline{\Gamma}_{\gamma,l,J}$ = GG, the average radiation width

$\overline{\Gamma}_{f,l,J}$ = GF, the average fission width

$\overline{D}_{l,J}$ = D, the average level spacing

The average neutron widths are defined in Section D.2.2.2, Equation (31c), where $\overline{\Gamma}_{nlJ} = \left\langle \Gamma_n(l,J) \right\rangle$. Degrees of freedom are discussed in Section 2.4.20.

The average total width, at energy E, is

$$\overline{\Gamma}_{l,J} = \overline{\Gamma}_{nl,J} + \overline{\Gamma}_{\gamma l,J} + \overline{\Gamma}_{fl,J} + \overline{\Gamma}_{xl,J} \text{ ,}$$

and all widths are evaluated at energy E. J=AJ, I=SPI, and l=L are given in File 2. The penetration factors and phase shifts are functions of a or AP, as describe earlier.

D.2.2. Definitions for the Unresolved Resonance Region

Editions of ENDF-102 prior to ENDF/B-V have had some errors in the "Definitions" section of Appendix D (previously Section D.2.1). To clarify the points and facilitate parallel reading with Gyulassy and Perkins, Reference 8, their parenthesized indices will be used. Section D.2.3 contains a table of equivalences to the notation used in D.2.1 and Section D.2.4 compares the present discussion with those previously given.

D.2.2.1. Sums and Averages

In an energy interval $\Delta\varepsilon$, let the resonances be identified by a subscript $\lambda = 1, 2, \ldots$ which goes over all the resonances. The present discussion is concerned with the ***combinatorial*** aspects of level sequences, hence λ enumerates ***all*** the resonances, whether their widths are observably large or not. One purpose of this section is to permit estimation of missed resonances by comparing observed level densities or strength functions with the theoretically-expected relations. The latter are concerned with the set of all resonances, and not just those that are observable in a particular experiment.

Let x denote a set of quantum numbers that label a subset of resonances in the interval. If there are N(x) such resonances, their level density is

$$\rho(x) = N(x)/\Delta\varepsilon\,, \tag{D.23}$$

and their level spacing is

$$D(x) = 1/\rho(x)\,. \tag{D.24}$$

If y_λ is some quantity associated with each resonance, λ, the sum of the y-values over the subset x is

$$\sum\nolimits_\lambda^x y_\lambda\,. \tag{D.25}$$

In this section, the summation index λ is written as a subscript, and the range of the summation is indicated by the superscript x. Equation (D.25) says "sum the quantity y over every resonance in the interval $\Delta\varepsilon$ which has the quantum numbers x." Usually, these resonances will possess other quantum numbers too, but it is the set x which determines whether they are included or not.

An ***average*** of the quantity y over the set x is

$$\langle y \rangle^x = \left[1/N(x)\right] \sum\nolimits_\lambda^x y_\lambda \tag{D.26}$$

D.2.2.2. Reduced Widths

In this section, reduced widths follow the experimental definition rather than the theoretical usage $\Gamma = 2P\gamma^2$. A partial width for the decay of a resonance into a particular channel carries many quantum numbers, but we need only three, the total and orbital angular momenta J and *l*, and the channel spin s. The reduced neutron width, $\Gamma^l_{n\lambda}(J,s)$, is defined by:

$$\Gamma_{n\lambda}(l,J,s) = \Gamma^l_{n\lambda}(J,s)\sqrt{E}\;\nu_l(E) \tag{D.27}$$

where $v_l = P_l/\rho$
$v_0 = 1$,
$v_1 = \rho^2/(1+\rho^2)$
$v_2 = \rho^4/(9+3\rho^2+\rho^4)$
and $\rho = ka$, *a* being the channel radius.

Assuming additivity of partial widths,

$$\Gamma^l_{n\lambda}(J) = \Sigma_s \Gamma^l_{n\lambda}(J,s) \tag{D.28}$$

where Σ_s is a summation over the 1 or 2 possible channel-spin values.

If we average over resonances, and assume that the average partial width is independent of channel spin,[5]

$$\left\langle \Gamma^l_n(J) \right\rangle = \sum\nolimits_s \left\langle \Gamma^l_n(J,s) \right\rangle = \mu_{l,J} \left\langle \Gamma^l_n(J,s) \right\rangle \tag{D.29}$$

[5] This is not true for the individual resonances

Equation (D.29) introduces the multiplicity $\mu_{l,J}$, which for neutrons can have the value 1 or 2, depending on whether the channel spin has one or two values. For l=0, or I=0, or J=0, $\mu_{l,J} = 1$. In other cases, s can take on the values I ±1/2 subject to the additional vector sum

$$\vec{s} = \vec{l} + \vec{J} \tag{D.30}$$

which may again restrict $\mu_{l,J}$ to the value one.[6]

The other new notation is the line through the quantum number s, meaning that the quantity $\left\langle \Gamma_n^l(j,\not{s}) \right\rangle$ does not depend on the value of s. This is ***not*** the same as omitting s from the parentheses, since ***that*** defines the left-hand side quantity. This is the primary source of confusion in previous discussions. Since v_l only depends on l,

$$\begin{aligned} \left\langle \Gamma_n(l,J) \right\rangle &= \left\langle \Gamma_n^l(J)\sqrt{E}v_l \right\rangle && \text{a.)} \\ &= \mu_{l,J} \left\langle \Gamma_n^l(J,\not{s})\sqrt{E}v_l \right\rangle && \text{b.)} \\ &= \mu_{l,J} \left\langle \Gamma_n^l(J,\not{s}) \right\rangle \overline{\sqrt{E}v_l} && \text{c.)} \end{aligned} \tag{D.31}$$

where the bar over $\sqrt{E}v_l$ denotes some average value appropriate to the interval.

D.2.2.3. Strength Function

The pole-strength function was originally introduced as an average over the R-matrix reduced widths for a given channel, γ_c^2. Using the experimental convention.

$$S(l,J,s) = \left\langle \Gamma_n^l(J,s) \right\rangle^{l,J,s} \Big/ D(l,J,s)\,. \tag{D.32}$$

Since the channel spin values are uniquely determined by J and l, together with the target spin I which is common to all the resonances, s is superfluous in defining the subset over which the average is taken, and

$$S(l,J,s) = \left\langle \Gamma_n^l(J,s) \right\rangle^{l,J} \Big/ D(l,J)\,. \tag{D.33}$$

If the parity π were used as an explicit quantum number, l could be dropped,

$$S(l,J,s) = \left\langle \Gamma_n^l(J,s) \right\rangle^{J,\pi} \Big/ D(J,\pi)\,, \tag{D.34}$$

because l and π are equivalent for labeling resonances. That is, every resonance with a given J and π will have channels labeled by the same set of l-values, whether their partial widths are observably large or not. Some authors go one step further and drop π, so that J ***means*** J,π, but that is an invitation to confusion.

Expressing S(l,J,s) as a sum over reduced widths gives

$$S\left(l,J,\not{s}\right) = \sum_{\lambda}^{l,J} \Gamma_{n\lambda}^{l}(J,s)/\Delta\varepsilon \tag{D.35}$$

where we use the assumed independence of $\left\langle \Gamma_n^l(J,\not{s}) \right\rangle$ on s to get the same result on the left-hand-side.

[6] For example, if I = 1/2, $\mu_{1,2} = 1$.

The strength function S(l,J) is defined as

$$\begin{aligned} S(l,J) &= \sum_s S(l,J,s) && \text{(a)} \\ &= \mu_{l,J}\, S(l,J,s) && \text{(b)} \end{aligned} \tag{D.36}$$

The corresponding sum and average forms are

$$\begin{aligned} S(l,J) &= \sum_{\lambda}^{l,J} \Gamma_{n\lambda}^{l}(J)\big/\Delta\varepsilon && \text{(a)} \\ &= \left\langle \Gamma_n^l(J)^{l,J} \right\rangle \Big/ D(l,J) && \text{(b)} \end{aligned} \tag{D.37}$$

The next "natural" summation would be to collect the different l-contributions to the total width, to form S(J), but this is not what is observable. Instead one defines S(l) as a weighted sum of the S(l,J,s):

$$S(l) = \frac{\sum_{Js} gS(l,J,s)}{\sum_{Js} g} \tag{D.38}$$

This equation occurs in Lynn, Reference 1, as 6.126, with a confusing typographical error, namely the index s is missing from S(l,J,s).

Actually, the strength function was introduced first in the "s-wave" form

$$S(0) = \sum_{\lambda}^{l=0} (g\Gamma_n^0)_\lambda \big/ D \;(l=0) \tag{D.39}$$

and later generalized by Saplakoglu et al. Reference 9, to the p-wave form

$$S(1) = (1/\Delta\varepsilon)(2l+1)^{-1} \sum_{\lambda}^{l=1} (g\Gamma_n^1)_\lambda \,. \tag{D.40}$$

For expository purposes, it is clearer to start from (31). The sum on J and s is for fixed l:

$$\sum_{Js} \;\equiv \sum_{s=I-\frac{1}{2}}^{I+\frac{1}{2}} \;\sum_{J=|l-s|}^{l+s} \;. \tag{D.41}$$

It is important to note that the outer sum on channel spin is correct as written. It goes over the values I±½ if I≥½ , and over the single value ½, if I=0. It is ***not*** further constrained by Equation (D.30) because now ***it*** is the "independent variable." The inner sum on J enumerates some J-values once, and some twice, the latter occurring when both s-values can produce that J-value. The number of times J occurs is the same $\mu_{l,J}$ that appeared previously.

If we are summing a quantity that is independent of s, then (D.41) can be rewritten:

$$\Sigma_{Js}\, y(\not{s}) = \widetilde{\Sigma}_{l,J}\, \mu_{lJ}\, y(\not{s}) \tag{D.42}$$

The multiplicity $\mu_{l,J}$ takes care of the sum on s, and the tilde over the sum on J, as emphasized by Gyulassy and Perkins, Reference 8, reminds us that J goes over its full range, "once-only":[7]

$$\begin{aligned} \sum_J^{\sim} &= \sum_{J=\left|l-I-\frac{1}{2}\right|}^{l+I+\frac{1}{2}} && \text{if } l \geq I \qquad \text{(a)} \\ &= \sum_{J=\left|I-l-\frac{1}{2}\right|}^{l+I+\frac{1}{2}} && \text{if } I \geq l \qquad \text{(b)} \end{aligned} \tag{D.43}$$

[7] Reference 8 has this written incorrectly.

The denominator in Equation (D.38) can be shown to be

$$\Sigma_{Js}\, g = 2l+1\,, \tag{D.44}$$

or, since g is independent of s,

$$\widetilde{\Sigma}_J\, \mu_{l,J}\, g = 2l+1\,. \tag{D.45}$$

G-P assume, and later approximately justify by comparison to experiment, that S(l,J,s) is also independent of J. With this, Equation (D.38) becomes

$$\begin{aligned} S(l) &= (2l+1)^{-1} \sum\nolimits_{Js}\; gS(l,\not{J},\not{s}) = S(l,\not{J},\not{s}) \quad \text{(a)} \\ &= S\left(l,J\right)\big/\mu_{l,J}\,, \qquad\qquad\qquad\quad \text{(b)} \end{aligned} \tag{D.46}$$

using Equation (D.36.b).

Note the peculiar fact that S(l) and S(l,J,s) are independent of J, but S(l,J) is not. This is a consequence of the fact that more than one channel spin value can contribute to S(l,J), inducing a "J-dependence" in the form of a possible factor of two.

As a sum over resonances,

$$\begin{aligned} S(l) &= (2l+1)^{-1}\; \sum\nolimits_{Js}\; gS(l,\not{J},\not{s}) \qquad\qquad \text{(a)} \\ &= (2l+1)^{-1} \sum\nolimits_{Js}\; \sum\nolimits_{\lambda}^{l,J} g\,\Gamma_{n\lambda}^{l}(J,s)/\Delta\varepsilon \qquad \text{(b)} \\ &= (2l+1)^{-1}\; \widetilde{\Sigma}_J\; \sum\nolimits_{\lambda}^{l,J} g\,\Gamma_{n\lambda}^{l}(J)/\Delta\varepsilon \quad\,, \qquad \text{(c)} \end{aligned} \tag{D.47}$$

The right hand side of Equation (D.47c) says to sum $\Gamma^{l}_{n\lambda}$(J) over all possible values of J, which is what is meant by Equations (D.39) and (D.40). We can suppress the explicit J's and write, as in Equation (D.40),

$$S(l) = (1/\Delta\varepsilon)\,(2l+1)^{-1}\; \Sigma_{\lambda}^{l}\,(g\Gamma_{n\lambda}^{l})_{\lambda} \tag{D.48}$$

but we have to remember that Γ^{l}_{n} is still Γ^{l}_{n}(J), and not a new quantity.

As an average, using the same convention,

$$S(l) = (2l+1)^{-1}\, \left\langle g\Gamma_{n}^{l} \right\rangle^{l} \Big/ D(l) \quad . \tag{D.49}$$

Otherwise, all the notation is correct: D(l) is the spacing of l-wave resonances without regard to their J-values, and the average $\langle\,\rangle^{l}$ goes over all resonances possessing the quantum number l, again without regard for their J-values. It is worth noting explicitly that although S(l,J) is "almost" independent of J, this is not true of $\left\langle \Gamma_{n}^{l}(J) \right\rangle$. As Equation (37b) shows, its J-dependence is canceled by the J-dependence of D(l,J), up to the factor $\mu_{l,J}$. This property is what makes strength functions useful.

D.2.2.4. Level Spacings

G-P emphasize that

$$\rho(l) = \widetilde{\Sigma}_J\, \rho(l,J) \tag{D.50}$$

which, together with the assumption

$$\rho(l,J) = K(l)(2J+1)\;, \tag{D.51}$$

leads to

$$\rho(l) = \rho(l,J)\,\frac{(2l+1)}{g}\,\omega_{I,l}\,, \tag{D.52}$$

where

$$\begin{aligned} \omega_{I,l} &= (l+1)/(2l+1) \quad \text{for } l \le I \\ &= (I+1)/(2I+1) \quad \text{for } l \ge I \end{aligned} \tag{D.53}$$

and is unity if l=0 or I=0.

The reader is referred to Reference 8 for a fuller discussion but here we can point out that, for a given parity, $\rho(l,J)$ is independent of l, by definition. As noted, every resonance with a given J and π has the same set of associated l-channels, whether it has an observable width or not. Hence

$$\begin{aligned} &\rho(0,J) = \rho(2,j) = \rho(4,j) = \ldots, \text{ and} \\ &\rho(1,J) = \rho(3,j) = \rho(5,j) = \ldots \end{aligned} \tag{D.54}$$

The further assumption of parity-independence makes $\rho(l,J)$ totally independent of l. As a result, G-P's K(l) from Equation (D.51) is independent of l, and

$$\rho(l) = C(2l+1)\,\omega_{I,l} \ , \tag{D.55}$$

where C depends on the nuclear species by not on any quantum numbers.

D.2.2.5. Gamma Widths

In the limited energy range of a few keV usually covered by the unresolved resonance region, the gamma width may be assumed to be constant and equal to that obtained from an analysis of the resolved resonances. If, however, the energy range is rather wide, an energy dependence as given by some of the well-known theoretical models, Reference 1, may be built in. Since the observed gamma width is the sum of a large number of primary gamma transitions, each assumed to have a chi-squared distribution of μ=1, the sum is found to have a $\mu \ge 20$. In effect this implies that the gamma width is a constant, since a chi-squared distribution with a large number of degrees of freedom approximates a δ-function.

D.2.2.6. Degrees of Freedom

For the reasons enumerated in Chapter 2, Section 2.4.20, the following values should be used:

1. Neutron width, $1. \le$ AMUN $\le 2.$, and specifically, AMUN= $\mu_{l,J}$.
2. Radiation width, AMUG=0.
3. Fission width, $1. \le$ AMUF $\le 4.$, to be determined by comparison with experiment. Only integral values are permitted, although non-integers occur in some analyses.
4. Competitive width, $1. \le$ AMUX $\le 2.$, because only a single inelastic level excitation is permitted as a competitive reaction. Specifically, AMUX= $\mu_{l',J}$, where J is the spin of the resonance, and l' is the orbital angular momentum of the inelastically scattered neutron. Since the daughter nucleus may have a spin $\tilde{I}$ different from the target spin, I, l' may be different from l and the number of channel spin values $\mu_{l',J}$ may be different from $\mu_{l,J}$.

D.2.3. Equivalent Quantities in Sections D.1 and D.2

Symbol in D.1	Symbol in D.2.1	Symbol in D.2.2	Definition
r	-	λ	This is a non-equivalence. λ enumerates ***all*** resonances. r enumerates those within a subset and hence ***implies*** a set of quantum numbers.
Γ_{nr}		$\Gamma_{n\lambda}(l,J)$	The neutron width, summed over channel spin.
$\Gamma_{\gamma r}$,Γ_{fr},...		-	Not used in D.2.2, but the same implication of l, J holds.
P_l		ρv_l	Penetration factor.
	$D_{l,J}$	$D(l,J)$	Average level spacing for a subset of resonances with given l and J.
	$\overline{\Gamma}^0_{nl,J}$	$\left\langle \Gamma^l_n(J) \right\rangle^{l,J}$	The l-wave reduced width, averaged over all resonances with given l and J.
	$\overline{\Gamma}_{nl,J}$	$\left\langle \Gamma_n(l,J) \right\rangle^{l,J}$	The average neutron width. In practice, the energy-dependence of this quantity is not averaged, but extracted before averaging.

D.2.4. Comparison with previous editions of ENDF-102

D.2.4.1. ENDF-102, October 1970 edition

1. Equation (1). $D_{observed}$ is $D(l)$.

2. Line 9. l is not the angular momentum of "the incident neutron." The incident neutrons carry all angular momenta. l is the orbital angular momentum of the resonance, or more precisely, of the channel or channels which are involved. The resonant l^{th} phase shift will interfere with the non-resonant ones in angular distributions, but not in angle-integrated cross sections.

3. Equation (2)

   ρ_J is $\rho(l,J)$; ρ_{obs} is $\rho(l)$; Σ is $\tilde{\Sigma}_J$.

4. Equation (3). D_J is $D(l,J)$ and the right-hand-side should have a factor $\omega_{l,l}$.

5. Page D-11, line 1. "Level-spacing" means $D(l,J)$. Line 8. The statement "If we assume the s-wave strength function is independent of J..."presumably means assuming S(0,J) is independent of J, since the s-wave strength function itself, S(0), is a sum over J-states and is therefore "independent" of J by definition.

   Equation 4 means

   $$S(0) = S(0,J,s) = S(0,J)/\mu_{0,J}$$

   which because $\mu_{0,J}$= 1 implies

   $$S(0) = S(0,J) = \langle \Gamma^0_n(J) \rangle^{0,J}/D(0,J) .$$

   Equation 5 is trickier because $\mu_{l,J}$ is not identically equal to 1, and the discussion appears to give the user the option of getting $D(l,J)$ from Equation (3) and "the corresponding reduced neutron width" from Equation (5), or of using the ENDF/B convention, Equation (6).

The problem lies in the failure to distinguish $\Gamma^l_n(J)$ from $\Gamma^l_n(J,s)$. Equation (6) states the "ENDF/B convention":

$$\left\langle \Gamma^l_{nJ} \right\rangle = \left\langle \Gamma^0_{nJ} \right\rangle \sqrt{E}\ \nu_l \mu_{lJ} \quad .$$

(Here and in the following, $\sqrt{E}$ and ν_l are average values appropriate to the energy interval.)

We know that the correct relationship is

$$\left\langle \Gamma_n(l,J) \right\rangle = \left\langle \Gamma^l_n(J,\not{s}) \right\rangle \sqrt{E}\ \nu_l \mu_{lJ}$$
$$= \left\langle \Gamma^l_n(J) \right\rangle \sqrt{E}\ \nu_l$$

If we assume that $\left\langle \Gamma^l_{nJ} \right\rangle$ in Equation (6) is to agree with experiment, $\left\langle \Gamma^{0l}_{nJ} \right\rangle$ then must be

$$\left\langle \Gamma^l_n(J,s) \right\rangle = \left\langle \Gamma^l_n(J) \right\rangle \Big/ \mu_{I,J} \ .$$

If we use a subscript E to denote an ENDF-convention quantity,

$$\left\langle \Gamma^{0l}_{nJ} \right\rangle \rightarrow \left\langle \Gamma^{0l}_{nJE} \right\rangle = \left\langle \Gamma^{0l}_{nJ}\ \text{actual} \right\rangle \Big/ \mu_{I,J}$$

and now

$$\frac{\left\langle \Gamma^0_{nJ} \right\rangle^l}{D_{l,J}} \text{ in (5) means } \frac{\left\langle \Gamma^{0l}_{nJE} \right\rangle}{D_{l,J}} = \frac{\left\langle \Gamma^0_n \,\text{actual} \right\rangle^l_J}{D_{l,J}\ \mu_{l,J}}$$

which is correct. Thus an ENDF reduced width $\left\langle \Gamma^{0l}_{nJE} \right\rangle$ will sometimes be half what an experimentalist would measure.

In the notation of D.2.2., Equation (24) is

$$\left\langle \Gamma_n(l,J) \right\rangle^{l,J} = \left\langle \Gamma^l_n(J,s) \right\rangle^{l,J} \sqrt{E}\ \nu_l\ \mu_{l,J}$$

and $\Gamma^l_n(J)$ is the reduced width determined by experiment.

For p-waves,

$$S(1) = S(1,J)/\mu_{1,J} = \left\langle \Gamma^1_n(J) \right\rangle^{1,J} / D(1,J)\mu_{1,J} \ ,$$

and Equation (5) would read:

$$S_1 = \frac{\left\langle \Gamma^1_n(J_1) \right\rangle^{1,J_1}}{D(1,J_1)\mu_{1,J_1}} = \frac{\left\langle \Gamma^1_n(J_2) \right\rangle^{1,J_2}}{D(1,J_2)\mu_{1,J_2}} = \ldots$$

6. The October 1970 edition uses three different symbols for the reduced width. In a unified notation:

page D-9 $\quad \overline{\Gamma}^0_{nl,J} = \left\langle \Gamma^l_n(J) \right\rangle_{l,J}$

page D-11 $\quad \left\langle \Gamma^0_n \right\rangle^{l=1}_J = \left\langle \Gamma^l_n(J) \right\rangle_{l,J}$

page D-12 $\quad \left\langle \Gamma^{0l}_{nJ} \right\rangle = \left\langle \Gamma^l_n(J,\not{s}) \right\rangle_{l,J}$

D.2.4.2. Comments on ENDF-102, October 1975 edition, Section D.2.1

1. Equation (1). $D_{l,\text{observed}}$ is D(l).
2. Same as comment 2 on the 1970 edition; above.
3. Equation (2). D_{obs} is D(l); $\rho_{l,obs}$ is $\rho(l)$; Σ_J is $\tilde{\Sigma}_J$.
4. "All allowed l-values label the same set of resonances" means $\rho(l,J)$ does not depend on l (for given parity).
5. Equation (3). $(2J + 1)^{-1}$ is missing from the right hand side.
6. Page D-12, second equation:

The quantity $\langle g\Gamma^l_n \rangle$ is $\left\langle g\Gamma^l_n(J)\right\rangle^l$. The bracket $\langle\rangle^l$ means summed over all J-values. The other two brackets are for particular J-values, *i.e.*,

$$\left\langle g\Gamma^l_n\right\rangle = \left\langle g\,\Gamma^l_n(J)\right\rangle^l$$
$$= \frac{g\left\langle\Gamma^l_n(J)\right\rangle^{l,J}}{\omega_{I,l}\,\mu_{l,J}} = \frac{g\left\langle\Gamma^l_n(J,\not{s})\right\rangle}{\omega_{I,l}}$$

7. "The strength functions for a given l-value but different J-values" means S(l,J). These are not all equal--it is the ratio $S(l,J)\mu_{l,J}$ which is independent of J.
8. Equation (D.6) should read:

$$\left\langle\Gamma_n(l,J)\right\rangle = \left\langle\Gamma^l_n(J,\not{s})\right\rangle\sqrt{E}\;\nu_l\,\mu_{l,J}$$
$$= \left[\left\langle\Gamma^l_n(J)\right\rangle\right]\sqrt{E}\;\nu_l$$

where Γ^l_n(J) is the reduced width determined by experiment. That is, the relation involving $\mu_{l,J}$ is only valid for an ***average*** width, and hence $\sqrt{E}\;\nu_l$ must also be some appropriate average value. The quantum number s should be exhibited when μ is used.

D.3 The Competitive Width

D.3.1 Penetrability Factor for the Competitive Width in the Resolved Resonance Region

A. <u>SLBW and MLBW</u>

For these formalisms, the only physical situation which can be handled without approximation is that in which a ***single*** inelastic competitive process is possible, because the formalism presently permits the definition of only ***one*** additional quantity. The most common case will occur when inelastic scattering to the first excited state of the target nucleus is energetically possible. Ignoring, as in the case of elastic scattering, the possibility that the partial widths depend on channel spin, the penetrability is identical to that for elastic scattering, but the energy is reduced by the excitation energy of the first excited state, corrected for recoil, so that

$$\Gamma_{xr}(E) = \Gamma_{n'r}(E) = \frac{P_l\left(E - E^*_1\right)\Gamma_{xr}\left(\left|E_r\right|\right)}{P_l\left(\left|E_r - E^*_1\right|\right)},\quad \text{if } E \geq E^*_1$$

and

$$\Gamma_{xr} = 0 \quad \text{if } E < E_1^*$$

where E_1^* is (AWRI+1)/AWRI times the excitation energy of the first excited state, E_1^{ex} ($E_1^{ex} = -QX$ in File 2).

This definition involves two conventions, both taken over from the elastic case. One is the way in which an "experimental" reduced width $\Gamma^l_{n'}$ is defined in terms of the theoretical reduced width γ^2, and the other is the way in which negative energy levels are treated. Neither of these problems arises in the theory, where $\Gamma=2P\gamma^2$ and all quantities are defined in terms of the channel energy. Note that the *l*-value to be used in the penetrability is not that of the incident neutron, but of the "exit" inelastically scattered neutron.

It is conceivable that an (n,α) or (n,p) reaction to the ground state of the daughter nucleus could be open, without inelastic competition, in which case the formula for Γ_{xr} would be the same, but the P_l would be a Coulomb penetrability, and the excitation energy E_l^* would be replaced by the approximate Q-value and reduced mass. The General R-matrix and Hybrid R-function formalisms allow for this possibility (see Sections D.1.5 and D.1.6).

If more than one competitive process is energetically possible, then the SLBW and MLBW formats are inadequate to give the correct energy dependence of the competitive width, since they supply only one number, and a partial width is required for each process. *E.g.*, when two inelastic levels can be reached,

$$\Gamma_{xr}(E) = \frac{P_{l_1}(E - E_1^*)\Gamma_{n_1' r}\left(\left|E_r\right|\right)}{P_{l_1}\left(\left|E_r - E_1^*\right|\right)} + \frac{P_{l_2}(E - E_2^*)\Gamma_{n_2' r}\left(\left|E_r\right|\right)}{P_{l_2}\left(\left|E_r - E_2^*\right|\right)},$$

with appropriate modification below each threshold. Note that the exit *l*-values are independent of the incident-neutron *l*-value.

For codes that presently approximate Γ as a constant in the denominator, a possible procedure is to substitute a step function

$$\begin{aligned} \Gamma_{xr}(E) &= 0 && \text{if } E < E_1^* \\ &= \Gamma_{xr}\left(\left|E_r\right|\right) && \text{if } E \geq E_1^* \end{aligned}$$

and then make some provision to handle the resultant discontinuity in the cross section.

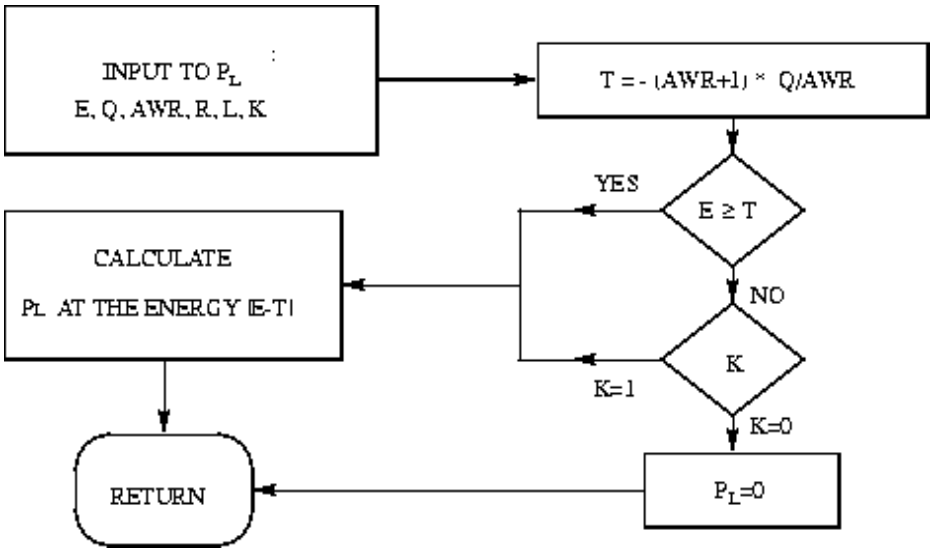
Users who are unable to handle this degree of complexity, and would like to use GT_R from File 2 as the total width without regard for whether the competitive process is energetically possible or not should at least be aware of the problem.

B. When the Adler-Adler and Reich-Moore formalisms are used for low-energy fissile materials, no recommendation concerning the treatment of Γ_{xr} need be given, and users can presume that it is zero. When Reich-Moore is used above the thermal region, the same comments apply as for the SLBW/MLBW formalism.

C. General R-matrix and Hybrid R-function formalisms allow multiple reaction channels, in addition to the elastic channel. The above discussion of penetrabilities pertains here also. For purposes of coding the penetrability factor as a subroutine, one possibility is to supply six arguments, an energy E, a Q-value Q, a mass ratio AWR, a radius R, an *l*-value L, and a sentinel K. Inside the subroutine, one calculates the threshold T= -(AWR +1.0) Q/AWR and then branches on K. If K=0, signaling an "incident" energy, the penetrability will be set to 0 if E is below threshold, but if K=1, signaling a "resonance" energy, the penetrability will be calculated at the absolute value of E-T. Thus an inelastic width would be calculated as

$$GINE\left(E\right) = GIN\left(\left|E_r\right|\right)\frac{P\left(E,Q=E^*,AWR,R,L,K=0\right)}{P\left(ER,Q=E^*,AWR,R,L,K=1\right)}$$

where P is a subroutine or function statement.



For both the R-formalisms, the evaluator must supply any Coulomb penetrabilities as tabulated functions of the incident neutron's laboratory energy. This choice keeps the energy consistent with that used in all other ENDF quantities and simplifies the problem of interpolating in the tables.

The evaluator will most likely calculate the Coulomb penetrabilities as functions of the center-of-mass energy in the exit channel, $E_{cm,exit}$. This is related to the center-of-mass energy in the incident channel by

$$E_{cm,inc} = E_{cm,exit} - Q$$

and the incident laboratory energy is

$$E_{lab,inc} = \frac{AWRI+1}{AWRI}E_{cm,inc} = \frac{AWRI+1}{AWRI}\left[E_{cm,exit} - Q\right] \quad .$$

In case the evaluator obtains his Coulomb penetrabilities as functions of the charged-particle laboratory energy, $E_{lab,exit}$, one more transformation is required:

$$E_{cm,exit} = \frac{\text{AWRIC}}{\text{AWRIC+ 1}}\ \text{E}_{\text{lab,exit}}\ ,$$

where AWRIC is the mass ratio in the exit channel.[8] In this case,

$$E_{lab,inc} = \left(\frac{\text{AWRI+1}}{\text{AWRI}}\right)\left[\frac{AWRIC}{AWRIC+1}E_{lab,exit} - Q\right]$$

These formulas enable the evaluator to supply the charged-particle penetrabilities as functions of the incident neutron's laboratory energy. This leaves to the user only the task of incorporating the dependence on the individual resonance energies, Section D.3.1.

D.3.2. Penetrability Factor for the Competitive Width in the Unresolved Resonance Region

Since many codes treat the average total width in the denominator of expressions like $\langle\Gamma_n\Gamma_\gamma/\Gamma\rangle$ as an energy-independent constant, the penetrability factor of the competitive width needs to be handled by specifying energy-dependent unresolved resonance parameters.

The formalism, which is a simple average over SBLW line shapes, takes account of the energy-dependence of the neutron widths in the numerator, by extracting their penetrability factors before the averaging is done. These then contribute to the energy-dependence of the average cross section. The energy-dependence of the neutron width in the denominator, i.e., in $\overline{\Gamma}$, is neglected. No such fix is readily available for the energy-dependence of the competitive width, whose penetrability factor will involve the threshold dependence of an inelastic cross section. The evaluator can circumvent this difficulty by specifying energy-dependent parameters and setting $\langle\Gamma_x\rangle$=0 below its threshold; then allowing it to build up according to the formulas given in Section D.3

The degrees of freedom, AMUX, should be 1.0 or 2.0. (See Section 2.4.20.)

D.3.3. Calculation of the Total Cross Section when a Competitive Reaction is Specified

When a competitive reaction is specified for SBLW or MLBW and Γ exceeds $\Gamma_n + \Gamma_\gamma + \Gamma_f$, the ENDF convention is that the scattering, capture, and fission cross sections will be calculated from the sum of File 2 and File 3 contributions, but the competitive reaction will be contained entirely in File 3, and no File 2 contribution should be added to it. The reason for this is that users can avoid problems in coding up resonant competitive widths. In the File 2 calculations, the correct total width Γ must be used in order to get the correct line shape.

[8] For an n,p reaction AWRIC = $M_{daughter}/m_p \approx$ AWRI; but for an n,α reaction, AWRIC = $M_{daughter}/m_\alpha \approx$ (AWRI-3)/4.

This puts the ***total*** cross section in a special category. If it is calculated as the sum of σ_n, σ_γ, σ_f, σ_x, then the above prescription works satisfactorily. However, if it is calculated from the SLBW formula,

$$\sigma_{n,t}(E) = \frac{\pi}{k^2}\sum_J g_J \frac{\Gamma_{nr}\Gamma_r}{\left(E - E_{r'}\right)^2 + \frac{1}{4}\left(\Gamma_r/2\right)^2},$$

as it is in some applications, then it will include the competitive reaction, and the user should not add the File 3 contribution to it. The ENDF convention presumes that $\sigma_{n,t}$ will be calculated by summing the partial reactions.

The General R-matrix and Hybrid R-function do not have this problem. The "competitive" reactions are treated normally, and File 2 and File 3 are added together for all reactions. That is because the total width is always the sum of the explicitly given partial widths. Depending on what non-elastic channels are specified, the total cross section may be calculated either as the sum of the partial cross sections, or from {1-ReU(*l*sJ)}, as described in Sections D.1.5.6 and D.1.6.4. If a File 3 contribution were specified for the total cross section, then it would be added to the {1-ReU} calculation, but not to the sum-of-parts calculation, as the latter would already include the File 3 contribution for each partial reaction. This assumes that the File 3 total is the sum of the File 3 partials.

REFERENCES

1. J.E. Lynn, **The Theory of Neutron Resonance Reactions**, Clarendon Press, Oxford (1958)
2. C.W. Reich and M.S. Moore, ***Phys. Rev.* 111**, 929 (1958)
3. F.T. Adler and D.B. Adler, *Interpretations of Neutron Cross Sections of the Fissionable Materials for the Resolved Resonance Region*, U.S. Atomic Energy Commission Report **CONF-660303**, ***Conf. on Neutron Cross Section Technology*** (1966), Book 2, p. 873
4. D.B. Adler and F.T. Adler, Argonne National Laboratory report **ANL-6792**, 695 (1963)
5. A.M. Lane and R.G. Thomas, ***Rev. Mod. Phys.* 30**, 257 (1958)
6. F.H. Fröhner, *Applied Neutron Resonance Theory*, Kernforschungszentrum, Karlsruhe report **KFK 2669** (1978)
7. J.M. Blatt and L.C. Biedenharn, ***Rev. Mod. Phys.* 24**, 258 (1952)
8. M. Gyulassy and S.T. Perkins, ***Nucl. Sci. Eng.* 53**, 482 (1974)
9. A. Saplakoglu, L. M. Bollinger, and R. E. Coté, ***Phys. Rev.* 109**, 1258 (1958)
10. F.H. Fröhner, *New Techniques for Multi-Level Cross Section Calculation and Fitting*, Brookhaven National Laboratory report **BNL-NCS-51363**, ***Proceedings of the Conference on Nuclear Data Evaluation, Methods and Procedures*** (1981), Vol. I, P. 375