VIII.A. EQUATIONS FOR UNRESOLVED RESONANCE REGION

The formulae for cross sections in the unresolved resonance region, as implemented in SAMMY, are presented in this section. The implementation is a modified form of that provided by Fritz Fröhner in his FITACS code [FF89]. (Please note that any mistakes in these formulae are attributable only to the author of this manual, not to Fröhner. The author is indebted to Herve Derrien for significant contributions both to the development of the code and to the composition of this section of the manual.)

Elastic cross section

The elastic cross section is given as the difference between the total cross section and the sum of all the non-elastic partial cross sections. The total cross section is given by Eqs. (VIII A.1) through (VIII A.4), and the non-elastic partial cross sections by Eqs. (VIII A.5) through (VIII A.20).

Total cross section

The average total cross section, for a given spin and parity and incident channel c, may be written in the form

$$\langle \sigma_c \rangle = \frac{2\pi g_c}{k_c^2}\left(1 - \mathrm{Re}\langle S_{cc} \rangle\right) \quad , \qquad \text{(VIII A.1)}$$

where, as usual, g_c is the spin factor and k_c is the center-of-mass momentum. The average scattering matrix $\langle S_{cc} \rangle$ is given by

$$\langle S_{cc} \rangle = e^{-2i\varphi_c} \, \frac{1 - \langle R_{cc} \rangle L_c^{0*}}{1 - \langle R_{cc} \rangle L_c^{0}} \quad , \qquad \text{(VIII A.2)}$$

and the average R-matrix can be written in the form

$$\langle R_{cc} \rangle = R_c^{\infty} + \; i\,\pi\, s_c \quad , \qquad \text{(VIII A.3)}$$

with parameters defined as follows:

R_c^{∞} = distant-level parameter (an input quantity);

φ_c = hard-sphere scattering phase shift, generated using matching radius a (an input quantity);

L_c^0 = $\left(S_c - B_c\right) + iP_c$ (see Section II.A), with boundary condition B_c chosen such that $S_c - B_c = 0$;

s_c = pole strength.

The pole strength is defined in terms of input quantities $\tilde{S}_c$ (the strength function, for which we have introduced the tilde to avoid confusion with the shift factor used in definition of L_c^0) and a_c (the R-matrix matching radius) as

$$s_c = \tilde{S}_c \sqrt{E} \big/ 2\rho \quad , \tag{VIII A.4}$$

where ρ is the center-of-mass momentum k_c multiplied by the channel radius a_c.

Non-elastic partial cross sections

The non-elastic partial cross sections may be written in terms of transmission coefficients T_x as

$$\left\langle \sigma_{ab} \right\rangle = \frac{\pi g_a}{k_a^2} \frac{T_a T_b}{T} \int_0^\infty dt \; e^{-iT_\gamma/T} \prod_{c \notin \gamma} \left(1 + \frac{2}{\nu_c} \frac{T_c}{T} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad , \tag{VIII A.5}$$

where the quantities to the left of the integral sign are the Hauser-Feshbach expression, and the integrand is the Moldauer prescription [PM80] for the width fluctuation correction factor. (A derivation of this expression, including the assumptions under which it is derived, is provided in Section VIII.A.1.) Here *a* represents the incident channel and *b* the exit channel; ν_c and T_c represent the number of degrees of freedom (multiplicity) and transmission coefficient, respectively, for channel *c*. Subscript γ refers to photon channels. *T* is defined as the sum over all channels:

$$T = \sum_c T_c \quad . \tag{VIII A.6}$$

The transmission coefficient for neutron channels is given by

$$T_c \; = \; 1 - \left| \left\langle S_{cc} \right\rangle \right|^2 \; = \; \frac{4\pi \; P_c \, s_c}{\left| 1 - \left\langle R_{cc} \right\rangle L_c \right|^2} \quad , \tag{VIII A.7}$$

where *c* is an incident channel, *P* and *L* are as defined in Section II.A, and the other quantities are given above. For photon and fission channels, the transmission coefficients for spin *J* are

$$T_\gamma = 2\pi \left\langle \Gamma_\gamma \right\rangle \big/ D_J \qquad \text{and} \qquad T_f = 2\pi \left\langle \Gamma_f \right\rangle \big/ D_J \quad , \tag{VIII A.8}$$

in which D_J is the mean level spacing for levels with this spin.

The *J*-dependence of the mean level spacing is set in SAMMY/FITACS via the Bethe formula (e.g., [FF83]):

$$\left(D_J\left(E\right)\right)^{-1}=\left(d\left(E\right)\right)^{-1}\left\{\exp\left[\frac{-J^2}{2\left(\sigma\left(E\right)\right)^2}\right]-\exp\left[\frac{-\left(J+1\right)^2}{2\left(\sigma\left(E\right)\right)^2}\right]\right\} \quad , \tag{VIII A.9}$$

where d (E) is independent of J, and σ is the spin cutoff parameter. The spin cutoff parameter is related to the level density parameter a and the energy E by the formula

$$\sigma^2=\left(0.14592\right)\left(A+1\right)^{2/3}\sqrt{a\left(E+BE-PE\right)} \quad , \tag{VIII A.10}$$

in which BE represents the neutron binding energy (an input parameter) and PE the pairing energy (also an input parameter). The value for a is determined from the input quantity D, which is the mean level spacing of the l = 0 resonances at E = 0; note that D includes both $J = I - i$ and $J = I + i$, where I is the spin of the target nucleus and i = ½ is the spin of the neutron. An expression for the inverse of D can be found from Eq. (VIII A.9) to be

$$\begin{aligned} D^{-1}&=\sum_J\left(D_J\left(E=0\right)\right)^{-1} \\ &=\left(d\left(0\right)\right)^{-1}\left\{\exp\left[\frac{-\left(I-\frac{1}{2}\right)^2}{2\sigma^2}\right]-\exp\left[\frac{-\left(I+\frac{3}{2}\right)^2}{2\sigma^2}\right]\right\} \quad ; \end{aligned} \tag{VIII A.11}$$

this expression is used to determine the value of σ^2 and hence of the level density parameter a.

The energy dependence of the mean level spacing is calculated with the Gilbert-Cameron composite formula [AG65]. Let E_x represent the excitation energy of the compound nucleus; this energy is equal to the sum of the incident neutron kinetic energy E and the neutron binding energy BE (which is an input quantity). That is to say,

$$E_x=E+BE \quad . \tag{VIII A.12}$$

The energy dependence for low excitation energies $\left(E_x<E_0\right)$, where E_0 is a matching energy, is given by the constant-temperature formula

$$D^{-1}\sim C_3\frac{\exp\left[C_2\sqrt{E_0-PE}\right]}{\left(E_0-PE\right)^{3/2}}\exp\left[\frac{E_x-E_0}{2}\left(\frac{C_2}{\sqrt{E_0-PE}}-\frac{3}{E_0-PE}\right)\right] \quad . \tag{VIII A.13}$$

In the code, the matching energy E_0 is set at

$$E_0 = \left[\frac{5}{2} + \frac{150}{(N+Z+1)} \right] \qquad \text{(VIII A.14)}$$

in units of MeV, with $N + Z$ being the mass number for the target nucleus. Values of the constants C_2 and C_3 are given by

$$C_2 = \sqrt{4a} \quad \text{and} \quad C_3 = \frac{1}{12\sqrt{2aq}} \quad , \qquad \text{(VIII A.15)}$$

with q defined as

$$q = 0.14592(N+Z+1)^{2/3} \quad , \qquad \text{(VIII A.16)}$$

where $N + Z$ is again the mass number for the target nucleus and a is the level density parameter.

At higher energies $(E_x > E_0)$, the energy dependence of the mean level spacing is calculated via the Fermi-Gas formula

$$D^{-1} \propto C_3 \frac{\exp\left[C_2 \sqrt{E_x - PE} \right]}{(E_x - PE)^{3/2}} \quad . \qquad \text{(VIII A.17)}$$

Note that the two formulae agree at the matching energy (i.e., at $E_x = E_0$).

Radiation widths $\langle \Gamma_\gamma \rangle$ are assumed to depend only on parity π and on E. The energy dependence is calculated with the giant dipole resonance model.

Fission widths $\langle \Gamma_f \rangle$ may vary with spin as well as parity and incident neutron energy E. Energy dependence is calculated with the Hill-Wheeler fission barrier transmission coefficients [DH53]. For a given J^π, the energy dependence of the fission widths is taken to be

$$\langle \Gamma_f(E) \rangle = \langle \Gamma_f(0) \rangle \frac{1 + \exp\left[E_{HW} / W_{HW} \right]}{1 + \exp\left[-(E - E_{HW}) / W_{HW} \right]} \quad , \qquad \text{(VIII A.18)}$$

where the Hill-Wheeler threshold energy E_{HW} and the Hill-Wheeler threshold width W_{HW} are input quantities. This equation may be written in more "standard" notation as

$$\left\langle \Gamma_f(E) \right\rangle = \left\langle \Gamma_f(0) \right\rangle \frac{1+\exp\left(2\pi\left(E_f - BE\right)/\hbar\omega\right)}{1+\exp\left(-2\pi\left(E_x - \left(E_f - BE\right)\right)/\hbar\omega\right)} \quad , \tag{VIII A.19}$$

where, as above, E_x is the excitation energy of the neutron and *BE* is the binding energy. Also, E_f is the fission barrier height, and $\hbar\omega$ the width of the fission barrier.

Finally, a few words regarding the derivation of Eq. (VIII A.5) are warranted. That derivation is based on several assumptions:

(1) The Moldauer prescription [PM80] for width fluctuations is used. That is, the width fluctuation correction factor is introduced to compensate for the non-unity of the ratio

$$\left\langle \frac{T_a T_b}{T} \right\rangle \Big/ \frac{\langle T \rangle}{\langle T_a \rangle \langle T_b \rangle} \quad . \tag{VIII A.20}$$

(2) Partial widths obey a chi-squared distribution with ν_c degrees of freedom (where the value of ν_c depends on the number of channels of this de-excitation); averages are therefore weighted with this distribution. In the Moldauer prescription for width fluctuations, simple channels have $1 < \nu_c < 1.78$; for lumped channels, ν_c is a function of T_c.

(3) Channels with the same transmission coefficients may be combined by introducing multiplicities.

The integral of Eq. (VIII A.5) is described by Fröhner as the "width fluctuation correction or Dresner factor." One (relatively modest) difference between SAMMY and the original FITACS coding is the algorithm for calculating the Dresner integral; in SAMMY, the coding has been refined to increase both speed and accuracy of calculation by using a non-uniform grid designed specifically for this task.

(Note: Prior to release 7 of the code, the Moldauer correction was inadvertently disabled in code. This has now been fixed.)