

Abstract

In 1980 the multilevel multichannel R-matrix code SAMMY was released for use in analysis of neutron-induced cross section data at the Oak Ridge Electron Linear Accelerator. Since that time, SAMMY has evolved to the point where it is now in use around the world for analysis of many different types of data. SAMMY is not limited to incident neutrons but can also be used for incident protons, alpha particles, or other charged particles; likewise, Coulomb exit channels can be included. Corrections for a wide variety of experimental conditions are available in the code: Doppler and resolution broadening, multiple-scattering corrections for capture or reaction yields, normalizations and backgrounds, to name but a few. The fitting procedure is Bayes' method, and data and parameter covariance matrices are properly treated within the code. Pre- and post-processing capabilities are also available, including (but not limited to) connections with the Evaluated Nuclear Data Files. Though originally designed for use in the resolved resonance region, SAMMY also includes a treatment for data analysis in the unresolved resonance region.

This document serves as a users' guide for SAMMY and many of its auxiliary codes.

Citations:

Citations for use of the SAMMY code should refer to this manual as

N. M. Larson, Updated Users' Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations, ORNL/TM-9179/R8, Oak Ridge National Laboratory, Oak Ridge, TN, USA (2008). Also ENDF-364/R2. The manual is available on the SAMMY web site at <https://info.ornl.gov/sites/publications/files/Pub13056.pdf>

CHAPTER 1

Introduction

This document serves as a users' guide to the multilevel multichannel R-matrix code SAMMY. Beginning with Revision 6, the organization of this manual has been redesigned in an effort to make it more legible, logical, and useful. A summary of the structure of this document is given here.

Introductions for the original version of this manual through the previous revision are available in Appendix A. An introduction specifically for the current revision, describing recent modifications and additions to the code and the manual, is found immediately following this general introduction. All SAMMY users are encouraged to read §I.A for an overview of recent developments.

Analysis of neutron cross-section data in the resolved resonance region (RRR) has three distinct aspects, each of which must be included in any analysis code: First, an appropriate formalism is needed for generating theoretical cross sections. Second, a plausible mathematical description must be provided for every experimental condition that affects the values of the quantities being measured. Third, a fitting procedure must be available to determine the parameter values which provide the “best” fit of theoretical to experimental numbers. These three aspects of the SAMMY code are described in §II (2), III (3), and IV (4) of this manual, respectively.

Calculation of the cross sections in the RRR is described in §II (2), with emphasis on the Reich-Moore approximation to R-matrix theory. Explicit equations are given for the various types of energy-differential cross sections (total, elastic, capture, fission, other reaction) and for the angle and energy-differential cross sections (elastic, reaction). Both Coulomb and non-Coulomb (neutron) formulae are shown.

Experimental modifications to the theoretical cross sections in the RRR are described in §III(3). Included here are such effects as Doppler and resolution broadening, normalization and backgrounds, finite-size corrections, and treatment of more than one nuclide in the target sample. SAMMY's fitting procedure is described in §IV(4). Bayes' equations are derived from Bayes' theorem plus assumptions about normality and linearity. The relationship between Bayes' equations and the more familiar least-squares equations is described.

Emphasis is placed on methodologies for properly including all measurement uncertainty in the analysis process, including the many SAMMY options for inclusion of data covariance information.

§V(5) describes such topics as post-processor options (calculating multigroup cross sections or other averages) and other miscellaneous features.

The input to SAMMY is detailed in §VI(6). Output is described in §VII(7).

SAMMY's treatment of the unresolved resonance region (URR) is discussed in §VIII(8).

The theoretical treatment was borrowed directly from Fritz Fröhner's FITACS program; subsequently, input/output and certain details of the calculation have been augmented to increase the functionality of this code.

§IX(9) describes the relationship of SAMMY to the Evaluated Nuclear Data Files (ENDF). Certain types of ENDF files can be used to provide resonance parameters, parameter covariance matrices, or experimental data as input to SAMMY. Likewise, SAMMY can produce ENDF files containing resonance parameters, point-wise cross sections, or uncertainty information.

A number of auxiliary programs are available for use with SAMMY input or output. §X(10) contains a brief description of those for which the SAMMY author has maintenance responsibility.

Advice for running SAMMY is presented in §XI(11). Even experienced SAMMY users are encouraged to read this section, as it contains information about recent developments that may be unfamiliar (but potentially useful) to long-time users. Novices are likely to find valuable suggestions in this section. Anyone requesting the author's help is expected to have read and followed the procedures outlined in §XI.B(11.2).

Sample runs are described in §XII(12). These include (1) tutorial exercises (designed to familiarize a novice user with running the code), (2) test cases (designed for quality control, to ensure that the code gives consistent answers from one platform to another and from one version to another, but also useful as examples of input for specific features of the code), and (3) simulations (Monte Carlo simulations of multiple-scattering corrections, designed to test the accuracy of the SAMMY treatment for those corrections).

§XIII(13) provides an introduction to the computer code itself, for the benefit of the code managers at various sites. The casual user will probably not need the information from this section.

CHAPTER 2

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][1]. 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][2] provides a more elementary introduction to the subject. One publication by Fröhner [FF80][3] 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][4] 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 assumptions¹:

- (1) the applicability of non-relativistic quantum mechanics;

¹In 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.

(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.

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 Fig. 2.1. 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 2.1, general equations of scattering theory are presented and their derivations discussed. The fundamental R-matrix equations are presented. Section II.A.12.1.1 gives a detailed derivation of the equations for a simple case. Section II.A.22.1.2 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.B2.2. The recommended choice for most applications is the Reich-Moore approximation, described in Section II.B.12.2.1. 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.22.2.2. Two historically useful but now obsolete approximations are single-level and multilevel Breit Wigner (SLBW and MLBW), discussed in Section II.B.32.2.3. Provisions for including non-compound (direct) effects are discussed in Section II.B.42.2.4.

In Section II.C2.3, 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.

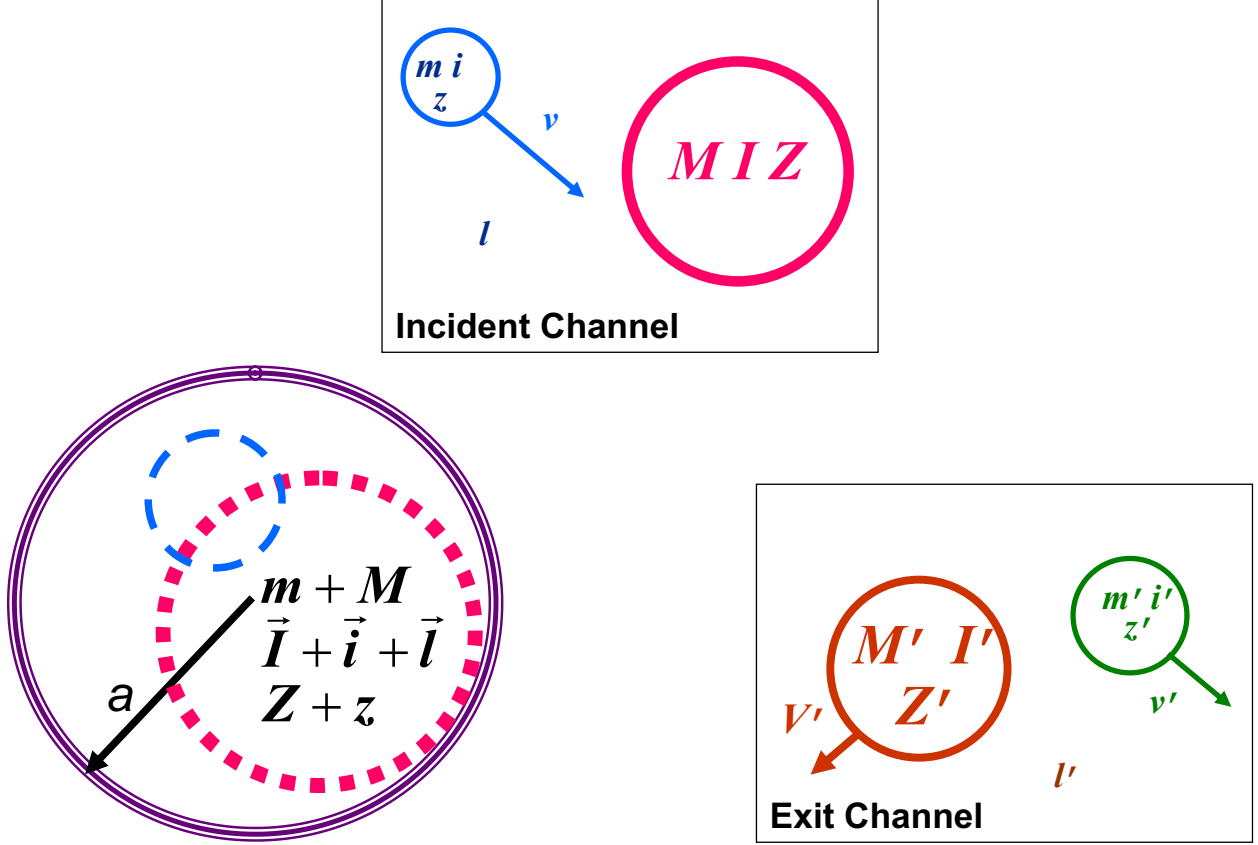


Figure 2.1: Schematic of entrance and exit channels as used in scattering theory. For the interior region (with separation distance $r < a$), no assumptions are made about the nature of the interaction. In the figure, m , i , and z refer to the mass, spin, and charge of the incident particle while M , 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.

2.1 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.12.1.1, 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 [1] for a detailed derivation in the general case, or to Section II.A.22.1.2 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

$$\sigma_{cc'} = \frac{\pi}{k_\alpha^2} g_{J\alpha} \left| e^{2iw_c} \delta_{cc'} - U_{cc'} \right|^2 \delta_{JJ'} , \quad (2.1)$$

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.4.2.3.4) The spin statistical factor $g_{J\alpha}$ is given by

$$g_{J\alpha} = \frac{2J+1}{(2i+1)(2I+1)} , \quad (2.2)$$

and center-of-mass momentum K_α by

$$K_\alpha^2 = (\hbar k_\alpha)^2 = \frac{2mM^2}{(m+M)^2} E. \quad (2.3)$$

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.22.3.2.

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

$$U_{cc'} = \Omega_c W_{cc'} \Omega_{c'}, \quad (2.4)$$

where Ω is given by

$$\Omega_c = e^{i(w_c - \phi_c)}. \quad (2.5)$$

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., [1]) and shown in Table 2.1. The matrix W in Eq. 2.4 is related to the R-matrix (in matrix notation with indices suppressed) via

$$W = P^{1/2} (I - RL)^{-1} (I - RL^*) P^{-1/2}. \quad (2.6)$$

The quantity I in this equation represents the identity matrix, and superscript $*$ indicates a complex conjugate. The form of the R-matrix is given in Section II.A.12.1.1 in general Section II.B2.2 for the versions used in SAMMY. The quantity L in Eq. 2.6 is given by

$$L = (S - B) + iP, \quad (2.7)$$

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 [5]).

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

$$P \rightarrow P_l(\rho) \quad \text{and} \quad S \rightarrow S_l(\rho), \quad (2.8)$$

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 a particle pair α , orbital angular momentum l , and channel radius a_c , ρ has the form

$$\rho = k_\alpha a_c = \frac{1}{\hbar} \sqrt{\frac{2m_\alpha M_\alpha}{m_\alpha + M_\alpha} \frac{M}{m + M}} \sqrt{(E - \Xi_\alpha)} a_c, \quad (2.9)$$

as shown in Section II.C.2 2.3.2. Here Ξ_α is the energy threshold for the 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 formulae² for P , S , and ϕ in the non-Coulomb case are shown in Table II.A.1 2.1. For two charged particles, formulae for the penetrabilities are given in Section II.C.4 2.3.4. 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 2.1: 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	$\rho^7/(225 + 45\rho^2 + 6\rho^4 + \rho^6)$	$-(675 + 90\rho^2 + 6\rho^4)/(225 + 45\rho^2 + 6\rho^4 + \rho^6)$	$\rho - \tan^{-1} [\rho(15 - \rho^2)/(15 - 6\rho^2)]$
l	$\frac{\rho^2 P_{l-1}}{(1 - S_{l-1})^2 + P_{l-1}^2}$	$\frac{\rho^2 (l - S_{l-1})}{(1 - S_{l-1})^2 + P_{l-1}^2} - l$	$\phi_{l-1} - \tan^{-1} (P_{l-1}/(l - S_{l-1}))^\dagger$

[†] The iterative formula for ϕ_l could also be defined by $B_l = (B_{l-1} + X_l)/(1 - B_{l-1}X_l)$ where $B_l = \tan(\rho - \phi_l)$ and $X_l = P_{l-1}/(l - S_{l-1})$

²To avoid ambiguity, it should be stated that below the channel threshold, that is, for $(E - \Xi_\alpha) < 0$, SAMMY uses the convention of Lane-Thomas, namely setting $P_c = 0$ and $S_c = \text{Re}(L_c) = L_c$, instead of using an analytical continuation of the shift and penetrability function in the complex plane by computing the expressions in Table 2.1 as a function of an imaginary ρ for which $iP_c(\rho)$ becomes real-valued, but separate from $S_c(\rho)$.

Formulae for a particular cross section type can be derived by summing over the terms in Eq. (II A.1)2.1. For the total cross section, the sum over all possible exit channels and all spin groups gives

$$\begin{aligned}
\sigma^{total} &= \sum_{\substack{\text{incident} \\ \text{channels} \\ c}} \sum_{\substack{\text{all} \\ \text{channels} \\ c'}} \sum_J \frac{\pi}{k_\alpha^2} g_J |\delta_{cc'} - U_{cc'}|^2 \\
&= \frac{\pi}{k_\alpha^2} \sum_J g_J \sum_{\substack{\text{incident} \\ \text{channels} \\ c}} \sum_{\substack{\text{all} \\ \text{channels} \\ c'}} (\delta_{cc'} - U_{cc'} \delta_{cc'} - U_{cc'}^* \delta_{cc'} + |U_{cc'}|^2) \\
&= \frac{2\pi}{k_\alpha^2} \sum_J g_J \sum_{\substack{\text{incident} \\ \text{channels} \\ c}} (1 - \text{Re}(U_{cc})).
\end{aligned} \tag{2.10}$$

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

$$\sigma_{\alpha\alpha} = \frac{\pi}{k_\alpha^2} \sum_J g_J \sum_{\substack{c=\text{incident} \\ \text{channel}}} \left(1 - 2\text{Re}(U_{cc}) + \sum_{\substack{c'=\text{incident} \\ \text{channel}}} |U_{cc'}|^2 \right). \tag{2.11}$$

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

$$\sigma_\alpha^{reaction} = \frac{\pi}{k_\alpha^2} \sum_J g_J \sum_{\substack{c=\text{incident} \\ \text{channel}}} \sum_{\substack{c'=\text{reaction} \\ \text{channel}}} |U_{cc'}|^2. \tag{2.12}$$

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

$$\sigma_\alpha^{reaction} = \frac{\pi}{k_\alpha^2} \sum_J g_J \sum_{\substack{c=\text{incident} \\ \text{channel}}} \left(1 - \sum_{\substack{c'=\text{all channels} \\ \text{except capture}}} |U_{cc'}|^2 \right). \tag{2.13}$$

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

2.1.1 R-Matrix and A-Matrix Equations

The R-matrix was introduced in Eq. 2.6 as

$$W = P^{1/2} (I - RL)^{-1} (I - RL^*) P^{-1/2}, \tag{2.14}$$

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

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_{\lambda} - E} \delta_{J,J'} , \quad (2.15)$$

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

$$\Gamma_{\lambda c} = 2\mathbf{P}_c \gamma_{\lambda c}^2. \quad (2.16)$$

Note that in Eq. 2.15 that energies and widths are given in laboratory frame of reference, while the derivation in §2.1.2 is in center-of-mass (please see Eq. 2.60 for the relationship of laboratory and center-of-mass parameters). The sum in Eq. (II A1.2)2.15 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

$$A_{\mu\lambda}^{-1} = (E_{\lambda} - E) \delta_{\mu\lambda} - \sum_c \gamma_{\mu c} L_c \gamma_{\lambda c}. \quad (2.17)$$

To see the relationship of the A-matrix to the R-matrix, we begin by multiplying both sides of Eq. (II A1.4)2.17 by A and summing over λ :

$$\sum_{\lambda} A_{\mu\lambda}^{-1} A_{\lambda\nu} = \sum_{\lambda} (E_{\lambda} - E) \delta_{\mu\lambda} A_{\lambda\nu} - \sum_c \gamma_{\mu c} L_c \gamma_{\lambda c} A_{\lambda\nu},$$

or

$$(2.18)$$

$$\delta_{\mu\nu} = (E_{\mu} - E) A_{\mu\nu} - \sum_c \gamma_{\mu c} L_c \sum_{\lambda} \gamma_{\lambda c} A_{\lambda\nu}.$$

Dividing by $(E_{\mu} - E)$, 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

$$\begin{aligned}
\sum_{\mu} \gamma_{\mu c'} (E_{\mu} - E)^{-1} \delta_{\mu\nu} \gamma_{\nu c''} &= \sum_{\mu} \gamma_{\mu c'} (E_{\mu} - E)^{-1} (E_{\mu} - E) A_{\mu\nu} \gamma_{\nu c''} \\
&\quad - \sum_{\mu} \gamma_{\mu c'} (E_{\mu} - E)^{-1} \sum_c \gamma_{\mu c} L_c \sum_{\lambda} \gamma_{\lambda c} A_{\lambda\nu} \gamma_{\nu c''},
\end{aligned} \tag{2.19}$$

which can be reduced to

$$\begin{aligned}
\gamma_{\nu c'} (E_{\nu} - E)^{-1} \gamma_{\nu c''} &= \sum_{\mu} \gamma_{\mu c'} A_{\mu\nu} \gamma_{\nu c''} \\
&\quad - \sum_c \left[\sum_{\mu} \gamma_{\mu c'} (E_{\mu} - E)^{-1} \gamma_{\mu c} \right] L_c \sum_{\lambda} \gamma_{\lambda c} A_{\lambda\nu} \gamma_{\nu c''}.
\end{aligned} \tag{2.20}$$

Summing over ν puts this into the form

$$\begin{aligned}
\left[\sum_{\nu} \gamma_{\nu c'} (E_{\nu} - E)^{-1} \gamma_{\nu c''} \right] &= \sum_{\mu\nu} \gamma_{\mu c'} A_{\mu\nu} \gamma_{\nu c''} \\
&\quad - \sum_c \left[\sum_{\mu} \gamma_{\mu c'} (E_{\mu} - E)^{-1} \gamma_{\mu c} \right] L_c \sum_{\lambda\nu} \gamma_{\lambda c} A_{\lambda\nu} \gamma_{\nu c''},
\end{aligned} \tag{2.21}$$

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

$$\begin{aligned}
R_{c'c''} &= \sum_{\mu\nu} \gamma_{\mu c'} A_{\mu\nu} \gamma_{\nu c''} - \sum_c R_{c'c} L_c \sum_{\lambda\nu} \gamma_{\lambda c} A_{\lambda\nu} \gamma_{\nu c''}, \\
&= \sum_c [\delta_{c'c} - R_{c'c} L_c] \sum_{\lambda\nu} \gamma_{\lambda c} A_{\lambda\nu} \gamma_{\nu c''}.
\end{aligned} \tag{2.22}$$

Solving for the summation, this equation can be rewritten as

$$[(I - RL)^{-1} R]_{cc''} = \sum_{\lambda\nu} \gamma_{\lambda c} A_{\lambda\nu} \gamma_{\nu c''}. \tag{2.23}$$

To relate this to the scattering matrix, we note that Eq. (II A.6)2.6 can be rewritten using Eq. (II A.7)2.7 into the form

$$\begin{aligned}
W &= P^{1/2} (I - RL)^{-1} (I - RL^*) P^{-1/2} \\
&= P^{1/2} (I - RL)^{-1} (I - RL + 2iRP) P^{-1/2} \\
&= P^{1/2} [(I - RL)^{-1} (I - RL) + 2i(I - RL)^{-1} RP] P^{-1/2} \\
&= P^{1/2} P^{-1/2} + 2iP^{1/2} (I - RL)^{-1} RPP^{-1/2} \\
&= I + 2iP^{1/2} (I - RL)^{-1} RP^{1/2}.
\end{aligned} \tag{2.24}$$

Comparing Eq. (II A1.10)2.23 to Eq. (II A1.11)2.24 gives, in matrix form,

$$W = I + 2iP^{1/2}\gamma A\gamma P^{1/2}. \tag{2.25}$$

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)2.17; assuming no level-level interference for the gamma channels (for example), this equation can be approximated as

$$A_{\mu\lambda}^{-1} \approx (E_\lambda - E)\delta_{\mu\lambda} - \left[\sum_{\substack{\gamma=\text{gamma} \\ \text{channels}}} \gamma_{\mu\gamma} L_\gamma \gamma_{\lambda\gamma} \right] \delta_{\mu\lambda} - \sum_{\substack{c=\text{particle} \\ \text{channels}}} \gamma_{\mu c} L_c \gamma_{\lambda c}. \tag{2.26}$$

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)2.26 becomes

$$A_{\mu\lambda}^{-1} \approx (E_\lambda - E - i\bar{\Gamma}_{\lambda\gamma}/2) \delta_{\mu\lambda} - \sum_{\substack{c=\text{particle} \\ \text{channels}}} \gamma_{\mu c} L_c \gamma_{\lambda c}. \tag{2.27}$$

The bar over $\bar{\Gamma}_{\lambda\gamma}$ 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)2.17 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

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_{\lambda} - E - i\bar{\Gamma}_{\lambda\gamma}/2} \delta_{JJ'}, \quad (2.28)$$

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.

2.1.2 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][6], presented at the SAMMY workshop in Paris in 2002, and Foderaro [AF71][2]. 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][1].

Schrödinger equation

The Schrödinger equation with a complex potential is

$$\left(\frac{-\hbar^2}{2\mu} \nabla^2 + V + iW \right) \psi = E^{(\text{CoM})} \psi, \quad (2.29)$$

in which one can consider that V causes scattering and W causes absorption and the reduced mass $\mu = \frac{mM}{m+M}$ (m and M defined as before). **Note that energies in §2.1.2 are in the center-of-mass (CoM) frame.** The wave function can be expanded in the usual fashion,

$$\psi(r, \cos(\theta)) = \sum_{l=0}^{\infty} \frac{u_l(r)}{r} P_l(\cos(\theta)), \quad (2.30)$$

for which the radial portion obeys the equation

$$\frac{d^2 u_l}{dr^2} + \left[k^2 - \frac{2\mu}{\hbar^2} (V + iW) - \frac{l(l+1)}{r^2} \right] u_l = 0, \quad (2.31)$$

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

$$u_l(r=0) = 0. \quad (2.32)$$

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

$$u_l(r) = I_l(r) - U_l O_l(r). \quad (2.33)$$

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:

$$\begin{aligned} |U_l|^2 &= 1 \text{ for } W = 0, \\ |U_l|^2 &< 1 \text{ for } W \neq 0. \end{aligned} \quad (2.34)$$

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 ,

$$E_\lambda^{(\text{CoM})} = \frac{\hbar^2 k_\lambda^2}{2\mu}, \quad (2.35)$$

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

$$\frac{d^2 w_{\lambda l}}{dr^2} + \left[k_\lambda^2 - \frac{2\mu}{\hbar^2} V - \frac{l(l+1)}{r^2} \right] w_{\lambda l} = 0, \quad (2.36)$$

for which the boundary conditions are

$$w_{\lambda l}(r=0) = 0 \quad \text{and} \quad \frac{a}{w_{\lambda l}(a)} \frac{dw_{\lambda l}}{dr} \Big|_{r=a} = B_l. \quad (2.37)$$

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

$$\begin{aligned} \int_0^a \left(\frac{d^2 w_{\lambda l}}{dr^2} w_{\mu l} - w_{\lambda l} \frac{d^2 w_{\mu l}}{dr^2} \right) dr &= \int_0^a \frac{d}{dr} \left(\frac{dw_{\lambda l}}{dr} w_{\mu l} - w_{\lambda l} \frac{dw_{\mu l}}{dr} \right) dr \\ &= \left[\frac{dw_{\lambda l}}{dr} w_{\mu l} - w_{\lambda l} \frac{dw_{\mu l}}{dr} \right]_0^a \\ &= \frac{dw_{\lambda l}}{dr} \Big|_{r=a} w_{\mu l}(a) - w_{\lambda l}(a) \frac{dw_{\mu l}}{dr} \Big|_{r=a} - [0] \\ &= \frac{B_l}{a} [w_{\lambda l}(a) w_{\mu l}(a) - w_{\lambda l}(a) w_{\mu l}(a)] = 0, \end{aligned} \quad (2.38)$$

in which both equations of (II A2.9)2.37 have been invoked. The integral in Eq. (II A2.10)2.38 can also be evaluated using Eq. (II A2.8)2.36, giving

$$\begin{aligned}
\int_0^a \left(\frac{d^2 w_{\lambda l}}{dr^2} w_{\mu l} - w_{\lambda l} \frac{d^2 w_{\mu l}}{dr^2} \right) dr &= \int_0^a \left(\left[-k_{\lambda}^2 - \frac{2\mu V}{\hbar^2} \right] w_{\lambda l} w_{\mu l} - w_{\lambda l} \left[-k_{\mu}^2 - \frac{2\mu V}{\hbar^2} \right] w_{\mu l} \right) dr \\
&= \int_0^a (-k_{\lambda}^2 w_{\lambda l} w_{\mu l} + k_{\mu}^2 w_{\lambda l} w_{\mu l}) dr \\
&= -(k_{\lambda}^2 - k_{\mu}^2) \int_0^a w_{\lambda l} w_{\mu l} dr.
\end{aligned} \tag{2.39}$$

Equating Eq. (II A2.10)2.38 to Eq. (II A2.11)2.39 gives

$$(k_{\lambda}^2 - k_{\mu}^2) \int_0^a w_{\lambda l} w_{\mu l} dr = 0. \tag{2.40}$$

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

$$\int_0^a w_{\lambda l} w_{\mu l} dr = 0 \quad \text{if} \quad \lambda \neq \mu. \tag{2.41}$$

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

$$\int_0^a w_{\lambda l} w_{\mu l} dr = \delta_{\lambda \mu}. \tag{2.42}$$

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

$$u_l(r) = \sum_{\lambda} c_{\lambda l} w_{\lambda l}(r) \quad \text{for } r \leq a, \tag{2.43}$$

with

$$c_{\lambda l} = \int_0^a u_l w_{\lambda l} dr. \tag{2.44}$$

This equation for $c_{\lambda l}$ is derived by multiplying Eq. (II A2.15)2.43 by $u_{\lambda l}(r)$, integrating, and applying Eq. (II A2.14)2.42.

Consider now the integral

$$\int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr, \quad (2.45)$$

which can be expanded by use of Eqs. (II A2.3)2.31 and (II A2.8)2.36 to give

$$\begin{aligned} & \int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr \\ &= \int_0^a \left(\left[k^2 - \frac{2\mu}{\hbar^2} (V + iW) - \frac{l(l+1)}{r^2} \right] u_l w_{\lambda l} + u_l \left[k_{\lambda}^2 - \frac{2\mu}{\hbar^2} V - \frac{l(l+1)}{r^2} \right] w_{\lambda l} \right) dr \quad (2.46) \\ &= (k_{\lambda}^2 - k^2) \int_0^a u_l w_{\lambda l} dr + \frac{2\mu}{\hbar} \int_0^a W u_l w_{\lambda l} dr. \end{aligned}$$

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

$$\overline{W}_{\lambda l} = \frac{\int_0^a W u_l w_{\lambda l} dr}{\int_0^a u_l w_{\lambda l} dr} \quad (2.47)$$

permits rewriting Eq. (II A2.18)2.46 in the form

$$\int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr = \left(k_{\lambda}^2 - k^2 + i \frac{2\mu}{\hbar^2} \overline{W}_{\lambda l} \right) \int_0^a u_l w_{\lambda l} dr. \quad (2.48)$$

Integrating the left-hand side of this equation gives

$$\begin{aligned} \int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr &= \left[\frac{du_l}{dr} w_{\lambda l} - u_l \frac{dw_{\lambda l}}{dr} \right]_0^a = \left[\frac{du_l}{dr} w_{\lambda l} - u_l \frac{dw_{\lambda l}}{dr} \right]_{r=a} \\ &= \left[\frac{du_l}{dr} w_{\lambda l} - u_l \frac{B_l}{a} w_{\lambda l} \right]_{r=a} = \left[a \frac{du_l}{dr} - u_l B_l \right]_{r=a} \frac{w_{\lambda l}(a)}{a}, \end{aligned} \quad (2.49)$$

in which we have again made use of the boundary condition of Eq. (II A2.9)2.37. Integrating the right-hand side of Eq. (II A2.20)2.48 by applying Eq. (II A2.16)2.44 gives

$$\left(k_{\lambda}^2 - k^2 + i \frac{2\mu}{\hbar^2} \overline{W}_{\lambda l} \right) \int_0^a u_l w_{\lambda l} dr = \left(k_{\lambda}^2 - k^2 + i \frac{2\mu}{\hbar^2} \overline{W}_{\lambda l} \right) c_{\lambda l}. \quad (2.50)$$

Equating Eqs. (II A2.21)2.49 and (II A2.22)2.50 therefore gives

$$\begin{aligned} \left[a \frac{du_l}{dr} - u_l B_l \right]_{r=a} \frac{w_{\lambda l}}{a} &= \left(k_{\lambda}^2 - k^2 + i \frac{2\mu}{\hbar^2} \overline{W}_{\lambda l} \right) c_{\lambda l}, \\ \left[a \frac{du_l}{dr} - u_l B_l \right]_{r=a} \frac{w_{\lambda l}}{a} &= \left(E_{\lambda}^{(\text{CoM})} - E^{(\text{CoM})} + i \overline{W}_{\lambda l} \right) \frac{2\mu c_{\lambda l}}{\hbar^2}, \end{aligned} \quad (2.51)$$

or

$$c_{\lambda l} = \frac{\hbar^2 w_{\lambda l}(a)}{2\mu a \left(E_{\lambda}^{(\text{CoM})} - E^{(\text{CoM})} - i \overline{W}_{\lambda l} \right)} \left[a \frac{du_l}{dr} - u_l B_l \right]_{r=a}. \quad (2.52)$$

Inserting this into Eq. (II A2.15)2.43 gives

$$u_l(r) = \sum_{\lambda} w_{\lambda l}(r) \frac{\hbar^2 w_{\lambda l}(a)}{2\mu a \left(E_{\lambda}^{(\text{CoM})} - E^{(\text{CoM})} - i \overline{W}_{\lambda l} \right)} \left[a \frac{du_l}{dr} - u_l B_l \right]_{r=a}, \quad (2.53)$$

which when evaluated at $r = a$, becomes

$$u_l(a) = \sum_{\lambda} \frac{\hbar^2 w_{\lambda l}^2(a)}{2\mu a \left(E_{\lambda}^{(\text{CoM})} - E^{(\text{CoM})} - i \overline{W}_{\lambda l} \right)} \left[a \frac{du_l}{dr} - u_l B_l \right]_{r=a}, \quad (2.54)$$

Rearranging, this becomes

$$\begin{aligned} u_l(a) &= \left[a \frac{du_l}{dr} - u_l B_l \right]_{r=a} \sum_{\lambda} \frac{\hbar^2 w_{\lambda l}^2(a)/2\mu a}{\left(E_{\lambda}^{(\text{CoM})} - E^{(\text{CoM})} - i \overline{W}_{\lambda l} \right)} \\ &= \left[a \frac{du_l}{dr} - u_l B_l \right]_{r=a} \sum_{\lambda} \frac{\gamma_{\lambda l}^2}{\left(E_{\lambda}^{(\text{CoM})} - E^{(\text{CoM})} - i \overline{\Gamma}_{\lambda l}/2 \right)}, \end{aligned} \quad (2.55)$$

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

$$\gamma_{\lambda l} \equiv \sqrt{\frac{\hbar^2 w_{\lambda l}^2(a)}{2\mu a}} \quad (2.56)$$

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

$$\Gamma_{\lambda l} \equiv 2\overline{W}_{\lambda l}. \quad (2.57)$$

If we then define the R -function as

$$R_l = \sum_{\lambda} \frac{\gamma_{\lambda l}^2}{\left(E_{\lambda}^{(\text{CoM})} - E^{(\text{CoM})} - i \overline{\Gamma}_{\lambda l}/2 \right)}, \quad (2.58)$$

then Eq. (II A2.27)2.55 can be written in the form

$$u_l = \left(a \frac{du_l}{dr} - u_l B_l \right) R_l, \quad (2.59)$$

in which everything is evaluated at the matching radius a . Note that the form of Eq. 2.58 (which is in the CoM frame) is the same as if it were in the laboratory frame of reference. This is because of canceling terms in the numerator and denominator of the R-matrix, e.g.

$$\begin{aligned} E &\equiv E^{(\text{lab})} = \frac{M}{m+M} E^{(\text{CoM})}, \\ E_\lambda &\equiv E_\lambda^{(\text{lab})} = \frac{M}{m+M} E_\lambda^{(\text{CoM})}, \\ \gamma_{\lambda,l}^2 &\equiv (\gamma_{\lambda,l}^{(\text{lab})})^2 = \frac{M}{m+M} (\gamma_{\lambda,l}^{(\text{CoM})})^2, \text{ and} \\ \Gamma_{\gamma,l} &\equiv \Gamma_{\gamma,l}^{(\text{lab})} = \frac{M}{m+M} \Gamma_{\gamma,l}^{(\text{CoM})}. \end{aligned} \quad (2.60)$$

Due to this relationship, Eq. 2.58 can be used for CoM or laboratory frame parameters. Conventional SAMMY parameterization is to use the laboratory frame.

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

Equation (II A2.31)2.59 can be converted into the usual R-matrix formulae by inserting Eq. (II A2.5)2.33,

$$u_l = I_l - U_l O_l, \quad (2.61)$$

yielding

$$I_l - U_l O_l = \left[a \left(\frac{dI_l}{dr} - U_l \frac{dO_l}{dr} \right) - B_l (I_l - U_l O_l) \right] R_l, \quad (2.62)$$

in which everything is again evaluated at the matching radius a . Solving Eq. (II A2.33)2.62 for U gives

$$U_l \left[-O_l + R_l \left(a \frac{dO_l}{dr} - B_l O_l \right) \right] = I_l - R_l \left(a \frac{dI_l}{dr} - B_l I_l \right), \quad (2.63)$$

or

$$U_l = \frac{I_l - R_l \left(a \frac{dI_l}{dr} - B_l I_l \right)}{\left[-O_l + R_l \left(a \frac{dO_l}{dr} - B_l O_l \right) \right]} = \frac{I_l}{O_l} \frac{1 - R_l \left(\frac{a}{I_l} \frac{dI_l}{dr} - B_l \right)}{1 - R_l \left(\frac{a}{O_l} \frac{dO_l}{dr} - B_l \right)}. \quad (2.64)$$

We define L_l as

$$L_l \equiv \frac{a}{O_l(a)} \frac{dO_l}{dr} \Big|_{r=a} \equiv S_l + iP_l. \quad (2.65)$$

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

$$\frac{a}{I_l(a)} \frac{dI_l}{dr} \Big|_{r=a} = L_l^* = S_l - iP_l \quad (2.66)$$

and

$$\frac{I_l}{O_l} = \frac{O_l^*}{O_l} = \frac{|O|e^{-i\phi}}{|O|e^{i\phi}} = e^{-2i\phi}. \quad (2.67)$$

Therefore Eq. (II A2.34)2.63 becomes

$$U_l = e^{-2i\phi} \frac{1 - R_l(L_l^* - B_l)}{1 - R_l(L_l - B_l)}, \quad (2.68)$$

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

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][2]. 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

$$\psi(r, \theta) = e^{ikz} + \frac{e^{ikr}}{r} f(\theta), \quad (2.69)$$

where f has the form

$$f(\theta) = \frac{1}{2ik} \sum_l (2l+1) [U_l - 1] P_l(\cos \theta). \quad (2.70)$$

The cross section is then given by

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2. \quad (2.71)$$

For angle-integrated cross sections, the equation found by inserting Eq. (II A2 a.2)2.70 into Eq. (II A2 a.3)2.71 can be integrated to give

$$\begin{aligned} \sigma &= \int \left[-\frac{1}{2ik} \sum_l (2l+1) [U_l^* - 1] P_l(\cos \theta) \right] \\ &\quad \times \left[\frac{1}{2ik} \sum_{l'} (2l'+1) [U_{l'} - 1] P_{l'}(\cos \theta) \right] d(\cos \theta) d\phi \\ &= \frac{1}{4k^2} \sum_{ll'} (2l+1)(2l'+1) [U_l^* - 1][U_{l'} - 1] \int_0^{2\pi} d\phi \int_{-1}^1 P_l(\cos \theta) P_{l'}(\cos \theta) d(\cos \theta) \quad (2.72) \\ &= \frac{1}{4k^2} \sum_{ll'} (2l+1)(2l'+1) [U_l^* - 1][U_{l'} - 1] 2\pi \frac{2}{2l+1} \delta_{ll'} \\ &= \frac{\pi}{k^2} \sum_l (2l+1) |U_l - 1|^2. \end{aligned}$$

This is analogous to the “standard” scattering theory equation shown in Eq. (II A.1)2.1.

2.2 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][7, 4].

Four versions of R-matrix theory are available in SAMMY: the Reich-Moore approximation (Section II.B.1)2.2.1, the single-level (SLBW) and multilevel Breit-Wigner (MLBW) approximations (Section II.B.3)2.2.3, and a variant on the Reich Moore which mimics the full R-matrix (Section II.B.2)2.2.2. An option to include a direct capture component is also provided (Section II.B.4)2.2.4.

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.” [4](pg. 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.22.2.2 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.42.2.4 for details.

Also available within SAMMY are both the SLBW and the MLBW formulations (Section II.B.3)2.2.3; 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][8] convention in which only the elastic cross section is truly multilevel, and all other types of cross section are single level.

2.2.1 Reich-Moore Approximation to Multilevel R-Matrix Theory

The Reich-Moore approximation [9] 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.12.1.1.

In the eliminated-channel approximation, the R-matrix of Eq. (II A.6)2.6 (for the spin group defined by total spin J and implicit parity π) has the form

$$R_{cc'} = \left[\sum_{\lambda} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_{\lambda} - E - i\bar{\Gamma}_{\lambda\gamma}/2} + R_c^{ext} \delta_{cc'} \right] \delta_{JJ'}, \quad (2.73)$$

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

The “external R-function” R_c^{ext} of Eq. (II B1.1)2.73 will be discussed at the end of Section II.B.1.d2.2.1.

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

$$\Gamma_{\lambda c} = 2\gamma_{\lambda c}^2 P_c(E), \quad (2.74)$$

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)2.74 becomes

$$\Gamma_{\lambda c} = 2\gamma_{\lambda c}^2 \quad (2.75)$$

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)2.7, to generate W , and from there calculating U and, ultimately, σ . However, while Eq. (II A.6)2.6 for W is correct, an equivalent form that is computationally more stable [10] is

$$W = I + 2iX, \quad (2.76)$$

where X is given in matrix notation by

$$X = P^{1/2} L^{-1} (L^{-1} - R)^{-1} R P^{1/2}. \quad (2.77)$$

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

$$X_{cc'} = P_c^{1/2} L_c^{-1} \sum_{c''} [(L^{-1} - R)^{-1}]_{cc''} R_{c''c'} P_{c'}^{1/2} \delta_{JJ'}. \quad (2.78)$$

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:

$$u_{E_\lambda} = \begin{cases} \sqrt{E_\lambda} & \text{for } E_\lambda > 0 \\ -\sqrt{-E_\lambda} & \text{for } E_\lambda < 0 \end{cases} \quad (2.79)$$

$$u_{\Gamma_{\lambda c}} = \gamma_{\lambda c} = \begin{cases} \sqrt{\frac{\Gamma_{\lambda c}}{2P_l(|E_\lambda - \Xi_c|)}} & \text{if } \Gamma_{\lambda c} > 0 \\ -\sqrt{\frac{|\Gamma_{\lambda c}|}{2P_l(|E_\lambda - \Xi_c|)}} & \text{if } \Gamma_{\lambda c} < 0 \end{cases} \quad \text{in the PARAmeter file,} \quad (2.80)$$

in which Ξ_c is the energy threshold for the channel (Section II.C.2)2.3.2. 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??), 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.

Energy-differential cross sections

The observable cross sections are found in terms of X by first substituting Eqs. (II A.42.4, II A.52.5, and II B1.32.76) into Eq. (II A.1)2.1, 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

$$\sigma_{\alpha,\alpha'}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[(\sin^2 \phi_c (1 - 2X_{cc}^i) - X_{cc}^r \sin(2\phi_c)) \delta_{\alpha,\alpha'} + \sum_{c'} (X_{cc'}^i{}^2 + X_{cc'}^r{}^2) \right]. \quad (2.81)$$

(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)2.81 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)2.81 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

$$\sigma_{total}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c [(\sin^2 \phi_c + X_{cc}^i \cos(2\phi_c) - X_{cc}^r \sin(2\phi_c))], \quad (2.82)$$

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

$$\sigma_{elastic}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[\sin^2 \phi_c (1 - 2X_{cc}^i) - X_{cc}^r \sin(2\phi_c) + \sum_{c'} \left(X_{cc'}^i{}^2 + X_{cc'}^r{}^2 \right) \right]. \quad (2.83)$$

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

$$\sigma_{reaction}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \sum_{c'} \left[X_{cc'}^i{}^2 + X_{cc'}^r{}^2 \right] \quad (2.84)$$

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

$$\sigma_{absorption}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[X_{cc}^i - \sum_{c'} \left(X_{cc'}^i{}^2 + X_{cc'}^r{}^2 \right) \right]. \quad (2.85)$$

Here both the sum over c and the sum over c' include all incident 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

$$\sigma_{capture}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_{inc\ c} \left[X_{cc}^i - \sum_{all\ c'} \left(X_{cc'}^i{}^2 + X_{cc'}^r{}^2 \right) \right]. \quad (2.86)$$

or may be found by subtracting the sum of all reaction cross sections from the absorption cross section. In Eq. (II B1 a.6)2.86, the sum over c includes all incident particle channels for the J^π spin group, and the sum over c' includes **all** particle channels, both incident and exit, for that spin group.

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 directly above 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)2.77 takes the form

$$\begin{aligned}
 X &= \sqrt{P} L^{-1} (L^{-1} - R)^{-1} R \sqrt{P} \\
 &= \begin{bmatrix} \frac{\sqrt{P_1}}{iP_1} & 0 \\ 0 & \frac{\sqrt{P_2}}{iP_2} \end{bmatrix} \begin{bmatrix} \frac{1}{iP_1} - \frac{\gamma_1^2}{D} & -\frac{\gamma_1\gamma_2}{D} \\ -\frac{\gamma_1\gamma_2}{D} & \frac{1}{iP_2} - \frac{\gamma_2^2}{D} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\gamma_1^2}{D} & \frac{\gamma_1\gamma_2}{D} \\ \frac{\gamma_1\gamma_2}{D} & \frac{\gamma_2^2}{D} \end{bmatrix} \begin{bmatrix} \sqrt{P_1} & 0 \\ 0 & \sqrt{P_2} \end{bmatrix}, \quad (2.87)
 \end{aligned}$$

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

2.2.2 Simulation of Full R-Matrix

2.2.3 Breit-Wigner Approximations

2.2.4 Direct Capture Component

2.3 Details and Conventions Used In Sammy

Note: Subject to change with inclusion of AMPX R-matrix engine!!!

2.3.1 Spin and Angular Momentum Conventions

2.3.2 Kinematics

2.3.3 Evaluation of Hard-Sphere Phase Shift

2.3.4 Modifications for Charged Particles

2.3.5 Inverse Reactions (Reciprocity)

2.4 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

2.4.1 Derivatives for Reich-Moore Approximation

2.4.2 Derivatives for MLBW and SLBW Approximations

2.4.3 Details Involving Derivatives

CHAPTER 3

Experimental Conditions

3.1 Theoretical Foundation For Numerical Broadening

3.2 Doppler Broadening

3.3 Resolution Broadening

3.4 Self-shielding And Multiple-scattering Corrections To Capture Or Fission Yields

The theoretical capture, fission, and other cross sections may be calculated directly from the equations in Sec. ?? using the Reich-Moore (or other) approximation to the multilevel R-matrix. However, in order to compare with experimental results, corrections must often be made for the finite (noninfinitesimal) size of the sample.

Both “self-shielding” and “multiple-scattering” effects must be included in the calculation. These corrections are most often needed for capture experiments; however, they may also be needed for fission, absorption, or other partial cross sections. For the rest of this section, “capture” will be taken to indicate whichever type of cross section is under investigation; the corrections described here apply in any case.

Derivation of the appropriate expressions for self-shielding and multiple-scattering corrections, including details of the methods of calculation, is nontrivial and will not be presented here. Results of comparison tests with Monte Carlo calculations indicate good agreement between Monte Carlo results and results obtained via SAMMY, as reported in [11]. See Section 10.13 for a description of the Monte Carlo code used for such comparisons.

The capture yield $Y(E)$ can be written as the sum of four components, each of which is described separately below; that is,

$$Y(E) = Y_0(E) + Y_1(E) + Y_2(E) + Y_n(E). \quad (3.1)$$

3.4.1 Self-Shielding

Self-shielding is the reduction in the observed capture cross section due to interactions of incident neutrons with other nuclei in front of the current position. The probability that capture will occur at depth z (within dz) can be written as

$$\frac{n}{D} e^{-n\sigma_t z/D} \sigma_c dz, \quad (3.2)$$

where n is the sample thickness in atoms/barn and D is the sample thickness in the same units as z . Subscripts t and c denote total and capture cross sections, respectively. Integrating over z (from 0 to D) gives the self-shielded capture yield

$$Y_0 = \frac{\sigma_c}{\sigma_t} (1 - e^{-n\sigma_t}). \quad (3.3)$$

(See the end of this section for a discussion of the normalization options for capture yields.)

3.4.2 Single Scattering

The scattering correction is the increase in the observed capture cross section due to capture of neutrons that have been scattered out of the original beam path. Calculation of the scattering effect is more complicated than the self-shielding because it involves the product of (1) the probability of reaching a position (x, y, z) inside the sample, (2) the probability of scattering from that position into solid angle Ω within $d\Omega$, (3) the probability of those scattered nuclei reaching position q within dq along that direction, and (4) the probability of being captured at that location. This product is then integrated over the position q , over solid angle Ω , and over the sample volume, giving the single-scattering result. If the z axis is defined by the beam line, this expression can be reduced to the form

$$Y_1(E) = \frac{1}{S} \int dx \int dy \frac{n}{D} \int dz e^{-(\frac{n}{D}\sigma_t z)} \int d\Omega \frac{d\sigma}{d\Omega} \sigma'_c \frac{n}{D} \int dq e^{-(\frac{n}{D}\sigma'_t q)}, \quad (3.4)$$

in which primes indicate the evaluation at the scattered energy, rather than at the incident energy of the neutron. The scattered energy is given by

$$E' = E \left[\frac{\cos(\theta)}{1+r} + \sqrt{\frac{1}{(1+1/r)^2} - \frac{\sin^2(\theta)}{(1+r)^2}} \right]^2, \quad (3.5)$$

where r is the ratio of the mass of the target nuclide³ to the mass of the neutron. (See Section II.C.2 and especially Eq. (II C2 b.3) for a derivation of this equation.)

Explicit evaluation of the expression in Eq. 3.4 requires detailed knowledge of the geometry of the sample and its positioning relative to the neutron beam, as shown in the sketch in Figure III D.1. In the case where the sample is a round disk, with a flat surface perpendicular to the beam, the expression can be reduced to

$$Y_1(E) = Y_{1\infty f} + Y_{1\infty b} + Y_{1cf} + Y_{1cb}, \quad (3.6)$$

where the subscripts f and b refer to forward and backward scattering, respectively. The subscript ∞ indicates that this term assumes the sample extends to infinity in the dimensions perpendicular to the beam; subscript c indicates that this term is the correction for finite size.

The “infinite” terms in Eq. 3.6 are one-dimensional integrals,

$$Y_{1\infty f}(E) = \frac{1}{2} \int_0^1 d\mu \frac{d\sigma}{d\Omega} \frac{\sigma'_c}{\sigma'_t} \left(\frac{1 - e^{-n\sigma_t}}{\sigma_t} + \frac{e^{-n\sigma_t} - e^{-n\sigma'_t/\mu}}{\sigma_t - \sigma'_t/\mu} \right), \quad (3.7)$$

and

$$Y_{1\infty b}(E) = \frac{1}{2} \int_{-1}^0 d\mu \frac{d\sigma}{d\Omega} \frac{\sigma'_c}{\sigma'_t} \left(\frac{1 - e^{-n\sigma_t}}{\sigma_t} + \frac{1 - e^{-n(\sigma_t - \sigma'_t/\mu)}}{\sigma_t - \sigma'_t/\mu} \right), \quad (3.8)$$

in which $\mu = \cos(\theta)$. The “finite” corrections involve four-dimensional integrals of the form

$$Y_{1cf}(E) = \frac{1}{2} \int_0^1 d\mu \frac{d\sigma}{d\Omega} \frac{\sigma'_c}{\sigma'_t} Q_f(\mu, \sigma_t, \sigma'_t) \quad (3.9)$$

and

$$Y_{1cb}(E) = \frac{1}{2} \int_{-1}^0 d\mu \frac{d\sigma}{d\Omega} \frac{\sigma'_c}{\sigma'_t} Q_b(\mu, \sigma_t, \sigma'_t). \quad (3.10)$$

Here the three-dimensional integral Q_f is given by

$$Q_f(\mu, \sigma_t, \sigma'_t) = \int dz e^{-n\sigma'_t D/z} \int d^2S \left(e^{-n\sigma_t(D-z)/(D\mu)} - e^{-n\sigma_t L/D} \right) \quad (3.11)$$

³There may, of course, be several different types of target nuclide, each with a different mass. While the equations in this section assume only one nuclide, the implementation in the SAMMY code includes summations over all nuclides in the sample.

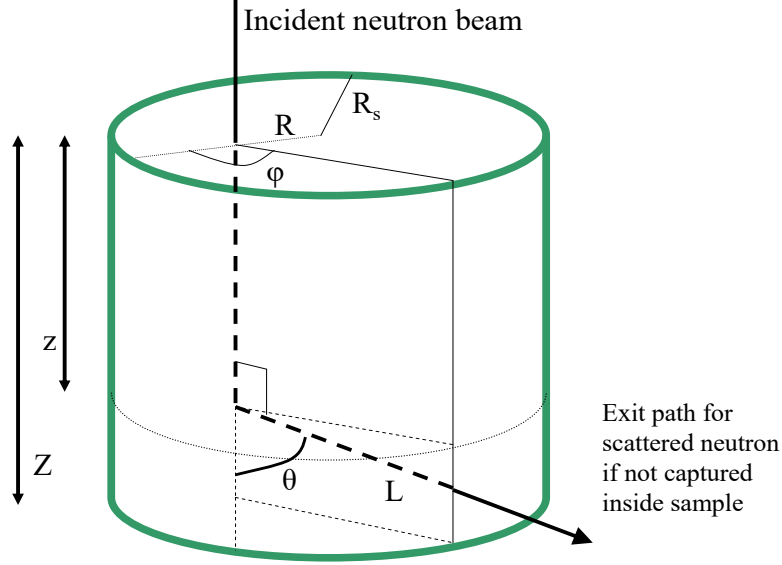


Figure 3.1: Geometry for the single-scattering correction to capture or fission yield, for a neutron incident on the flat surface of a cylindrical sample.

and Q_b by

$$Q_b(\mu, \sigma_t, \sigma'_t) = \int dz e^{-n\sigma'_t(D-z)/z} \int d^2S \left(e^{-n\sigma_t(D-z)/(D\mu)} - e^{-n\sigma_t L/D} \right), \quad (3.12)$$

where L is the actual path length, within the sample, available for travel by the scattered neutron; note that L is geometry dependent. The integration over d^2S in this expression for $Q_{f,b}$ is over the beam cross section; the integration over z is over the thickness of the sample. SAMMY evaluates Q on a separate grid and interpolates to produce the required values for Eqs. 3.9 and 3.10.

Values for Q are generated in advance (in segment SAMPAR) and stored in a file named SAMMY.SSM. This file may be renamed and reused for subsequent runs, as long as the geometry remains the same.

3.4.3 More than one scatter

Derivation of the effect of two or more scatters followed by capture is accomplished in a similar manner to the derivation of the single-scattering effect. The exact expression for k scatters involves $(3k + 3)$ embedded integrations; it is therefore necessary to make severe

approximations in order to derive an expression that can be calculated in a finite amount of time. The approximation currently employed by SAMMY is borrowed from Moxon [12], based on a derivation by Case et al. [13]; an independent derivation was developed in preparation for implementation into the SAMMY code. The approximation assumes that after two scatterings, neutrons are uniformly distributed both in direction of motion and in position within the sample⁴. To quantify this approximation, we assume that the escape probability for a neutron after k scatterings (i.e., at energy $E(k)$) depends only on the energy; specifically, the escape probability is given by the formula

$$p_{escape}(E^{(k)}) = \frac{1}{n\sigma_t^{(k)}} \left[\frac{1}{2} - \int_1^\infty \mu^{-3} e^{-n\sigma_t^{(k)}\mu} d\mu \right] \frac{1 + 2n\sigma_t^{(k)}}{1 + \frac{2n\sigma_t^{(k)}}{1+Z/R}}, \quad (3.13)$$

where R is the radius of the sample. With this approximation, one can recursively define a function y via

$$y_{j-1} = \int d\Omega_j \frac{d\sigma_t^{(j-1)}}{d\Omega_j} (\sigma_c^{(j)} + y_j) (1 - p_{escape}(E^{(j)})), \quad (3.14)$$

in which the superscript denotes the energy at which the cross section is to be calculated. The initial estimate for a neutron scattered k times is

$$y_{k-1} \approx 2\pi \int d\mu_k \frac{d\sigma_t^{(k-1)}}{d\Omega_k} \sigma_c^{(k)} (1 - p_{escape}(E^{(k)})). \quad (3.15)$$

This function y can then be used to estimate the capture yield for two or more scatterings:

$$Y_2(E) = \frac{1}{S} \int dx \int dy \frac{n}{E} \int dz e^{-\frac{n}{D}\sigma_t z} \int d\Omega \frac{d\sigma_t}{d\Omega} y_l \frac{n}{D} \int dq e^{-\frac{n}{D}\sigma_t' q}. \quad (3.16)$$

In this form the multiple-scattering capture yield has the same mathematical properties as the single-scattering capture yield of Eq. 3.4. Similar computational techniques can therefore be used to evaluate both quantities.

3.4.4 Alternative for more than one scatter

For very thick samples and/or very strong resonances, the crude approximation described above for double-plus scattering may be woefully inadequate. For those situations,

⁴This approximation has the effect of decoupling $2k$ of the embedded integrals, so that they can be performed separately from the others.

tabulated values can be used for Y_2 . The tabulated values are generated with a series of three runs, first SAMMY with the command

```
PREPARE INPUT FOR MONte carlo simulation, or simply
MONTE CARLO
```

Next, the SAMSMC code is run to perform the Monte Carlo calculation. Then SAMGY2 reads the output from SAMSMC, smooths the Y_2 curve, and creates a file named SAMY2.DAT that contains the tabulated Y_2 values for use in the next SAMMY run. For that run, the command

```
Y2 VALUES ARE TABULAted
```

is inserted into the INPut file, and the name of the file must be included in the input stream.

Only the values of Y_2 are given in this manner; derivatives are still generated as though the original form were used. **Caution must be exercised when using this option**, especially when varying resonance parameters, since (1) the tabulated values of Y_2 do not change unless the entire process is repeated and (2) derivatives are inaccurate.

Simulation sim009 makes use of this option.

3.4.5 Neutron sensitivity

In capture experiments, not only gamma rays but also scattered neutrons reach the detector. The detector is not always able to distinguish between the two; hence, it may be necessary to make corrections for the neutron sensitivity of the detector. These corrections are temporarily unavailable in SAMMY, pending further study.

3.4.6 Normalization and input options

Capture yield data may be normalized in a variety of ways; therefore, SAMMY allows the user to choose which normalization is to be taken. The normalization generally referred to as capture “yield” is the one shown in the equations in this section; this choice has the property that values are in the range from 0 to 1. Another commonly used normalization requires dividing by thickness n ; in this case, the value approaches the capture cross section in the limit of zero thickness. Finally, the data may be normalized as $(1 - e^{-n\sigma_t}) \sigma_t$, that is, by multiplying the yield by the total cross section. To use these options, the appropriate phrase must be included in the alphanumeric section of the INPut file:

```
NORMALIZE AS YIELD Rather than cross section
```

NORMALIZE AS CROSS Section rather than yield

NORMALIZE AS (1-E)Sigma

No default is assumed for normalization; instead, SAMMY requires that one of the above options be specified by the user.

The default mode in SAMMY is to not include self-shielding and multiple-scattering corrections; therefore, to invoke these corrections, users will need to include one or more of the following phrases in their INPut file.

For self-shielding but no multiple-scattering correction:

USE SELF SHIELDING Only, no scattering, or
SELF SHIELD

For self-shielding, single-scattering (with edge-effects), and no double-scattering correction:

USE SINGLE SCATTERING plus self shielding, or SINGLE

For self-shielding, single-scattering (infinite slab approximation), and no double-scattering corrections, two commands are required:

SINGLE and INFINITE SLAB

For self-shielding, single-scattering (with edge-effects correction), and multiple-scattering corrections:

INCLUDE DOUBLE SCATTERING plus single scattering, or MULTIPLE SCATTERING or
DOUBLE

For self-shielding, single-scattering (infinite-slab approximation), and multiple-scattering corrections, two commands are needed:

DOUBLE and INFINITE SLAB

When finite-size corrections (for single scattering) are wanted, additional input is needed to express the geometric properties of the beam and of the sample. These include the dimensions of the sample, the cross-sectional dimensions of the beam if smaller than the sample, and integers that determine the accuracy to which the functions $Q_{f,b}$ will be calculated. Details are given in Table VI A.1, card set 11.

Examples using multiple-scattering corrections can be found in test cases tr039, tr052, tr064, tr099, and others.

3.5 Other Experimental Corrections

CHAPTER 4

Fitting Procedure

- 4.1 Derivation Of Bayes' Equations**
- 4.2 Implementation Of Bayes' Equations**
- 4.3 Constructing The Parameter Set**
- 4.4 Treatment Of Data Covariance Matrices**
- 4.5 Miscellaneous Topics Related To Covariances**

CHAPTER 5

Miscellaneous

- 5.1 Reconstructing Point-wise Cross Sections
- 5.2 Integral Quantities
- 5.3 Averaging The Cross Sections
- 5.4 Stellar-averaged Capture Cross Sections
- 5.5 Pseudo Cross Sections For Testing
- 5.6 Summed Strength Function

CHAPTER 6

Input

6.1 The INPut File

6.2 The PARameter File

6.3 The DATA and Data CoVariance Files

6.4 Integral Data File

6.5 Interactive Input To Sammy

6.6 Other Input Files For Sammy

CHAPTER 7

Output

7.1 Line-printer Output

7.2 Output To Be Used As Input

7.3 Plot Output

7.4 Complete Set Of Partial Derivatives For Resonance Parameters

7.5 Compact Format For Parameter Covariance Information

7.6 Publication Aids

7.7 Other Output Files

CHAPTER 8

Unresolved Resonance Region

As a first step towards expansion into the unresolved resonance region, Fritz Fröhner's code FITACS [14] has been obtained and inserted into SAMMY. FITACS uses Hauser-Feshbach theory with width fluctuations. The adjustable parameters are neutron strength functions, distant-level parameters, average radiation widths (at $E = 0$), and average fission widths (at $E = 0$). The energy dependence of the radiation widths is specified via the giant dipole model, of the fission widths via Hill-Wheeler fission barrier transmission coefficients, and of the mean level spacing for s-waves via the Gilbert-Cameron composite formula. Mean spacings for $l > 0$ are given via the Bethe formula. Moldauer's prescription is used for partial cross sections. Details of the theory are presented in Section 8.1.

Initially (for release M2 of the code), FITACS was incorporated into SAMMY (as segments SAMFFF and SAMACS) in a limited fashion only. Internal changes were made, to be consistent with SAMMY notation and to use dynamic dimensioning of arrays. The M + W version of Bayes' method has replaced the fitting procedure used in FITACS. Calculation of penetrabilities was extended to all l values (FITACS had used only s, p, d, and f-waves). The output included files from which plots can be made. Results were reported in SAMMY.PAR in the same format as is used in the input file (as well as in more human-legible fashion in SAMMY.LPT).

Subsequently, additional modifications, improvements, and new features have been made in the SAMMY URR treatment:

- Partial derivatives with respect to varied parameters are calculated exactly rather than approximately.
- A more efficient integration routine has been written for the Dresner integral, Eq. (VIII A.5) ??.
- It is possible to include (and vary, if desired) a normalization for each data set.
- Elastic cross section data may be fitted.

- There is no limit on the number or type of experimental data sets. Data may be kept in separate files rather than appended to the parameter file.
- The output has been modified to conform more closely to SAMMY conventions.
- An “annotated” PARAmeter file, including key-word-based input, is the default input option, and the only option available for output. (Files in the original format can still be used for input, but options are limited with that format.)
- Different sets of average resonance parameters can be used in different energy ranges.
- Output can be produced in ENDF/B format, for both File 2 (resonance parameters) and File 32 (covariance matrices). ENDF files cannot be used for input, because the ENDF format requires a more limited theoretical description than does FITACS/SAMMY.
- The fitting procedure can be performed sequentially, in similar fashion as in the resolved resonance region. That is, output PARAmeter and COVariance files from the fit to one data set may be used as input to another run which fits another data set. [Initially, only simultaneous fitting of all data sets was permitted.]
- “No-Bayes” runs can be made: cross sections will be calculated from the resonance parameters, but no fitting will be done.

Additions being considered for future revisions of the code include the following:

- Multiple nuclides in the sample
- An option to calculate multigroup cross sections and covariances
- An option to include integral quantities in the fit
- Extensions to the theory
- Additional ENDF capability (requiring ENDF format changes)
- A link between the resolved resonance parameters and those for the unresolved region, in order to provide more consistent evaluated cross sections

- Methodologies for retroactive generation of covariance matrices, similar to that used in the resolved resonance region

Input for analysis of data in the unresolved resonance region is described in Section VIII.B. Output is described in Section VIII.C. The relationship between ENDF parameters and SAMMY/URR parameters is discussed in Section VIII.D. For an example of the use of SAMMY/URR, see [15] and test cases 73, 88, 127, 133, 134, 142, and 145.

8.1 Equations For Unresolved Resonance Region

The formulae for cross sections in the unresolved resonance region, as implemented in SAMMY, are presented in this section. The implementation is a modified form of that provided by Fritz Fröhner in his FITACS code [14]. (Please note that any mistakes in these formulae are attributable only to the author of this manual, not to Fröhner. The author is indebted to Herve Derrien for significant contributions both to the development of the code and to the composition of this section of the manual.)

Elastic cross section

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

Total cross section

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

$$\langle \sigma_c \rangle = \frac{2\pi g_c}{k_c^2} (1 - \text{Re} \langle S_{cc} \rangle) , \quad (8.1)$$

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

$$\langle S_{cc} \rangle = e^{-2i\phi_c} \frac{1 - \langle R_{cc} \rangle L_c^{0*}}{1 - \langle R_{cc} \rangle L_c^0} , \quad (8.2)$$

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

$$\langle R_{cc} \rangle = R_c^\infty + i\pi s_c, \quad (8.3)$$

with parameters defined as follows:

R_c^∞ = distant-level parameter (in input quantity);

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

$L_c^0 = (S_c - B_c) + iP_c$ (see Section 2.1) with boundary condition B_c chosen such that $S_c - B_c = 0$;

s_c = pole strength.

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

$$s_c = \tilde{S}_c \sqrt{E}/2\rho \quad (8.4)$$

where ρ is the center-of-mass momentum k_c multiplied by the channel radius a_c . **Please note that many authors choose to report \tilde{S}_c in units of 10^{-4} !**[16]

Non-elastic partial cross sections

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

$$\langle \sigma_{ab} \rangle = \frac{\pi g_a T_a T_b}{k_a^2 T} \int_0^\infty dt e^{-T_\gamma/T} \Pi \left(1 + \frac{2 T_c}{\nu_c T} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}}, \quad (8.5)$$

where the quantities to the left of the integral sign are the Hauser-Feshbach expression, and the integrand is the Moldauer prescription [17] for the width fluctuation correction factor. (A derivation of this expression, including the assumptions under which it is derived, is provided in Section ??.) Here a represents the incident channel and b the exit channel; ν_c and T_c represent the number of degrees of freedom (multiplicity) and transmission coefficient, respectively, for channel c . Subscript γ refers to photon channels. T is defined as the sum over all channels:

$$T = \sum_c T_c . \quad (8.6)$$

The transmission coefficient for neutron channels is given by

$$T_c = 1 - |\langle S_{cc} \rangle|^2 = \frac{4\pi P_c s_c}{|1 - \langle R_{cc} \rangle L_c|^2} , \quad (8.7)$$

where c is an incident channel, P and L are as defined in Section 2.1, and the other quantities are given above. For photon and fission channels, the transmission coefficients for spin J are

$$T_\gamma = 2\pi \langle \Gamma_\gamma \rangle / D_J \quad \text{and} \quad T_f = 2\pi \langle \Gamma_f \rangle / D_J , \quad (8.8)$$

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

The J -dependence of the mean level spacing is set in SAMMY/FITACS via the Bethe formula (e.g., [3]):

$$(D_J(E))^{-1} = (d(E))^{-1} \left\{ e^{\frac{-J^2}{2(\sigma(E))^2}} - e^{\frac{-(J+1)^2}{2(\sigma(E))^2}} \right\} , \quad (8.9)$$

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

$$\sigma^2 = (0.14592)(A+1)^{2/3} \sqrt{a(E + BE - PE)} , \quad (8.10)$$

in which BE represents the neutron binding energy (an input parameter) and PE the pairing energy (also an input parameter). The value for a is determined from the input quantity D , which is the mean level spacing of the $l = 0$ resonances at $E = 0$; note that D includes both $J = I - i$ and $J = I + i$, where I is the spin of the target nucleus and $i = 1/2$ is the spin of the neutron. An expression for the inverse of D can be found from Eq. 8.9 to be

$$\begin{aligned} D^{-1} &= \sum_J (D_J(E=0))^{-1} \\ &= (d(0))^{-1} \left\{ e^{\frac{-(I-\frac{1}{2})^2}{2\sigma^2}} - e^{\frac{-(I+\frac{3}{2})^2}{2\sigma^2}} \right\} ; \end{aligned} \quad (8.11)$$

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

The energy dependence of the mean level spacing is calculated with the Gilbert-Cameron composite formula [18]. Let E_x represent the excitation energy of the compound nucleus; this energy is equal to the sum of the incident neutron kinetic energy E and the neutron binding energy BE (which is an input quantity). That is to say,

$$E_x = E + BE . \quad (8.12)$$

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

$$D^{-1} \sim C_3 \frac{\exp [C_2 \sqrt{E_0 - PE}]}{(E_0 - PE)^{3/2}} \exp \left[\frac{E_x - E_0}{2} \left(\frac{C_2}{\sqrt{E_0 - PE}} - \frac{3}{E_0 - PE} \right) \right] . \quad (8.13)$$

In the code, the matching energy E_0 is set at

$$E_0 = \left[\frac{5}{2} + \frac{150}{(N + Z + 1)} \right] \quad (8.14)$$

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

$$C_2 = \sqrt{4a} \quad \text{and} \quad C_3 = \frac{1}{12\sqrt{2aq}} , \quad (8.15)$$

with q defined as

$$q = 0.14592(N + Z + 1)^{2/3} , \quad (8.16)$$

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

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

$$D^{-1} \propto C_3 \frac{\exp [C_2 \sqrt{E_x - PE}]}{(E_x - PE)^{3/2}} . \quad (8.17)$$

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

Radiation widths $\langle \Gamma_\gamma \rangle$ are assumed to depend only on parity π and on E . The energy dependence is calculated with the giant dipole resonance model. Fission widths $\langle \Gamma_f \rangle$ may vary with spin as well as parity and incident neutron energy E . Energy dependence is calculated with the Hill-Wheeler fission barrier transmission coefficients [19]. For a given J^π , the energy dependence of the fission widths is taken to be

$$\langle \Gamma_f(E) \rangle = \langle \Gamma_f(0) \rangle \frac{1 + \exp [E_{HW}/W_{HW}]}{1 + \exp [-(E - E_{HW})/W_{HW}]} , \quad (8.18)$$

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

$$\langle \Gamma_f(E) \rangle = \langle \Gamma_f(0) \rangle \frac{1 + \exp [2\pi(E_f - BE)/\hbar\omega]}{1 + \exp [-2\pi(E_x - (E_f - BE))/\hbar\omega]} , \quad (8.19)$$

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

Finally, a few words regarding the derivation of Eq. 8.5 are warranted. That derivation is based on several assumptions:

1. The Moldauer prescription [17] for width fluctuations is used. That is, the width fluctuation correction factor is introduced to compensate for the non-unity of the ratio

$$\left\langle \frac{T_a T_b}{T} \right\rangle / \frac{\langle T \rangle}{\langle T_a \rangle \langle T_b \rangle} . \quad (8.20)$$

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

The integral of Eq. 8.5 is described by Fröhner as the “width fluctuation correction or Dresner factor.” One (relatively modest) difference between SAMMY and the original

FITACS coding is the algorithm for calculating the Dresner integral; in SAMMY, the coding has been refined to increase both speed and accuracy of calculation by using a non-uniform grid designed specifically for this task. (Note: Prior to release 7 of the code, the Moldauer correction was inadvertently disabled in code. This has now been fixed.)

8.1.1 Derivation of Non-Elastic Average Cross Section

8.2 Input For Analysis Of Data In Unresolved Resonance Region

Two or more input files are required for analysis in the unresolved resonance region (URR). The first is comparable to the usual SAMMY INPut file, which may contain as few as three lines: Card set 1 of Table VIA.1?? (the title line), card set 2 (nuclide name, atomic weight, and energy range), and (at least) one line for card set 3 (alphanumeric information). Options for alphanumeric commands in the URR are

```
UNRESOLVED RESONANCE region
EXPERIMENTAL DATA ARe in separate files
ANNOTATED PARAMETER file for urr
NO ANNOTATED PARAMETER file for urr input
ENDF/B-VI FILE 2 IS wanted
PUT COVARIANCE MATRIx into endf file 32
COVARIANCE MATRIX FRom old run is used
GENERATE FILE 3 POINT-wise cross sections
DEBUG
DO NOT SOLVE BAYES Equations
USE ENERGY LIMITS AS given in the input file
PRINT PARTIAL DERIVAtives
INCLUDE MIN \& MAX ENergies when creating endf file
```

The first of these is required, as the SAMMY default is the resolved resonance region (RRR). The other alphanumeric commands are optional; their effects are described below.

The second file, the URR PARAmeter file, contains the unresolved resonance parameters. In the URR, there are several differences from the usual SAMMY conventions: To inform the code that a parameter is to be varied, FITACS assumes that, if the uncertainty is given as zero for a given parameter, then that parameter is not varied. (Hence there is no

means of providing a default value for uncertainty.) This procedure is in contrast with the usual SAMMY procedure of assigning a value (generally 1) to a flag for each varied parameter; in the future, the formats for input to the FITACS portion of SAMMY will perhaps be modified to conform to SAMMY standards.

SAMMY permits several types of modifications to the original FITACS-style PARAmeter file: (1) Experimental data may be kept in separate files. (2) Normalizations can be included (and varied) for each data set. (3) ENDF File 2 and File 32 can be produced. (4) ENDF File 3 can be produced. (5) The PARAmeter file itself may be “annotated” in order to be more legible to humans. (6) Units may be specified for various quantities. (7) Different parameters may be specified in different energy regions. (8) Direct inelastic and/or direct capture components may be added. (9) Sequential analyses may be performed. (10) The analysis may be restricted to an energy range smaller than that for which the data are defined. Options (6) through (9) are available only with the annotated PARAmeter file.

Each of the 10 options is described separately below; details are given in Tables 8.1 and 8.2. Table ?? provides a guide for the various types of energy ranges encountered during a URR analysis.

1. When the INPut file contains the phrase

EXPERIMENTAL DATA ARE in separate files,

experimental data are kept in separate file(s) rather than included as a portion of the URR PARAmeter file. Files names for individual data sets are given on the lines immediately following the INPut and PARAmeter file names in the interactive input stream. See, for example, test case tr073 run y.

2. Normalizations can be included and varied (i.e., fitted) for each data set. That is, the theoretical calculation of the cross section is modified by

$$Theory = norm \times \sigma_{calculated}, \quad (8.21)$$

where *norm* is given by the formula

$$norm = a + bE^c \quad (8.22)$$

and a , b , and c are input parameters, specified in the PARAmeter file. Note that one set of values for a , b , and c is given for each data set. Note also that there is no possibility to specify b and c unless

EXPERIMENTAL DATA ARE in separate files.

See tr073 for examples.

3. When output in ENDF File 2 format is wanted, the phrase

ENDF/B-VI FILE 2 IS wanted

must be present in the INPut file. Also include the command

DEBUG

if you wish to create an annotated file SAMMY.NDX. This annotated file contains comments that define which parameters' values are given; except for the annotations, this file is identical to the SAMMY.NDF.

One additional SAMMY input file must be provided; the name for this file is given in the input stream after the name of the PARAmeter file (or after the COVariance file if it exists) and before the name(s) of any data files. This NDF file provides information regarding the specifics of the ENDF file to be created. The NDF file is in key word format, and contains only the following parameters:

Z = charge

A = atomic number

Mat = ENDF material number

NUmber of energy points = number

Energy number 1 = value of energy-point

Only the one or two characters in capitals are required; others are optional. The value is given following the equal sign. One or the other of NU...= and E...= must be present. (If both are present, NU...= will be ignored.)

The number of energy points specifies at how many equally spaced points per energy region the parameter values will be printed into the ENDF file. Values may also be printed at Emin and Emax, the limits of the analysis, if the phrase

`INCLUDE MIN & MAX ENergies in endf file`

is given in the INPut file. For example, for 3 points per region and 5 regions, a total of $3 \times 5 + 2 = 17$ sets of values would be given in the ENDF file.

If, instead of having a certain number of points for each energy range, specific values of energy are wanted in the ENDF file, then the alternative `E...=` should be specified. Subsequent energies are given one per line, with or without the key word `E...=` prior to the value. These energy values should be the last entries in this file.

See test cases tr073 and tr127 for examples. Runs a, b, e, and f of tr127 use `NU...=` key word, while run g uses the `E...=` key word.

To also obtain the associated covariance file (ENDF File 32), include the phrase

`PUT COVARIANCE MATRix into endf file 32`

in the INPut file. See test case tr128 runs j and k for examples.

4. ENDF File 3 output (point-wise cross sections, in file SAMMY.FL3) can be generated when the command

`GENERATE FILE 3 POINt-wise cross sections`

is included in the INPut file. The energy grid for this cross section is as defined by the input data sets. If the `DEBUG` command is also used, an annotated ENDF File 3 (SAMMY.FLX) output file is also produced. See test case tr073, runs n through t, for examples.

5. Two modes, annotated and unannotated, are available for the URR PARAmeter file:

The unannotated mode is essentially equivalent to Fröhner's original FITACS file (which includes both parameters and data). Formats for this file are described in Table 8.1; all numbers, both integer and real, are specified with F10 formats. To use this mode, the INPut file must contain the command

`NO ANNOTATED PARAMETER file for urr input`

Test case tr073 has examples of this input mode.

The annotated PARAmeter file is described in detail in Table 8.2; this is the default mode for SAMMY. With this option, some parameters are entered by key word; other

parameter lists have headings to define which parameters are in the list. See, for example, test case tr073 run g, or test cases tr128.

6. Units may be specified for various energy-related quantities by including the phrase “in eV”, “in keV”, or “in MeV” in the appropriate location in the PARAmeter file. (Note that, as always with SAMMY input, capitalization is irrelevant.) If units are not specified, defaults are as given in Table 8.2 (i.e., MeV for binding energy and pairing energy, eV for all others). The quantities for which units may be specified are as follows:

excitation energies for inelastic states

binding energy

pairing energy

energy maxima for the different ranges (see (7) below)

energies for direct inelastic contribution (see (8) below)

See in particular tr128 run l (letter “l” not number “one”) for examples.

7. Different parameter values may be used in different energy ranges; see Table 8.2, card sets 4-7, for input details. See test case tr128 for examples.
8. A direct inelastic component may be added to the inelastic and total cross sections, and/or a direct capture component added to the capture and total cross sections. These components are specified numerically on grids chosen by the user; SAMMY interpolates linearly between grid points. See card set 11 of Table 8.2 for details. Examples are in tr088 and tr134.
9. Although many data sets can be analyzed simultaneously in URR, SAMMY also permits sequential runs similar to those used in the RRR. For details, see the description of the SAMMY.COV file in the next section, §8.3. For examples, see test case tr073 runs a and g.
10. The default choice for energy range in the URR is to include all energies for which data are available. However, the analysis may be restricted to a smaller energy range by including the command

USE ENERGY LIMITS AS given in the input file

in the INPut file. See test case tr073 runs j, k, l for examples.

Table 8.1: Formats for original PARAmeter file for treatment of the unresolved resonance region

Card Set	Line No.	Description
1	1-4	First four lines are alphanumeric title
2	1	Number of iterations, fitting tolerance (essentially delta chi squared). Note that integers are to be specified as real numbers. All formats are F10.
	2	Mass in amu, radius in Fermi (or use default), neutron binding energy in MeV, pairing energy PE in MeV. Again, formats are F10; note that the energy units are MeV, as opposed to the usual SAMMY standard of eV.
3	1,2,...	Center-of-mass excitation energy (in eV), spin, and parity for the n th target level (beginning with ground state). Repeat as many times as needed.
	Last	(Blank)
4	1	Strength function \tilde{S}_c , uncertainty, distant-level parameter R_c^∞ , uncertainty, radiation width $\langle\Gamma_\gamma\rangle$ in eV, uncertainty, mean level spacing D in eV for $l = 0$ <i>Note: Some authors choose to list strength function in units of 10^{-4}[16]</i>
	2	Strength function, uncertainty, distant-level parameter, uncertainty, radiation width in eV, uncertainty, for $l = 1$
	3	Strength function, uncertainty, distant-level parameter, uncertainty, radiation width in eV, uncertainty, for $l = 2$
	4,5,...	As above, for higher l values as needed
	Last	(Blank)
5	1	For the lowest J value for $l = 0$, - Average fission width $\langle\Gamma_f\rangle$ (eV) - Degree of freedom ν_f for fission width distribution - Hill-Wheeler threshold energy E_{HW} - Hill-Wheeler threshold width W_{HW} - Uncertainty on the average fission width
	2,3,...	Repeat line 1 for each possible value of J for $l = 0$.

	4,5,...	<p>Repeat lines 1-3 for each possible value of J for $l = 1, 2, \dots$</p> <p>For a given spin J and parity (even or odd l), only one set of values is actually used for $\langle \Gamma_f \rangle$ and the other parameters. Nevertheless, all J and l must be included in this list. Only the values associated with the lowest l value will be used for the calculations; the other values will be ignored.</p> <p>For example, the ground state of ^{235}U is $7/2^-$.</p> <ul style="list-style-type: none"> - For $l = 0$, $J^\pi = 3^-, 4^-$. - For $l = 1$, $J^\pi = 2^+, 3^+, 4^+, 5^+$. - For $l = 2$, $J^\pi = 1^-, 2^-, 3^-, 4^-, 5^-, 6^-$. - The 3^- and 4^- values used in the calculations will be those given for $l = 0$. The values given for $J^\pi = 3^-$ and 4^- with $l = 2$ will be ignored.
	Last	(Blank)
6	1	Type of cross-section data (TOTAL , CAPTURE , FISSION , or INELASTIC)
	2	Uncertainties are RELATIVE or ABSOLUTE
	3	Energy, cross section, and uncertainty for first data point. Normalization and uncertainty (a and Δa) for this data set.
	4, ...	Energy, cross section, uncertainty. (Note: if RELATIVE then these need to be specified only for first data point; the others are assumed to be the same.)
	Last	(Blank)
6x	All	Repeat card set 6 as many times as needed, in any order
7	1	The single word “ NORMALIZATION ”. (Card set 7 is present only if the command “ EXPERIMENTAL DATA ARE in separate files ” appears in card set 3 of the INPUT file.)
	2	Type of cross section, normalization parameters $a, \Delta a, b, \Delta b, c, \Delta c$, where the normalization for this data set is given by $norm = a + bE^c$
	3, etc.	Repeat Line 2 once for each data set. Normalizations must appear in the same order in which the data sets appear. SAMMY will check to be sure the data types are consistent.

Table 8.2: Formats for annotated PARAmeter file for treatment of the unresolved resonance region

Card Set	Line No.	Description															
1	1,2,...	Alphanumeric title, as many lines as desired. Printed but otherwise ignored.															
	Last	----- (First four characters must be hyphens [minus signs]; this ends the title. Other characters on this line are printed but ignored.)															
2	1,2,...	Key word = Value. Possible keywords here are <table> <thead> <tr> <th>Key word</th><th>Meaning</th><th>Default</th></tr> </thead> <tbody> <tr> <td>ITERations</td><td>number of iterations</td><td>3</td></tr> <tr> <td>TOLerance</td><td>fitting tolerance</td><td>0.005</td></tr> <tr> <td>RADius</td><td>radius in F</td><td>1.23 AW1/3+0.8</td></tr> <tr> <td>AW (atomic weight)</td><td>mass in amu</td><td>(no default)</td></tr> </tbody> </table> Only the letters in capitals are required; the values may be in any format.	Key word	Meaning	Default	ITERations	number of iterations	3	TOLerance	fitting tolerance	0.005	RADius	radius in F	1.23 AW1/3+0.8	AW (atomic weight)	mass in amu	(no default)
Key word	Meaning	Default															
ITERations	number of iterations	3															
TOLerance	fitting tolerance	0.005															
RADius	radius in F	1.23 AW1/3+0.8															
AW (atomic weight)	mass in amu	(no default)															
	Last	(Blank)															
3	0	“----” An optional line of minus signs may be inserted; this line will be ignored by the code.															
	1	“ELAStic and inelastic states”. Only the first four characters are necessary, others are optional. Units of excitation energy are eV unless specified anywhere on this line (after the first four characters) as “in eV”, “in keV”, or “in MeV”.															
	2,3,...	Center-of-mass excitation energy, spin, and parity for the n th target level (beginning with ground state). Format must be 3F10 (ten characters per number, three numbers on a line, decimal points must be included).															
	Last	(blank)															
4	0	“----” Optional.															
	1,2,...	Key word = Value. Possible keywords here are <table> <thead> <tr> <th>Key word</th><th>Meaning</th><th>Default</th></tr> </thead> <tbody> <tr> <td>BINDing energy</td><td>neutron binding energy (MeV)</td><td>(none)</td></tr> <tr> <td>PAIring energy</td><td>pairing energy (MeV)</td><td>(none)</td></tr> </tbody> </table> Only the letters in capitals are required; the values may be in any format. To override the default units, insert a phrase “in eV”, “in keV”, or “in MeV” after the key word and before the equal sign. Examples: Binding Energy (in eV) = 6536000. Pairing energy in eV = 1610000.	Key word	Meaning	Default	BINDing energy	neutron binding energy (MeV)	(none)	PAIring energy	pairing energy (MeV)	(none)						
Key word	Meaning	Default															
BINDing energy	neutron binding energy (MeV)	(none)															
PAIring energy	pairing energy (MeV)	(none)															
	Last	(blank)															
5	0	“----” Optional.															
	1	“STReng del_s distnt del_d gamma width del_g bethed” (Only first three characters are necessary. This line indicates that strength functions, distant-level parameters, etc., are coming next.)															

	2	Strength function \tilde{S}_c , uncertainty, distant-level parameter R_c^∞ , uncertainty, radiation width $\langle\Gamma_\gamma\rangle$ in eV, uncertainty, mean level spacing D in eV for $l = 0$. F10 formats. <i>Note: Some authors choose to list strength function in units of 10^{-4}[16]</i>
	3	Strength function, uncertainty, distant-level parameter, uncertainty, radiation width in eV, uncertainty, for $l = 1$
	4	Strength function, uncertainty, distant-level parameter, uncertainty, radiation width in eV, uncertainty, for $l = 2$
	5,6,...	As above, for higher l values as needed
	Last	(blank)
6	0	“----” Optional.
	1	“FISSion width fnu ethr wthr del_fission width” (Only first three characters are necessary. This line indicates that fission parameters are coming next.)
	2	For the lowest J value for $l = 0$, Average fission width $\langle\Gamma_f\rangle$ (eV) Degree of freedom ν_f for fission width distribution Hill-Wheeler threshold energy E_{HW} Hill-Wheeler threshold width W_{HW} Uncertainty on the average fission width J, l The first line contains the lowest J value associated with $l = 0$. Formats are F10 for everything except the l -value, which is I5 (i.e., the right-most column is # 65). Inclusion of J and l in the input file is optional but recommended.
	3,4,...	Repeat line 2 for each possible value of J for $l = 0$
	5,6,...	Repeat lines 2-4 for each possible value of J for $l = 1, 2, \dots$. For a given spin J and parity (even or odd l), only one set of values is actually used for $\langle\Gamma_f\rangle$ and the other parameters. Nevertheless, all J and l must be included in this list. Only the values associated with the lowest l value will be used for the calculations; the other values will be ignored. For example, the ground state of ^{235}U is $7/2^-$. For $l = 0$, $J^\pi = 3^-, 4^-$. For $l = 1$, $J^\pi = 2^+, 3^+, 4^+, 5^+$. For $l = 2$, $J^\pi = 1^-, 2^-, 3^-, 4^-, 5^-, 6^-$. The 3^- and 4^- values used in the calculations will be those given for $l = 0$. The values given for $J^\pi = 3^-$ and 4^- with $l = 2$ will be ignored.
	Last	(blank)
7	0	“----” optional line

	1	<p>Key word = Value. Only one possible keyword is permitted here:</p> <table> <tr> <th><u>Key word</u></th><th><u>Meaning</u></th><th><u>Default</u></th></tr> <tr> <td>ENERgy maximum</td><td>maximum energy in this region (eV)</td><td>(none)</td></tr> </table> <p>Only the letters in capitals are required; the values may be in any format.</p> <p>To override the default units, insert a phrase “in eV”, “in keV”, or “in MeV” after the key word and before the equal sign.</p> <p>Examples: Energy maximum in MeV = 0.15.</p>	<u>Key word</u>	<u>Meaning</u>	<u>Default</u>	ENERgy maximum	maximum energy in this region (eV)	(none)
<u>Key word</u>	<u>Meaning</u>	<u>Default</u>						
ENERgy maximum	maximum energy in this region (eV)	(none)						
4-7	all	Repeat card sets 4-7, once for each energy region, as many times as needed. Alternatively, repeat only line 1 of card set 7, in which case the starting parameter values are assumed to be identical to those in the previous energy region.						
8		In either case, end with a line saying “END of resonance parameter description”.						
9	0	“----” optional line						
	1	<p>Type of cross-section data (TOTAL, CAPTure, FISSion, or INELastic).</p> <p>Card set 9 will be omitted from this file if the command “EXPERIMENTAL DATA ARE in separate files” appears in the INPut file.</p>						
	2	Uncertainties are RELAtive or ABSOLute. (Only “RELA” or “ABSO” is needed.)						
	3	<p>Energy (eV), cross section (barn), uncertainty (barn if ABSOLute, dimensionless if RELAtive) for first data point.</p> <p>Norm and unc (a and Δa) for this data set.</p> <p>Format is 3F10.</p>						
	4,5,...	Energy, cross section, uncertainty (Note: if RELAtive, then need specify only for first data point, rest are assumed to be the same.)						
	Last	(blank)						
9x	all	Repeat card set 9 as many times as needed, in any order						
10	0	“----” optional line						
	1	“NORMAlization”. [Card set 10 may be present only if INPut file specifies “experimental data are in separate files”.]						
	2	Type of cross section, normalization parameters $a, \Delta a, b, \Delta b, c, \Delta c$, where the normalization for this data set is given by $norm = a + bE^c$						
	3,4,...	Repeat once for each data set. Note that normalizations must appear in the same order in which the data sets appear. SAMMY will check to be sure the data types are consistent.						
	Last	(blank)						
10a	0	“----” optional line						
	1	“EARLier normalization”. [Card set 10a, an alternative to card set 10, is to be used only if an earlier SAMMY run has produced a covariance file.]						

	2	N1, N2, ... Nlast, in [40I2] format. Here N1 is the ordering of the first data set for this run, as it appeared in previous SAMMY runs; see test case tr145 for illustrative examples.						
	Last	(blank)						
11	0	“----” optional line						
	1	“DIRECT Inelastic contribution”, <i>or</i> “DIRECT Capture contribution”. Note that eight characters (rather than the usual four) are required here.						
	2	<p>Energy = value, Sigma = value. Both key words (and both values) must be on the same line.</p> <table><tr><td><u>Key word</u></td><td><u>Meaning</u></td></tr><tr><td>Energy</td><td>Energy in (eV)</td></tr><tr><td>Sigma</td><td>Direct inelastic cross section (b) at that energy</td></tr></table> <p>To use different units, insert a phrase “in eV”, “in keV”, or “in MeV” after the key word “Energy”.</p>	<u>Key word</u>	<u>Meaning</u>	Energy	Energy in (eV)	Sigma	Direct inelastic cross section (b) at that energy
<u>Key word</u>	<u>Meaning</u>							
Energy	Energy in (eV)							
Sigma	Direct inelastic cross section (b) at that energy							
	3,4,...	<p>Repeat line 2 as many times as required.</p> <p>Note that card set 11 may be omitted if the contribution of the direct inelastic cross section is negligible or unknown.</p>						

8.3 Output From Analysis In Unresolved Resonance Region

As with the resolved resonance region, each SAMMY/URR run may produce several output files:

1. The SAMMY.LPT file contains details of the calculations.
2. For runs which involve the solution of Bayes' equations and hence the generation of updated parameter values (a "Bayes run" as opposed to a "no-Bayes run" which simply calculates cross sections), an output file SAMMY.PAR is provided in the annotated form described in Table 8.2. (This file, of course, is quite different from the file by the same name produced in a resolved resonance region run.)
3. For Bayes runs, a COVariance file SAMMY.COV is produced, which contains (among other things) the final parameter covariance matrix; see below for more detail.
4. Files SAMMY.NDF and SAMMY.N32 contain the URR portion of ENDF File 2 and 32, respectively; these files are produced when the appropriate command is in the INPut file.
5. Files SAMMY.NDX and SAMMY.N3X contain the same information as in SAMMY.NDF and SAMMY.N32 respectively, but also include comment lines defining the parameters whose values are given. Only the uncertainty values are given in SAMMY.N3X; correlations are printed only in SAMMY.N32.

The binary COVariance file SAMMY.COV can be used as input to a subsequent SAMMY run that uses the same R-matrix parameters but different data sets and different normalizations, in a similar fashion to sequential runs in the RRR. There are slight differences, however, in the usage of this COVariance file; no auxiliary program comparable to SAMAMR is required here, as there is only one type of data-reduction parameter (the normalizations). The user must simply rename and modify the SAMMY.PAR file to contain the appropriate normalization parameters for the data sets about to be analyzed. The output PARameter file will contain card set 10a of Table 8.2; PARameter files to be used as input will use either card set 10 (for new data sets for which the normalizations have not yet been defined) or card set 10a (to re-use normalizations already defined for the current data sets). See test case tr145 for examples.

To use an output SAMMY.PAR file as input to a new run without the accompanying COV file, it is necessary to delete the first line of the file; this line reads as follows:

`COVARIANCE MATRIX FRom old run is used`

When the COV file is to be used (for sequential runs), keep this line in the PARameter file. Test cases tr073, tr088, tr127, tr128, tr133, tr145, and others provide sample input and output for URR calculations.

CHAPTER 9

Evaluation Connection

9.1 CSEWG Constants

CHAPTER 10

Auxiliary Programs

- 10.1 angodf: Convert From Energy/Angle To Angle/Energy
- 10.2 convrt: Convert From Refit Input to Sammy or Vice Versa
- 10.3 samamr: Add, Mix, or Recover Variables
- 10.4 samamx: Modify a Single Value
- 10.5 samcpr: Compare Results
- 10.6 samdis: Statistical Distributions
- 10.7 samftz: Fix TZERO (t_0)
- 10.8 samort: Plot The Oak Ridge Resolution Function
- 10.9 samplt: Alternative Form For Plot Files
- 10.10 samqua: Resonance Quantum Numbers
- 10.11 samrpt: Plot RPI Resolution Function
- 10.12 samrst: Plot Resolution Function
- 10.13 samsmc: Monte Carlo Multiple Scattering
- 10.14 samsta: Staircase Plots
- 10.15 samthn: Thinning Data
- 10.16 suggel: Estimating L and J
- 10.17 samrml: Calculate Cross Sections From Endf File 2
- 10.18 samgy2: Smooth The Tabulated Y2 Function

CHAPTER 11

Helpful Hints

- 11.1 Strategy For Data Evaluation With Sammy**
- 11.2 Procedures To Follow When You Have Problems**
- 11.3 Miscellaneous Comments And Suggestions**

CHAPTER 12

Examples

12.1 Tutorial

12.2 Test Cases

12.3 Monte Carlo Simulations of Multiple-scattering Corrections

CHAPTER 13

Computer Code

Use of the more modern CMake system should remove most of computer dependence now.

- 13.1 Dynamic Allocation Of Array Storage
- 13.2 Use Of Temporary Data Files To Store Intermediate Results
- 13.3 Division Of The Program Into Autonomous Segments
- 13.4 Computer-specific Features
- 13.5 ORELA Data Format
- 13.6 Configuration And Distribution System

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CHAPTER 14

Appendices