## VIII.A.1. Derivation of Non-Elastic Average Cross Section

Derivations shown in this section are based on (1) notes provided by Fritz Fröhner [FF99] and (2) discussions with Herve Derrien [HD00a]. Any errors in these pages are the responsibility of the SAMMY author alone.

The interpretation of the transmission coefficient $T_c$ in terms of average resonance parameters is straightforward if one assumes that the resonant cross section can be approximated by the single-level Breit Wigner formula, i.e.,

$$\sigma_{ab} = \frac{\pi g_a}{k_a^2} \sum_\lambda \frac{\Gamma_{\lambda a}\, \Gamma_{\lambda b}}{\left(E - E_\lambda\right)^2 + \left(\Gamma_\lambda / 2\right)^2} \quad , \tag{VIII A1.1}$$

in which total width $\Gamma_\lambda$ is the sum of all partial widths. The corresponding average cross section in an energy interval containing a large number of resonances may be written as

$$\left\langle \sigma_{ab} \right\rangle = \frac{\pi g_a}{k_a^2} 2\pi \rho_a \left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle \quad , \tag{VIII A1.2}$$

where $\rho$ is the level density, and the brackets refer to averages. (Note that the subscript $\lambda$ has been dropped for simplicity's sake.) The calculation of the average quantity $\left\langle \Gamma_a \Gamma_b / \Gamma \right\rangle$ is not straightforward, since the known parameters are $\left\langle \Gamma_a \right\rangle$ and $\left\langle \Gamma_b \right\rangle$ (from the statistical properties of the resonance parameters). One has to take into account the fluctuations of the partial widths of the resonances from the chi-squared distribution of the parameters.

A method of calculating the average $\left\langle \Gamma_a \Gamma_b / \Gamma \right\rangle$ from the known entities $\left\langle \Gamma_a \right\rangle \left\langle \Gamma_b \right\rangle / \left\langle \Gamma \right\rangle$ was proposed by Dresner [FF99]. He suggested making the substitution

$$\left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle = \left\langle \frac{\Gamma_a \Gamma_b}{\sum\limits_{all\ c} \Gamma_c} \right\rangle = \left\langle \Gamma_a \Gamma_b \int_0^\infty dq \exp\left( -q \sum_c \Gamma_c \right) \right\rangle \quad , \tag{VIII A1.3}$$

which follows from the identity

$$\int_0^\infty d\,q\, e^{-qQ} = \frac{1}{Q} \int_0^\infty d\,y\, e^{-y} = \frac{1}{Q} \quad . \tag{VIII A1.4}$$

The product of partial widths in Eq. (VIII A1.3) can be rearranged as

$$\left\langle \Gamma_a \Gamma_b \int_0^\infty d\,q \exp\left( -q \sum_c \Gamma_c \right) \right\rangle = \left\langle \int_0^\infty d\,q \;\; \Gamma_a \, e^{-q\Gamma_a} \;\; \Gamma_b \, e^{-q\Gamma_b} \;\; \prod_{c \neq a,b} e^{-q\Gamma_c} \right\rangle \, . \quad \text{(VIII A1.5)}$$

Because the channels *a*, *b*, and *c* are independent, the average of the product is equal to the product of the averages. Likewise integration over $q$ is independent of the averaging process; hence Eq. (VIII A1.3) can be rewritten as

$$\left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle = \int_0^\infty d\,q \; \left\langle \Gamma_a \, e^{-q\Gamma_a} \right\rangle \left\langle \Gamma_b \, e^{-q\Gamma_b} \right\rangle \prod_{c \neq a,b} \left\langle e^{-q\Gamma_c} \right\rangle \quad . \qquad \text{(VIII A1.6)}$$

One assumes the partial widths obey a chi-squared distribution with $\nu$ degrees of freedom, which has the form

$$\rho(x,\nu)dx = \left[ \mathbf{\Gamma}\left(\frac{\nu}{2}\right) \right]^{-1} \left(\frac{\nu x}{2}\right)^{\nu/2-1} e^{-\nu x/2} \, \frac{\nu}{2} \, dx \quad , \qquad \text{(VIII A1.7)}$$

where $\mathbf{\Gamma}$ in this expression refers to the gamma function. Note that $\nu = 1$ corresponds to the Porter-Thomas distribution for a single neutron channel; $\nu = 2$ corresponds to two channels. For fission, the value of $\nu$ depends on the number of open or partially open fission channels; $\nu_f$ is an input parameter in SAMMY (and in FITACS).

Applying this distribution to the average quantity needed in Eq. (VIII A1.6), with $x = \Gamma_c \,/ \left\langle \Gamma_c \right\rangle$, gives

$$\begin{aligned} \left\langle e^{-q\Gamma_c} \right\rangle &= \int_0^\infty e^{-q \langle \Gamma_c \rangle x} \; \rho(x,\nu) \, dx \\ &= \frac{1}{\mathbf{\Gamma}(\nu/2)} \left(\frac{\nu}{2}\right)^{\frac{\nu}{2}-1} \int_0^\infty e^{-q \langle \Gamma_c \rangle x} \; x^{\frac{\nu}{2}-1} \; e^{-\nu x/2} \, \frac{\nu}{2} \, dx \quad , \end{aligned} \qquad \text{(VIII A1.8)}$$

which can be rewritten into the form

$$\left\langle e^{-q\Gamma_c}\right\rangle = \frac{1}{\mathbf{\Gamma}(\nu/2)}\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}} \int_0^\infty e^{-\left(q\langle\Gamma_c\rangle+\nu/2\right)x}\; x^{\frac{\nu}{2}-1}\,dx$$

$$= \frac{1}{\mathbf{\Gamma}(\nu/2)}\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}\left(\frac{\nu}{2}+q\left\langle\Gamma_c\right\rangle\right)^{-\frac{\nu}{2}} \int_0^\infty e^{-w}\; w^{\frac{\nu}{2}-1}\,dw \qquad \text{(VIII A1.9)}$$

$$= \frac{1}{\mathbf{\Gamma}(\nu/2)}\left(1+\frac{2}{\nu}q\left\langle\Gamma_c\right\rangle\right)^{-\frac{\nu}{2}}\Gamma(\nu/2) = \left(1+\frac{2}{\nu}q\left\langle\Gamma_c\right\rangle\right)^{-\frac{\nu}{2}} .$$

Likewise, $\left\langle \Gamma_a\, e^{-q\Gamma_a}\right\rangle$ from Eq. (VIII A1.6) has the form

$$\left\langle \Gamma_a\, e^{-q\Gamma_a}\right\rangle = \int_0^\infty \left\langle\Gamma_a\right\rangle x\, e^{-q\langle\Gamma_a\rangle x}\; \rho(x,\nu)\,dx$$

$$= \frac{\left\langle\Gamma_a\right\rangle}{\mathbf{\Gamma}(\nu/2)}\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}-1} \int_0^\infty e^{-q\langle\Gamma_a\rangle x}\; x^{\frac{\nu}{2}}\; e^{-\nu x/2}\,\frac{\nu}{2}\,dx$$

$$= \frac{\left\langle\Gamma_a\right\rangle}{\mathbf{\Gamma}(\nu/2)}\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}\left(\frac{\nu}{2}+q\left\langle\Gamma_a\right\rangle\right)^{-\frac{\nu}{2}-1} \int_0^\infty e^{-w}\; w^{\frac{\nu}{2}}\,dw$$

$$= \frac{\left\langle\Gamma_a\right\rangle}{\mathbf{\Gamma}(\nu/2)}\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}\left(\frac{\nu}{2}+q\left\langle\Gamma_a\right\rangle\right)^{-\frac{\nu}{2}-1} \mathbf{\Gamma}\left(\frac{\nu}{2}+1\right)$$

$$= \frac{\left\langle\Gamma_a\right\rangle}{\mathbf{\Gamma}(\nu/2)}\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}\left(\frac{\nu}{2}+q\left\langle\Gamma_a\right\rangle\right)^{-\frac{\nu}{2}-1} \frac{\nu}{2}\mathbf{\Gamma}\left(\frac{\nu}{2}\right)$$

$$= \left\langle\Gamma_a\right\rangle\left(1+\frac{2}{\nu}q\left\langle\Gamma_a\right\rangle\right)^{-\frac{\nu}{2}-1} \qquad \text{(VIII A1.10)}$$

and similarly for $\left\langle \Gamma_b\, e^{-q\Gamma_b}\right\rangle$. Hence Eq. (VIII A1.6) can be expressed as

$$\left\langle\frac{\Gamma_a\Gamma_b}{\Gamma}\right\rangle = \left\langle\Gamma_a\right\rangle\left\langle\Gamma_b\right\rangle \int_0^\infty dq\; \prod_c \left(1+\frac{2}{\nu_c}q\left\langle\Gamma_c\right\rangle\right)^{-\nu_c/2-\delta_{ac}-\delta_{bc}} , \qquad \text{(VIII A1.11)}$$

in which the correspondence of $\nu$ with channel $c$ is made explicit by the addition of the subscript.

Making a change of variable from $q$ to $t = \langle \Gamma \rangle \, q$ gives

$$\left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle = \frac{\langle \Gamma_a \rangle \langle \Gamma_b \rangle}{\langle \Gamma \rangle} \int_0^\infty dt \, \prod_c \left( 1 + \frac{2}{\nu_c} \frac{\langle \Gamma_c \rangle}{\langle \Gamma \rangle} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad . \qquad \text{(VIII A1.12)}$$

The "transmission coefficients" are related to the average widths by

$$T_c = 2\pi \, \rho_c \, \langle \Gamma_c \rangle \quad . \qquad \text{(VIII A1.13)}$$

Note the equality of the level densities, $\rho_a = \rho_b = \rho_c = \rho_J$, since all refer to the same spin and parity. Hence Eq. (VIII A1.12) can be rewritten as

$$2\pi \, \rho_a \left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle = \frac{T_a T_b}{T} \int_0^\infty dt \, \prod_c \left( 1 + \frac{2}{\nu_c} \frac{T_c}{T} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad , \qquad \text{(VIII A1.14)}$$

so that the cross section can be expressed as

$$\langle \sigma_{ab} \rangle = \frac{\pi g_a}{k_a^2} \frac{T_a T_b}{T} \int_0^\infty dt \, \prod_c \left( 1 + \frac{2}{\nu_c} \frac{T_c}{T} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad . \qquad \text{(VIII A1.15)}$$

For photon channels, the limit of non-fluctuating radiation widths, $\nu_{c=\gamma} \to \infty$ gives

$$\lim_{\nu \to \infty} \left( 1 + \frac{2}{\nu_c} \frac{T_c}{T} t \right)^{-\nu_c/2} = e^{-t \, T_\gamma / T} \quad . \qquad \text{(VIII A1.16)}$$

Therefore our expression for the cross section, Eq. (VIII A1.15), takes the form

$$\langle \sigma_{ab} \rangle = \frac{\pi g_a}{k_a^2} \frac{T_a T_b}{T} \int_0^\infty dt \; e^{-i T_\gamma / T} \prod_{c \notin \gamma} \left( 1 + \frac{2}{\nu_c} \frac{T_c}{T} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad , \qquad \text{(VIII A1.17)}$$

which is equivalent to Eq. (VIII A1.6) combined with Eq. (VIII A1.2). This concludes the derivation of the formula given in Eq. (VIII A.5).

Evaluation of this expression for the average cross section in SAMMY (and in FITACS) assumes further simplification: First, we make the change of variable from $t$ to $q = t\,T_\gamma / T$ :

$$\left\langle \sigma_{ab} \right\rangle = \frac{\pi\, g_a}{k_a^2} \frac{T_a T_b}{T_\gamma} \int_0^\infty dq \; e^{-q} \prod_{c \notin \gamma} \left( 1 + \frac{2}{\nu_c} \frac{T_c}{T_\gamma} q \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \cdot \tag{VIII A1.18}$$

Second, we change variable from $q$ to $u = e^{-q}$ to obtain

$$\left\langle \sigma_{ab} \right\rangle = \frac{\pi\, g_a}{k_a^2} \frac{T_a T_b}{T_\gamma} \int_0^1 du \prod_{c \notin \gamma} \left( 1 - \frac{2}{\nu_c} \frac{T_c}{T_\gamma} \ln u \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad . \tag{VIII A1.19}$$

Next, define parameters $b_c$ via

$$b_c = \frac{2}{\nu_c} \frac{T_c}{T_\gamma} \quad , \tag{VIII A1.20}$$

substitute into Eq. (VIII A1.19), and sum over incident (neutron) channels $a$ and reaction channels $b$, to give

$$\left\langle \sigma_{nx} \right\rangle = \frac{\pi\, g}{k^2} T_\gamma \sum_{a \in n} \sum_{b \in x} \frac{\nu_a b_a}{2} \frac{\nu_b b_b}{2} \int_0^1 du \prod_{c \notin \gamma} \left( 1 - b_c \ln u \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad . \tag{VIII A1.21}$$

This can be written as

$$\left\langle \sigma_{nx} \right\rangle = \frac{\pi\, g}{k^2} T_\gamma \, Q_{nx} \quad , \tag{VIII A1.22}$$

where $Q$ is defined as

$$Q_{nx} = \sum_{a \in n} \sum_{b \in n} \frac{\nu_a b_a}{2} \frac{\nu_b b_b}{2} I_{ab} \tag{VIII A1.23}$$

with

$$I_{ab} = \int_0^1 du \prod_{c \notin \gamma} \left( 1 - b_c \ln u \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad . \tag{VIII A1.24}$$

This expression for $I_{ab}$ is denoted the "Dresner integral." Evaluation of this integral is accomplished in SAMMY by (1) choosing a grid for $u$ in which the spacing between points increases as the integrand flattens and (2) using a quadratic quadrature scheme. This integration scheme was tested with a wide range of plausible values for $b$'s and $\nu$'s, comparing results for various values of $N$ (where $N$ is the number of points in the $u$-grid). Results were good to six digits of accuracy, for all tested values of $b$'s and v's, using as few as 201 points in the grid.