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UPDATED USERS' GUIDE FOR SAMMY: MULTILEVEL R-MATRIX FITS TO NEUTRON DATA USING BAYES' EQUATIONS

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II. SCATTERING THEORY

Details of scattering theory have been well understood since the middle of the previous century, when they were summarized in a review article by Lane and Thomas [AL58]. A wealth of additional reference material is available to the student of scattering theory; only a few are listed here. The text by Foderaro [AF71] provides a more elementary introduction to the subject. One publication by Fröhner [FF80] is based on lectures presented at the International Centre for Theoretical Physics (ICTP) Winter Courses on Nuclear Physics and Reactors, 1978; this is a comprehensive and useful guide to applied neutron resonance theory. It includes a variety of topics, including preparation of data, various approximations to scattering theory, Doppler broadening, experimental complications, data-fitting procedures, and statistical tests. Another Fröhner paper [FF00] is somewhat more theoretical, and covers many aspects of data fitting in the resonance region.

The particular aspect of scattering theory with which we are concerned is the R-matrix formalism. A summary of the underlying principles is given here.

R-matrix theory is a mathematically rigorous phenomenological description of what is actually seen in an experiment (i.e., the measured cross section). The theory is not a model of neutron-nucleus interaction, in the sense that it makes no assumptions about the underlying physics of the interaction. Instead it parameterizes the measurement in terms of quantities such as the interaction radii and boundary conditions, resonance energies and widths, and quantum numbers; values for these parameters may be determined by fitting theoretical calculations to observed data. The theory is mathematically correct, in that it is analytic, unitary, and rigorous; nevertheless, in practical applications, the theory is always approximated in some fashion.

R-matrix theory is based on the following assumptions: (1) the applicability of non-relativistic quantum mechanics; (2) the absence or unimportance of all processes in which more than two product nuclei are formed; (3) the absence or unimportance of all processes of creation or destruction; and (4) the existence of a finite radial separation beyond which no nuclear interactions occur, although Coulomb interactions are given special treatment. [In practical applications two of these four assumptions may be violated in one degree or another: (1) The theory may be used for relativistic neutron energies, and corrected for relativistic effects; nevertheless, non-relativistic quantum mechanics is assumed. (2) A fission experiment with more than two final products is treated as a two-step process. That is, the immediate result of the neutron-nuclide interaction is assumed to be limited to two final products, at least one of which decays prior to detection.]

R-matrix theory is expressed in terms of channels, where a channel is defined as a pair of (incoming or outgoing) particles, plus specific information relevant to the interaction between the two particles. A schematic depicting entrance and exit channels is shown in Figure II.1. Note that entrance channels can also occur as exit channels, but some exit channels (e.g., fission channels) do not occur as entrance channels. Two interacting particles are shown in the portion of the figure that is labeled “Interior Region”; here the particles are separated by less than the interaction radius *a*.

In Section II.A, general equations of scattering theory are presented and their derivations discussed. The fundamental R-matrix equations are presented. Section II.A.1 gives a detailed derivation of the equations for a simple case. Section II.A.2 shows the relationship between the R-matrix and the A-matrix, which is another common representation of scattering theory.

The approximations to R-matrix theory available in the SAMMY code are detailed in Section II.B. The recommended choice for most applications is the Reich-Moore approximation, described in Section II.B.1. For some applications, the Reich-Moore approximation is inadequate; for those cases, a method for using SAMMY's Reich-Moore approximation to mimic the full (exact) R-matrix is presented Section II.B.2. Two historically useful but now obsolete approximations are single-level and multilevel Breit Wigner (SLBW and MLBW), discussed in Section II.B.3. Provisions for including non-compound (direct) effects are discussed in Section II.B.4.

In Section II.C, details are given for the SAMMY nomenclature and other conventions, for transformations to the center-of-momentum system, and for the calculation of penetrability, shift factors, and hard-sphere phase shifts in both Coulomb and non-Coulomb cases.

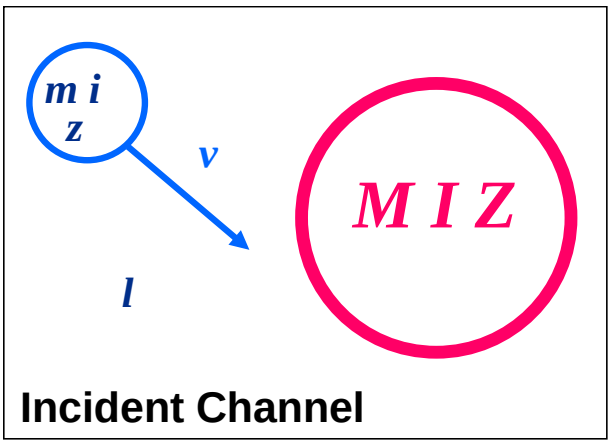
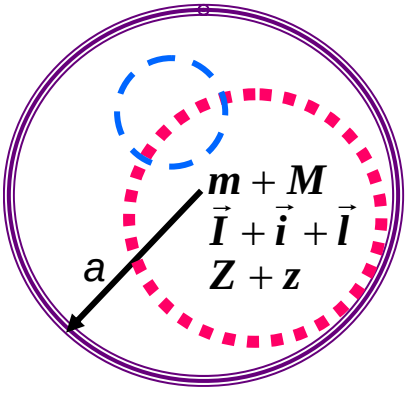
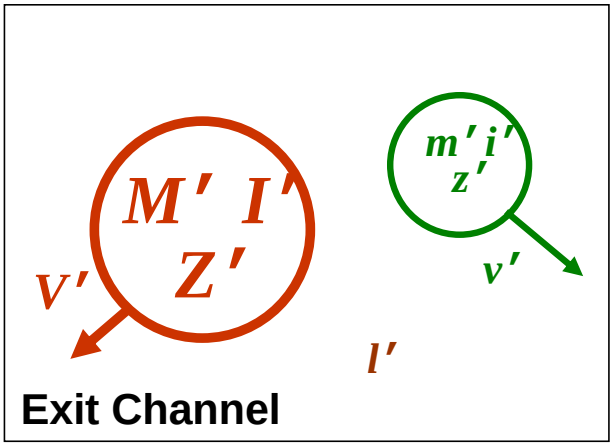


Figure II.1. Schematic of entrance and exit channels as used in scattering theory. For the interior region (with separation distance $r < a$), no assumptions are made about the nature of the interaction. In the figure, m, i, and z refer to the mass, spin, and charge of the incident particle while M, I and Z refer to the target particle. Orbital angular momentum is denoted by l and velocity by v. Primes are used for post-collision quantities.





II. A. EQUATIONS FOR SCATTERING THEORY

In this section, equations for scattering theory are presented but not derived. Specifics for the R-matrix formulation of scattering theory are presented in Section II.A.1, which provides a discussion of an alternative formulation (the A-matrix). Readers interested in the derivation of the equations for scattering theory are referred to the Lane and Thomas article [AL58] for a detailed derivation in the general case, or to Section II.A.2 of this document for a simplified version.

In scattering theory, a channel may be defined by $c = (\alpha, l, s, J)$, where the following definitions apply:

- α represents the two particles making up the channel; α includes mass (m and M), charge (z and Z), spin (i and I) with associated parities, and all other quantum numbers for each of the two particles, plus the Q-value (equivalent to the negative of the threshold energy in the center of momentum system).

- l is the orbital angular momentum of the pair, and the associated parity is given by $(-1)^l$.

- s represents the channel spin (including the associated parity); that is, s is the quantized vector sum of the spins of the two particles of the pair: $\vec{s} = \vec{i} + \vec{I}$.

- J is the total angular momentum (and associated parity); that is, J is the quantized vector sum of l and s: $\vec{J} = \vec{l} + \vec{s}$.

Only J and its associated parity π are conserved for any given interaction. The other quantum numbers may differ from channel to channel, as long as the sum rules for spin and parity are obeyed. Within this document and within the SAMMY code, the set of all channels with the same J and π are called a "spin group."

In all formulae given below, spin quantum numbers (e.g., J) are implicitly assumed to include the associated parity. Quantized vector sum rules are implicitly assumed to be obeyed. Readers unfamiliar with these sum rules are referred to Section II.C.1.a for a mini-tutorial on the subject.

Let the angle-integrated cross sections from entrance channel c to exit channel c' with total angular momentum J be represented by $\sigma_{cc'}$. This cross section is given in terms of the scattering matrix $U_{cc'}$ as

$$\sigma_{cc'} = \frac{\pi}{k_a^2} g_{J\alpha} \left| e^{2iw_c} \delta_{cc'} - U_{cc'} \right|^2 \delta_{JJ'} \quad , \qquad \text{(II A.1)}$$

where k_α is the wave number (and $K_\alpha = \hbar k_\alpha$ = center-of-mass momentum) associated with incident particle pair α, $g_{J\alpha}$ is the spin statistical factor, and w_c is the Coulomb phase-shift

difference. Note that w_c is zero for non-Coulomb channels. (Details for the charged-particle case are presented in Section II.C.4.) The spin statistical factor g is given by

$$g_{J\alpha} = \frac{2J+1}{(2i+1)\,(2I+1)} \quad , \tag{II A.2}$$

and center-of-mass momentum K_α by

$$K_\alpha^2 = \left(\hbar k_\alpha\right)^2 = \frac{2m\,M^2}{\left(m+M\right)^2} E \quad . \tag{II A.3}$$

Here E is the laboratory kinetic energy of the incident (moving) particle. A derivation of this value for K_α is given in Section II.C.2.

The scattering matrix U can be written in terms of matrix W as

$$U_{cc'} = \Omega_c\, W_{cc'}\, \Omega_{c'} \quad , \tag{II A.4}$$

where Ω is given by

$$\Omega_c = e^{i\,(w_c - \varphi_c)} \quad . \tag{II A.5}$$

Here again, w_c is zero for non-Coulomb channels, and the potential scattering phase shifts for non-Coulomb interactions φ_c are defined in many references (e.g., [AL58]) and shown in Table II A.1. The matrix W in Eq. (II A.4) is related to the R-matrix (in matrix notation with indices suppressed) via

$$W = P^{1/2}(I - RL)^{-1}(I - RL^*)P^{-1/2} \quad . \tag{II A.6}$$

The quantity I in this equation represents the identity matrix. The form of the R-matrix is given in Section II.A.1 in general and in Section II.B for the versions used in SAMMY. The quantity L in Eq. (II A.6) is given by

$$L = (S - B) + iP \quad , \tag{II A.7}$$

with P being the penetration factor (penetrability) S the shift factor, and B the arbitrary boundary constant at the channel radius a_c. P and S are functions of energy E, and also depend on the orbital angular momentum l and the channel radius a_c. Formulae for P and S are found in many references (see, for example, Eq. (2.9) in [JL58]).

For non-Coulomb interactions, the penetrability and shift factor have the form

$$P \to P_l\left(\rho\right) \quad \text{and} \quad S \to S_l\left(\rho\right) \quad , \tag{II A.8}$$

where ρ is related to the center-of-mass momentum which in turn is related to the laboratory energy of the incident particle (E). For arbitrary channel c with particle pair α, orbital angular momentum l, and channel radius a_c, ρ has the form

$$\rho = k_\alpha a_c = \frac{1}{\hbar}\sqrt{\frac{2m_\alpha M_\alpha}{(m_\alpha + M_\alpha)}\frac{M}{(m+M)}}\sqrt{(E-\Xi_\alpha)}\ \ a_c \quad , \qquad \text{(II A.9)}$$

as shown in Section II.C.2. Here Ξ_α is the energy threshold for particle pair α, m_α and M_α are the masses of the two particles of particle pair α, and m and M are the masses of the incident particle and target nuclide, respectively.

Appropriate formulae for P, S, and φ in the non-Coulomb case are shown in Table IIA.1. For two charged particles, formulae for the penetrabilities are given in Section II.C.4.

The energy dependence of fission and capture widths is negligible over the energy range of these calculations. Therefore, a penetrability of unity may be used.

Table II A.1. Hard-sphere penetrability (penetration factor) *P*, level shift factor *S*, and potential-scattering phase shift φ for orbital angular momentum *l*, wave number *k*, and channel radius a_c, with $\rho = ka_c$

l	P_l	S_l	φ_l
0	ρ	0	ρ
1	$\rho^3/(1+\rho^2)$	$-1/(1+\rho^2)$	$\rho - \tan^{-1}\rho$
2	$\rho^5/(9+3\rho^2+\rho^4)$	$-(18+3\rho^2)/(9+3\rho^2+\rho^4)$	$\rho - \tan^{-1}[3\rho/(3-\rho^2)]$
3	$\rho^7/(225+45\rho^2)+6\rho^4+\rho^6)$	$-(675+90\rho^2+6\rho^4)/(225+45\rho^2+6\rho^4+\rho^6)$	$\rho - \tan^{-1}[\rho(15-\rho^2)/(15-6\rho^2)]$
4	$\rho^9/(11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8$	$-(44100+4725\rho^2+270\rho^4+10\rho^6)/(11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8)$	$\rho - \tan^{-1}[\rho(105-10\rho^2)/(105-45\rho^2+\rho^4)]$
l	$\dfrac{\rho^2 P_{l-1}}{(l-S_{l-1})^2+P_{l-1}^2}$	$\dfrac{\rho^2(l-S_{l-1})}{(l-S_{l-1})^2+P_{l-1}^2} - l$	$\varphi_{l-1} - \tan^{-1}\left((P_{l-1}/(l-S_{l-1})\right)$ or $B_l = (B_{l-1}+X_l)/(1-B_{l-1}X_l)$ with $B_l = \tan(\rho-\varphi_l)$ and $X_l = (P_{l-1})/(l-S_{l-1})$

Formulae for a particular cross section type can be derived by summing over the terms in Eq. (II A.1). For the total cross section, the sum over all possible exit channels and all spin groups gives

$$\begin{aligned}\sigma^{total} &= \sum_{\substack{incident\\channels\\c}} \sum_{\substack{all\\channels\\c'}} \sum_{J} \frac{\pi}{k_\alpha^2} g_\alpha \left|\delta_{cc'} - U_{cc'}\right|^2 \\ &= \frac{\pi}{k_\alpha^2} \sum_{J} g_J \sum_{\substack{incident\\channels\\c}} \sum_{\substack{all\\channels\\c'}} \left(\delta_{cc'} - U_{cc'}\delta_{cc'} - U_{cc'}^{*}\delta_{cc'} + \left|U_{cc'}\right|^2\right) \qquad \text{(II A.10)} \\ &= \frac{2\pi}{k_\alpha^2} \sum_{J} g_J \sum_{\substack{incident\\channels\\c}} \left(1 - \mathrm{Re}\left(U_{cc}\right)\right) \quad .\end{aligned}$$

For non-charged incident particles, the elastic (or scattering) cross section is given by

$$\sigma_{\alpha\alpha} = \frac{\pi}{k_\alpha^2} \sum_{J} g_J \sum_{\substack{c=incident\\channel}} \left(1 - 2\,\mathrm{Re}\left(U_{cc}\right) + \sum_{\substack{c'=incident\\channel}} \left|U_{cc'}\right|^2\right) \quad . \qquad \text{(II A.11)}$$

Similarly, the cross section for any non-elastic reaction can be written

$$\sigma_\alpha^{reaction} = \frac{\pi}{k_\alpha^2} \sum_{J} g_J \sum_{\substack{c=incident\\channel}} \sum_{\substack{c'=reaction\\channel}} \left|U_{cc'}\right|^2 \quad . \qquad \text{(II A.12)}$$

In particular, the capture cross section could be written as the difference between the total and all other cross sections,

$$\sigma^{capture} = \frac{\pi}{k_\alpha^2} \sum_{J} g_J \sum_{\substack{c=incident\\channel}} \left(1 - \sum_{\substack{c'=all\ channels\\except\ capture}} \left|U_{cc'}\right|^2\right) \quad . \qquad \text{(II A.13)}$$

(This form will be used later, in Section II.B.1.a, when the capture channels are treated in an approximate fashion.)

II.A.1. R-Matrix and A-Matrix Equations

The R-matrix was introduced in Eq. (II A.6) as

$$W = P^{1/2}(I - RL)^{-1}(I - RL^{*})P^{-1/2} \quad , \tag{II A1.1}$$

but the formula for the R-matrix was not given there. If λ represents a particular resonance (or level), then the general form for the R-matrix is

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c}\,\gamma_{\lambda c'}}{E_{\lambda} - E}\,\delta_{JJ'} \quad , \tag{II A1.2}$$

where E_{λ} represents the energy of the resonance, and the reduced width amplitude γ is related to the partial width Γ by

$$\Gamma_{\lambda \boldsymbol{c}} = 2\,\boldsymbol{P_c}\,\gamma_{\lambda \boldsymbol{c}}^{2} \quad . \tag{II A1.3}$$

The sum in Eq. (II A1.2) contains an infinite number of levels. All channels, including the "gamma channel" for which one of the particles is a photon, are represented by the channel indices.

The R-matrix is not the only possibility for parameterization of the scattering matrix. In the R-matrix formulation, equations are expressed in terms of channel-channel interactions. It is also possible to formulate scattering theory in terms of level-level interactions; this formulation uses what is called the A-matrix, which is defined as

$$A^{-1}_{\mu\lambda} = \left(E_{\lambda} - E\right)\delta_{\mu\lambda} - \sum_{c} \gamma_{\mu c}\,L_c\,\gamma_{\lambda c} \quad . \tag{II A1.4}$$

To see the relationship of the A-matrix to the R-matrix, we begin by multiplying both sides of Eq. (II A1.4) by A and summing over λ:

$$\begin{aligned} &\sum_{\lambda} A^{-1}_{\mu\lambda}\,A_{\lambda\nu} = \sum_{\lambda}\left(E_{\lambda} - E\right)\delta_{\mu\lambda}\,A_{\lambda\nu} - \sum_{c}\gamma_{\mu c}\,L_c \sum_{\lambda}\gamma_{\lambda c}\,A_{\lambda\nu} \quad , \\ \text{or} \qquad &\delta_{\mu\nu} = \left(E_{\mu} - E\right)A_{\mu\nu} - \sum_{c}\gamma_{\mu c}\,L_c \sum_{\lambda}\gamma_{\lambda c}\,A_{\lambda\nu} \quad . \end{aligned} \tag{II A1.5}$$

Dividing by $\left(E_{\mu} - E\right)$, multiplying on the left by $\gamma_{\mu c'}$ and on the right by $\gamma_{\nu c''}$, and summing over μ puts this equation into the form

$$\begin{aligned} \sum_{\mu}\gamma_{\mu c'}\left(E_{\mu} - E\right)^{-1}\delta_{\mu\nu}\,\gamma_{\nu c''} = &\sum_{\mu}\gamma_{\mu c'}\left(E_{\mu} - E\right)^{-1}\left(E_{\mu} - E\right)A_{\mu\nu}\,\gamma_{\nu c''} \\ &-\sum_{\mu}\gamma_{\mu c'}\left(E_{\mu} - E\right)^{-1}\sum_{c}\gamma_{\mu c}\,L_c \sum_{\lambda}\gamma_{\lambda c}A_{\lambda\nu}\,\gamma_{\nu c''} \quad , \end{aligned} \tag{II A1.6}$$

which can be reduced to

$$\gamma_{\nu c'}\left(E_\nu - E\right)^{-1}\gamma_{\nu c''} = \sum_\mu \gamma_{\mu c'} A_{\mu\nu}\gamma_{\nu c''} - \sum_c \left[\sum_\mu \gamma_{\mu c'}\left(E_\mu - E\right)^{-1}\gamma_{\mu c}\right] L_c \sum_\lambda \gamma_{\lambda c} A_{\lambda\nu}\gamma_{\nu c''} \quad . \tag{II A1.7}$$

Summing over *v* puts this into the form

$$\left[\sum_\nu \gamma_{\nu c'}\left(E_\nu - E\right)^{-1}\gamma_{\nu c''}\right] = \sum_{\mu\nu} \gamma_{\mu c'} A_{\mu\nu}\gamma_{\nu c''} - \sum_c \left[\sum_\mu \gamma_{\mu c'}\left(E_\mu - E\right)^{-1}\gamma_{\mu c}\right] L_c \sum_{\lambda\nu} \gamma_{\lambda c} A_{\lambda\nu}\gamma_{\nu c''} \quad , \tag{II A1.8}$$

in which we can replace the quantities in square brackets by the R-matrix, giving

$$\begin{aligned} R_{c'c''} &= \sum_{\mu\nu}\gamma_{\mu c'} A_{\mu\nu}\gamma_{\nu c''} - \sum_c R_{c'c} L_c \sum_{\lambda\nu}\gamma_{\lambda c} A_{\lambda\nu}\gamma_{\nu c''} \\ &= \sum_c \left[\delta_{c'c} - R_{c'c}L_c\right]\sum_{\lambda\nu}\gamma_{\lambda c} A_{\lambda\nu}\gamma_{\nu c''} \quad . \end{aligned} \tag{II A1.9}$$

Solving for the summation, this equation can be rewritten as

$$\left[\left(I - RL\right)^{-1} R\right]_{cc''} = \sum_{\lambda\nu}\gamma_{\lambda c} A_{\lambda\nu}\gamma_{\nu c''} \quad . \tag{II A1.10}$$

To relate this to the scattering matrix, we note that Eq. (II A.6) can be rewritten using Eq. (II A.7) into the form

$$\begin{aligned} W &= P^{1/2}\left(I - RL\right)^{-1}\left(I - RL^*\right)P^{-1/2} \\ &= P^{1/2}\left(I - RL\right)^{-1}\left(I - RL + 2iRP\right)P^{-1/2} \\ &= P^{1/2}\left[\left(I - RL\right)^{-1}\left(I - RL\right) + 2i\left(I - RL\right)^{-1} RP\right]P^{-1/2} \\ &= P^{1/2}P^{-1/2} + 2iP^{1/2}\left(I - RL\right)^{-1} RPP^{-1/2} \\ &= I + 2iP^{1/2}\left(I - RL\right)^{-1} RP^{1/2} \quad . \end{aligned} \tag{II A1.11}$$

Comparing Eq. (II A1.10) to Eq. (II A1.11) gives, in matrix form,

$$W = I + 2iP^{1/2}\gamma A\gamma P^{1/2} \quad . \tag{II A1.12}$$

These equations are exact; no approximations have been made.

One common approximation should be discussed here: the "eliminated channel" approximation, for which one particular type of channel is treated in aggregate and assumed to not interfere from level to level. This is most easily understood in the A-matrix definition, Eq. (II A1.4); assuming no level-level interference for the gamma channels (for example), this equation can be approximated as

$$A^{-1}_{\mu\lambda} \approx \left(E_\lambda - E\right)\delta_{\mu\lambda} - \left[\sum_{\substack{\gamma=\text{gamma}\\ \text{channels}}} \gamma_{\mu\gamma}\, L_\gamma\, \gamma_{\lambda\gamma}\right]\delta_{\mu\lambda} - \sum_{\substack{c=\text{particle}\\ \text{channels}}} \gamma_{\mu c}\, L_c\, \gamma_{\lambda c} \quad . \qquad \text{(II A1.13)}$$

The quantity in square brackets corresponds to those channels for which the level-level interference is to be neglected; that is, only the interactions within one level are important. For gamma channels, $L = S+iP$ reduces to $L= i$, so Eq. (II A1.13) becomes

$$A^{-1}_{\mu\lambda} \approx \left(E_\lambda - E - i\overline{\Gamma}_{\lambda\gamma}/2\right)\delta_{\mu\lambda} - \sum_{\substack{c=\text{particle}\\ \text{channels}}} \gamma_{\mu c}\, L_c\, \gamma_{\lambda c} \quad . \qquad \text{(II A1.14)}$$

The bar over $\overline{\Gamma}_{\lambda\gamma}$ is used to indicate the special treatment for this channel.

In this form, our expression for A is analogous to the exact expression in Eq. (II A1.4) with two modifications: the additional imaginary term is added to the energy difference, and the sum over the channels includes only the "particle channels" (non-eliminated channels). It is therefore possible to immediately write the R-matrix formula for the eliminated-channel approximation as

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c}\, \gamma_{\lambda c'}}{E_\lambda - E - i\overline{\Gamma}_{\lambda\gamma}/2}\, \delta_{JJ'} \quad , \qquad \text{(II A1.15)}$$

where the channel indices c and c' refer only to particle channels, not to the gamma channels. This formula for the R-matrix is the Reich-Moore approximation and is the form which is used in the SAMMY code. See Section II.B.1 for more about this formulation of R-matrix theory.

II.A.2. Derivation of Scattering Theory Equations

Many authors have given derivations of the equations for the scattering matrix in terms of the R-matrix. Sources for the derivation shown here are unpublished lecture notes of Fröhner [FF02], presented at the SAMMY workshop in Paris in 2002, and Foderaro [AF71]. This derivation is valid for only the simple case of spinless projectiles and target nuclei, assuming only elastic scattering and absorption. For the general case, the reader is referred to Lane and Thomas [AL58].

Schrödinger equation

The Schrödinger equation with a complex potential is

$$\left(\frac{-\hbar^2}{2m} \nabla^2 + V + iW \right) \psi = E\psi \quad , \tag{II A2.1}$$

in which one can consider that V causes scattering and W causes absorption. The wave function can be expanded in the usual fashion,

$$\psi(r, \cos\theta) \; = \; \sum_{l=0}^{\infty} \frac{u_l(r)}{r} P_l(\cos\theta) \quad , \tag{II A2.2}$$

for which the radial portion obeys the equation

$$\frac{d^2 u_l}{dr^2} \; + \; \left[k^2 - \frac{2m}{\hbar^2}(V + iW) - \frac{l(l+1)}{r^2} \right] u_l \; = \; 0 \quad , \tag{II A2.3}$$

subject to the conditions that $|\psi|^2$ is everywhere finite and that

$$u_l(r = 0) = 0 \quad . \tag{II A2.4}$$

In the external region, $r > a$, the nuclear forces are zero ($V = W = 0$), so the solution has the form

$$u_l(r) \; = \; I_l(r) - U_l O_l(r) \quad . \tag{II A2.5}$$

I_l represents an incoming free wave, and O_l represents an outgoing free wave. U_l is the "collision function" or "S function" that describes the effects of the nuclear interaction, giving both the attenuation and the phase shift of the outgoing wave:

and

$$\begin{aligned} |U_l|^2 &= 1 \text{ for } W = 0 \quad , \\ |U_l|^2 &< 1 \text{ for } W \neq 0 \quad . \end{aligned} \tag{II A2.6}$$

Our goal is to determine an appropriate analytic form for U_l.

Orthogonal eigenvectors in interior region

For the interior region $r < a$, we define eigenfunctions $w_{\lambda l}(r)$ and eigenvalues E_λ,

$$E_\lambda = \frac{\hbar^2 k_\lambda^2}{2m} \quad , \tag{II A2.7}$$

for the wave equation without absorption ($W = 0$),

$$\frac{d^2 w_{\lambda l}}{dr^2} + \left[k_\lambda^{\,2} - \frac{2m}{\hbar^2} V - \frac{l(l+1)}{r^2} \right] w_{\lambda l} = 0 \quad , \tag{II A2.8}$$

for which the boundary conditions are

$$w_{\lambda l}(r=0) = 0 \qquad \text{and} \qquad \frac{a}{w_{\lambda l}(a)} \left. \frac{d w_{\lambda l}}{dr} \right|_{r=a} = B_l \quad . \tag{II A2.9}$$

Note that $w_{\lambda l}(r)$ is real if the boundary parameter B_l is chosen to be real. The eigenfunctions are orthogonal, since

$$\begin{aligned} \int_0^a \left(\frac{d^2 w_{\lambda l}}{dr^2} w_{\mu l} - w_{\lambda l} \frac{d^2 w_{\mu l}}{dr^2} \right) dr &= \int_0^a \frac{d}{dr} \left(\frac{d w_{\lambda l}}{dr} w_{\mu l} - w_{\lambda l} \frac{d w_{\mu l}}{dr} \right) dr \\ &= \left[\frac{d w_{\lambda l}}{dr} w_{\mu l} - w_{\lambda l} \frac{d w_{\mu l}}{dr} \right]_0^a \\ &= \left. \frac{d w_{\lambda l}}{dr} \right|_{r=a} w_{\mu l}(a) \; - \; w_{\lambda l}(a) \left. \frac{d w_{\mu l}}{dr} \right|_{r=a} - \; [0] \\ &= \frac{B_l}{a} \left[w_{\lambda l}(a) w_{\mu l}(a) - w_{\lambda l}(a) w_{\mu l}(a) \right] \; = \; 0 \quad , \end{aligned} \tag{II A2.10}$$

in which both equations of (II A2.9) have been invoked. The integral in Eq. (II A2.10) can also be evaluated using Eq. (II A2.8), giving

$$
\begin{aligned}
&\int_0^a \left(\frac{d^2 w_{\lambda l}}{dr^2} w_{\mu l} - w_{\lambda l} \frac{d^2 w_{\mu l}}{dr^2} \right) dr \\
&\quad = \int_0^a \left(\left[-k_\lambda^2 - \frac{2mV}{\hbar^2} \right] w_{\lambda l} w_{\mu l} - w_{\lambda l} \left[-k_\mu^2 - \frac{2mV}{\hbar^2} \right] w_{\lambda l} \right) dr \\
&\quad = \int_0^a \left(-k_\lambda^2 w_{\lambda l} w_{\mu l} + k_\mu^2 w_{\lambda l} w_{\mu l} \right) dr \\
&\quad = -\left(k_\lambda^2 - k_\mu^2 \right) \int_0^a w_{\lambda l} w_{\mu l} \, dr \quad .
\end{aligned}
\tag{II A2.11}
$$

Equating Eq. (II A2.10) to Eq. (II A2.11) gives

$$
\left(k_\lambda^2 - k_\mu^2 \right) \int_0^a w_{\lambda l} w_{\mu l} \, dr = 0 \quad . \tag{II A2.12}
$$

For $\lambda \neq \mu$, assuming no degenerate states, it therefore follows that

$$
\int_0^a w_{\lambda l} w_{\mu l} \, dr = 0 \ \text{ if } \lambda \neq \mu \quad . \tag{II A2.13}
$$

The orthogonality of the eigenvectors is therefore established. We assume that these wave functions are normalized such that

$$
\int_0^a w_{\lambda l} \, w_{\mu l} \ dr \ = \ \delta_{\lambda \mu} \quad . \tag{II A2.14}
$$

Matching at the surface

The internal wave function for the true potential (including the imaginary part *iW*) can be expanded in terms of the eigenfunctions as

$$
u_l(r) = \sum_\lambda c_{\lambda l} \, w_{\lambda l}(r) \quad \text{for } r \leq a \quad , \tag{II A2.15}
$$

with

$$
c_{\lambda l} = \int_0^a u_l \, w_{\lambda l} \ dr \quad . \tag{II A2.16}
$$

This equation for $c_{\lambda l}$ is derived by multiplying Eq. (II A2.15) by $u_{\lambda l}(r)$, integrating, and applying Eq. (II A2.14).

Consider now the integral

$$\int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr \quad , \tag{II A2.17}$$

which can be expanded by use of Eqs. (II A2.3) and (II A2.8) to give

$$\begin{aligned} &\int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr \\ &\quad = \int_0^a \left(-\left[k^2 - \frac{2m}{\hbar^2}(V + iW) - \frac{l(l+1)}{r^2} \right] u_l \, w_{\lambda l} + u_l \left[k_\lambda{}^2 - \frac{2m}{\hbar^2} V - \frac{l(l+1)}{r^2} \right] w_{\lambda l} \right) dr \qquad \text{(II A2.18)} \\ &\quad = \left(k_\lambda{}^2 - k^2 \right) \int_0^a u_l w_{\lambda l} \, dr \quad + \quad \frac{2m}{\hbar^2} \int_0^a W u_l w_{\lambda l} \, dr \quad . \end{aligned}$$

Defining $\bar{W}_{\lambda l}$ as

$$\bar{W}_{\lambda l} \quad = \quad \int_0^a W u_l \, w_{\lambda l} \, dr \Big/ \int_0^a u_l \, w_{\lambda l} \, dr \tag{II A2.19}$$

permits rewriting Eq. (II A2.18) in the form

$$\int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr = \left(k_\lambda{}^2 - k^2 + i \frac{2m}{\hbar^2} \bar{W}_{\lambda l} \right) \int_0^a u_l \, w_{\lambda l} \, dr \quad . \tag{II A2.20}$$

Integrating the left-hand side of this equation gives

$$\begin{aligned} \int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr \; &= \left[\frac{du_l}{dr} w_{\lambda l} - u_l \frac{dw_{\lambda l}}{dr} \right]_0^a \; = \left[\frac{du_l}{dr} w_{\lambda l} - u_l \frac{dw_{\lambda l}}{dr} \right]_{r=a} \\ &= \left[\frac{du_l}{dr} w_{\lambda l} - u_l \frac{B_l}{a} w_{\lambda l} \right]_{r=a} = \left[a \frac{du_l}{dr} - u_l B_l \right]_{r=a} \frac{w_{\lambda l}(a)}{a} \quad , \end{aligned} \tag{II A2.21}$$

in which we have again made use of the boundary condition of Eq. (II A2.9). Integrating the right-hand side of Eq. (II A2.20) by applying Eq. (II A2.16) gives

$$\left(k_\lambda{}^2 - k^2 + i\frac{2m}{\hbar^2}\bar{W}_{\lambda l}\right)\int_0^a u_l\, w_{\lambda l}\, dr \;=\; \left(k_\lambda{}^2 - k^2 + i\frac{2m}{\hbar^2}\bar{W}_{\lambda l}\right)c_{\lambda l} \quad . \tag{II A2.22}$$

Equating Eqs. (II A2.21) and (II A2.22) therefore gives

$$\begin{aligned}\left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a}\frac{w_{\lambda l}}{a} &= \left(k_\lambda{}^2 - k^2 + i\frac{2m}{\hbar^2}\bar{W}_{\lambda l}\right)c_{\lambda l} \quad , \\ \left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a}\frac{w_{\lambda l}}{a} &= \left(E_\lambda - E + i\bar{W}_{\lambda l}\right)\frac{2m\, c_{\lambda l}}{\hbar^2} \quad ,\end{aligned} \tag{II A2.23}$$

or

$$c_{\lambda l} = \frac{\hbar^2\, w_{\lambda l}(a)}{2ma\left(E_\lambda - E + i\bar{W}_{\lambda l}\right)}\left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a} \quad . \tag{II A2.24}$$

Inserting this into Eq. (II A2.15) gives

$$u_l(r) = \sum_\lambda w_{\lambda l}(r)\frac{\hbar^2 w_{\lambda l}(a)}{2ma\left(E_\lambda - E + i\bar{W}_{\lambda l}\right)}\left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a} \quad , \tag{II A2.25}$$

which, when evaluated at $r = a$, becomes

$$u_l(a) = \sum_\lambda \frac{\hbar^2 w_{\lambda l}^2(a)}{2ma\left(E_\lambda - E + i\bar{W}_{\lambda l}\right)}\left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a} \quad . \tag{II A2.26}$$

Rearranging, this becomes

$$\begin{aligned}u_l(a) &= \left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a}\sum_\lambda \frac{\left[\hbar^2 w_{\lambda l}^2(a)/2ma\right]}{\left(E_\lambda - E + i\bar{W}_{\lambda l}\right)} \\ &= \left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a}\sum_\lambda \frac{\gamma_{\lambda l}^2}{\left(E_\lambda - E + i\Gamma_{\lambda l}/2\right)} \quad ,\end{aligned} \tag{II A2.27}$$

in which the decay amplitude $\gamma_{\lambda l}$ is defined as

$$\gamma_{\lambda l} \equiv \sqrt{\frac{\hbar^2 w_{\lambda l}^2(a)}{2ma}} \tag{II A2.28}$$

and the absorption width $\Gamma_{\lambda l}$ as

$$\Gamma_{\lambda l} \equiv 2W_{\lambda l} \quad . \tag{II A2.29}$$

If we then define the R-function as

$$R_l = \sum_\lambda \frac{\gamma_{\lambda l}^2}{\left(E_\lambda - E + i\Gamma_{\lambda l}/2\right)} \quad , \qquad \text{(II A2.30)}$$

then Eq. (II A2.27) can be written in the form

$$u_l = \left(a\frac{du_l}{dr} - u_l B_l \right) R_l \quad , \qquad \text{(II A2.31)}$$

in which everything is evaluated at the matching radius *a*.

Scattering matrix in terms of R-matrix (neutrons only)

Equation (II A2.31) can be converted into the usual R-matrix formulae by inserting Eq. (II A2.5),

$$u_l = I_l - U_l O_l \quad , \qquad \text{(II A2.32)}$$

yielding

$$I_l - U_l O_l = \left[a\left(\frac{dI_l}{dr} - U_l \frac{dO_l}{dr} \right) - B_l \left(I_l - U_l O_l \right) \right] R_l \quad , \qquad \text{(II A2.33)}$$

in which everything is again evaluated at the matching radius *a*. Solving Eq. (II A2.33) for *U* gives

$$U_l \left[-O_l + R_l \left(a\frac{dO_l}{dr} - B_l O_l \right) \right] = I_l - R_l \left(a\frac{dI_l}{dr} - B_l I_l \right) \quad , \qquad \text{(II A2.34)}$$

or

$$U_l = \frac{I_l - R_l \left(a\frac{dI_l}{dr} - B_l I_l \right)}{\left[-O_l + R_l \left(a\frac{dO_l}{dr} - B_l O_l \right) \right]} = \frac{I_l}{O_l} \frac{1 - R_l \left(\frac{a}{I_l}\frac{dI_l}{dr} - B_l \right)}{1 - R_l \left(\frac{a}{O_l}\frac{dO_l}{dr} - B_l \right)} \quad . \qquad \text{(II A2.35)}$$

We define L_l as

$$L_l \equiv \frac{a}{O_l(a)} \left. \frac{dO_l}{dr} \right|_{r=a} \equiv S_l + i P_l \quad . \qquad \text{(II A2.36)}$$

For spinless particles, $I_l^* = O_l$, so that

$$\frac{a}{I_l(a)}\frac{dI_l}{dr}\bigg|_{r=a} = L_l^* = S_l - iP_l \qquad \text{(II A2.37)}$$

and

$$\frac{I_l}{O_l} = \frac{O_l^*}{O_l} = \frac{|O|e^{-i\varphi}}{|O|e^{i\varphi}} = e^{-2i\varphi} \quad . \qquad \text{(II A2.38)}$$

Therefore Eq. (II A2.34) becomes

$$U_l \;=\; e^{-2i\varphi}\,\frac{1-R_l\left(L_l^*-B_l\right)}{1-R_l\left(L_l-B_l\right)} \quad , \qquad \text{(II A2.39)}$$

which is the usual form for the scattering matrix in terms of the R-matrix in this simple case.

II.A.2.a. Relating the scattering matrix to the cross sections

The relationship between the scattering matrix *U* and the cross section σ is also described by many authors; see, for example, [AF71]. Here we provide a summary for the simplest case.

The wave function for a spinless particle far from the scattering source can be written as

$$\psi(r,\theta) = e^{ikz} + \frac{e^{ikr}}{r} f(\theta) \quad , \tag{II A2 a.1}$$

where *f* has the form

$$f(\theta) = \frac{1}{2ik}\sum_l (2l+1)\left[U_l - 1\right] P_l(\cos\theta) \quad . \tag{II A2 a.2}$$

The cross section is then given by

$$\frac{d\sigma}{d\Omega} = \left| f(\theta) \right|^2 \quad . \tag{II A2 a.3}$$

For angle-integrated cross sections, the equation found by inserting Eq. (II A2 a.2) into Eq. (II A2 a.3) can be integrated to give

$$\begin{aligned}
\sigma &= \int \left[-\frac{1}{2ik}\sum_l (2l+1)\left[U_l^* - 1\right] P_l(\cos\theta) \right] \\
&\qquad \times \left[\frac{1}{2ik}\sum_{l'} (2l'+1)\left[U_{l'} - 1\right] P_{l'}(\cos\theta) \right] d(\cos\theta)\, d\varphi \\
&= \frac{1}{4k^2}\sum_{ll'} (2l+1)(2l'+1)\left[U_l^* - 1\right]\left[U_{l'} - 1\right] \int_0^{2\pi} d\varphi \int_{-1}^{1} P_l(\cos\theta) P_{l'}(\cos\theta)\, d(\cos\theta) \qquad \text{(II A2 a.4)} \\
&= \frac{1}{4k^2}\sum_{ll'} (2l+1)(2l'+1)\left[U_l^* - 1\right]\left[U_{l'} - 1\right] 2\pi \frac{2}{2l+1}\delta_{ll'} \\
&= \frac{\pi}{k^2}\sum_l (2l+1)\left|U_l - 1\right|^2 \quad .
\end{aligned}$$

This is analogous to the "standard" scattering theory equation shown in Eq. (II A.1).

II. B. VERSIONS OF MULTILEVEL R-MATRIX THEORY

Many representations of multilevel R-matrix theory have been developed over the years. For a summary of the more common versions, the reader is referred to the works of Fröhner [FF80, FF00].

Four versions of R-matrix theory are available in SAMMY: the Reich-Moore approximation (Section II.B.1), the single-level (SLBW) and multilevel Breit-Wigner (MLBW) approximations (Section II.B.3), and a variant on the Reich Moore which mimics the full R-matrix (Section II.B.2). An option to include a direct capture component is also provided (Section II.B.4).

The Reich-Moore approximation is the preferred method for most modern evaluations; it is the default formalism for SAMMY runs.

Fröhner, in fact, suggests that the Reich-Moore approximation is universally applicable to all cases: "Experience has shown that with this approximation [Reich Moore] all resonance cross section data can be described in detail, in the windows as well as in the peaks, even the weirdest multilevel interference patterns . . . It works equally well for light, medium-mass and heavy nuclei, fissile and nonfissile." [FF00, page 60]

For most purposes, Reich Moore is indeed indistinguishable from the exact formulation. Notable exceptions are situations where interference effects exist between capture and other channels. For those cases, small modifications to the SAMMY input will permit the user to mimic the effect of the non-approximated R-matrix; see Section II.B.2 for details.

Occasionally it is not possible to properly describe a cross section within the confines of R-matrix theory, because the reaction includes a direct component. SAMMY has provisions for the user to provide a numerical description of this component; see Section II.B.4 for details.

Also available within SAMMY are both the SLBW and the MLBW formulations (Section II.B.3); these are included for the sake of completeness, for comparison purposes, and because many of the evaluations in the nuclear data files were performed with Breit-Wigner formulae. However, it is strongly recommended that only Reich Moore be used for new evaluations, for several reasons: MLBW is often inadequate; SLBW is almost always inadequate. When it is correct, MLBW gives identical results to Reich Moore. "Ease of Programming" is no longer a valid excuse for using MLBW, since the programming has already been accomplished. Similarly, a slow computer is no longer a legitimate excuse, since modern computers can readily handle the more rigorous formulae.

Finally, it should be noted that SAMMY's implementation of MLBW does not correspond to the usual definition of MLBW. Instead, SAMMY uses the ENDF [ENDF-102] convention in which only the elastic cross section is truly multilevel, and all other types of cross section are single level.

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

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

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 $\overline{\Gamma}_{\lambda\gamma}$ 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

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

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

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

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.

II. B. 1. a. Energy-differential cross sections

The observable cross sections are found in terms of X by first substituting Eqs. (II A.4, II A.5, and II B1.3) into Eq. (II A.1), summing over spin groups (i.e., over J^π), and then summing over all channels corresponding to those particle pairs and spin groups. If X^r represents the real part and X^i the imaginary part of X, then the angle-integrated (but energy-differential) cross section for the interaction that leads from particle pair α to particle pair α' has the form

$$\sigma_{\alpha,\alpha'}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[\left(\sin^2\varphi_c \left(1 - 2X^i_{cc}\right) - X^r_{cc} \sin\left(2\varphi_c\right) \right) \delta_{\alpha,\alpha'} + \sum_{c'} \{ X^{i\,2}_{cc'} + X^{r\,2}_{cc'} \} \right] . \quad \text{(II B1 a.1)}$$

(This formula is accurate only for cases in which one of particles in α is a neutron; however, both particles in α' may be charged.)

In Eq. (II B1 a.1) the summations are over those channels c and c' {of the spin group defined by J^π} for which the particle pairs are, respectively, α and α'. More than one "incident channel" $c = (\alpha, l, s, J)$ can contribute to this cross section, for example when both $l = 0$ and $l = 2$ are possible, or when, in the case of incident neutrons and non-zero spin target nuclei, both channel spins are allowed. Similarly, there may be several "exit channels" $c' = (\alpha', l', s', J')$, depending on the particular reaction being calculated (e.g., elastic, inelastic, fission).

The total cross section (for non-Coulomb initial states) is the sum of Eq. (II B1 a.1) over all possible final-state particle-pairs α', assuming the scattering matrix is unitary (i.e., assuming that the sum over c' of $|U_{cc'}|^2 = 1$). Written in terms of the X matrix, the total cross section has the form

$$\sigma_{total}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[\sin^2\varphi_c + X^i_{cc} \cos(2\varphi_c) - X^r_{cc} \sin(2\varphi_c) \right] , \quad \text{(II B1 a.2)}$$

where again the sum over c includes only those channels of the J^π spin group for which the particle pair is α.

The angle integrated elastic cross section is given by

$$\sigma_{elastic}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[\sin^2\varphi_c \left(1 - 2X^i_{cc}\right) - X^r_{cc} \sin\left(2\varphi_c\right) + \sum_{c'} \left\{ X^{i\,2}_{cc'} + X^{r\,2}_{cc'} \right\} \right] . \quad \text{(II B1 a.3)}$$

In this case, both c and c' are limited to those channels of the J^π spin group for which the particle-pair is α; again, there may be more than one such channel for a given spin group.

Similarly, the reaction cross section from particle pair α to particle pair α' (where α' is not equal to α) is

$$\sigma_{reaction}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \sum_{c'} \left[X^{i\ 2}_{cc'} + X^{r\ 2}_{cc'} \right] \quad . \qquad \text{(II B1 a.4)}$$

Here c is restricted to those channels of the J^π spin group from which the particle pair is α, and c' to those channels for which the particle-pair is α'.

The absorption cross section has the form

$$\sigma_{absorption}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[X^i_{cc} - \sum_{c'} \left\{ X^{i\ 2}_{cc'} + X^{r\ 2}_{cc'} \right\} \right] \quad . \qquad \text{(II B1 a.5)}$$

Here both the sum over c and the sum over c' include <u>all</u> <u>incident</u> particle channels (i.e., particle pair α only) for the J^π spin group.

The capture cross section for the eliminated radiation channels can be calculated directly as

$$\sigma_{capture}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_{inc\,c} \left[X^i_{cc} - \sum_{all\,c'} \left\{ X^{i\ 2}_{cc'} + X^{r\ 2}_{cc'} \right\} \right] \quad , \qquad \text{(II B1 a.6)}$$

or may be found by subtracting the sum of all reaction cross sections from the absorption cross section. In Eq. (II B1 a.6), the sum over c includes all incident particle channels for the J^π spin group, and the sum over c' includes <u>all</u> particle channels, both incident and exit, for that spin group.

II.B.1.a.i. One-level two-channel case

For a simple one-level, two-channel case for which the shift factor is set to zero, the various cross sections defined in Section II.B.1.a can easily be expressed in terms of resonance parameters. Users are reminded that SAMMY is by no means restricted to this simple case and can be used with as many levels and as many channels as are needed to describe the particular physical situation. Nevertheless, it is useful to examine the cross section equations for this simple case: while these equations are a crude over-simplification for most physical situations, there is often physical insight to be gained by examination of these equations.

For this simple case, the *X* matrix of Eq. (II B1.4) takes the form

$$\begin{aligned} X &= \sqrt{P}L^{-1}\left(L^{-1}-R\right)^{-1}R\sqrt{P} \\ &= \begin{bmatrix} \frac{\sqrt{P_1}}{iP_1} & 0 \\ 0 & \frac{\sqrt{P_2}}{iP_2} \end{bmatrix} \begin{bmatrix} \frac{1}{iP_1}-\frac{\gamma_1^2}{D} & -\frac{\gamma_1\gamma_2}{D} \\ -\frac{\gamma_1\gamma_2}{D} & \frac{1}{iP_2}-\frac{\gamma_2^2}{D} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\gamma_1^2}{D} & \frac{\gamma_1\gamma_2}{D} \\ \frac{\gamma_1\gamma_2}{D} & \frac{\gamma_2^2}{D} \end{bmatrix} \begin{bmatrix} \sqrt{P_1} & 0 \\ 0 & \sqrt{P_2} \end{bmatrix}, \end{aligned} \qquad \text{(II B1 ai.1)}$$

in which the subscript on the penetrabilities denotes the channel number (not the angular momentum), the symbol *D* has been used for $E_\lambda - E - i\overline{\gamma}_{\lambda\gamma}^2$, and the subscript λ has been omitted from the reduced-width amplitudes for simplicity's sake. This equation can be rewritten as

$$X = \frac{iP_1P_2D}{iD} \begin{bmatrix} \frac{1}{\sqrt{P_1}} & 0 \\ 0 & \frac{1}{\sqrt{P_2}} \end{bmatrix} \begin{bmatrix} P_2\left(D-iP_1\gamma_1^2\right) & -iP_1P_2\gamma_1\gamma_2 \\ -iP_1P_2\gamma_1\gamma_2 & P_1\left(D-iP_2\gamma_2^2\right) \end{bmatrix}^{-1} \begin{bmatrix} \gamma_1^2 & \gamma_1\gamma_2 \\ \gamma_1\gamma_2 & \gamma_2^2 \end{bmatrix} \begin{bmatrix} \sqrt{P_1} & 0 \\ 0 & \sqrt{P_2} \end{bmatrix}$$

$$= \frac{P_1P_2}{P_1P_2\left(D^2-iP_1\gamma_1^2D-iP_2\gamma_2^2D\right)} \begin{bmatrix} \frac{1}{\sqrt{P_1}} & 0 \\ 0 & \frac{1}{\sqrt{P_2}} \end{bmatrix} \begin{bmatrix} P_1\left(D-iP_2\gamma_2^2\right) & iP_1P_2\gamma_1\gamma_2 \\ iP_1P_2\gamma_1\gamma_2 & P_2\left(D-iP_1\gamma_1^2\right) \end{bmatrix} \times \begin{bmatrix} \gamma_1^2 & \gamma_1\gamma_2 \\ \gamma_1\gamma_2 & \gamma_2^2 \end{bmatrix} \begin{bmatrix} \sqrt{P_1} & 0 \\ 0 & \sqrt{P_2} \end{bmatrix},$$

or

$$X = \frac{1}{\left(D^2 - iP_1\gamma_1^2 D - iP_2\gamma_2^2 D\right)} \begin{bmatrix} \frac{1}{\sqrt{P_1}} & 0 \\ 0 & \frac{1}{\sqrt{P_2}} \end{bmatrix}$$

$$\times \begin{bmatrix} P_1\gamma_1^2 D - iP_1P_2\gamma_1^2\gamma_2^2 + iP_1P_2\gamma_1^2\gamma_2^2 & P_1 D\gamma_1\gamma_2 - iP_1P_2\gamma_1\gamma_2^3 + iP_1P_2\gamma_1\gamma_2^3 \\ iP_1P_2\gamma_1^3\gamma_2 + P_2 D\gamma_1\gamma_2 - iP_1P_2\gamma_1^3\gamma_2 & iP_1P_2\gamma_1^2\gamma_2^2 + P_2\gamma_2^2 D - iP_1P_2\gamma_1^2\gamma_2^2 \end{bmatrix} \begin{bmatrix} \sqrt{P_1} & 0 \\ 0 & \sqrt{P_2} \end{bmatrix}$$

$$= \frac{1}{\left(D^2 - iP_1\gamma_1^2 D - iP_2\gamma_2^2 D\right)} \begin{bmatrix} \frac{1}{\sqrt{P_1}} & 0 \\ 0 & \frac{1}{\sqrt{P_2}} \end{bmatrix} \begin{bmatrix} P_1\gamma_1^2 D & P_1 D\gamma_1\gamma_2 \\ P_2 D\gamma_1\gamma_2 & P_2\gamma_2^2 D \end{bmatrix} \begin{bmatrix} \sqrt{P_1} & 0 \\ 0 & \sqrt{P_2} \end{bmatrix}$$

$$= \frac{1}{\left(D - iP_1\gamma_1^2 - iP_2\gamma_2^2\right)} \begin{bmatrix} P_1\gamma_1^2 & \sqrt{P_1P_2}\gamma_1\gamma_2 \\ \sqrt{P_1P_2}\gamma_1\gamma_2 & P_2\gamma_2^2 \end{bmatrix} ,$$

or, finally,

$$\begin{aligned} X &= \frac{1}{\left(E_\lambda - E - i\bar{\gamma}_\gamma^2 - iP_1\gamma_1^2 - iP_2\gamma_2^2\right)} \begin{bmatrix} P_1\gamma_1^2 & \sqrt{P_1P_2}\gamma_1\gamma_2 \\ \sqrt{P_1P_2}\gamma_1\gamma_2 & P_2\gamma_2^2 \end{bmatrix} \\ &= \frac{1}{\left(E_\lambda - E - i\Gamma/2\right)} \begin{bmatrix} \Gamma_1/2 & \sqrt{\Gamma_1\Gamma_2}/2 \\ \sqrt{\Gamma_1\Gamma_2}/2 & \Gamma_2/2 \end{bmatrix} , \end{aligned} \qquad \text{(II B1 ai.2)}$$

in which Γ is the sum of the partial widths $\Gamma_1 + \Gamma_2 + \Gamma_\gamma$.

In this form, *X* can be substituted into the equations for the various cross sections. Assuming the second channel is a reaction channel, Eq. (II B1 a.2) for the total cross section becomes

$$\begin{aligned} \sigma_{total}(E) &= \frac{4\pi}{k_\alpha^2}\, g_J \left[\sin^2\varphi_c + \frac{\Gamma\Gamma_1}{4d}\cos\,(2\varphi_c) - \frac{\left(E - E_\lambda\right)\Gamma_1}{2d}\sin\,(2\varphi_c) \right] \\ &= \frac{2\pi}{k_\alpha^2}\, g_J \left[1 - \left(1 - \frac{\Gamma\Gamma_1}{2d}\right)\cos\,(2\varphi_c) - \frac{\left(E - E_\lambda\right)\Gamma_1}{d}\sin\,(2\varphi_c) \right] , \end{aligned} \qquad \text{(II B1 ai.3)}$$

in which *d* has been used to represent $\left|\left(E_\lambda - E - i\Gamma/2\right)\right|^2 = \left(E - E_\lambda\right)^2 + \left(\Gamma/2\right)^2$. Similarly, the elastic cross section, Eq. (II B1 a.3), can be expressed as

$$\sigma_{elastic}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[\sin^2\varphi_c \left(1 - 2\frac{\Gamma\Gamma_1}{4d}\right) - \frac{\left(E-E_\lambda\right)\Gamma_1}{2d}\sin\left(2\varphi_c\right) + \left(\frac{\Gamma\Gamma_1}{4d}\right)^2 + \left(\frac{\left(E-E_\lambda\right)\Gamma_1}{2d}\right)^2 \right] , \quad \text{(II B1 ai.4)}$$

which reduces to

$$\sigma_{elastic}(E) = \frac{2\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[1 - \cos 2\varphi_c \left(1 - \frac{\Gamma\Gamma_1}{2d}\right) - \sin 2\varphi_c \frac{\left(E-E_\lambda\right)\Gamma_1}{d} - \frac{\Gamma_1\left(\Gamma_\gamma + \Gamma_2\right)}{2d} \right] . \quad \text{(II B1 ai.5)}$$

The reaction cross section, Eq. (II B1 a.4), becomes

$$\sigma_{reaction}(E) = \frac{4\pi}{k_\alpha^2}\, g \left[\left(\frac{\Gamma\sqrt{\Gamma_1\Gamma_2}}{4d}\right)^2 + \left(\frac{\left(E-E_\lambda\right)\sqrt{\Gamma_1\Gamma_2}}{2d}\right)^2 \right] = \frac{\pi g}{k_\alpha^2}\left[\frac{\Gamma_1\Gamma_2}{d}\right] , \quad \text{(II B1 ai.6)}$$

and, finally, the capture cross section, Eq. (II B1 a.6), is

$$\sigma_{capture}(E) = \frac{4\pi g}{k_\alpha^2} \left[\frac{\Gamma\Gamma_1}{4d} - \left\{ \left(\frac{\Gamma\Gamma_1}{4d}\right)^2 + \left(\frac{\left(E-E_\lambda\right)\Gamma_1}{2d}\right)^2 + \left(\frac{\Gamma\sqrt{\Gamma_1\Gamma_2}}{4d}\right)^2 + \left(\frac{\left(E-E_\lambda\right)\sqrt{\Gamma_1\Gamma_2}}{2d}\right)^2 \right\} \right] \quad \text{(II B1 ai.7)}$$

$$= \frac{4\pi g}{k_\alpha^2} \left[\frac{\Gamma\Gamma_1}{4d} - \left\{ \frac{\Gamma_1^2}{4d} + \frac{\Gamma_1\Gamma_2}{4d} \right\} \right] = \frac{\pi g}{k_\alpha^2}\left[\frac{\Gamma_1\bar{\Gamma}_\gamma}{d}\right] .$$

II.B.1.b. Angular distributions

Angular distributions (elastic, inelastic, or other reaction) cross sections for incident neutrons can be calculated from Reich-Moore resonance parameters. Following Blatt and Biedenharn [JB52] with some notational changes, the angular distribution cross section in the center-of-mass system may be written

$$\frac{d\sigma_{\alpha\alpha'}}{d\Omega_{CM}} = \sum_{L} B_{L\alpha\alpha'}(E)\, P_L(\cos\beta) \quad , \qquad \text{(II B1 b.1)}$$

in which the subscript $\alpha\alpha'$ indicates which type of cross section is being considered (i.e., α represents the entrance particle pair and α' represents the exit pair). P_L is the Legendre polynomial of degree L, and β is the angle of the outgoing neutron (or other particle) relative to the incoming neutron in the center-of-mass system. The coefficients $B_{L\alpha\alpha'}(E)$ are given by

$$B_{L\alpha\alpha'}(E) = \frac{1}{4k_\alpha^2} \sum_{J_1} \sum_{J_2} \sum_{l_1 s_1} \sum_{l'_1 s'_1} \sum_{l_2 s_2} \sum_{l'_2 s'_2} \frac{1}{(2i+1)(2I+1)} \times G_{\{l_1 s_1 l'_1 s'_1 J_1\}\{l_2 s_2 l'_2 s'_2 J_2\} L} \quad \mathrm{Re}\left[(\delta_{c_1 c'_1} - U_{c_1 c'_1})(\delta_{c_2 c'_2} - U^*_{c_2 c'_2})\right] \quad , \qquad \text{(II B1 b.2)}$$

in which the various summations are to be interpreted as follows:

(1) sum over all spin groups defined by spin J_1 and the implicit associated parity

(2) sum over all spin groups defined by spin J_2 and the implicit associated parity

(3) sum over the entrance channels c_1 belonging to the J_1 spin group and having particle pair α, with orbital angular momentum l_1 and channel spin s_1 [i.e., $c_1 = (\alpha, l_1, s_1, J_1)$]

(4) sum over the exit channels c'_1 in J_1 spin group with particle-pair α', orbital angular momentum l'_1, and channel spin s'_1 [i.e., $c'_1 = (\alpha', l'_1, s'_1, J_1)$]

(5) sum over entrance channels c_2 in J_2 spin group where $c_2 = (\alpha, l_2, s_2, J_2)$

(6) sum over exit channels c'_2 in J_2 spin group where $c'_2 = (\alpha', l'_2, s'_2, J_2)$

Also note that i and I are the spins of the two particles (projectile and target nucleus) in particle-pair α.

The geometric factor G can be exactly evaluated as a product of terms

$$G_{\{l_1 s_1 l'_1 s'_1 J_1\}\{l_2 s_2 l'_2 s'_2 J_2\} L} = A_{l_1 s_1 l'_1 s'_1; J_1}\, A_{l_2 s_2 l'_2 s'_2; J_2}\, D_{l_1 s_1 l'_1 s'_1 l_2 s_2 l'_2 s'_2; L J_1 J_2} \quad , \qquad \text{(II B1 b.3)}$$

where the factor $A_{l_1 s_1 l'_1 s'_1; J_1}$ is of the form

$$A_{l_1 s_1 l'_1 s'_1; J_1} = \sqrt{(2l_1+1)(2l'_1+1)}\,(2J_1+1)\,\Delta(l_1 J_1 s_1)\,\Delta(l'_1 J_1 s'_1) \quad . \qquad \text{(II B1 b.4)}$$

The expression for D is

$$D_{l_1 s_1 l'_1 s'_1 l_2 s_2 l'_2 s'_2; L J_1 J_2} = (2L+1)\ \Delta^2(J_1 J_2 L)\ \Delta^2(l_1 l_2 L)\ \Delta^2(l'_1 l'_2 L)$$
$$\times w(l_1 J_1 l_2 J_2, s_1 L)\ w(l'_1 J_1 l'_2 J_2, s'_1 L)\ \delta_{s_1 s_2}\ \delta_{s'_1 s'_2}\ (-1)^{s_1 - s'_1} \qquad \text{(II B1 b.5)}$$
$$\times \frac{n!\ (-1)^n}{(n-l_1)!\ (n-l_2)!\ (n-L)!}\ \frac{n'!\ (-1)^{n'}}{(n'-l'_1)!\ (n'-l'_2)!\ (n'-L)!}\ ,$$

in which n is defined by

$$2n = l_1 + l_2 + L \quad ; \qquad \text{(II B1 b.6)}$$

D is zero if l_1+l_2+L is an odd number. A similar expression defines n'. The Δ^2 term is given by

$$\Delta^2(abc) = \frac{(a+b-c)!\ (a-b+c)!\ (-a+b+c)!}{(a+b+c+1)!}\ , \qquad \text{(II B1 b.7)}$$

for which the arguments a, b, and c are to be replaced by the appropriate values given in Eqs. (II B1 b.4) and (II B1 b.5). The expression for $\Delta^2(abc)$ implicitly includes a selection rule for the arguments; that is, the quantized vector sum must hold,

$$\vec{a} + \vec{b} = \vec{c} \qquad \text{or} \qquad |a-b| \le c \le a+b \qquad \text{(II B1 b.8)}$$

with c being either integer or half-integer. The quantity w in Eq. (II B1 b.5) is defined as

$$w(l_1 J_1 l_2 J_2, sL) = \sum_{k=kmin}^{kmax} \frac{(-1)^{k+l_1+J_1+l_2+J_2}\ (k+1)!}{(k-(l_1+J_1+s))!\ (k-(l_2+J_2+s))!}$$
$$\times \frac{1}{(k-(l_1+l_2+L))!\ (k-(J_1+J_2+L))!} \qquad \text{(II B1 b.9)}$$
$$\times \frac{1}{(l_1+J_1+l_2+J_2-k)!\ (l_1+J_2+s+L-k)!\ (l_2+J_1+s+L-k)!}$$

(and similarly for the primed expression), where *kmin* and *kmax* are chosen such that none of the arguments of the factorials are negative. That is,

$$kmin = \max\{(l_1+J_1+s),\ (l_2+J_2+s),\ (l_1+l_2+L),\ (J_1+J_2+L)\}$$
$$kmax = \min\{(l_1+J_1+l_2+J_2),\ (l_1+J_2+s+L),\ (l_2+J_1+s+L)\}\ . \qquad \text{(II B1 b.10)}$$

Single-channel case

For some situations, these equations can be greatly simplified. When the target spin is zero and there are no possible reactions (no fission, no inelastic, no other reactions), then each spin group will consist of a single channel (the elastic channel). In this case, the coefficients $B_{L\alpha\alpha'}(E)$ reduce to

$$B_{L\alpha\alpha}(E) = \frac{1}{4k_\alpha^2} \sum_{J_1} \sum_{J_2} \sum_{c_1=(\alpha\, l_1\, s_1\, J_1)} \sum_{c_2=(\alpha\, l_2\, s_2\, J_2)} G_{\{l_1 s_1 l_1 s_1 J_1\}\,\{l_2 s_2 l_2 s_2 J_2\}\,L} \times \frac{1}{(2i_a+1)\,(2i_b+1)} \mathrm{Re}\left[\,(1-U_{c_1 c_1})\;(1-U^*_{c_2 c_2})\,\right] , \qquad \text{(II B1 b.11)}$$

where the existence of only one channel requires that the primed quantities of Eq.(II B1 b.2) be equal to the unprimed (e.g., $\alpha = \alpha'$). The geometric factor *G* becomes

$$G_{\{l_1 s_1 l_1 s_1 J_1\}\,\{l_2 s_2 l_2 s_2 J_2\}\,L} = A_{l_1 s_1 l_1 s_1;\, J_1}\; A_{l_2 s_2 l_2 s_2;\, J_2}\; D_{l_1 s_1 l_1 s_1 l_2 s_2 l_2 s_2;\, L\, J_1\, J_2} , \qquad \text{(II B1 b.12)}$$

in which the factor *A* reduces to the simple form

$$A_{l_1 s_1 l_1 s_1; J_1} = (2l_1+1)\;(2J_1+1)\;\Delta^2(l_1\, J_1\, s_1) , \qquad \text{(II B1 b.13)}$$

and the expression for *D* reduces to

$$D_{l_1 s_1 l_1 s_1 l_2 s_2 l_2 s_2;\, L\, J_1\, J_2} = (2L+1)\;\Delta^2(J_1\, J_2\, L)\;\Delta^4(l_1\, l_2\, L) \times w^2(l_1\, J_1\, l_2\, J_2, s_1\, L)\;\delta_{s_1 s_2} \left[\frac{n!}{(n-l_1)!\;(n-l_2)!\;(n-L)!}\right]^2 , \qquad \text{(II B1 b.14)}$$

in which *n* is again defined as in Eq. (II B1 b.6).

II. B.1.c. Specifying individual reaction types

Early versions of SAMMY permitted users to specify "inelastic", "fission", and "reaction" data. However, the tacit assumption was that all the exit channels are relevant to the type of data being used. If, for example, three exit channels were specified as (1) inelastic, (2) first fission channel, and (3) second fission channel, then any calculation for "inelastic", "fission", or "reaction" data types would automatically include all three exit channels in the final state.

Hence, in early versions of SAMMY, true inelastic cross sections (for example) would be calculated only if all of the following conditions were met:

1. Either "inelastic", "fission", or "reaction" was specified as the data type in the INPut file, card set 8.

2. The exit channel description was appropriate for inelastic channels: The INPut file noted that penetrabilities were to be calculated (LPENT = 1 on line 2 of card set 10.1) and also provided a non-zero value for the excitation energy.

3. No fission channel (or other exit channel) was defined in the INPut file (and PARameter file).

Beginning with release M5 of the SAMMY code, it is now possible to include only a subset of the exit channels in the outgoing final state. The third condition in the list above is no longer necessary, but is replaced by another (less restrictive) condition:

3. Exit channels that are not inelastic have a flag ("1" in column 18 of line 2 of card set 10.1 or card set 10.2 of the INPut file), denoting that this channel does not contribute to the final state.

(Similar considerations hold, of course, for any other reaction type, not only for inelastic.)

With release 7.0.0 of the SAMMY code in 2006, a more intuitive input is possible. When channels are specified using either of the particle-pair options (see card set 4 or 4a of Table VIA.1), then the data type line (card set 8 of Table VIA.1) may be used to specify the name(s) of the particle pair(s) to be included in the final-state reaction. Specifically, beginning in the first column of card set 8, include the phrase

FINAL-state particle pairs are

or

PAIRS in final state =

(Only the first five characters are required, the others are optional.) Elsewhere on the same line, give the eight-character designation of the particle pair(s) to be included in the final-state reaction. Only channels involving those particle pairs will be included in the final state; any channels not involving those particle pairs will not be included. (Caution: The particle pair name must be *exactly* as it appears in the INPut file, including capitalization.)

The same two command lines may be used for angular distributions with specific final states, provided the phrase “ANGULar distribution” is given later on the same line.

See test case tr159 for an example which includes three reactions, one being (n,α) and the other two inelastic (n,n'). Various options for input are given in this test case.

Run “k” of test case tr112 shows an example for the angular distribution of a reaction cross section.

II.B.1.d. External R-function

When generating cross sections via R-matrix theory, it is important to include contributions from *all* resonances, even those outside the energy range of the data. Tails from negative-energy resonances (which may correspond to bound states) and from higher-lying resonances can contribute significantly to the "background" of the R-matrix and must therefore not be omitted. There are infinitely many of these resonances, so approximations must be made.

The usual approximation is to use pseudo or dummy resonances to approximate the effect of the infinite number of outlying resonances. The energy associated with a dummy resonance must be outside the energy region for which the analysis is valid.

For discussion regarding two different philosophies for determining appropriate choices of dummy resonances, see Leal et al. [LL99] and Fröhner and Bouland [FF01].

Any number of additional possibilities exist for approximating the contribution of the external resonances to the tail of the R-matrix. A logarithmic parameterization of the R-function is implemented in SAMMY; note that this is properly denoted as a *function* rather than *a matrix*, because it is diagonal with respect to the channels. The form used in the code is

$$R_c^{ext}(E) = \overline{R}_{con,c} + \overline{R}_{lin,c} E + \overline{R}_{q,c} E^2 - s_{lin,c}\left(E_c^{up} - E_c^{down}\right) - \left(s_{con,c} + s_{lin,c} E\right) \ln\left[\frac{E_c^{up} - E}{E - E_c^{down}}\right] \quad . \qquad \text{(II B1 d.1)}$$

Any or all of the seven free parameters may be varied during a SAMMY analysis (see Table VI B.2, card set 3, and card set 3a). Note that R_c^{ext} is strictly real in this parameterization.

The *u*-parameters (i.e., the parameters on which Bayes' equations will operate, as described in Section IV.C) associated with the external R-function are given by

$$\begin{array}{lll} u\left(E_c^{down}\right) = E_c^{down} & u\left(E_c^{up}\right) = E_c^{up} & \\ u\left(\overline{R}_{con,c}\right) = \overline{R}_{con,c} & u\left(\overline{R}_{lin,c}\right) = \overline{R}_{lin,c} & u\left(\overline{R}_{q,c}\right) = \overline{R}_{q,c} \\ u\left(s_{con,c}\right) = \sqrt{s_{con,c}} & u\left(s_{lin,c}\right) = s_{lin,c} & \end{array} \quad . \qquad \text{(II B1 d.2)}$$

Of the current ENDF formats [ENDF-102], only new LRF = 7 format permits this type of parameterization of the R-function. The more commonly used LRF = 3 format (the so-called Reich Moore format) allows only the dummy-resonance option.

II.B.2. Simulation of Full R-Matrix

While SAMMY does not yet have the ability to calculate the full (unapproximated) R-matrix of Lane and Thomas [AL58], it is possible to use the Reich-Moore approximation in such a way that it mimics the full R-matrix with a high degree of accuracy. This is necessary, for example, in cases where there are interference effects between the (incident) neutron channel and a gamma channel – that is, for some low-mass nuclides.

The Reich-Moore approximation involves an aggregate treatment ("excluded channels") for the gamma widths (capture widths). Therefore, to approximate the full R-matrix, one sets the Reich-Moore gamma width to a very small number and uses an exit channel to define the actual gamma channel:

1. Set the SAMMY gamma-channel widths to a very small number, perhaps 0.001.

2. Define an exit channel to be the actual capture channel and assign appropriate values for the widths. Quantum numbers for this channel will be the same as those for fission channels (in particular, set LPENT = 0).

3. When calculating capture cross sections, set the IFEXCL flag to 1 for all other (non-gamma) exit channels. (See Section II.B.1.c and card set 10.1 or 10.2 of Table VIA.1 for details.) When calculating other reaction cross sections, set the IFEXCL flag to 0 for the reaction channels of interest, to1 for the capture channels, and to 1 for any other reaction channels to be excluded.

When utilizing this option, SAMMY users should take care that results are not unduly influenced by the approximation in step 1 above. To test this, make radical changes in the value used for the gamma widths (e.g., set the value to 100.0 or 10^{-6}) and recalculate the cross section. Note that it is not possible to set these values to zero; doing so results in numerical overflow problems (because computers do not know how to calculate zero divided by zero).

Comparisons between cross sections calculated by SAMMY and those generated by the R-matrix code EDA [GH75] using the same R-matrix parameters have shown agreement to ~5 significant digits [INDC03]. Some of the runs for those comparisons are now assembled into SAMMY test case tr125.

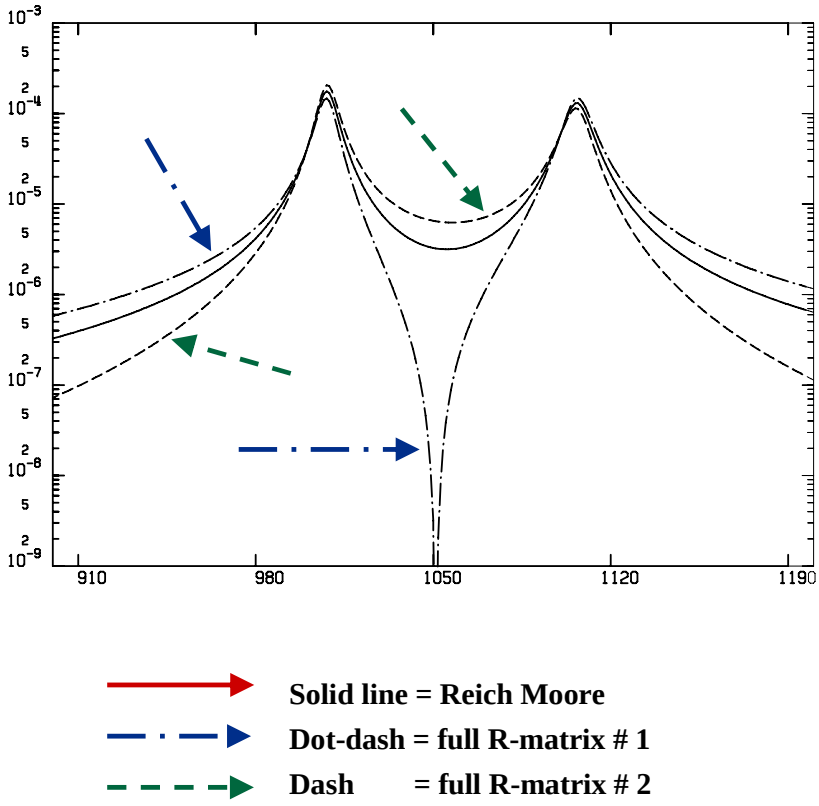
Test case tr110 shows an artificial but extreme example of a situation in which use of the Reich-Moore approximation gives very different results from those obtained via the full R-matrix. For this example, there are two resonances with parameter values as shown in Table II B2.1; plots of the curves calculated with those parameters are shown in Figure II B2.1. As evident from the figure, the Reich-Moore curve lies between the two extreme R-matrix curves which show constructive (dashed curve) and destructive (dot-dash curve) interference.

Table II B2.1. Parameter values used to illustrate Reich-Moore vs. full R-matrix calculations

	λ	Energy (MeV)	$\bar{\Gamma}_{\lambda\gamma}$ (eV)	$\Gamma_{\lambda n}$ (eV)	Sign $\times \Gamma_{\lambda\gamma}$ (eV)[a]
Reich Moore	1	1.0	1.0	10000.	
	2	1.1	1.1	11000.	
Pseudo-full R-matrix # 1	1	1.0	10^{-8}	10000.	1.0
	2	1.1	10^{-8}	11000.	1.1
Pseudo-full R-matrix # 2	1	1.0	10^{-8}	10000.	1.0
	2	1.1	10^{-8}	11000.	−1.1

[a] Remember that the value given in the SAMMY PARameter file is not the partial width Γ (which is always a positive number); rather, it is the sign of the reduced-width amplitude γ multiplied by the partial width Γ. Hence, the negative sign in the final entry of this table is actually associated with the reduced-width amplitude for the capture channel. See Section II.B.1 for further discussion.

Figure II B2.1. Reich-Moore approximation vs. full R-matrix for artificial example of test case tr110.



Different treatments for different capture channels

Occasionally it may be convenient to treat certain gamma widths individually while treating most gamma widths in aggregate fashion. This can be accomplished by defining "particle" channels for the individual widths (as described above), and using the Reich-Moore capture channel (eliminated width) for the aggregate width.

To calculate the capture cross section in this situation, it is not sufficient to specify the data type as "CAPTURE", because that would give only the contribution from the aggregate width. To obtain the contribution from the individual widths, specify the data type as "REACTION" or (preferably) as "FINAL state pairs =" followed by the exact names specified for the gamma-channel particle-pairs. (See card sets 4 and 8 of Table VI 8.1 and Section II.B.1.c for details.)

To calculate the complete capture cross section, use "FINAL state pairs =" for the data type, and add the command line

```
ADD ELIMINATED CAPTUre channel to final state
```

This will cause SAMMY to add the contributions from the individual capture channels plus the contribution from the aggregate channels.

The formula used to calculate the capture cross section is similar to Eq. (II B1 a.6), with only the non-capture exit channels included in the summation over c',

$$\sigma_{capture}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[X^i_{cc} - \sum_{\substack{c' = \text{non-capture} \\ \text{exit channels}}} \left\{ X^{i\ 2}_{cc'} + X^{r\ 2}_{cc'} \right\} \right] \quad . \qquad \text{(II B2.1)}$$

II.B.3. Breit-Wigner Approximation

In addition to the preferred Reich-Moore formalism, SAMMY also offers the option to calculate cross sections using either the multilevel Breit-Wigner (MLBW) or the single-level Breit-Wigner (SLBW) [GB36]. This has the advantage that the calculation occurs more rapidly because fewer computations are required; however, it also has the disadvantage that unphysical cross sections may be generated. Use of this option is discouraged for new analyses; the option is included within SAMMY for completeness' sake, to permit use of SAMMY with most ENDF resonance parameter information, and to facilitate comparisons with older codes such as SIOB [GD78].

Formulae for MLBW and SLBW cross sections are presented in Section II.B.3.a; these are identical to those used in ENDF files [ENDF-102], although they are not necessarily programmed in this fashion. Formulae for derivatives are given in Section II.D.2.

The reader should be aware that the ENDF version of MLBW (and hence, SAMMY's version of MLBW) does not correspond to the usual definition of multilevel Breit Wigner. Instead, only the elastic cross section is calculated with the multilevel formula; other partial cross sections for the MLBW format are actually *single*-level.

A note regarding broadening: Historically, the Breit-Wigner formulations had the great advantage that the cross sections could be Doppler broadened analytically, using the high-energy approximation to the free-gas model of Doppler broadening (Section III.B.3). Results were written in terms of χ and ψ functions, and computation was relatively rapid. However, with the advent of modern computers, more accurate cross sections and more accurate Doppler-broadening computations can be accomplished rapidly, without resorting to these rather crude approximations. In SAMMY, Doppler and resolution broadening are accomplished numerically, in the same manner for MLBW and SLBW cross sections as for Reich-Moore cross sections, as described in Section III of this manual.

II.B.3.a. Single and multilevel Breit-Wigner cross sections

The MLBW elastic (scattering) cross section may be written in the form

$$\sigma^{elastic} = \frac{\pi}{k^2}\sum_J g_J \sum_c \left\{ \left(1-\cos 2\varphi\right)\left(2 - \sum_\lambda \Gamma_{\lambda c}\Gamma_\lambda / d_\lambda \right) \right.$$
$$+ 2\sin 2\varphi \sum_\lambda \Gamma_{\lambda c}\left(E - E_\lambda\right)/d_\lambda \qquad \text{(II B3 a.1)}$$
$$\left. + \left(\sum_\lambda \Gamma_{\lambda c}\left(E-E_\lambda\right)/d_\lambda \right)^2 + \left(\sum_\lambda \Gamma_{\lambda c}\Gamma_\lambda / 2d_\lambda \right)^2 \right\} \quad ,$$

in which the summation over *c* includes only incident (i.e., neutron) channels. For SLBW, the level-level interference terms in this equation are dropped; that is, the summations over λ in the last line are outside, rather than inside, the parentheses. The total width Γ_λ in Eq. (II B3 a.1) is given by

$$\Gamma_\lambda = \sum_c \Gamma_{\lambda c} + \overline{\Gamma}_{\lambda\gamma} \quad , \qquad \text{(II B3 a.2)}$$

in which the sum over *c* includes **all** particle channels (i.e., over all channels except the eliminated capture channel). Partial widths $\Gamma_{\lambda c}$ and $\overline{\Gamma}_{\lambda\gamma}$ are related to amplitudes $\gamma_{\lambda c}$ and $\overline{\gamma}_\lambda$, as in the Reich-Moore approximation, by

$$\Gamma_{\lambda c}^{neutron} = 2\gamma_{\lambda c}^2 P_c$$
$$\Gamma_{\lambda c}^{fission} = 2\gamma_{\lambda c}^2 \qquad \text{(II B3 a.3)}$$
$$\text{and} \qquad \overline{\Gamma}_{\lambda\gamma} = 2\overline{\gamma}_{\lambda\gamma}^2 \quad .$$

(Note that we have again adopted the convention that the gamma channel be denoted by a bar over the symbol, even though it is not really treated differently from particle channels in the Breit Wigner approximations.) The denominator d_λ in Eq. (II B3 a.1) represents

$$d_\lambda = \left(E - E_\lambda\right)^2 + \left(\Gamma_\lambda / 2\right)^2 \quad . \qquad \text{(II B3 a.4)}$$

For both MLBW and SLBW, the fission cross section is given by

$$\sigma^{fission} = \frac{\pi}{k^2}\sum_J g_J \sum_c \sum_{c'} \sum_\lambda \frac{\Gamma_{\lambda c}\Gamma_{\lambda c'}}{d_\lambda} \quad , \qquad \text{(II B3 a.5)}$$

in which the sum over *c* includes only incident (neutron) channels, d_λ is again given by Eq. (II B3 a.4), and the sum over *c´* includes all exit channels. Caution: In principle, Eq. (II B3 a.5) could be used to describe any reaction channel, where term "reaction" encompasses any non-elastic,

non-capture channel. However, the only reaction channel permitted in ENDF is fission; for SLBW only one fission channel is permitted, and for MLBW two fission channels may be used. In addition, ENDF allows only one neutron channel (i.e., only one entrance channel). Because SAMMY's Breit-Wigner options were created solely for use with ENDF evaluations (for comparison purposes), similar restrictions apply to the use of the Breit-Wigner approximations in SAMMY. (For the more general case involving other reactions such as inelastic, (n,p), (n,α), or fission with more than two channels, use the Reich-Moore approximation as discussed in Section II.B.1.c.)

The Breit-Wigner form for the capture cross section is

$$\sigma^{capture} = \frac{\pi}{k^2} \sum_J g_J \sum_c \sum_\lambda \frac{\Gamma_{\lambda c} \overline{\Gamma}_{\lambda\gamma}}{d_\lambda} \quad , \qquad \text{(II B3 a.6)}$$

where, again, the sum over *c* includes only incident (neutron) channels. Total and absorption cross sections are given by the appropriate sums of the other three cross sections,

$$\sigma^{total} = \sigma^{elastic} + \sigma^{fission} + \sigma^{capture} \qquad \text{(II B3 a.7)}$$

and

$$\sigma^{absorption} = \sigma^{fission} + \sigma^{capture} \quad . \qquad \text{(II B3 a.8)}$$

As noted in Section IV.C, it is the *u*-parameters on which Bayes' equations operate. The *u*-parameters associated with the MLBW and SLBW resonances are defined similarly to those for Reich-Moore resonances:

$$u\left(E_\lambda\right) = \pm\sqrt{\left|E_\lambda\right|} \quad , \qquad \text{(II B3 a.9)}$$

where the negative sign is chosen if $E_\lambda < 0$,

$$u\left(\Gamma_{\lambda c}\right) = \gamma_{\lambda c} \qquad \text{(II B3 a.10)}$$

and

$$u\left(\overline{\Gamma}_{\lambda\gamma}\right) = \overline{\gamma}_{\lambda\gamma} \quad . \qquad \text{(II B3 a.11)}$$

(The reduced-width amplitudes $\gamma_{\lambda c}$ and $\overline{\gamma}_{\lambda\gamma}$ may be either positive or negative. However, the sign is irrelevant in the Breit-Wigner equations, for which the reduced-width amplitudes enter only as squared quantities.)

The matching radius a_c may also be varied (i.e., treated as a *u*-parameter) with the Breit-Wigner approximations.

II.B.4. Direct Capture Component

An externally generated direct capture component may be added to the appropriate cross section types (capture, absorption, and total) by including the phrase

```
ADD DIRECT CAPTURE Component to capture, total, and absorption cross section
```

in the alphanumeric command section of the INPut file. When this command is present, the direct capture component for at least one of the nuclides is provided as a numerical function of energy, in a separate file (the "DRC file"). SAMMY will linearly interpolate as needed between the energy points given.

The format of the DRC file is as follows:

First line:	key word "NUClide Number", followed by an equal sign "=", followed by the nuclide number as specified in the PARameter file.
Second line:	energy (eV), value of direct capture component (barn), in 2F20 format.
Third line:	repeat second line as many times as needed.
Last line:	blank.

These lines may be repeated for each nuclide as needed. Not all nuclides need to be included, but those which are included should be given in the same order as in the PARameter file. (For example, give the direct capture component for nuclides number 2, 4, and 7, rather than 4, 7, and 2.)

The actual value of the direct capture component added to the capture (and total and absorption) cross section for any given nuclide is the product of the value determined from the DRC file and a constant (energy-independent) coefficient whose value is specified as miscellaneous parameter DRCAP. See Table VI B.2 for details.

Test case tr076 contains examples.

II.C. DETAILS AND CONVENTIONS USED IN SAMMY

Details of cross section evaluation are often a matter of convention: for example, should one use *l-s* or *j-j* coupling for spin assignments? The spin conventions used in SAMMY are described in Section II.C.1.

Section II.C.2 describes the conversion of energy and momentum from the laboratory reference system to the center-of-mass system.

The method used for computing $\sin 2\varphi$ and $\cos 2\varphi$, where φ is hard-sphere phase shift, is described in Section II.C.3.

Modifications are needed to the cross section equations when a channel contains two charged particles. These are described in Section II.C.4.

When data from an inverse reaction are used in an evaluation, modifications to either the measured data or the R-matrix parameters are needed. These are described in Section II.C.5.

II.C.1. Spin and Angular Momentum Conventions

For any analysis or evaluation, the analyst bears ultimate responsibility for including the proper spin-group definitions.

This is not the responsibility of the SAMMY program nor of the SAMMY author. SAMMY will issue warnings for obvious errors, but it is the responsibility of the user to notice and heed those warnings. It is also the responsibility of the user to ensure that the set of spin groups is complete; program SAMQUA, described in Section X.J, can be used for guidance in that effort.

It is worthwhile to discuss what is meant by "complete." Clearly, it is neither necessary nor possible to include all legitimate values of all of the quantum numbers (*l*, *s*, and *J*), because an infinite number of spin groups is available. Generally, one should include low values of *l*, *l* = 0 being always required and *l* = 1, 2, 3, … being included when the experimental data require their inclusion. For each *l*, the user should determine (using SAMQUA or by hand) all possible *s*-values leading to all possible *J*-values. In general, all such channels and spin groups should be included in the analysis. When the hard-sphere phase shift values are sufficiently large that there is a noticeable contribution to the cross section from the hard-sphere phase shift, all such channels must be included. On rare occasions, there may be one resonance (or several) whose high *l*-value dictates the presence of a particular channel in a particular spin group, but for which the hard-sphere phase shift is negligible for all energies of interest in this experiment. In this case, it would be reasonable to omit other channels and spin groups with this same *l*-value, without degrading the quality of the evaluation.

The spin and angular momentum conventions used in SAMMY (and in its predecessor MULTI [GA74]) are described in Table II C1.1. Recall that the word "channel" refers to the physical configuration (e.g., the particular particles involved) as well as to the quantum numbers given here. For example, an incident channel might consist of a neutron (intrinsic spin i = ½) impinging on a target (sample) whose spin is I, so that the channel spin is s, where $\vec{s} = \vec{i} + \vec{I}$. The relative orbital angular momentum of this channel (neutron plus target) is l, and total spin is J, where $\vec{J} = \vec{s} + \vec{l}$. For elastic scattering, the exit channel is the same as the entrance channel. For a reaction such as (n,p), the exit channel contains a proton (spin i' = ½) and another nuclide (spin I'); the channel spin is s', where $\vec{s}' = \vec{i}' + \vec{I}'$. The relative angular momentum proton-nuclide system is $\boldsymbol{l}'$, and the total J must satisfy $\vec{J} = \vec{s}' + \vec{l}'$.

Readers unfamiliar with vector sum rules are referred to Section II.C.1.a for a short summary of the basic principles.

Table II C1.1. Spin and angular momentum conventions used in SAMMY [a]

Symbol	FORTRAN name used in SAMMY	Meaning	Value or range of values
i or i'		Intrinsic spin of incident or outgoing particle	½ for neutron; in general, integer or half-integer
I or I'	SPINI	Spin of target [i.e., sample] or residual nuclei	Integer or half-integer
l or l'	LSPIN (channel 1, group number) *or* LSPIN (whatever channel, group number)	Orbital angular momentum in incident or outgoing channel	Non-negative integer
s or s'	CHSPIN (channel 1, group number) *or* CHSPIN (whatever channel, group number)	Incident or outgoing channel spin, equal to the vector sum of the spins of the two particles in the channel	$\vec{s} = \vec{I} + \vec{i}$ or $\vec{s}' = \vec{I}' + \vec{i}'$
J	SPINJ (group number)	(1) Spin of resonance (2) Spin of excited level in the compound nucleus (3) Total angular momentum quantum number	$\vec{J} = \vec{I} + \vec{s}$ $= \vec{I}' + \vec{s}'$

[a] Note: The channel spin s (s') was denoted by j (j') in early versions of this manual.

The spin statistical factor g_J appearing in the equations for cross section (see Section II.A) is given in terms of the spins *i* and *I* of the two particles in the entrance channel and the total spin *J* of the particular channel; that is

$$g_J = \frac{(2J+1)}{(2i+1)(2I+1)} \qquad \text{(II C1.1)}$$

in the general case, and

$$g_J = \frac{(2J+1)}{2(2I+1)} \qquad \text{(II C1.2)}$$

when the incident particle is a neutron or proton.

A few words of discussion about the use of these quantum numbers in SAMMY are warranted here, to avoid possible confusion:

(1) Values for the spin *i* of the projectile and spin *I* of the target particle are specified in the particle-pair definitions, card set 4 of the INPut file (see Section VI.A). Values for spins i' and I' (for exit particles) are also given in card set 4.

(2) With older input formats, incident spin *i* is assumed to be ½ unless otherwise specified (in card set 3). *I* is given as SPINI in card set 10.1. Values for spins i' and I' are not specified.

(3) Projectile spin *i* and target spin *I* are required for evaluation of the spin statistical factor *g*, and in calculation of the channel spin *s*. Exit particle spins are used to calculate channel spin s' but are otherwise unused.

(4) Channel spins *s* and s' are used as channel descriptors in the output (LPT or IO file; see Section VII). SAMMY will issue a warning statement (but not abort) if these values are inconsistent (if, for example, $\vec{s} \neq \vec{i} + \vec{I}$).

(5) The orbital angular momentum *l* is used for generating penetrabilities, shift factors, and potential phase shifts.

(6) To the extent that it is possible (depending on which input format is used), SAMMY will warn of inconsistent spin or parity values, and abort when obvious errors occur. Users should read through the SAMMY.LPT file, especially at the beginning of an evaluation, to check for warning messages.

(7) Finally, users are urged to review the discussion in the first two paragraphs of this section, to read and heed the suggestions in Section XI (especially those under the heading "Step 2. Preparation of INPut and PARameter files"), and to make use of the auxiliary code SAMQUA when preparing the spin group information.

II.C.1.a. Quantum vector algebra

For a complete description of sum rules for quantum vectors, the reader is referred to textbooks on elementary quantum mechanics. Here we simply state the vector sum rules without detailed explanation.

Let $\vec{a}$ be a quantized vector. The value of this vector, generally written either a or $|\vec{a}|$, is either a positive half-integer or a positive integer. That is to say, a can have any of the values 0, 1/2, 1, 3/2, 2, 5/2, etc. For example, the spin of a neutron or proton is 1/2, and the spin of an alpha particle is 0. The orbital angular momentum l for a pair of particles is integral, l = 0, 1, 2, 3, etc.

Given two quantized vectors $\vec{a}$ and $\vec{b}$, and let $\vec{c} = \vec{a} + \vec{b}$ be the sum of the two vectors. The possible values for c are then

$$|a - b| \leq c \leq a + b \quad , \qquad \text{(II C1 a.1)}$$

where the allowed values of c are separated by one unit. Examples are shown in Table II C1 a.1. Values of a and b are in the left-most column and the uppermost row; values for c are in the other cells of the table. Because Eq. (II C1 a.1) is symmetric with respect to a and b, entries are made only in the lower triangular half of the table.

Each spin vector has an associated parity, which can be positive or negative. For example, protons, neutrons, and alpha particles have positive parity; many nuclides have negative parity. The parity associated with angular momentum l is $(-1)^l$. Parity is conserved when two vectors are added; the product of the parities of the two components is the parity of the resulting vector. A vector which is formed as the sum of two positive-parity vectors will have positive parity, a vector which is formed as the sum of two negative-parity vectors will have positive parity, and a vector which is formed as the sum of one positive-parity vector and one negative-parity vector will have negative parity. In other words, if a and b have the same parity, c has positive parity. If f a and b have different parity, c has negative parity.

Table II C1 a.1. Allowed values for the sum of two quantized vectors

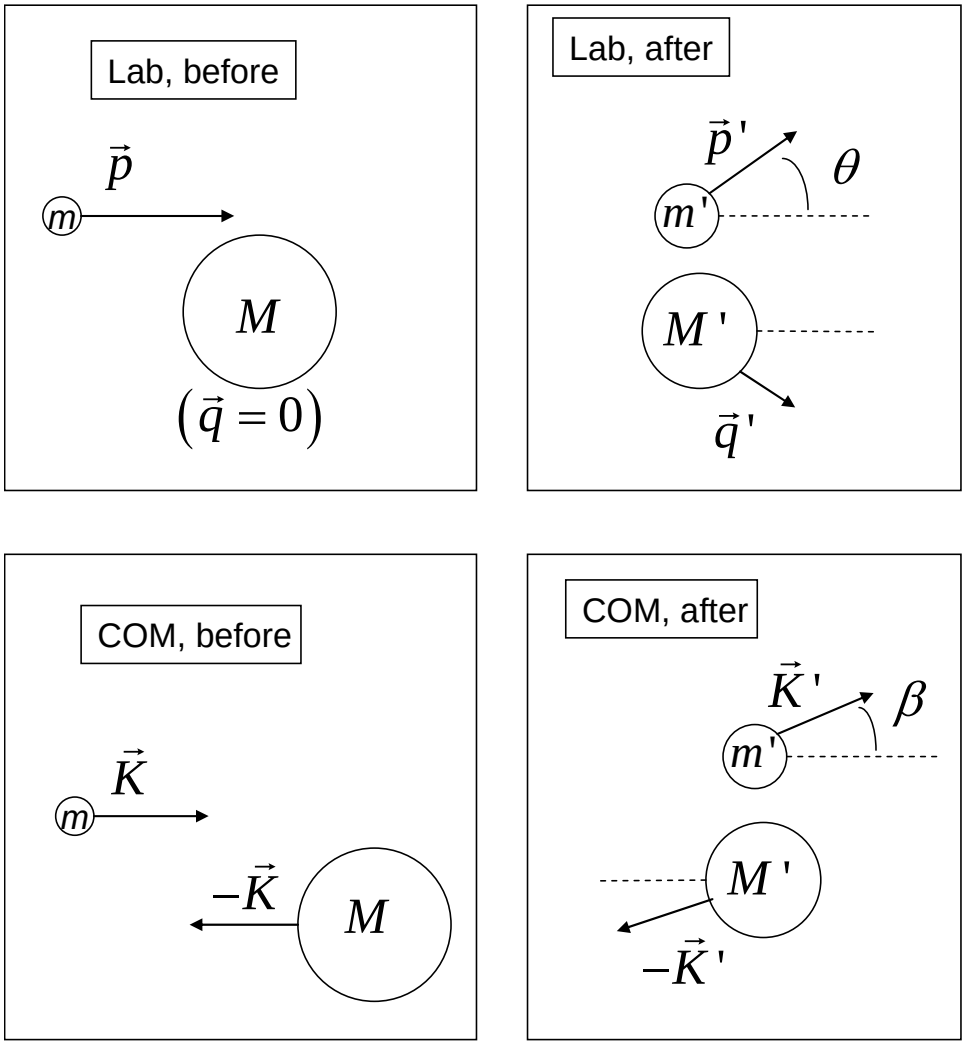
	0	½	1	3/2	2	5/2	3	7/2	4	9/2
0	0									
1/2	1/2	0, 1								
1	1	1/2, 3/2	0, 1, 2							
3/2	3/2	1, 2	1/2, 3/2, 5/2	0, 1, 2, 3						
2	2	3/2, 5/2	1, 2, 3	1/2, 3/2, 5/2, 7/2	0, 1, 2, 3, 4					
5/2	5/2	2, 3	3/2, 5/2, 7/2	1, 2, 3, 4	1/2, 3/2, 5/2, 7/2, 9/2	0, 1, 2, 3, 4, 5				
3	3	5/2, 7/2	2, 3, 4	3/2, 5/2, 7/2, 9/2	1, 2, 3, 4, 5	1/2, 3/2, 5/2, 7/2, 9/2, 11/2	0, 1, 2, 3, 4, 5, 6			
7/2	7/2	3, 4	5/2, 7/2, 9/2	2, 3, 4, 5	3/2, 5/2, 7/2, 9/2, 11/2	1, 2, 3, 4, 5, 6	1/2, 3/2, 5/2, 7/2, 9/2, 11/2, 13/2	0, 1, 2, 3, 4, 5, 6, 7		
4	4	7/2, 9/2	3, 4, 5	5/2, 7/2, 9/2, 11/2	2, 3, 4, 5, 6	3/2, 5/2, 7/2, 9/2, 11/2, 13/2	1, 2, 3, 4, 5, 6, 7	1/2, 3/2, 5/2, 7/2, 9/2, 11/2, 13/2, 15/2	0, 1, 2, 3, 4, 5, 6, 7, 8	
9/2	9/2	4, 5	7/2, 9/2, 11/2	3, 4, 5, 6	5/2, 7/2, 9/2, 11/2, 13/2	2, 3, 4, 5, 6, 7	3/2, 5/2, 7/2, 9/2, 11/2, 13/2, 15/2	1, 2, 3, 4, 5, 6, 7, 8	1/2, 3/2, 5/2, 7/2, 9/2, 11/2, 13/2, 15/2, 17/2	0, 1, 2, 3, 4, 5, 6, 7, 8, 9

II.C.2. Kinematics

The center-of-mass (COM) momenta, $K = \hbar k$ (initial) and $K' = \hbar k'$ (after the interaction), needed in the formulae for cross sections (see Section II.A) may be found in terms of laboratory energies E and E' by utilizing conservation of energy and momentum. The interaction is shown schematically in Figure II C 2.1, in both the laboratory (lab) and COM systems.

In this section we summarize the relevant equations relating the various momenta, energies, and angles involved in the description of the reaction. Details of the derivations are given in Section II.C.2.a.

Figure II C 2.1. Schematic of particle pairs for kinematics calculation.



Nomenclature: The two particles have mass *m* and *M* before the interaction (i.e., in the incident channel); the exit channel may contain completely different particles. The initial momentum of the incident particle is $\vec{p}$; the target particle is stationary (momentum $\vec{q} = 0$); in the COM, the initial momentum of the incident particle is $\vec{K} = \hbar \vec{k}$, and the target particle's momentum is $-\vec{K}$. Primes refer to values after the interaction (in the exit channel). Quantities measured during an experiment are incident laboratory energy $E = p^2 / 2m$, laboratory energy of the exiting particle $E' = p'^2 / 2m'$, and laboratory angle θ relative to the incident direction. All other quantities will be specified in terms of these quantities.

Equation numbers in the rest of this section relate to the derivation in the following section.

The Q-value, Eq. (II C2 a.6), is defined as

$$Q \equiv m + M - m' - M' \qquad \text{(II C2.1)}$$

and is related to the laboratory threshold energy , Eq. (II C2 a.24), here denoted by Ξ, via

$$\Xi = -\frac{m+M}{M} Q \quad . \qquad \text{(II C2.2)}$$

The initial momentum *K* in the COM, Eq. (II C2 a.2), is given by

$$K = \hbar k = \frac{M}{m+M} \sqrt{2mE} \quad , \qquad \text{(II C2.3)}$$

and the final COM momentum K', Eq. (II C2 a.8), by

$$K' = \sqrt{\frac{2m'M'}{(m'+M')} \frac{M}{(m+M)} \left[E - \Xi\right]} \quad . \qquad \text{(II C2.4)}$$

The laboratory energy of the outgoing particle, Eq. (II C2 a.25), is equal to

$$E' = \frac{M'}{(m'+M')} \frac{M}{(m+M)} \left\{ \gamma \mu + \sqrt{1 - \gamma^2 \left(1 - \mu^2\right)} \right\}^2 \left[E - \Xi\right] \quad , \qquad \text{(II C2.5)}$$

in which $\mu = \cos\theta$, and γ is given in Eq. (II C2 a.26) as

$$\gamma^2 = \frac{m'}{M'} \frac{m}{M} \frac{m'+M'}{m+M} \frac{E}{E-\Xi} \quad . \qquad \text{(II C2.6)}$$

The relationships between the COM and lab angles are, from Eqs. (II C2 a.29) and (II C2 a.31)

$$\nu = -\gamma\left(1-\mu^2\right)+\mu\sqrt{1-\gamma^2\left(1-\mu^2\right)} \qquad \text{(II C2.7)}$$

and

$$\mu = \frac{\nu+\gamma}{\sqrt{1+\gamma^2+2\gamma\nu}} \quad , \qquad \text{(II C2.8)}$$

where $\nu = \cos\beta$ and β is the COM angle. The transformation of angle-differential cross sections from COM to lab involves the derivative of ν with respect to μ, as given by Eq. (II C2 a.33):

$$\frac{d\nu}{d\mu} = \frac{\left(\mu\gamma+\sqrt{1-\gamma^2\left(1-\mu^2\right)}\right)^2}{\sqrt{1-\gamma^2\left(1-\mu^2\right)}} \quad . \qquad \text{(II C2.9)}$$

See Section II.B.1.b for details on the calculations of angular distributions with the Reich-Moore formulation of R-matrix theory.

In older versions of input to the SAMMY code (when particle-pair input is not used), the excitation energy can be specified either in the laboratory system (as in Eq. (II C2.2)) or in the center-of-mass system (as $-Q$); SAMMY will make the appropriate conversions. The default is laboratory. Users who wish to override the default (or who wish to keep a reminder handy) should include (in INPut file) the phrase

```
CM NON-COULOMB EXCITation energies, or
LAB NON-COULOMB EXCItation energies
```

as needed for the non-Coulomb case and

```
CM COULOMB EXCITATIOn energies, or
LAB COULOMB EXCITATIon energies
```

for use with charged-particle channels.

When using the key-word particle-pair input option (card set 4 of Table VI A.1), it is possible to specify the Q-value (equivalent to the negative of the center-of-mass excitation energy) rather than the excitation energy. It is recommended that Q-value rather than excitation energy be given, to avoid any ambiguity when more than one nuclide is present in the target.

Within SAMMY, the conversion factors from laboratory energy to COM momenta are calculated in subroutine Fixrad in segment/subdirectory "old" (and also used in segment "new") and stored in an array "Zke" which must then be multiplied by the square root of the energy (minus the adjusted Q value) to give k or k'. Appropriate numerical constants are included to facilitate conversion from units of eV (for energy) to inverse Fermi (for wave number, which is momentum divided by $\hbar$). Values for constants are described in Section IX.A of this report.

II.C.2.a. Derivation of kinematics equations

Let $\vec{V}$ represent the velocity of the center-of-mass (COM) system relative to the laboratory system. Before the interaction, the relationships between the velocities are

$$\frac{\vec{p}}{m} = \frac{\vec{K}}{m} + \vec{V} \quad \text{and} \quad 0 = -\frac{\vec{K}}{M} + \vec{V} \quad , \tag{II C2 a.1}$$

from which we can solve for $\vec{V}$ and $\vec{K}$ in terms of $\vec{p}$:

$$\vec{V} = \frac{\vec{K}}{M} \quad \text{and} \quad \vec{\mathrm{K}} = \frac{\mathrm{M}}{\mathrm{m+M}}\vec{p} \ , \quad \text{which implies} \quad \vec{V} = \frac{\vec{p}}{(m+M)} \quad . \tag{II C2 a.2}$$

The total energy in the lab must equal the energy *in* the COM plus the energy *of* the COM. Before the interaction, this gives us

$$\begin{aligned} E_{\text{lab}} &= E_{\text{of COM}} + E_{\text{in COM}} \\ \frac{p^2}{2m} + m + M &= \frac{(m+M)V^2}{2} + \frac{K^2}{2m} + \frac{K^2}{2M} + m + M \quad , \end{aligned} \tag{II C2 a.3}$$

which is clearly true, as can be seen by substitution of the expressions in Eq. (II C2 a.2) into (II C2 a.3). We are using non-relativistic energies but nevertheless including the masses because they may be different before and after the interaction. Within the COM, conservation of energy requires that the initial and final energies are equal:

$$\begin{aligned} E_{\text{in com}} &= E'_{\text{in com}} \\ \frac{K^2}{2m} + \frac{K^2}{2M} + m + M &= \frac{K'^2}{2m'} + \frac{K'^2}{2M'} + m' + M' \quad . \end{aligned} \tag{II C2 a.4}$$

Solving for K' in terms of K gives

$$\begin{aligned} \frac{K'^2}{2}\left(\frac{1}{m'} + \frac{1}{M'}\right) &= \frac{K^2}{2}\left(\frac{1}{m} + \frac{1}{M}\right) + \left(m + M - \left(m' + M'\right)\right) \quad \text{or} \\ \frac{K'^2}{2}\left(\frac{m'+M'}{m'M'}\right) &= \frac{K^2}{2}\left(\frac{m+M}{mM}\right) + (Q) \quad , \end{aligned} \tag{II C2 a.5}$$

in which we have defined the Q-value as

$$Q = m + M - m' - M' \quad . \tag{II C2 a.6}$$

Rewriting Eq. (II C2 a.5) using the value for K from Eq. (II C2 a.2) gives

$$\begin{aligned} K'^2 &= \frac{2m'M'}{m'+M'}\left[K^2\left(\frac{m+M}{2mM}\right)+Q\right] \\ &= \frac{2m'M'}{m'+M'}\left[\left\{p\frac{M}{m+M}\right\}^2\left(\frac{m+M}{2mM}\right)+Q\right] \\ &= \frac{2m'M'}{m'+M'}\left[\frac{p^2}{2m}\frac{M}{(m+M)}+Q\right] \quad . \end{aligned} \tag{II C2 a.7}$$

This can also be written as

$$K'^2 = \frac{2m'M'}{m'+M'}\left[E\frac{M}{(m+M)}+Q\right] \quad , \tag{II C2 a.8}$$

in which E is equal to the kinetic energy of the incident particle in the laboratory system,

$$E = \frac{p^2}{2m} \quad . \tag{II C2 a.9}$$

This definition of E is used throughout this manual; cross sections are always specified in terms of this energy unless otherwise noted explicitly.

The transformation from COM to laboratory gives values for momenta after the interaction. Again, we add velocities, similar to Eq. (II C2 a.1), using Eq. (II C2 a.2) for $\vec{V}$:

$$\frac{\vec{p}'}{m'} = \frac{\vec{K}'}{m'} + \vec{V} = \frac{\vec{K}'}{m'} + \frac{\vec{p}}{(m+M)} \quad . \tag{II C2 a.10}$$

(An analogous set of equations holds for the second particle,

$$\frac{\vec{q}'}{M'} = -\frac{\vec{K}}{M} + \vec{V} = -\frac{\vec{K}}{M} + \frac{\vec{p}}{(m+M)} \quad , \tag{II C2 a.11}$$

but we shall not be concerned with this particle now.)

Setting $\mu = \cos\theta$ and $\nu = \cos\beta,$ we can write Eq. (II C2 a.10) in terms of components

$$\frac{p'\cos\theta}{m'} = \frac{K'\cos\beta}{m'} + \frac{p}{(m+M)} \quad \text{and} \quad \frac{p'\sin q}{m'} = \frac{K'\sin\beta}{m'} + 0 \qquad \text{(II C2 a.12)}$$

or

$$p'\mu = K'\nu + \frac{m'p}{(m+M)} \quad \text{and} \quad p'\sqrt{1-\mu^2} = K'\sqrt{1-\nu^2} \quad , \qquad \text{(II C2 a.13)}$$

in which we have set $\mu = \cos\theta$ and $\nu = \cos\beta.$ Squaring and adding the two equations in (II C2 a.13) gives

$$\left(\frac{p'\mu}{m'}\right)^2 + \left(\frac{p'\sqrt{1-\mu^2}}{m'}\right)^2 = \left(\frac{K'\nu}{m'}\right)^2 + \left(\frac{K'\sqrt{1-\nu^2}}{m'}\right)^2 + 2\frac{K'\nu}{m'}\frac{p}{(m+M)} + \left(\frac{p}{(m+M)}\right)^2, \qquad \text{(II C2 a.14)}$$

or

$$\frac{p'^2}{m'^2} = \frac{K'^2}{m'^2} + \frac{2K'\nu p}{m'(m+M)} + \frac{p^2}{(m+M)^2} \quad . \qquad \text{(II C2 a.15)}$$

Replacing $K'\nu$ with its equivalent from Eq. (II C2 a.13) puts Eq. (II C2 a.15) into the form

$$\frac{p'^2}{m'^2} = \frac{K'^2}{m'^2} + \frac{2p}{m'(m+M)}\left\{p'\mu - \frac{m'p}{m+M}\right\} + \frac{p^2}{(m+M)^2} \quad , \qquad \text{(II C2 a.16)}$$

which can be rearranged as

$$p'^2 = K'^2 + \frac{2m'p\mu}{(m+M)}p' - \frac{m'^2p^2}{(m+M)^2} \quad . \qquad \text{(II C2 a.17)}$$

Solving for p' in terms of other quantities gives

$$p' = \frac{m'}{m+M}p\mu + \sqrt{\left(\frac{m'}{m+M}\right)^2 p^2\mu^2 - \left(\frac{m'}{m+M}\right)^2 p^2 + K'^2}$$
$$= \frac{m'}{m+M}\left\{p\mu + \sqrt{p^2\left(\mu^2-1\right) + \left(\frac{m+M}{m'}\right)^2 K'^2}\right\} \quad . \qquad \text{(II C2 a.18)}$$

(Consideration of the $p = 0$ limit confirms that this choice of sign for the radical is appropriate.)

From Eq. (II C2 a.7), we know K' in terms of p. Therefore, to simplify Eq. (II C2 a.18), we define ξ as

$$\xi = \left(\frac{m'}{m+M} \right) \frac{p}{K'} \quad . \tag{II C2 a.19}$$

Using this definition of ξ, Eq. (II C2 a.18) can be put into the form

$$\begin{aligned} p' &= \frac{m'}{m+M} \left\{ p\mu + \sqrt{p^2 \left(\mu^2 - 1 \right) + \xi^{-2} p^2} \right\} \\ &= \frac{m'}{m+M} \frac{p}{\xi} \left\{ \xi \mu + \sqrt{1 - \xi^2 \left(1 - \mu^2 \right)} \right\} \quad . \end{aligned} \tag{II C2 a.20}$$

The quantity outside the curly brackets is exactly equal to K'; making this substitution gives

$$p' = K' \left\{ \xi \mu + \sqrt{1 - \xi^2 \left(1 - \mu^2 \right)} \right\} \quad . \tag{II C2 a.21}$$

The laboratory energy of the outgoing particle can then be found as

$$E' = \frac{p'^2}{2m'} = \frac{K'^2}{2m'} \left\{ \xi \mu + \sqrt{1 - \xi^2 \left(1 - \mu^2 \right)} \right\}^2 \quad , \tag{II C2 a.22}$$

or, using Eq. (II C2 a.8) for K',

$$E' = \frac{M'}{m' + M'} \left\{ \xi \mu + \sqrt{1 - \xi^2 \left(1 - \mu^2 \right)} \right\}^2 \left[E \frac{M}{(m+M)} + Q \right] \quad . \tag{II C2 a.23}$$

It is customary to define the laboratory threshold energy, here denoted by Ξ, as

$$\Xi \equiv - \frac{m+M}{M} Q \quad . \tag{II C2 a.24}$$

In terms of Ξ, Eq. (II C2 a.23) for E' becomes

$$E' = \frac{M'}{m' + M'} \frac{M}{(m+M)} \left\{ \xi \mu + \sqrt{1 - \xi^2 \left(1 - \mu^2 \right)} \right\}^2 \left[E - \Xi \right] \quad . \tag{II C2 a.25}$$

Equation (II C2 a.19) for ξ can also be written in terms of Ξ, using Eq. (II C2 a.8), as

$$\xi^2 = \frac{\left(\frac{m'}{m+M}\right)^2 2mE}{\frac{2m'M'}{m'+M'}\left[E\frac{M}{(m+M)}+Q\right]} = \frac{m'}{M'}\frac{m}{M}\frac{m'+M'}{m+M}\frac{E}{E-\Xi} \quad . \qquad \text{(II C2 a.26)}$$

Next, we consider the transformation of angle from laboratory θ to COM β and vice versa. From Eq. (II C2 a.13) we have

$$p'\mu = K'\nu + \frac{m'p}{(m+M)} = K'\nu + K'\xi \quad , \qquad \text{(II C2 a.27)}$$

in which we have made use of Eq. (II C2 a.19). Substituting Eq. (II C2 a.21) into this equation gives

$$p'\mu = K'\left\{\xi\mu + \sqrt{1-\xi^2\left(1-\mu^2\right)}\ \right\}\mu = K'\nu + K'\xi \quad , \qquad \text{(II C2 a.28)}$$

which reduces to

$$\nu = -\xi\left(1-\mu^2\right) + \mu\sqrt{1-\xi^2\left(1-\mu^2\right)} \quad . \qquad \text{(II C2 a.29)}$$

This equation can be inverted to give μ in terms of ν as follows:

$$\begin{aligned}
\left[\nu + \xi\left(1-\mu^2\right)\right]^2 &= \mu^2\left[1-\xi^2\left(1-\mu^2\right)\right] \quad , \\
\nu^2 + 2\xi\nu\left(1-\mu^2\right) + \xi^2\left(1-2\mu^2+\mu^4\right) &= \mu^2 - \xi^2\mu^2 + \xi^2\mu^4 \quad , \\
\mu^2\left(1+\xi^2+2\xi\nu\right) &= \nu^2 + 2\xi\nu + \xi^2 \quad , \\
\mu^2 &= \frac{\nu^2+2\xi\nu+\xi^2}{\left(1+\xi^2+2\xi\nu\right)} \quad ,
\end{aligned} \qquad \text{(II C2 a.30)}$$

or, finally, as

$$\mu = \frac{\nu+\xi}{\sqrt{1+\xi^2+2\xi\nu}} \quad . \qquad \text{(II C2 a.31)}$$

The transformation of cross section from COM to lab requires the derivative of ν with respect to μ; this is found from Eq. (II C2 a.29):

$$\begin{aligned}\frac{d\nu}{d\mu} &= \frac{d}{d\mu}\left\{-\xi\left(1-\mu^2\right)+\mu\sqrt{1-\xi^2\left(1-\mu^2\right)}\ \right\} \\ &= 2\mu\xi+\sqrt{1-\xi^2\left(1-\mu^2\right)}+\frac{\mu\,2\mu\,\xi^2\,\frac{1}{2}}{\sqrt{1-\xi^2\left(1-\mu^2\right)}} \qquad \text{(II C2 a.32)} \\ &= \frac{2\mu\xi\sqrt{1-\xi^2\left(1-\mu^2\right)}+1-\xi^2\left(1-\mu^2\right)+\mu^2\xi^2}{\sqrt{1-\xi^2\left(1-\mu^2\right)}}\ ,\end{aligned}$$

giving, finally, the expression for the derivative

$$\frac{d\nu}{d\mu}=\frac{\left(\mu\xi+\sqrt{1-\xi^2\left(1-\mu^2\right)}\right)^2}{\sqrt{1-\xi^2\left(1-\mu^2\right)}}\ . \qquad \text{(II C2 a.33)}$$

II.C.2.b. Kinematics for elastic scattering

In the case of elastic scattering, primed quantities are exactly equal to unprimed, and the Q-value is zero. The equations of Section II.C.2 therefore simplify to the forms shown here.

The initial momentum *K* in the center-of-mass (COM) system is found from Eq. (II C2.3) to be

$$K = \hbar k = \frac{M}{m+M}\sqrt{2mE} \quad , \tag{II C2 b.1}$$

and the final COM momentum K' is found in Eq. (II C2.4) to be

$$K' = \frac{M}{m+M}\sqrt{2mE} \quad . \tag{II C2 b.2}$$

The laboratory energy of the outgoing particle is found from Eqs. (II C2.5) and (II C2.6) to be

$$E' = \left[\frac{1}{m+M}\left\{m\mu + \sqrt{M^2 - m^2\left(1-\mu^2\right)}\ \right\}\right]^2 E \quad , \tag{II C2 b.3}$$

with $\mu = \cos\theta$.

The relationships between the COM and lab angles, Eqs. (II C2.7) and (II C2.8), become

$$\nu = -\frac{m}{M}\left(1-\mu^2\right) + \mu\sqrt{1-\left(\frac{m}{M}\right)^2\left(1-\mu^2\right)} \tag{II C2 b.4}$$

and

$$\mu = \frac{M\nu + m}{\sqrt{M^2 + m^2 + 2mM\nu}} \quad , \tag{II C2 b.5}$$

where $\nu = \cos\beta$ and β is the COM angle. The derivative of ν with respect to μ, Eq. (II C2.9), is

$$\frac{d\nu}{d\mu} = \frac{\left(\mu m + \sqrt{M^2 - m^2\left(1-\mu^2\right)}\right)^2}{\sqrt{M^2 - m^2\left(1-\mu^2\right)}} \quad . \tag{II C2 b.6}$$

II.C.3. Evaluation of Hard-Sphere Phase Shift

Formulae for the hard-sphere phase shift (otherwise known as the potential-scattering phase shift) are given in Table II A.1 for non-Coulomb interactions. What is actually needed in SAMMY is not, however, the phase shifts φ themselves but rather $\cos(2\varphi)$ and $\sin(2\varphi)$. Since evaluation of φ requires the inverse tangent function, results for $\cos(2\varphi)$ and $\sin(2\varphi)$ are more readily generated with fewer computer round-off errors by using trigonometric relationships to generate formulae for $\cos(2\varphi)$ and $\sin(2\varphi)$ directly.

For all l, it is clear from Table II A.1 that φ may be written in the form

$$\varphi = \rho - X \quad , \tag{II C3.1}$$

where

$$X = \tan^{-1} f \tag{II C3.2}$$

and f is a different function of ρ for each value of l. From Eq. (II C3.1), using elementary trigonometric relationships, we find

$$\cos\varphi \;=\; \cos\rho\ \cos X \;+\; \sin\rho\ \sin X \tag{II C3.3}$$

and

$$\sin\varphi \;=\; -\cos\rho\ \sin X \;+\; \sin\rho\ \cos X \quad . \tag{II C3.4}$$

Thus, $\cos(2\varphi)$ becomes

$$\begin{aligned} \cos(2\varphi) \;&=\; 2\cos^2\varphi - 1 = 2\cos^2\rho\ \ \cos^2 X\ \left(1+\tan\rho\ \tan X\right)^2 - 1 \\ &= 2\ \frac{\cos^2\rho}{1+f^2}\ \left(1+f\ \tan\rho\right)^2 - 1 \quad . \end{aligned} \tag{II C3.5}$$

Similarly, $\sin(2\varphi)$ can be written

$$\begin{aligned} \sin(2\varphi) \;&=\; 2\cos\varphi\sin\varphi \;=\; 2\cos^2\rho\ \cos^2 X\ (1+\tan\rho\tan X)(-\tan X+\tan\rho) \\ &=\; 2\frac{\cos^2\rho}{1+f^2}(1+f\ \tan\rho)(-f+\tan\rho) \quad . \end{aligned} \tag{II C3.6}$$

Equations (II C3.5) and (II C3.6) are the form used in SAMMY to evaluate the hard-sphere phase shift terms for non-Coulomb situations.

II.C.4. Modifications for Charged Particles

The penetrabilities P_l, shift factors S_l, and potential-scattering phase shifts φ_l defined in Table II A.1 apply only to non-Coulomb interactions such as those involving incident neutrons. Often, however, the two particles in a channel will both have a positive charge; examples are the exit channels for (n,α) or (n,p) interactions, and the incident channels in the inverse (reciprocal) measurements (α,n) and (p,n). In this case the expressions for penetrabilities, shift factors, and phase shifts must be modified to include the long-range interaction; see, for example, the discussion of Lane and Thomas [AL58].

An extension for SAMMY to include Coulomb penetrabilities, shift factors, and phase shifts was developed by R. O. Sayer [RS00] (and modified by the SAMMY author) and used first for analysis of ^{16}O data [LL98, RS00]. FORTRAN routines used for this purpose are a modified version of the routine COULFG of Barnett [AB82].

Additional changes were required to calculate the cross sections for incident charged particles; details are given in Section II.C.4.a. Because the Coulomb interaction is long range, only the angle-differential cross sections are calculable; the angle-integrated cross sections are infinite.

Expressions for P_l, S_l, and φ_l for particle pair α involve the parameter η_α, which is defined as

$$\eta_\alpha = \frac{z_\alpha Z_\alpha e^2 \mu_\alpha}{\hbar^2 k_\alpha} \quad , \tag{II C4.1}$$

where z and Z are the charge numbers for the two particles in the particle pair. The reduced mass μ_α is defined in the usual manner as

$$\mu_\alpha = \frac{m_\alpha M_\alpha}{m_\alpha + M_\alpha} \quad , \tag{II C4.2}$$

where m_α and M_α are the masses of the two particles in channel α. The center-of-mass (COM) momentum $\hbar k_\alpha$ is defined in the same manner as in Eq. (II C2 a.8), as

$$\hbar^2 k_\alpha^2 = \frac{2 m_\alpha M_\alpha}{\left(m_\alpha + M_\alpha\right)} \frac{M}{\left(m + M\right)} \left(E - \Xi\right) \quad . \tag{II C4.3}$$

In Eq. (II C4.3), the masses of particles in the incident channel are denoted without subscripts; these masses may be different from the masses in particle pair α. If the excitation energy is given in the COM system, this expression takes the form

$$\hbar^2 k_\alpha^2 = \frac{2 m_\alpha M_\alpha}{\left(m_\alpha + M_\alpha\right)} \frac{M}{\left(m + M\right)} \left(E - \left[\frac{m + M}{M} \right] \Xi_{\text{com}} \right) \quad . \tag{II C4.4}$$

In the SAMMY input, the user can specify the value of the excitation energy either in the laboratory system [as in Eq. (II C4.3)] or in the COM system; SAMMY will make the appropriate conversions. The default is laboratory. Users who wish to provide COM values should include the phrase "CM COULOMB EXCITATION ENERGIES" as needed.

The reaction Q-value is the negative of variable Ξ_{COM} = ECHAN (in the COM system) in card set 10.1 or 10.2 of Table VI A.1. When using the particle-pair input, card set 4 or 4a of Table VIA.1, it is possible to give the Q-value directly; this is the recommended input format.

Recall that a channel is defined by the particle pair (with mass, spin, and charge for each of the two particles, plus the Q-value) plus the spin quantum numbers *l*, *s*, and *J*. Quantities defined above in Eqs. (II C4.1) through (II C4.4) depend only on the particle pair α and not on the spin quantum numbers. Other quantities (below) depend also on the value of *l*.

If a_c is the channel radius for this channel, we again define ρ as

$$\rho = k_\alpha a_c \qquad \text{(II C4.5)}$$

The penetrabilities $P_l(\eta,\rho)$, shift factors $S_l(\eta,\rho)$, and phase shifts $\varphi_l(\eta,\rho)$ are then calculated as functions of $F_l(\eta,\rho)$ and $G_l(\eta,\rho)$, the regular and irregular Coulomb wave functions, respectively. The equations are as follows:

$$P_l = \frac{\rho}{A_l^2}, \qquad S_l = \frac{\rho}{A_l}\frac{\partial A_l}{\partial \rho}, \qquad \text{and} \quad \cos\varphi_l = \frac{G_l}{A_l} \quad , \qquad \text{(II C4.6)}$$

where

$$A_l^2 = F_l^2 + G_l^2 \quad . \qquad \text{(II C4.7)}$$

In Eqs. (II A.1) and (II A.5), the Coulomb phase-shift difference w_c is required for charged-particle interactions. From Lane and Thomas [AL58], this quantity has the value

$$w_c = \begin{cases} 0 & l = 0 \\ \sum_{n=1}^{l} \tan^{-1}\left(\frac{\eta_\alpha}{n}\right) & l \neq 0 \end{cases} \quad . \qquad \text{(II C4.8)}$$

Finally, we note that an alternative version of the Coulomb functions is available in SAMMY. This alternative, modified from files provided by Hale [GH02], requires longer run time but appears to be more accurate at low values of ρ (and corresponding high values of η). SAMMY will automatically switch to the more accurate version when it discerns the need. To invoke this alternative for all calculations, include the phrase "USE ALTERNATIVE COULomb functions" in the INPut file.

II.C.4.a. Charged-particle initial states

To derive the equations for the angle-differential cross sections for charged-particle incident channels, we begin with the Lane and Thomas [AL58] expression [page 292, Eq. (2.6)]. When this expression is corrected (for a missing complex conjugate, a missing minus sign, and missing delta functions), summed over the exit channel spins s', and averaged over the incident channel spins s, the resulting equation for the angle-differential cross section is

$$\begin{aligned}\frac{d\sigma_{\alpha\alpha'}}{d\Omega_{CM}} &= \sum_L B_{L\alpha\alpha'}(E) P_L(\cos\beta) + \frac{\pi}{k_\alpha^2}\left|C_\alpha(\beta)\right|^2 \delta_{\alpha\alpha'} \\ &+ \frac{\sqrt{4\pi}}{k_\alpha^2}\sum_{Jsl} g_J \,\mathrm{Re}\left[-i\left(\frac{e^{2iw_{l\alpha}}-U_{cc}}{2}\right)C_\alpha^*\, P_l(\cos\beta)\right]\delta_{\alpha\alpha'} \quad .\end{aligned} \tag{II C4 a.1}$$

Here we have again used the convention that $c=\{\alpha,l,s,J\}$. For the charged-particle case, the definition of $B_{L\alpha\alpha'}(E)$ is modified slightly from the non-Coulomb case [Eq. (II B1 b.2)] to give

$$\begin{aligned}B_{L\alpha\alpha'}(E) = \frac{1}{4k_\alpha^2} &\sum_{J_1}\sum_{J_2}\sum_{l_1 s_1}\sum_{l'_1 s'_1}\sum_{l_2 s_2}\sum_{l'_2 s'_2} \\ &\times G_{\{l_1 s_1 l'_1 s'_1 J_1\}\{l_2 s_2 l'_2 s'_2 J_2\} L}\ \frac{1}{(2i+1)(2I+1)} \\ &\times \mathrm{Re}\left[(e^{2iw_{l\alpha}}\delta_{c_1 c'_1}-U_{c_1 c'_1})(e^{-2iw_{l\alpha}}\delta_{c_2 c'_2}-U^*_{c_2 c'_2})\right] \quad .\end{aligned} \tag{II C4 a.2}$$

In the final line of Eq. (II C4 a.2), the quantity c_1 is substituted for the expression $\{\alpha,l_1,s_1,J_1\}$, c_2 for $\{\alpha,l_2,s_2,J_2\}$, c'_1 for $\{\alpha',l'_1,s'_1,J_1\}$, and c'_2 for $\{\alpha',l'_2,s'_2,J_2\}$. The geometric term G in Eq. (II C4 a.2) is the same as for the non-Coulomb case and is defined in Eqs. (II B1 b.3) to (II B1 b.10). Notation for summation indices is the same as in the non-Coulomb case.

What is different here is the presence of the exponential involving the Coulomb phase-shift difference $w_{l\alpha}$, defined in Eq. (II C4.7). Also, the scattering matrix contains the $w_{l\alpha}$ in the definition of Ω; the Sommerfeld parameter η_α in Eq. (II C4.1) is defined as

$$\eta_\alpha = \frac{z\,Z\,e^2\mu_\alpha}{\hbar^2 k_\alpha} \quad . \tag{II C4 a.3}$$

The additional terms in Eq. (II C4 a.1) involve the function C_α, which is defined as

$$C_\alpha = \frac{1}{\sqrt{4\pi}} \eta_\alpha \ \text{cosec}^2\left(\frac{\beta}{2}\right) e^{-2i\eta_\alpha \ln\left[\sin\left(\frac{\beta}{2}\right)\right]} \quad . \qquad \text{(II C4 a.4)}$$

It is this term which is infinite at $\beta = 0$ (forward scattering) and which causes the (angle-integrated) elastic-scattering cross section to be infinite.

Center-of-mass vs Laboratory

Angular distribution cross sections are sometimes reported as if measured in the center-of-mass system rather than in the laboratory system; hence, SAMMY can calculate either version. To specify which is wanted, insert one of the phrases

```
USE CENTER OF MASS Cross sections
USE LABORATORY CROSS sections
```

into your INPut file (see Tables VI A.1 and VI A1.2). Center-of-mass is the default.

Acknowledgements

The author is grateful to SAMMY users Jeff Blackmon and Olivier Bouland for uncovering bugs in early implementations of charged-particle elastic scattering, and to Eric Berthoumieux (author of the ANARKI R-matrix code) for providing calculations to assist in debugging this portion of SAMMY.

II.C.5. Inverse Reactions (Reciprocity)

Occasionally a user may wish to include data from an inverse reaction in the same evaluation as the forward reaction. For example, for an evaluation of the ^{16}O resonance parameters, Sayer [RS00] wanted to include ^{16}O(n,α)^{13}C data. No such data existed, but ^{13}C(α,n)^{16}O data were available.

Unfortunately SAMMY does not have the capability of including reciprocal data in the same evaluation (using the same resonance parameters). SAMMY was designed with the intent of treating one incident particle (originally a neutron) and many different types of nuclides within the target. Other codes (e.g., EDA [GH75]) were designed with a different philosophy: to simultaneously treat all interactions leading to the same compound nucleus. Eventually the SAMMY author hopes to add similar capabilities to the SAMMY code.

Meanwhile, two alternatives are available: (1) The SAMMY user can convert the data using reciprocal relationships, and include the converted data within his or her evaluation. (2) If there is no need for simultaneous* fitting, resonance parameter values can be converted to those appropriate for the reciprocal reaction. Either of these two can be accomplished by application of the principle of detailed balance.

To convert the cross section from the $A'(a',a)A$ reaction to the $A(a,a')A'$ reaction, we first consider the center-of-mass (COM) system, in which the energies are easily related by

$$E_{COM} = E'_{COM} - Q \quad . \qquad \text{(II C5.1)}$$

Elementary kinematics (as illustrated in Figure II C5.1) gives the conversion to the laboratory values E and E',

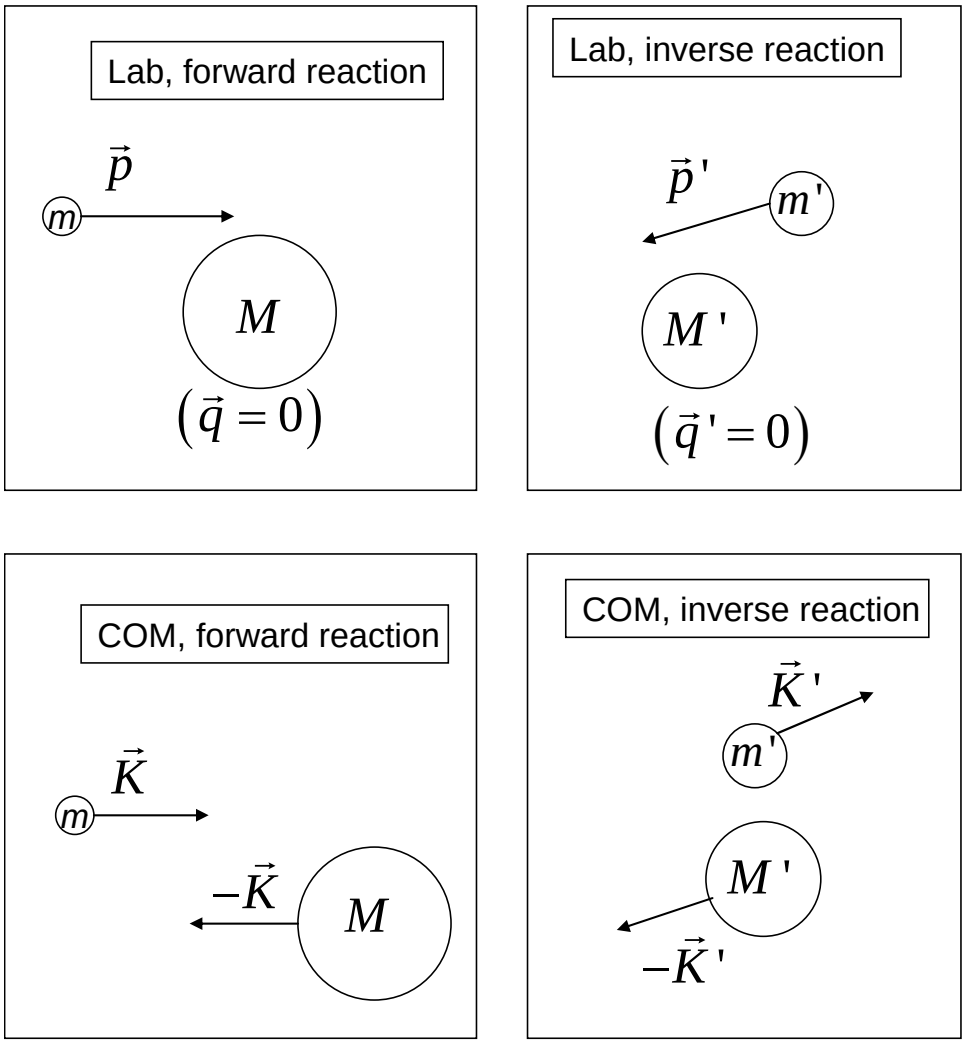
$$E_{COM} = \frac{M}{m+M} E \quad , \qquad E'_{COM} = \frac{M'}{m'+M'} E' \quad , \qquad Q = -\frac{M}{m+M} \Xi_{lab} \quad , \qquad \text{(II C5.2)}$$

and algebra then gives

$$E' = \left(E - \Xi_{lab}\right) \frac{M}{m+M} \frac{m'+M'}{M'} \quad . \qquad \text{(II C5.3)}$$

* By "simultaneous" is meant either (1) truly simultaneous or (2) "sequential using the covariance matrix from one SAMMY run fitting one data set as input to another run fitting another data set." See Section IV of this manual for details of both possibilities.

Figure II C5.1. Schematic of kinematics for inverse reactions.



The R-matrix for the $A'(a',a)A$ system must have the same value (at comparable energies) as the R-matrix for the $A(a,a')A'$ system. Hence

$$R'_{cc''} = \sum_{\lambda} \frac{\gamma'_{\lambda c}\gamma'_{\lambda c''}}{E'_{\lambda} - E' - i\Gamma'_{\lambda\gamma}/2}$$

$$= \sum_{\lambda} \frac{\gamma'_{\lambda c}\gamma'_{\lambda c''}}{E'_{\lambda} - \left[\left(E - \Xi_{lab}\right)\frac{M}{m+M}\frac{m'+M'}{M'}\right] - i\Gamma'_{\lambda\gamma}/2} = \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c''}}{E_{\lambda} - E - i\Gamma_{\lambda\gamma}/2} = R_{cc''} \quad . \tag{II C5.4}$$

In order for the equality on the bottom line of Eq. (II C5.4) to hold, the unprimed resonance parameters must be defined as follows:

$$E_\lambda = E'_\lambda\, q + \Xi_{lab} \ , \qquad \Gamma_{\lambda c} = \Gamma'_{\lambda c}\, q \ , \qquad \gamma_{\lambda c} = \gamma'_{\lambda c}\sqrt{q} \ , \tag{II C5.5}$$

where

$$q = \left[\frac{m+M}{M}\right]\left[\frac{M'}{m'+M'}\right] \tag{II C5.6}$$

(for c = any channel, for example neutron, fission, or capture). These equations may be used to convert the resonance parameters.

To convert the experimental data, recall that there is a multiplicative kinematic factor of $1/K^2$, where K is the momentum of the incident particle in the COM frame. For $A'(a',a)A$, this term is

$$\frac{1}{K'^2} = \frac{(m'+M')^2}{2m'(M')^2 E'} \ , \tag{II C5.7}$$

and for $A(a,a')A'$, the term is

$$\frac{1}{K^2} = \frac{(m+M)^2}{2mM^2 E} \ . \tag{II C5.8}$$

The experimental cross sections must be multiplied by the ratio of these two values, and appropriate energy substitutions made.

Another multiplicative factor that must be adjusted is the spin statistical factor, which also reflects the parameters of the incident channel. Since the compound nuclear spin J is the same in either system, the correct multiplier is the ratio of the two:

$$\frac{g_{J:A(aa')A'}}{g_{J:A'(a'a)A}} = \frac{(2i'+1)(2I'+1)}{(2i+1)(2I+1)} \ . \tag{II C5.9}$$

With these changes, the cross section for the $A(a,a')A'$ reaction may be written in terms of the cross section for the $A'(a',a)A$ reaction as

$$\sigma_{A(aa')A'}(E) = \frac{(2i'+1)(2I+1)}{(2i+1)(2I+1)}\frac{m'M'^2}{mM^2}\frac{(m+M)^2}{(m'+M')^2}\frac{E'}{E}\sigma_{A'(a'a)A}(E') \ . \tag{II C5.10}$$

II.D. DERIVATIVES

In order to make use of sophisticated fitting procedures such as Bayes' equations (Section IV of this manual), it is necessary to know the partial derivatives of the theory with respect to the parameters to be fitted (the "varied parameters"). The easiest method for calculating derivatives of cross sections with respect to resonance parameters is to use a numerical difference approximation, of the form

$$\frac{\partial\sigma}{\partial P} \approx \frac{\sigma\left(P+\Delta P\right)-\sigma\left(P\right)}{\Delta P} \quad , \tag{II D.1}$$

or, to avoid problems from the asymmetry of that approximation,

$$\frac{\partial\sigma}{\partial P} \approx \frac{\sigma\left(P+\Delta P\right)-\sigma\left(P-\Delta P\right)}{2\Delta P} \quad . \tag{II D.2}$$

Numerical methods, however, are neither as accurate nor as efficient or rapid as analytic derivatives. For that reason, SAMMY uses analytic derivatives wherever possible. In particular, derivatives of cross sections with respect to resonance parameters are all calculated analytically.

To reiterate: SAMMY does NOT use numerical derivatives of the form (II D.1). When a numerical derivative is absolutely necessary, the form (II D.2) is used. For R-matrix parameters, analytic derivatives are always used. (The only exception to this rule is for charged-particle shift factors and penetrabilities, for which calculations of both the functions and the derivatives require numerical techniques.)

The R-matrix equations are expressed in terms of the reduced-width amplitude γ rather than the partial width Γ. In the SAMMY code, the amplitudes are the parameters to be varied. In general, SAMMY distinguishes between "*u*-parameters" and "*p*-parameters": The *u*-parameter is the variable whose value is sought by the fitting procedure. The *p*-parameter is the parameter whose value is given in the SAMMY input and output files. There is a well-defined relationship between the two, but the relationship is not necessarily one to one. For example, the value for the neutron width specified in the input PARameter file (see Table VI B.2 in Section VI.B) is related to three parameters, any or all of which might be varied:

$$\Gamma_{\lambda n} = 2P_l(\rho)\gamma_{\lambda n}^2 \quad ,$$

$$\rho_\lambda = k_\lambda a_n \quad , \tag{II D.3}$$

and

$$\hbar k_\lambda = \frac{M}{m+M}\sqrt{2mE_\lambda} \quad .$$

Here γ_λ, a_n, and E_λ all may be varied parameters. In the SAMMY input, varied parameters are indicated by a flag, whose value (0, 1, or 3) indicates how that parameter is to be treated. The

convention is that a flag on Γ denotes the status of the γ parameter, because the other two (the radius and the energy) are separately flagged.

Throughout this document, when the varied *u*-parameter is different from the flagged *p*-parameter, the equations relating the two are given explicitly. For the R-matrix (in all its various guises), the *u*-parameter associated with the resonance energy is

$$u\left(E_\lambda\right) = \pm\sqrt{\left|E_\lambda\right|} \quad , \tag{II D.4}$$

where the negative sign is chosen if E_λ is negative, and the *u*-parameter associated with the width is

$$u\left(\Gamma_{\lambda c}\right) = \gamma_{\lambda c} \quad . \tag{II D.5}$$

In the following sections, equations are given for the derivatives of the cross section with respect to the R-matrix parameters for the Reich-Moore approximation (Section II.D.1) and for the Breit-Wigner approximations (Section II.D.2). Additional details are in Section II.D.3.

II.D.1. Derivatives for Reich-Moore Approximation

The derivative of the cross section with respect to a resonance parameter is found by making use of the chain rule:

$$\frac{\partial \sigma}{\partial u_i} = \sum_{\substack{\mu \le \nu \\ \omega \le \tau}} \frac{\partial R_{\mu\nu}}{\partial u_i} \frac{\partial W_{\omega\tau}}{\partial R_{\mu\nu}} \frac{\partial U_{\omega\tau}}{\partial W_{\omega\tau}} \frac{\partial \sigma}{\partial U_{\omega\tau}} \quad , \qquad \text{(II D1.1)}$$

where the index J has been suppressed, since it is fixed for a given parameter u. Each term in this expression is evaluated separately.

Derivatives of cross sections with respect to the scattering matrix U, derivatives of U with respect to W, and derivatives of W with respect to R are found in Section II.D.1.a. Derivatives of R with respect to resonance parameters are given in Section II.D.1.b.

Derivatives of the cross sections with respect to the channel radius require additional terms beyond those in Eq. (II D1.1), because the radius is also used to determine the hard-sphere phase shift. These derivatives are discussed in Section II.D.1.c.

Derivatives of R with respect to the variables of the logarithmic parameterization of the external R-function (defined in Section II.B.1.d) are given in Section II.D.1.d.

II.D.1.a. Derivatives with respect to R-matrix

For resonance and R^{ext} parameters, the derivative of the cross section may be written as

$$\frac{\partial \sigma}{\partial u_i} = \sum_{\substack{c \le d \\ e \le f}} \frac{\partial R_{cd}}{\partial u_i} \frac{\partial W_{ef}}{\partial R_{cd}} \frac{\partial U_{ef}}{\partial W_{ef}} \frac{\partial \sigma}{\partial U_{ef}} \quad , \qquad \text{(II D1 a.1)}$$

where the index J has been suppressed, since it is fixed for a given parameter u. Indices c, d, e, and f denote channels. The restriction $c \le d$ indicates that the sum includes, for example, only terms with indices $c_1 c_2$ and not terms with indices $c_2 c_1$ (for $c_1 \ne c_2$); this restriction results from the symmetry of R and W (or X) with respect to interchange of indices.

Each term in the expression (II D1 a.1) will be evaluated separately, starting with the right-most term. All except $\partial R / \partial u$ are evaluated in this section; $\partial R / \partial u$ is discussed in subsequent sections.

The derivatives of cross section with respect to the real part of U can be expressed as

$$\frac{\partial \sigma}{\partial U^r} = \frac{\partial \sigma}{\partial U}\frac{\partial U}{\partial U^r} + \frac{\partial \sigma}{\partial U^*}\frac{\partial U^*}{\partial U^r} = \frac{\partial \sigma}{\partial U} + \frac{\partial \sigma}{\partial U^*} = 2\,\mathrm{Re}\left[\frac{\partial \sigma}{\partial U}\right] \quad , \qquad \text{(II D1 a.2)}$$

where the asterisk implies complex conjugate, and U and U^* are treated as independent entities. Similarly the derivative with respect to the imaginary part of U is given by

$$\frac{\partial \sigma}{\partial U^i} = \frac{\partial \sigma}{\partial U}\frac{\partial U}{\partial U^i} + \frac{\partial \sigma}{\partial U^*}\frac{\partial U^*}{\partial U^i} = i\frac{\partial \sigma}{\partial U} - i\frac{\partial \sigma}{\partial U^*} = -2\,\mathrm{Im}\left[\frac{\partial \sigma}{\partial U}\right] . \qquad \text{(II D1 a.3)}$$

It follows that the derivative of the cross section with respect to U can be written as

$$\frac{\partial \sigma}{\partial U} = \mathrm{Re}\left[\frac{\partial \sigma}{\partial U}\right] + i\,\mathrm{Im}\left[\frac{\partial \sigma}{\partial U}\right] = \frac{1}{2}\left(\frac{\partial \sigma}{\partial U^r} - i\frac{\partial \sigma}{\partial U^i}\right) . \qquad \text{(II D1 a.4)}$$

Using Eq. (II D1 a.4), values for the partial derivative of σ with respect to U are found from Eqs. (II A.8) to (II A.11), which give

$$\frac{\partial \sigma^{total}}{\partial U_{ef}} = -\frac{\pi g}{k^2}\delta_{ef} \quad , \qquad \text{(II D1 a.5)}$$

$$\frac{\partial \sigma_{\alpha\alpha}}{\partial U_{ef}} = -\frac{\pi g}{k^2}\left(\delta_{ef} - U^*_{ef}\right) \quad , \qquad \text{(II D1 a.6)}$$

$$\frac{\partial \sigma_{\alpha\alpha'}}{\partial U_{ef}} = \frac{\pi g}{k^2} U^*_{ef} \qquad \text{for } \alpha' \neq \alpha, \tag{II D1 a.7}$$

and

$$\frac{\partial \sigma^{\,capture}}{\partial U_{ef}} = -\frac{\pi g}{k^2} U^*_{ef} \quad . \tag{II D1 a.8}$$

Derivatives of a complex variable (such as U) with respect to another complex variable (such as W) may be generated directly, without separately considering the real and imaginary parts of each variable; this is demonstrated explicitly in Section II.D.3. Here, we make use of this result to evaluate $\partial U / \partial W$ and $\partial W / \partial R$.

Derivatives of U_{ef} with respect to W_{ef} are formed directly from Eq. (II A.4), which may be expressed as

$$U_{ef} = \Omega_e W_{ef} \Omega_f \quad , \tag{II D1 a.9}$$

so that

$$\frac{\partial U_{ef}}{\partial W_{ef}} = \Omega_e \Omega_f \quad . \tag{II D1 a.10}$$

Derivatives of W with respect to R are formed from Eqs. (II B1.3) and (II B1.4), which we rewrite as

$$\begin{aligned} W = I + 2iX &= I + 2i\left(\sqrt{P}L^{-1}\left(L^{-1}-R\right)^{-1}R\sqrt{P}\right) \\ &= I + 2i\sqrt{P}L^{-1}\left(L^{-1}-R\right)^{-1}\left[R-L^{-1}+L^{-1}\right]\sqrt{P} \\ &= I + 2i\sqrt{P}L^{-1}\left(L^{-1}-R\right)^{-1}\left[R-L^{-1}\right]\sqrt{P} + 2i\sqrt{P}L^{-1}\left(L^{-1}-R\right)^{-1}\left[L^{-1}\right]\sqrt{P} \\ &= I - 2i\sqrt{P}L^{-1}\sqrt{P} + 2i\sqrt{P}L^{-1}\left(L^{-1}-R\right)^{-1}L^{-1}\sqrt{P} \quad . \end{aligned} \tag{II D1 a.11}$$

Explicitly displaying the indices, Eq. (II D1 a.11) takes the form

$$W_{ef} = I - 2i\delta_{ef}P_eL_f^{-1} + 2i\sqrt{P_e}\,L_e^{-1}Y_{ef}\,L_f^{-1}\sqrt{P_f} \quad , \tag{II D1 a.12}$$

where we have set

$$Y_{ef} = \left[\left(L^{-1}-R\right)^{-1}\right]_{ef} \quad . \tag{II D1 a.13}$$

In [NL80, Appendix A] and also in Section II.D.3 of this manual, we show that the derivative of Y with respect to R is given by

$$\frac{\partial Y_{ef}}{\partial R_{cd}} = Y_{ec}Y_{df} + Y_{ed}Y_{cf}\left(1-\delta_{cd}\right) \quad . \qquad \text{(II D1 a.14)}$$

Substitution of this expression into the derivative of Eq. (II D1 a.12) gives

$$\frac{\partial W_{ef}}{\partial R_{cd}} = 2i\sqrt{P_e}\, L_e^{-1}\left[Y_{ec}Y_{df} + Y_{ed}Y_{cf}\left(1-\delta_{cd}\right)\right] L_f^{-1}\sqrt{P_f} \quad . \qquad \text{(II D1 a.15)}$$

Alternatively, we may write

$$\frac{\partial X_{ef}}{\partial R_{cd}} = \sqrt{P_e}\, L_e^{-1}\left[Y_{ec}Y_{df} + Y_{ed}Y_{cf}\left(1-\delta_{cd}\right)\right] L_f^{-1}\sqrt{P_f} \quad , \qquad \text{(II D1 a.16)}$$

which is the more practically useful form in SAMMY.

Derivatives of R with respect to u depend upon which particular u-parameter is being considered. Parameters of the external R-matrix, resonance parameters, and channel radii are described in the next subsections.

II.D.1.b. Derivatives with respect to resonance parameters

From Eq. (II B1.1), the derivatives of the real and imaginary part of *R* with respect to the resonance *u*-parameter associated with the resonance energy are

$$\frac{\partial \mathrm{Re}\left[R_{\mu\nu}\right]}{\partial\sqrt{E_\lambda}} = \left[2\,\gamma_{\lambda\mu}\gamma_{\lambda\nu}\sqrt{E_\lambda}\right]\left[\left\{-\left(E_\lambda - E\right)^2 + \left(\overline{\gamma}_{\lambda\gamma}^2\right)^2\right\}/d_\lambda^2\right] \qquad \text{(II D1 b.1)}$$

and

$$\frac{\partial \mathrm{Im}\left[R_{\mu\nu}\right]}{\partial\sqrt{E_\lambda}} = \left[-4\,\gamma_{\lambda\mu}\gamma_{\lambda\nu}\sqrt{E_\lambda}\right]\left[\left\{\left(E_\lambda - E\right)\overline{\gamma}_{\lambda\gamma}^2\right\}/d_\lambda^2\right] \quad . \qquad \text{(II D1 b.2)}$$

The derivatives of *R* with respect to the *u*-parameter associated with the eliminated capture width can be written as

$$\frac{\partial \mathrm{Re}\left[R_{\mu\nu}\right]}{\partial\overline{\gamma}_{\lambda\gamma}} = \left[-4\,\gamma_{\lambda\mu}\gamma_{\lambda\nu}\overline{\gamma}_{\lambda\gamma}\right]\left[\left\{\left(E_\lambda - E\right)\overline{\gamma}_{\lambda\gamma}^2\right\}/d_\lambda^2\right] \qquad \text{(II D1 b.3)}$$

and

$$\frac{\partial \mathrm{Im}\left[R_{\mu\nu}\right]}{\partial\overline{\gamma}_{\lambda\gamma}} = \left[2\,\gamma_{\lambda\mu}\gamma_{\lambda\nu}\overline{\gamma}_{\lambda\gamma}\right]\left[\left\{\left(E_\lambda - E\right)^2 - \left(\overline{\gamma}_{\lambda\gamma}^2\right)^2\right\}/d_\lambda^2\right] \quad . \qquad \text{(II D1 b.4)}$$

The derivatives for the particle widths are

$$\frac{\partial \mathrm{Re}\left[R_{\mu\nu}\right]}{\partial\gamma_{\lambda\mu}} = \left[\gamma_{\lambda\nu}\left(1+\delta_{\mu\nu}\right)\right]\left[\left(E_\lambda - E\right)/d_\lambda\right] \qquad \text{(II D1 b.5)}$$

and

$$\frac{\partial \mathrm{Im}\left[R_{\mu\nu}\right]}{\partial\gamma_{\lambda\mu}} = \left[\gamma_{\lambda\nu}\left(1+\delta_{\mu\nu}\right)\right]\left[\overline{\gamma}_{\lambda\gamma}^2/d_\lambda\right] \quad . \qquad \text{(II D1 b.6)}$$

In the expressions above, the denominator term *d* is defined as

$$d_\lambda = \left(E_\lambda - E\right)^2 + \overline{\gamma}_{\lambda\gamma}^{\,4} \quad . \qquad \text{(II D1 b.7)}$$

In each of these equations, the first square bracket contains an energy-independent factor; in the code SAMMY, this factor (times 2) is evaluated outside the energy loop in subroutine BABB and is stored as BR($\mu\nu$,*i*) for the derivative of the real part of $R_{\mu\nu}$ with respect to the i^{th} parameter, and BI($\mu\nu$,*i*) for the derivative of the imaginary part of $R_{\mu\nu}$. The quantity in the second square bracket is energy dependent but channel independent. Therefore, it must be generated for each energy and is temporarily stored as UPR(*i*) and UPI(*i*) in subroutine ABPART.

One legacy from early versions of SAMMY should be explained in some detail.

To avoid problems arising from the computer's limited precision, and to minimize computing time, partial derivatives for non-*s*-wave ($l > 0$) resonances are truncated to zero far away from the resonance. The working definition of "far away" is 20 times the sum of the partial widths for that resonance, plus 3 times the sum of the Doppler- and resolution-broadening widths, that is, far beyond the region where a resonance should produce any noticeable effect. Specifically, the derivative of the cross section at energy E is set to zero for resonance level λ, if

$$\left|E - E_\lambda\right| > 20\left[\sum\nolimits_c \Gamma_{\lambda c} + \bar{\Gamma}_{\lambda\gamma}\right] + 3\left(D + r\right) \qquad \text{(II D1 b.8)}$$

for resonances with $l > 0$, where D represents the Doppler and r the resolution width. Moreover, the contribution to the imaginary part of R is set to zero whenever the distance from level λ is greater than 100 times that specified in Eq. (II D1 b.8). (The contribution to the *real* part of R is never assumed to be negligible.)

For s-wave resonances ($l = 0$), the user has the option of setting derivatives equal to zero beyond a certain distance, where the distance is twice that specified for non-*s*-waves. To invoke this option, include the command

```
USE S-WAVE CUTOFF
```

in the INPut file. CAUTION: Though the cross-section segment in SAMMY may run slightly faster with the cutoff option invoked, results will not be as accurate. Use of this option is not encouraged.

With the advent of modern computer systems, use of the non-*s*-wave cutoff feature is no longer a necessity. Furthermore, use of this cutoff may lead to problems; in particular, inaccuracies have been noted in the calculation of uncertainties on multigroup averages.

The command

```
USE NO CUTOFFS FOR Derivatives or cross sections
```

can be used to eliminate the non-*s*-wave cutoff. It is recommended that, prior to completion of an analysis, the SAMMY user compare results obtained with and without the cutoff, to determine whether results are sufficiently accurate with the cutoff invoked.

II.D.1.c. Derivatives with respect to channel radius

Derivatives with respect to channel radius *a* require modification of the procedure outlined in Section II.D.1.b, since phase shifts φ and penetrabilities *P* also depend on channel radius (sometimes called "matching radius"). All dependence on *a* is via ρ, where

$$\rho = k\,a \quad , \tag{II D1 c.1}$$

and momentum $\hbar k$ in the center-of-mass reference frame is described in Section II.C.2; *k* is the wave number in units of inverse length. The derivative of the cross section with respect to the radius can be written

$$\frac{\partial\sigma}{\partial a} = \frac{\partial\sigma}{\partial\rho}\frac{\partial\rho}{\partial a} = k\frac{\partial\sigma}{\partial\rho} \quad . \tag{II D1 c.2}$$

Our problem therefore reduces to finding $\partial\sigma/\partial\rho$.

The derivative of the cross section with respect to ρ may be formed from Eq. (II A.1):

$$\begin{aligned}\frac{\partial\sigma_{cc'}}{\partial\rho} &= \frac{\pi}{k_c^2}g_c\left[\left(\delta_{cc'}-U_{cc'}\right)\frac{\partial U^{*}_{cc'}}{\partial\rho} + \left(\delta_{cc'}-U^{J*}_{cc'}\right)\frac{\partial U_{cc'}}{\partial\rho}\right] \\ &= \frac{2\pi}{k_c^2}g_c\left[\delta_{cc'}\frac{\partial\,\mathrm{Re}\left(U_{cc'}\right)}{\partial\rho} - \mathrm{Re}\left(U^{J*}_{cc'}\frac{\partial U_{cc'}}{\partial\rho}\right)\right] \quad .\end{aligned} \tag{II D1 c.3}$$

From the definitions of Ω and φ, Eqs. (II A.4) and (II A.5), the partial of *U* with respect to ρ may be written as

$$\frac{\partial U_{cc'}}{\partial\rho} = -i\frac{\partial\varphi_c}{\partial\rho}U_{cc'} + \Omega_c\frac{\partial W_{cc'}}{\partial\rho}\Omega_{c'} - i\,U_{cc'}\frac{\partial\varphi_{c'}}{\partial\rho} \quad . \tag{II D1 c.4}$$

Equation (II D1 c.3) can therefore be written as

$$\begin{aligned}\frac{\partial\sigma_{cc'}}{\partial\rho} = \frac{2\pi}{k_c^2}g_c\Bigg\{&\delta_{cc'}\,\mathrm{Re}\left(-2i\frac{\partial\varphi_c}{\partial\rho}U_{cc}+\Omega_c^2\frac{\partial W_{cc}}{\partial\rho}\right) \\ &-\mathrm{Re}\left(U^{*}_{cc'}\left[-i\left(\frac{\partial\varphi_c}{\partial\rho}+\frac{\partial\varphi_{c'}}{\partial\rho}\right)U^{J}_{cc'}+\Omega_c\frac{W_{cc'}}{\partial\rho}\Omega_{c'}\right]\right)\Bigg\} \quad ,\end{aligned} \tag{II D1 c.5}$$

or

$$\frac{\partial \sigma_{cc'}}{\partial \rho} = \frac{2\pi}{k_c^2} g_c \left\{ \delta_{cc'} \mathrm{Re}\left(-2i \frac{\partial \varphi_c}{\partial \rho} U^J_{cc} + \Omega_c^2 \frac{\partial W_{cc}}{\partial \rho} \right) - \mathrm{Re}\left(\Omega_c^* W^*_{cc'} \Omega^*_{c'} \left[-i \left(\frac{\partial \varphi_c}{\partial \rho} + \frac{\partial \varphi_{c'}}{\partial \rho} \right) \Omega_c W_{cc'} \Omega_{c'} + \Omega_c \frac{W_{cc'}}{\partial \rho} \Omega_{c'} \right] \right) \right\} . \quad \text{(IID1c.6)}$$

Because $\Omega_c \, \Omega^*_c = 1$, this simplifies to the form

$$\frac{\partial \sigma_{cc'}}{\partial \rho} = \frac{2\pi}{k_c^2} g_c \ \mathrm{Re}\left\{ \delta_{cc'} \Omega_c^2 \left(-2i \frac{\partial \varphi_c}{\partial \rho} W_{cc} + \frac{\partial W_{cc}}{\partial \rho} \right) - \left(W^*_{cc'} \left[-i \left(\frac{\partial \varphi_c}{\partial \rho} + \frac{\partial \varphi_{c'}}{\partial \rho} \right) W_{cc'} + \frac{\partial W_{cc'}}{\partial \rho} \right] \right) \right\} . \quad \text{(II D1 c.7)}$$

Derivatives of hard-sphere phase shifts φ are formed by direct differentiation of the formulae in Table II A.1 for non-Coulomb and of the equations in Section II.C.4 for Coulomb.

The derivatives of *W* are found in similar fashion to the derivatives with respect to resonance parameters, beginning with Eq. (II D1 a.11):

$$\begin{aligned} \frac{\partial W_{cc'}}{\partial \rho} &= -2i \delta_{cc'} L_c^{-1} \frac{\partial P_c}{\partial \rho} + 2i \delta_{cc'} P_c L_c^{-2} \left(\frac{\partial S_c}{\partial \rho} + i \frac{\partial P_c}{\partial \rho} \right) \\ &+ 2i \frac{\partial P_c}{\partial \rho} \frac{1}{2\sqrt{P_c}} L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} L_{c'}^{-1} \sqrt{P_{c'}} \\ &+ 2i \sqrt{P_c} \left(-L_c^{-2} \right) \left(\frac{\partial S_c}{\partial \rho} + i \frac{\partial P_c}{\partial \rho} \right) \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} L_{c'}^{-1} \sqrt{P_{c'}} \\ &+ 2i \sqrt{P_c} L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} \left(\frac{\partial S_{c'}}{\partial \rho} + i \frac{\partial P_{c'}}{\partial \rho} \right) \left(L_{c'}^{-2} \right) \sqrt{P_{c'}} \\ &+ 2i \sqrt{P_c} L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} L_{c'}^{-1} \frac{\partial P_{c'}}{\partial \rho} \frac{1}{2\sqrt{P_{c'}}} \\ &+ 2i \sum_{c''} \sqrt{P_c} L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc''} L_{c''}^{-1} \left(\frac{\partial S_{c''}}{\partial \rho} + i \frac{\partial P_{c''}}{\partial \rho} \right) \\ &\qquad \times L_{c''}^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{c''c'} L_{c'}^{-1} \sqrt{P_{c'}} . \end{aligned} \quad \text{(II D1 c.8)}$$

This expression can be greatly simplified by setting

$$\vartheta_{cc'} = \sqrt{P_c}\, L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} L_{c'}^{-1} \sqrt{P_{c'}} - P_c L_c^{-1} \delta_{cc'} \quad , \qquad \text{(II D1 c.9)}$$

which gives

$$\begin{aligned} \frac{\partial W_{cc'}^{J}}{\partial \rho} \;=\; + \; i \, \frac{\partial P_c}{\partial \rho} \, \frac{1}{P_c} \vartheta_{cc'} \; + \; i \, \vartheta_{cc'} \, \frac{1}{P_{c'}} \, \frac{\partial P_{c'}}{\partial \rho} \\ + \; 2i \sum_{c''} \vartheta_{cc''} \, P_{c''}^{-1} \left(\frac{\partial S_{c''}}{\partial \rho} + i \frac{\partial P_{c''}}{\partial \rho} \right) \vartheta_{c''c'} \quad . \end{aligned} \qquad \text{(II D1 c.10)}$$

Derivatives of penetrabilities P_c and shift factors S_c are found by direct differentiation of the formulae in Table II A.1 for non-Coulomb and Section II.C.4 for Coulomb. Derivatives of the cross sections with respect to ρ are then found by substituting results from Eq. (II D1 c.10) into Eq. (II D1 c.7).

II.D.1.d. Derivatives of logarithmic external R-function

Derivatives of R^{ext} with respect to the u-parameters are found from Eqs. (II B1 d.1) and (II B1 d.2) to be of the form

$$\frac{\partial R_c^{ext}}{\partial E_c^{up}} = -\frac{s_{con,c} + s_{lin,c}\, E_c^{up}}{E_c^{up} - E} \quad , \tag{II D1 d.1}$$

$$\frac{\partial R_c^{ext}}{\partial E_c^{down}} = -\frac{s_{con,c} + s_{lin,c}\, E_c^{down}}{E - E_c^{down}} \quad , \tag{II D1 d.2}$$

$$\frac{\partial R_c^{ext}}{\partial \bar{R}_{con,c}} = 1 \quad , \tag{II D1 d.3}$$

$$\frac{\partial R_c^{ext}}{\partial \bar{R}_{lin,c}} = E \quad , \tag{II D1 d.4}$$

$$\frac{\partial R_c^{ext}}{\partial \bar{R}_{q,c}} = E^2 \quad , \tag{II D1 d.5}$$

$$\frac{\partial R_c^{ext}}{\partial \sqrt{s_{con,c}}} = -2\sqrt{s_{con,c}}\, \ln\left[\frac{E_c^{up} - E}{E - E_c^{down}}\right] \quad , \tag{II D1 d.6}$$

and

$$\frac{\partial R_c^{ext}}{\partial s_{lin,c}} = -\left(E_c^{up} - E_c^{down}\right) - E\, \ln\left[\frac{E_c^{up} - E}{E - E_c^{down}}\right] \quad . \tag{II D1 d.7}$$

II.D.1.e. Derivatives with respect to *p*-parameters

As described in Section II.B.1, internally SAMMY operates in terms of the *u*-parameters, these being the parameters whose values are to be fitted via Bayes' equations (see Section IV). The *u*-parameters are related, but not necessarily equal, to the parameters whose values are given in the INPut and/or PARameter files, which are denoted as *p*-parameter.

When only the SAMMY code is used for calculations, there is no confusion arising from switching between *u*- and *p*-parameters. The transformation from *u*- to *p*-parameters also poses no difficulties in communicating parameter *values* between SAMMY and other codes (e.g., via ENDF files). However, in communicating uncertainty, covariance, or sensitivity (partial derivative) information, care must be taken to ensure that transformations are properly made.

In particular, the transformations involving the resonance energy and the partial widths must be calculated carefully.* The *p*-parameter for a particle width Γ, for example, is related to the corresponding *u*-parameter γ via the transformation [see Eq. (II B1.7)]

$$u_{\Gamma_{\lambda c}} = \gamma_{\lambda c} = \pm \sqrt{\frac{\Gamma_{\lambda c}}{2P_l\left(\left|E_\lambda - \Xi_c\right|\right)}} \quad , \qquad \text{(II D1 e.1)}$$

where P in this equation is the penetrability (with the appropriate angular momentum l for this channel) evaluated at E_λ, the energy of the resonance.

From Eqs. (II A.8) and (II A.9), P has the form

$$P_l = P_l(\rho) \qquad \text{with} \qquad \rho = \beta\, a_c \sqrt{\left(\left|E_\lambda - \Xi\right|\right)} \quad , \qquad \text{(II D1 e.2)}$$

in which β is a mass factor given explicitly in Eq. (II A.9), a_c is the channel radius, and Ξ represents the threshold energy. The ± sign in Eq. (II D1 e.1) is as given in the PARameter file (Table VI B.2). E_λ is another *p*-parameter, for which the corresponding *u*-parameter is

$$u_{E_\lambda} = \begin{cases} \sqrt{E_\lambda} & \text{for } E_\lambda > 0 \\ -\sqrt{-E_\lambda} & \text{for } E_\lambda < 0 \quad , \end{cases} \qquad \text{(II D1 e.3)}$$

from Eq. (II B1.6).

In the following discussion, most subscripts are omitted, for simplicity's sake. Equations for negative-energy resonances are indicated within square brackets.

* In early versions of SAMMY, these transformations were done incorrectly. These mistakes have been corrected in release R7 of this manual and in sammy-7.0.0 and subsequent releases of the code.

Consider a function f of the two u-parameters γ and u (which we take to be the u-parameter associated with the resonance energy). This function might be the cross section, or some other function such as transmission or average cross section. The equations of transformation to the two p-parameters Γ and E_λ are given above. The derivatives of f with respect to the p-parameters are therefore

$$\frac{\partial f}{\partial \Gamma} = \frac{\partial \gamma}{\partial \Gamma}\frac{\partial f}{\partial \gamma} + \frac{\partial u}{\partial \Gamma}\frac{\partial f}{\partial u} \qquad \text{(II D1 e.4)}$$

and

$$\frac{\partial f}{\partial E_\lambda} = \frac{\partial \gamma}{\partial E_\lambda}\frac{\partial f}{\partial \gamma} + \frac{\partial u}{\partial E_\lambda}\frac{\partial f}{\partial u} \quad . \qquad \text{(II D1 e.5)}$$

The partial derivatives of the u-parameters with respect to the p-parameter Γ can readily be found from Eqs. (II D1 e.1) and (II D1 e.3) as

$$\frac{\partial \gamma}{\partial \Gamma} = \pm \frac{1}{\sqrt{2P}}\frac{1}{2}\Gamma^{-1/2} = \pm\frac{1}{2}\sqrt{\frac{\Gamma}{2P}}\frac{1}{\Gamma} = \frac{\gamma}{2\Gamma} \quad , \qquad \text{(II D1 e.6)}$$

and

$$\frac{\partial u}{\partial \Gamma} = 0 \quad . \qquad \text{(II D1 e.7)}$$

The derivative of u with respect to E_λ is relatively straight forward:

$$\frac{\partial u}{\partial E_\lambda} = \frac{1}{2}E_\lambda^{-1/2} = \frac{1}{2u} = \frac{u}{2E_\lambda}$$
$$\left[\frac{\partial u}{\partial E_\lambda} = \frac{1}{2}\left(-E_\lambda\right)^{-1/2} = -\frac{1}{2u} = \frac{u}{2E_\lambda} \text{ if } E_\lambda < 0\right]. \qquad \text{(II D1 e.8)}$$

The derivative of γ with respect to E_λ is somewhat more complicated, having the form

$$\frac{\partial \gamma}{\partial E_\lambda} = \pm\sqrt{\frac{\Gamma}{2}}\left(-\frac{1}{2}\right)P^{-3/2}\frac{dP}{d\rho}\frac{\partial \rho}{\partial E_\lambda} = \mp\frac{1}{2}\sqrt{\frac{\Gamma}{2P}}\frac{P'}{P}\frac{\partial \rho}{\partial E_\lambda} = -\frac{\gamma P'}{2P}\frac{\partial \rho}{\partial E_\lambda} \quad , \text{(II D1 e.9)}$$

in which we have defined P' to be $dP/d\rho$. From Eq. (II D1 e.2), for $E_\lambda > \Xi$, it follows that

$$\frac{\partial \gamma}{\partial E_\lambda} = -\frac{\gamma P'}{2P}\frac{\beta a}{2\sqrt{\left(E_\lambda - \Xi\right)}} = -\frac{\gamma P'}{4P}\frac{\rho}{\left(E_\lambda - \Xi\right)} \quad . \qquad \text{(II D1 e.10)}$$

Similarly, for $E_\lambda < \Xi$, we find

$$\frac{\partial\gamma}{\partial E_\lambda} = -\frac{\gamma P'}{2P}\frac{\partial}{\partial E_\lambda}\beta a\sqrt{-(E_\lambda-\Xi)} = -\frac{\gamma P'}{2P}\frac{\beta a(-1)}{2\sqrt{-(E_\lambda-\Xi)}}$$
$$= +\frac{\gamma P'}{4P}\frac{\beta a\sqrt{-(E_\lambda-\Xi)}}{-(E_\lambda-\Xi)} = -\frac{\gamma P'}{4P}\frac{\rho}{(E_\lambda-\Xi)} \quad . \qquad \text{(II D1 e.11)}$$

Equations (II D1 e.4) and (II D1 e.5) can therefore be rewritten as

$$\frac{\partial f}{\partial\Gamma} = \frac{\gamma}{2\Gamma}\frac{\partial f}{\partial\gamma} + 0 \qquad \text{(II D1 e.12)}$$

and

$$\frac{\partial f}{\partial E_\lambda} = -\frac{\gamma P'}{4P}\frac{\rho}{(E_\lambda-\Xi)}\frac{\partial f}{\partial\gamma} + \frac{u}{2E_\lambda}\frac{\partial f}{\partial u} \quad . \qquad \text{(II D1 e.13)}$$

Similarly, if the function *f* is defined in terms of *p*-parameters, the derivatives of *f* with respect to the *u*-parameters are given by

$$\frac{\partial f}{\partial\gamma} = \frac{\partial\Gamma}{\partial\gamma}\frac{\partial f}{\partial\Gamma} + \frac{\partial E_\lambda}{\partial\gamma}\frac{\partial f}{\partial E_\lambda} \qquad \text{(II D1 e.14)}$$

and

$$\frac{\partial f}{\partial u} = \frac{\partial\Gamma}{\partial u}\frac{\partial f}{\partial\Gamma} + \frac{\partial E_\lambda}{\partial u}\frac{\partial f}{\partial E_\lambda} \quad . \qquad \text{(II D1 e.15)}$$

That is, the inverse transformation (from *p*-space to *u*-space) requires the use of the partial derivatives of *p*-parameters with respect to the *u*-parameters. These derivatives have the form

$$\frac{\partial\Gamma}{\partial\gamma} = \pm 2P\ 2\gamma = \pm 4P\gamma = \frac{2\Gamma}{\gamma} \quad , \qquad \text{(II D1 e.16)}$$

$$\frac{\partial E_\lambda}{\partial\gamma} = 0 \quad , \qquad \text{(II D1 e.17)}$$

and

$$\frac{\partial E_\lambda}{\partial u} = 2u = \frac{2E_\lambda}{u} \qquad \left[\frac{\partial E_\lambda}{\partial u} = -2u = \frac{2E_\lambda}{u} \text{ if } E_\lambda < 0\right] . \qquad \text{(II D1 e.18)}$$

The partial derivative of Γ with respect to u requires special care to evaluate correctly. For $u^2 = E_\lambda > \Xi$, this derivative has the form

$$\begin{aligned}\frac{\partial\Gamma}{\partial u} &= 2\frac{\partial P}{\partial u}\gamma^2 = \frac{2P\gamma^2}{P}\frac{dP}{d\rho}\frac{\partial\rho}{\partial u} = \Gamma\frac{P'}{P}\frac{\partial}{\partial u}\left(\beta a\sqrt{\left(u^2-\Xi\right)}\right) \\ &= \Gamma\frac{P'}{P}\frac{\beta a 2u}{2\sqrt{\left(u^2-\Xi\right)}} = \Gamma\frac{P'}{P}\frac{\beta a\sqrt{\left(u^2-\Xi\right)}\,u}{\left(E_\lambda-\Xi\right)} = \Gamma\frac{P'}{P}\frac{\rho}{\left(E_\lambda-\Xi\right)}\frac{E_\lambda}{u}\ .\end{aligned} \tag{II D1 e.19}$$

If $0 < E_\lambda = u^2 < \Xi$, this partial derivative takes the form

$$\begin{aligned}\frac{\partial\Gamma}{\partial u} &= 2\frac{\partial P}{\partial u}\gamma^2 = \frac{2P\gamma^2}{P}\frac{dP}{d\rho}\frac{\partial\rho}{\partial u} = \Gamma\frac{P'}{P}\frac{\partial}{\partial u}\left(\beta a\sqrt{-\left(u^2-\Xi\right)}\right) \\ &= \Gamma\frac{P'}{P}\frac{\beta a(-2u)}{2\sqrt{-\left(u^2-\Xi\right)}} = \Gamma\frac{P'}{P}\frac{\beta a\sqrt{-\left(u^2-\Xi\right)}\,(-u)}{-\left(u^2-\Xi\right)} \\ &= \Gamma\frac{P'}{P}\frac{\rho}{\left(E_\lambda-\Xi\right)}\frac{E_\lambda}{u}\ .\end{aligned} \tag{II D1 e.20}$$

[Finally, if $0 > E_\lambda = -u^2$, then

$$\begin{aligned}\frac{\partial\Gamma}{\partial u} &= 2\frac{\partial P}{\partial u}\gamma^2 = \frac{2P\gamma^2}{P}\frac{dP}{d\rho}\frac{\partial\rho}{\partial u} = \Gamma\frac{P'}{P}\frac{\partial}{\partial u}\left(\beta a\sqrt{-\left(-u^2-\Xi\right)}\right) \\ &= \Gamma\frac{P'}{P}\frac{\beta a(2u)}{2\sqrt{\left(u^2+\Xi\right)}} = \Gamma\frac{P'}{P}\frac{\beta a\,u\sqrt{\left(u^2+\Xi\right)}}{(-)\left(-u^2-\Xi\right)} \\ &= \Gamma\frac{P'}{P}\frac{\rho}{\left(E_\lambda-\Xi\right)}\frac{E_\lambda}{u}\ ,\end{aligned} \tag{II D1 e.21}$$

in a form which is compatible with the other versions.]

Substituting Eqs. (II D1 e.16) through (II D1 e.19) into Eqs. (II D1 e.14) and (II D1 e.15) gives

$$\frac{\partial f}{\partial\gamma} = \frac{2\Gamma}{\gamma}\frac{\partial f}{\partial\Gamma} + 0 \tag{II D1 e.22}$$

and

$$\frac{\partial f}{\partial u} = \Gamma\frac{P'}{P}\frac{\rho}{\left(E_\lambda-\Xi\right)}\frac{E_\lambda}{u}\frac{\partial f}{\partial\Gamma} + \frac{2E_\lambda}{u}\frac{\partial f}{\partial E_\lambda}\ . \tag{II D1 e.23}$$

Using the formulae in Eqs. (II D1 e.22) and (II D1 e.23), it is possible to demonstrate that the second transformation is the inverse of the first. That is, if one substitutes the expressions for $\partial f / \partial \Gamma$ and $\partial f / \partial E_\lambda$ from Eqs. (II D1 e.22) and (II D1 e.23) into Eqs. (II D1 e.12) and (II D1 e.13), or vice-versa, the resulting equations are identities.

Consider, now, the definition of the covariance matrix associated with a particular set of values. The covariance matrix associated with the *u*-parameters is denoted (as in Section IV) as matrix *M*, where

$$M_{ij} = \left\langle \delta u_i \, \delta u_j \right\rangle \quad , \qquad \text{(II D1 e.24)}$$

in which δu_i represents a small increment in the value of parameter u_i , and the angle brackets represent the "expectation value." Diagonal elements of this matrix are the square of the uncertainties on the parameter values; off-diagonal elements describe the connectedness between different parameters.

To communicate SAMMY results to ENDF files, it is necessary to generate the covariance matrix associated with the *p*-parameters (here this matrix is denoted by *Q*). This matrix is generated by making use of the relationship between a small increment in a *p*-parameter and a small increment in each of the *u*-parameters:

$$\delta p_k = \sum_i \frac{\partial p_k}{\partial u_i} \delta u_i \quad , \qquad \text{(II D1 e.25)}$$

so that Q becomes

$$Q_{kl} = \left\langle \delta p_k \, \delta p_l \right\rangle = \sum_{i,j} \frac{\partial p_k}{\partial u_i} \left\langle \delta u_i \, \delta u_j \right\rangle \frac{\partial p_l}{\partial u_j} \quad . \qquad \text{(II D1 e.26)}$$

The expansion of this covariance matrix for the two-parameter example discussed above will not be given here, but is proposed as an exercise for the student.

Reminder: It is the *p*-parameters (not the *u*-parameters) that are listed in the SAMMY PARameter files (input and output) and in the SAMMY output file (SAMMY.LPT). Likewise, it is the *p*-parameters* which are listed in ENDF File 2.** Therefore, the covariance matrix elements given in ENDF File 32 must correspond to the *Q* matrix defined above; that is, the covariance matrix listed in ENDF File 32 must be the appropriate covariance matrix for the resonance parameters.

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* For the LRF=7 format, an option exists to list the reduced width amplitudes γ rather than the partial widths Γ. In this case, no transformation from *u*- to *p*-parameter space is necessary for the partial widths, but only for the resonance energies.

** Caveat: When a reduced-width amplitude is negative, it is not Γ but $G = -\Gamma$ that is listed in the ENDF file. ENDF covariance matrices are expressed in terms of *G*, not Γ.

When the cross section is calculated as a function of the *u*-parameters, a small increment in the calculated cross section is given by

$$\delta\sigma = \sum_n \frac{\partial\sigma}{\partial u_n}\delta u_n \quad . \tag{II D1 e.27}$$

Therefore the covariance matrix $\boldsymbol{C_{ij}}$ for the cross section is found from

$$C_{ij} = \left\langle \delta\sigma_i \, \delta\sigma_j \right\rangle = \left\langle \sum_n \left(\frac{\partial\sigma_i}{\partial u_n}\delta u_n \right) \sum_m \left(\frac{\partial\sigma_j}{\partial u_m}\delta u_m \right) \right\rangle$$

$$= \sum_{n,m} \frac{\partial\sigma_i}{\partial u_n} \left\langle \delta u_n \, \delta u_m \right\rangle \frac{\partial\sigma_j}{\partial u_m} \tag{II D1 e.28}$$

$$= \sum_{n,m} \frac{\partial\sigma_i}{\partial u_n} M_{nm} \frac{\partial\sigma_j}{\partial u_m} \quad ,$$

in which *M* is again defined as the covariance matrix for the *u*-parameters. In order to print the covariance matrix resonance parameters for the *p*-parameters into the ENDF formats, it is necessary to transform the parameter covariance matrix from *M* to *Q*. That transformation is made by inserting the formulae

$$\frac{\partial\sigma_i}{\partial u_n} = \sum_k \frac{\partial p_k}{\partial u_n} \frac{\partial\sigma_i}{\partial p_k} \tag{II D1 e.29}$$

and

$$\frac{\partial\sigma_j}{\partial u_m} = \sum_l \frac{\partial p_l}{\partial u_m} \frac{\partial\sigma_j}{\partial p_l} \tag{II D1 e.30}$$

into the previous expression, Eq. (II D1 e.28), yielding

$$C_{ij} = \sum_{n,m,k,l} \frac{\partial\sigma_i}{\partial p_k} \frac{\partial p_k}{\partial u_n} M_{nm} \frac{\partial p_l}{\partial u_m} \frac{\partial\sigma_j}{\partial p_l} \tag{II D1 e.31}$$

or

$$C_{ij} = \sum_{k,l} \frac{\partial\sigma_i}{\partial p_k} Q_{kl} \frac{\partial\sigma_j}{\partial p_l} \quad , \tag{II D1 e.32}$$

where *Q* is given by

$$Q_{kl} = \sum_{n,m} \frac{\partial p_k}{\partial u_n} M_{nm} \frac{\partial p_l}{\partial u_m} \quad . \tag{II D1 e.33}$$

For the case in which only one elastic width contains an energy-dependent penetrability, the *p*-parameter covariance matrix must be modified for all elements involving a width having energy-dependent penetrability.

II.D.2. Derivatives for MLBW and SLBW Approximations

From the form of the cross sections in Eqs. (II B3 a.1), (II B3 a.5), and (II B3 a.6), we note that there are only four expressions in which the resonance energies or widths occur. These expressions are denoted as follows:

$$A_{1c\lambda} = \Gamma_{\lambda c}\left(E - E_\lambda\right)/d_\lambda \quad , \tag{II D2.1}$$

$$A_{2c\lambda} = \Gamma_{\lambda c}\bar{\Gamma}_{\lambda\gamma}/d_\lambda \quad , \tag{II D2.2}$$

$$A_{3cc'\lambda} = \Gamma_{\lambda c}\Gamma_{\lambda c'}/d_\lambda \quad , \tag{II D2.3}$$

and

$$A_{4c\lambda} = \Gamma_{\lambda c}\Gamma_\lambda/d_\lambda \quad , \tag{II D2.4}$$

where d is given by Eq. (II B3 a.4) as

$$d_\lambda = \left(E - E_\lambda\right)^2 + \left(\Gamma_\lambda/2\right)^2 \quad . \tag{II D2.5}$$

Equation (II D2.4) is actually redundant, since

$$A_{4c\lambda} = \sum_{c'} A_{3cc'\lambda} + A_{2c\lambda} \quad . \tag{II D2.6}$$

As discussed in Section II.D, the assumption in the SAMMY code is that the u-parameters are independent and the p-parameters are derived quantities. Thus we need only evaluate partial derivatives of $A_{1c\lambda}$, $A_{2c\lambda}$, and $A_{3c\lambda}$ with respect to the u-parameters (i.e., with respect to the partial-width amplitudes and to the square root of the resonance energy). These derivatives may be written as follows:

$$\frac{\partial A_{1c\lambda}}{\partial\sqrt{E_\lambda}} = 2\sqrt{E_\lambda}\Gamma_{\lambda c}\left\{-1 + 2\left(E - E_\lambda\right)^2/d_\lambda\right\}/d_\lambda \quad , \tag{II D2.7}$$

$$\frac{\partial A_{2c\lambda}}{\partial\sqrt{E_\lambda}} = 4\sqrt{E_\lambda}\Gamma_{\lambda c}\bar{\Gamma}_{\lambda\gamma}\left(E - E_\lambda\right)/d_\lambda^2 \quad , \tag{II D2.8}$$

$$\frac{\partial A_{3cc'\lambda}}{\partial\sqrt{E_\lambda}} = 4\sqrt{E_\lambda}\,\Gamma_{\lambda c}\Gamma_{\lambda c'}\left(E - E_\lambda\right)/d_\lambda^2 \quad , \tag{II D2.9}$$

$$\frac{\partial A_{1c\lambda}}{\partial \overline{\gamma}_{\lambda\gamma}} = -2\overline{\gamma}_{\lambda\gamma}\Gamma_{\lambda c}\left(E - E_\lambda\right)\Gamma_\lambda / d_\lambda^2 \quad , \tag{II D2.10}$$

$$\frac{\partial A_{2c\lambda}}{\partial \overline{\gamma}_{\lambda\gamma}} = 2\,\overline{\gamma}_{\lambda\gamma}\,\Gamma_{\lambda c}\left\{\,2 - \overline{\Gamma}_{\lambda\gamma}\,\Gamma_\lambda / d_\lambda\right\} / d_\lambda \quad , \tag{II D2.11}$$

$$\frac{\partial A_{3cc'\lambda}}{\partial \overline{\gamma}_{\lambda\gamma}} = -2\,\overline{\gamma}_{\lambda\gamma}\,\Gamma_{\lambda c}\,\Gamma_{\lambda c'}\,\Gamma_\lambda / d_\lambda^2 \quad , \tag{II D2.12}$$

$$\frac{\partial A_{1c\lambda}}{\partial \gamma_{\lambda c''}} = 2\Gamma_{\lambda c}\left(E - E_\lambda\right)\left\{\delta_{cc''} - \Gamma_{\lambda c}\,\Gamma_{\lambda c''} / \left(2d_\lambda\right)\right\} / \left\{\gamma_{\lambda c''}\,d_\lambda\right\} \quad , \tag{II D2.13}$$

$$\frac{\partial A_{2c\lambda}}{\partial \gamma_{\lambda c''}} = 2\Gamma_{\lambda c}\,\overline{\Gamma}_{\lambda\gamma}\left\{\,\delta_{cc''} - \Gamma_{\lambda c}\,\Gamma_{\lambda c''} / \left(2d_\lambda\right)\right\} / \left\{\gamma_{\lambda c''}\,d_\lambda\right\} \quad , \tag{II D2.14}$$

and

$$\frac{\partial A_{3cc''\lambda}}{\partial \gamma_{\lambda c''}} = 2\Gamma_{\lambda c}\,\Gamma_{\lambda c'}\left\{\delta_{cc''} + \delta_{c'c''} - \Gamma_\lambda\,\Gamma_{\lambda c''} / \left(2d_\lambda\right)\right\} / \left\{\gamma_{\lambda c''}\,d_\lambda\right\} \quad , \tag{II D2.15}$$

All other derivatives are zero.

II.D.3. Details Involving Derivatives

In this section are presented some of the algebraic details relating to the partial derivatives. We first consider the derivative of one complex variable with respect to another, and then the derivative of the inverse of a matrix quantity. Both are needed in Section II.D.1.a.

Derivative of one complex variable with respect to another

Given any two complex variables $A = A^r + iA^i$ and $B = B^r + iB^i$, where A is an analytical function of B, the derivative of the components of A with respect to the components of B may be expressed as follows:

$$\frac{\partial A^r}{\partial B^r} = \mathrm{Re}\frac{\partial A}{\partial B^r} = \mathrm{Re}\frac{\partial A}{\partial B}\frac{\partial B}{\partial B^r} = \mathrm{Re}\frac{\partial A}{\partial B} \quad , \tag{II D3.1}$$

$$\frac{\partial A^r}{\partial B^i} = \mathrm{Re}\frac{\partial A}{\partial B^i} = \mathrm{Re}\frac{\partial A}{\partial B}\frac{\partial B}{\partial B^i} = \mathrm{Re}\frac{\partial A}{\partial B}(i) = -\mathrm{Im}\frac{\partial A}{\partial B} \quad , \tag{II D3.2}$$

$$\frac{\partial A^i}{\partial B^r} = \mathrm{Im}\frac{\partial A}{\partial B^r} = \mathrm{Im}\frac{\partial A}{\partial B}\frac{\partial B}{\partial B^r} = \mathrm{Im}\frac{\partial A}{\partial B} \quad , \tag{II D3.3}$$

and

$$\frac{\partial A^i}{\partial B^i} = \mathrm{Im}\frac{\partial A}{\partial B^i} = \mathrm{Im}\frac{\partial A}{\partial B}\frac{\partial B}{\partial B^i} = \mathrm{Im}\frac{\partial A}{\partial B}(i) = \mathrm{Re}\frac{\partial A}{\partial B} \quad . \tag{II D3.4}$$

Also, the usual chain rule applies:

$$\begin{aligned}\frac{\partial A^r}{\partial C^r} &= \frac{\partial A^r}{\partial B^r}\frac{\partial B^r}{\partial C^r} + \frac{\partial A^r}{\partial B^i}\frac{\partial B^i}{\partial C^r} \\ &= \left[\mathrm{Re}\left(\frac{\partial A}{\partial B}\right)\right]\left[\mathrm{Re}\left(\frac{\partial B}{\partial C}\right)\right] + \left[-\mathrm{Im}\left(\frac{\partial A}{\partial B}\right)\right]\left[\mathrm{Im}\left(\frac{\partial B}{\partial C}\right)\right] = \mathrm{Re}\left[\frac{\partial A}{\partial B}\frac{\partial B}{\partial C}\right] \quad ,\end{aligned} \tag{II D3.5}$$

$$\begin{aligned}\frac{\partial A^r}{\partial C^i} &= \frac{\partial A^r}{\partial B^r}\frac{\partial B^r}{\partial C^i} + \frac{\partial A^r}{\partial B^i}\frac{\partial B^i}{\partial C^i} \\ &= \left[\mathrm{Re}\left(\frac{\partial A}{\partial B}\right)\right]\left[-\mathrm{Im}\left(\frac{\partial B}{\partial C}\right)\right] + \left[-\mathrm{Im}\left(\frac{\partial A}{\partial B}\right)\right]\left[\mathrm{Re}\left(\frac{\partial B}{\partial C}\right)\right] = -\mathrm{Im}\left[\frac{\partial A}{\partial B}\frac{\partial B}{\partial C}\right] \quad ,\end{aligned} \tag{II D3.6}$$

$$\frac{\partial A^i}{\partial C^r} = \frac{\partial A^i}{\partial B^r}\frac{\partial B^r}{\partial C^r} + \frac{\partial A^i}{\partial B^i}\frac{\partial B^i}{\partial C^r}$$
$$= \left[\mathrm{Im}\left(\frac{\partial A}{\partial B}\right)\right]\left[\mathrm{Re}\left(\frac{\partial B}{\partial C}\right)\right] + \left[\mathrm{Re}\left(\frac{\partial A}{\partial B}\right)\right]\left[\mathrm{Im}\left(\frac{\partial B}{\partial C}\right)\right] = \mathrm{Im}\left[\frac{\partial A}{\partial B}\frac{\partial B}{\partial C}\right] \quad , \tag{II D3.7}$$

and

$$\frac{\partial A^i}{\partial C^i} = \frac{\partial A^i}{\partial B^r}\frac{\partial B^r}{\partial C^i} + \frac{\partial A^i}{\partial B^i}\frac{\partial B^i}{\partial C^i}$$
$$= \left[\mathrm{Im}\left(\frac{\partial A}{\partial B}\right)\right]\left[-\mathrm{Im}\left(\frac{\partial B}{\partial C}\right)\right] + \left[\mathrm{Re}\left(\frac{\partial A}{\partial B}\right)\right]\left[\mathrm{Re}\left(\frac{\partial B}{\partial C}\right)\right] = \mathrm{Re}\left[\frac{\partial A}{\partial B}\frac{\partial B}{\partial C}\right] \quad . \tag{II D3.8}$$

Derivative of the inverse of a matrix

In Eq. (II D1 a.13), the quantity *Y* is defined as

$$Y_{ef} = \left[\left(L^{-1} - R\right)^{-1}\right]_{ef} \quad . \tag{II D3.9}$$

To find the derivative of *Y* with respect to *R*, we first note that

$$\sum_a Y_{ea} Y_{ab}^{-1} = \delta_{eb} \quad , \tag{II D3.10}$$

so that the derivative is zero; that is,

$$0 = \frac{\partial}{\partial R_{cd}}\left[\sum_a Y_{ea} Y_{ab}^{-1}\right] = \sum_a \frac{\partial Y_{ea}}{\partial R_{cd}} Y_{ab}^{-1} + \sum_a Y_{ea}\frac{\partial Y_{ab}^{-1}}{\partial R_{cd}}$$
$$= \sum_a \frac{\partial Y_{ea}}{\partial R_{cd}} Y_{ab}^{-1} + \sum_a Y_{ea}\left\{-\delta_{ac}\delta_{bd} - \delta_{ad}\delta_{bc}\left(1-\delta_{cd}\right)\right\} \quad . \tag{II D3.11}$$

The quantity in curly brackets comes from the symmetry of the R-matrix and from the stipulation that only unique matrix elements are to be considered [$c \le d$, $e \le f$ in Eq. (II D1.1) and Eq. (II D1 a.1)]. Multiplying both terms by Y_{bf}, summing over *b*, and rearranging give

$$\sum_a \frac{\partial Y_{ea}}{\partial R_{cd}} \sum_b Y_{ab}^{-1} Y_{bf} \;=\; \sum_{a,b} Y_{ea} \left\{ \delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc}\left(1-\delta_{cd}\right) \right\} Y_{bf} \quad ,$$

$$\sum_a \frac{\partial Y_{ea}}{\partial R_{cd}} \delta_{af} = Y_{ec} Y_{df} + Y_{ed} Y_{cf} \left(1-\delta_{cd}\right) \quad , \qquad \text{(II D3.12)}$$

or, finally,

$$\frac{\partial Y_{ef}}{\partial R_{cd}} = Y_{ec} Y_{df} + Y_{ed} Y_{cf} \left(1-\delta_{cd}\right) \quad . \qquad \text{(II D3.13)}$$

This is the derivative used in Eq. (II D1 a.14).