II. B. 1. Reich-Moore Approximation to Multilevel R-Matrix Theory

The Reich-Moore approximation [CR58] is based on the idea that capture channels behave quite differently from particle channels. The particle-pair configuration for a capture channel consists of a gamma "particle" plus a nucleus with one more neutron than the target nucleus. For most physical situations, there are a multitude of such capture channels, whose behavior can be treated in an aggregate or average manner. It is assumed that there is no net interference between the aggregate capture channel and other channels, and the level-level interference of gamma channels is negligible, so that terms describing such interference may be eliminated from the R-matrix formulae. The mathematical derivation of this "eliminated-channel approximation" is discussed in Section II.A.1.

In the eliminated-channel approximation, the R-matrix of Eq. (II A.6) (for the spin group defined by total spin J and implicit parity π) has the form

$$R_{cc'} = \left[\sum_{\lambda} \frac{\gamma_{\lambda c}\, \gamma_{\lambda c'}}{E_{\lambda} - E - i\bar{\Gamma}_{\lambda\gamma}/2} + R_c^{ext} \delta_{cc'} \right] \delta_{JJ'} \quad , \tag{II B1.1}$$

where all levels (resonances) of that spin group are included in the sum. Subscript λ designates the particular level; subscripts c and c' designate channels (including particle pairs and all the relevant quantum numbers). The width $\bar{\Gamma}_{\lambda\gamma}$ occurring in the denominator corresponds to the "eliminated" non-interfering capture channels of the Reich-Moore approximation; we use the bar to indicate that this width is treated differently from other "particle" widths.

The "external R-function" R_c^{ext} of Eq. (II B1.1) will be discussed in Section II.B.1.d.

The channel width $\Gamma_{\lambda c}$ is given in terms of the reduced-width amplitude $\gamma_{\lambda c}$ by

$$\Gamma_{\lambda c} = 2\,\gamma_{\lambda c}^2\, P_c\left(E\right) \quad , \tag{II B1.2}$$

where P_c is the penetrability, whose value is a function of the type of particles in the channel, of the orbital angular momentum l, and of the energy E. The reduced-width amplitude $\gamma_{\lambda c}$ is always independent of energy, but the width $\Gamma_{\lambda c}$ may depend on energy via the penetration factor. For fission and for gamma channels, Eq. (II B1.2) becomes

$$\Gamma_{\lambda c} = 2\,\gamma_{\lambda c}^2 \quad ,$$

that is, the penetrability is effectively 1. (Note: In this manual, the reduced-width amplitude for the eliminated-channel capture width will be denoted by a bar above the symbol γ.)

Cross sections may be calculated by using the above expressions for R, with L given by Eq. (II A.7), to generate W, and from there calculating U and, ultimately, σ. However, while Eq. (II A.6) for W is correct, an equivalent form that is computationally more stable [NL92] is

$$W = I + 2i\,X \quad , \tag{II B1.3}$$

where X is given in matrix notation by

$$X = P^{1/2} L^{-1} \left(L^{-1} - R \right)^{-1} R\, P^{1/2} \quad . \tag{II B1.4}$$

When the suppressed indices and implied summations are inserted, the expression for X becomes

$$X_{c\,c'} = P_c^{1/2} L_c^{-1} \sum_{c''} \left[(L^{-1} - R)^{-1} \right]_{c\,c''} R_{c''c'}\; P_{c'}^{1/2}\; \delta_{J\,J'} \quad . \tag{II B1.5}$$

The various cross sections are then written in terms of X.

All calculations internally within SAMMY are expressed in terms of so-called "u-parameters," as distinguished from "p-parameters," which are the input quantities. The u-parameters associated with the resonance p-parameters are as follows:

$$u_{E_\lambda} = \begin{cases} \sqrt{E_\lambda} & \text{for } E_\lambda > 0 \\ -\sqrt{-E_\lambda} & \text{for } E_\lambda < 0 \quad , \end{cases} \tag{II B1.6}$$

and

$$u_{\Gamma_{\lambda c}} = \gamma_{\lambda c} = \begin{cases} \sqrt{\dfrac{\Gamma_{\lambda c}}{2P_l\left(\left|E_\lambda - \Xi_c\right|\right)}} & \text{if } \Gamma_{\lambda c} > 0 \\ -\sqrt{\dfrac{\left|\Gamma_{\lambda c}\right|}{2P_l\left(\left|E_\lambda - \Xi_c\right|\right)}} & \text{if } \Gamma_{\lambda c} < 0 \text{ in the PARameter file} \quad , \end{cases} \tag{II B1.7}$$

in which Ξ_c is the energy threshold for the channel (Section II.C.2).

It is important to note that the partial-width parameter $\Gamma_{\lambda c}$ is always a positive quantity, while the reduced-width amplitude $\gamma_{\lambda c}$ can be either positive or negative. Nevertheless, in the original SAMMY input or output PARameter file (and also in the ENDF File 2 formats [ENDF-102]), partial widths may appear with negative signs. The convention is that the sign given in those files is associated with the amplitude $\gamma_{\lambda c}$ rather than with the partial width $\Gamma_{\lambda c}$.

As of revision 8 of this document and release sammy-8.0.0 of the code, the reduced-width amplitudes and square root of resonance energy may be used as input to SAMMY; see Table VI B.2 for details. To use this option, include the command "`REDUCED WIDTH AMPLITUdes are used for input`" in card set 2 of the INPut file. An output file SAMMY.RED is created in this format whenever output file SAMMY.PAR is created.