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Updated Users' Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations

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ACKNOWLEDGMENTS FOR REVISION 1

Special thanks go to Sue Damewood for typing and assembling this document, and to Gerard de Saussure, without whose patient insistence many of the improvements described in this report would not have been made.

ABSTRACT

In 1980 the multilevel multichannel R-matrix code SAMMY was released for use in analysis of neutron data at the Oak Ridge Electron Linear Accelerator. Since that time, SAMMY has undergone significant modifications: (1) User-friendly options have been incorporated to streamline common operations and to protect a run from common user errors. (2) The Reich-Moore formalism has been extended to include an optional logarithmic parameterization of the external R-matrix, for which any or all parameters may be varied. (3) The ability to vary sample thickness, effective temperature, matching radius, and/or resolution-broadening parameters has been incorporated. (4) To avoid loss of information (i.e., computer round-off errors) between runs, the "covariance file" now includes precise values for all variables. (5) Unused but correlated variables may be included in the analysis.

Because of these and earlier changes, the 1980 SAMMY manual is now hopelessly obsolete. This report is intended to be complete documentation for the current version of SAMMY. Its publication in looseleaf form will permit updates to the manual to be made concurrently with updates to the code itself, thus eliminating most of the time lag between update and documentation.

ABSTRACT FOR REVISION 1

In August of 1984 the users' guide for version P of the multilevel multichannel R-matrix code SAMMY was published. Recently, major changes within SAMMY have led to the creation of version O, which is documented in this report. Among these changes are: (1) an alternative matrix-manipulation method for use in certain special cases; (2) division of theoretical cross-section generation and broadening operations into separate segments of the code; (3) an option to use the multilevel Breit-Wigner approximation to generate theoretical cross sections; (4) new input options; (5) renaming all temporary files as SAM??.DAT; (6) more sophisticated use of temporary files to maximize the number of data points that may be analyzed in a single run; and (7) significant internal restructuring of the code in preparation for changes described here and for planned future changes.

INTRODUCTION TO REVISION 1

Changes documented in this revision are as follows:

1. An alternative matrix-manipulation method, the *(I+Q)* inversion scheme, has been devised (see Sect. II). Use of this scheme requires that the data covariance matrix be diagonal, and that the number of data points be much larger than the number of varied parameters. When these two requirements are met, the *(I+Q)* inversion scheme uses significantly less computer core than does the original method, the *(N+V)* inversion scheme.
2. Cross-section calculations and broadening operations are now performed in two separate stand-alone segments of the computer code, since they are in fact two distinct operations. Within the broadening segment, the various broadening procedures have been sufficiently disentangled that one can, e.g., Doppler-broaden but not resolution-broaden.
3. The multilevel Breit-Wigner approximation may be used to generate cross sections; see Sect. III.C.
4. New input options are explained in the tables of Sect. VI. NOTE: No input has been changed; a user need not fear that his or her old INP or PAR files are obsolete.
5. All temporary files are now called SAM??.DAT with the question marks replaced by FORTRAN unit numbers. Thus if a run bombs or is aborted, all SAMMY files may be deleted with the single command "DEL SAM??.DAT". CAUTION: If you wish to discuss with the author why your job bombed, it would be best *not* to delete these files first. See Sect. X.B.
6. It is now sometimes possible to analyze very large data sets, of a thousand or more points, in one shot. This is due to the invention of a sophisticated "bookkeeping" system to use temporary files rather than in-core storage for larger arrays. To decide whether your particular case will fit into the PDP10, run the code SAMEST; i.e., type "R SAMEST" interactively, and answer the questions asked. Caveat: array sizes given are estimates only, not to be trusted absolutely.
7. The internal FORTRAN coding of SAMMY, version O, is considerably different from version P. (While users of the code will not notice these changes, anyone wishing to implement SAMMY on his or her own computer is warned to use one version or the other and not intermix them.) A consistent nomenclature for the several types of varied parameters has been developed. Subroutines have been subdivided so that each routine deals with a single well-defined operation. Attempts have been made to standardize FORTRAN usage, to minimize necessary changes when converting to another computer. Many of these changes were designed in preparation for future revisions, including (a) more correct treatment of resolution broadening, (b) inclusion of data parameters (such as normalization or background subtraction) as varied parameters, and (c) proper treatment of multiple isotopes.

II.A.1. Outline of Derivation of Bayes' Equations

Bayes' theorem may be written in the form

$$p(P|DX) \propto p(P|X)p(D|PX) \qquad \text{(IIA1.1)}$$

where

1. P represents the parameters of the (extended) R-matrix theory and D represents the experimental data to be analyzed.
2. X represents "background" or "prior" information such as the data from which prior knowledge of the parameters P was derived. X is assumed to be independent of D.
3. $p(P|DX)$ is the probability for the value of the parameters conditional upon the new data D and is what we seek. It is conventional to call $p(P|DX)$ the posterior probability. Since P represents several parameters, $p(P|DX)$ is a joint probability density function (joint pdf). The expectation values of P times $p(P|DX)$ are taken as the new estimates for the parameters; the associated covariance matrix gives us a measure of how well the parameters are determined and of the inter-dependencies of those determinations.
4. $p(D|PX)$ is the probability density function for observing the data D given that the parameters P are correct. It is a function of the parameters P of the model and is proportional to the likelihood function of the data D.
5. $p(P|X)$ is the joint pdf for the value of the parameters P of the model, prior to consideration of the new data D; it is known as the prior joint pdf. The expectation values of P times $p(P|X)$ are the prior estimates for the values of the parameters; the associated covariance matrix gives a measure of how well the parameters are known before consideration of the new data.
6. The constant of proportionality in Eq. (IIA1.1) can be determined from the normalization condition.

Let $P=\{P_k\}$ for $k=1$ to K be the set of all parameters of the theoretical model to be considered. The joint pdf $p(P|X)$ is assumed to be a joint normal pdf having as expectation value the vector $\bar{P}$ and the covariance matrix M. Under this assumption the pdf may be written

$$p(P|X) \propto \exp\left[-\tfrac{1}{2}(P-\bar{P})^t\ M^{-1}\ (P-\bar{P})\right] , \qquad \text{(IIA1.2)}$$

where the superscript t denotes the transpose.

The experimental data is represented by a data vector D whose components D_l are the L data points. The experimental conditions are assumed to be such that the data D (i.e., the D_l's) have a joint normal distribution with mean $T=T(P)$ and covariance matrix V. The likelihood function is then

$$p(D|PX) \propto \exp[-\tfrac{1}{2}(D-T)^t\ V^{-1}(D-T)] . \qquad \text{(IIA1.3)}$$

Here T represents theory (i.e., calculated values of cross section or transmission), and the covariance matrix V represents not only the experimental "errors" of the data, but also any theoretical "errors" resulting from approximations used in calculating T. Obviously V need not be diagonal.

Combining Eqs. (IIA1.1, .2, and .3) gives an expression for the pdf of P after consideration of new data D [i.e., for $p(P|DX)$], expressed in terms of the "true" value T. What is needed, however, is an expression for $p(P|DX)$ expressed in terms of the parameters P. This is obtained formally by considering T a function of P, performing a Taylor expansion about $\bar{P}$ [the expectation value of $p(P|X)$], and keeping only the linear terms:

$$T(P) \simeq \bar{T} + G(P-\bar{P}) \ , \tag{IIA1.4}$$

where $\bar{T}$ is equal to $T(\bar{P})$. The elements of G are the partial derivatives of T_n with respect to the parameters P_k, evaluated at $P=\bar{P}$.:

$$G_{nk} = \left.\frac{\partial T_n}{\partial P_k}\right|_{P=\bar{P}} \qquad \begin{array}{l} \text{for } n=1,2,\ldots,L \\ \text{for } k=1,2,\ldots,K \end{array} \tag{IIA1.5}$$

Since T is a vector of dimension L (equal to the number of data points), and P is a vector of dimension K (equal to the number of parameters), this "sensitivity matrix" G is of dimension $L \times K$.

Substituting Eq. (IIA1.4) into Eq. (IIA1.3) and using Eq. (IIA1.2), we obtain for the posterior joint pdf [Eq. (IIA1.1)]:

$$p(P|DX) \propto \exp[-\tfrac{1}{2}\{(P-\bar{P})^t M^{-1}(P-\bar{P}) + \tag{IIA1.6}$$

$$(D-\bar{T}-G(P-\bar{P}))^t V^{-1} (D-\bar{T}-G(P-\bar{P}))\}] \ .$$

Because of the three basic assumptions we have made, i.e.,

i. the prior joint pdf is a joint normal,

ii. the likelihood function is a joint normal, and

iii. the true value is a linear function of the parameters,

it follows that the posterior joint pdf is also a joint normal. Denoting its expectation value by $\bar{P}'$ and its covariance matrix by M', we may write:

$$p(P|DX) \propto \exp\ [-\tfrac{1}{2}(P-\bar{P}')^t\ M'^{-1}\ (P-\bar{P}')] \ . \tag{IIA1.7}$$

As shown in the next subsection, equating the linear and quadratic terms of the exponents in Eqs. (IIA1.6) and (IIA1.7) yields our final results, hereafter referred to as Bayes' equations:

$$\bar{P}' - \bar{P} = MG^t\ (N + V)^{-1}\ (D-T) \ , \tag{IIA1.8}$$

$$M-M' = MG^t\ (N + V)^{-1}\ G\ M \ , \tag{IIA1.9}$$

where the $L \times L$ matrix N is defined as

$$N = G\ M\ G^t \ . \tag{IIA1.10}$$

The matrix N is the covariance matrix of the joint pdf for the true value of the data based upon our prior pdf for the value of the parameters. Since this form of Bayes' equations involves the inverse of $(N + V)$, within SAMMY it is known as the "$(N + V)$ inversion scheme" (see Table VIA.2); this is the form implemented in all earlier versions of SAMMY.

An alternative form for Bayes' equations is

$$\bar{P}' = \bar{P} + M(I + Q)^{-1}G'V^{-1}(D - T) \qquad \text{(IIA1.11)}$$

$$M' = M(I + Q)^{-1} \qquad \text{(IIA1.12)}$$

where the $K \times K$ nonsymmetric matrix Q is defined as

$$Q = G'V^{-1}GM \qquad \text{(IIA1.13)}$$

This set of equations is known within SAMMY as the "$(I + Q)$ inversion scheme."

In the limit where the matrix M is diagonal and its elements tend to infinity, Bayes' equations become the familiar least-squares equations. Algebraic details for the $(N + V)$ inversion scheme [i.e., for Eqs. (IIA1.8) through (IIA1.10)] are given in [NL82].

Because the linearity condition [Eq. (IIA1.4)] may be only approximately correct, it is necessary to alter Bayes' equations slightly to permit iteration to an accurate solution. (Details are given in Subsection II.A.3.) It is the iterative form of Bayes' equations which is implemented in the code SAMMY.

Finally, we note that the derivation of Bayes' equations which we present in Subsection II.A.2 is not the only possible derivation. Alternative derivations can be found in [JM80] and [AG73].

II.A.2. Details of the Derivation

In Subsection II.A.1, we stated that Bayes' equations may be derived directly from Bayes' theorem,

$$p(P|DX) \propto p(P|X)p(D|PX), \tag{IIA2.1}$$

provided the three basic assumptions are met. These assumptions are:

i. the prior pdf is a joint normal. That is, the pdf for the parameters, prior to consideration of the data D, is

$$p(P|X) \propto \exp\{-\tfrac{1}{2}(P-\bar{P})'M^{-1}(P-\bar{P})\} \tag{IIA2.2}$$

ii. the likelihood function is a joint normal. That is, the pdf for the experimental data is

$$p(D|PX) \propto \exp\{-\tfrac{1}{2}(D-T)'V^{-1}(D-T)\} \tag{IIA2.3}$$

where T is a function of the parameter P.

iii. the true value is a linear function of the parameters. That is, a Taylor expansion of the theoretical values around the prior expectation values of the parameters truncates after the linear term:

$$T = \bar{T} + G(P-\bar{P}) \tag{IIA2.4}$$

where the sensitivity matrix G is defined by

$$G_{ik} = \left.\frac{\partial T_i}{\partial P_k}\right|_{P=\bar{P}} \tag{IIA2.5}$$

and the theoretical value $\bar{T}_i$ (i.e., $\bar{T}$ for data point i) is also evaluated at $P=\bar{P}$.

Given these three assumptions, the posterior pdf $p(P|DX)$ is also a joint normal distribution and may be written

$$p(P|DX) \propto \exp\{-\tfrac{1}{2}(P-\bar{P}')'(M')^{-1}(P-\bar{P}')\}\ . \tag{IIA2.6}$$

Substituting Eq. (IIA2.2) through (IIA2.6) into Eq. (IIA2.1) and equating the exponents yield, in matrix form,

$$(P-\bar{P}')'(M')^{-1}(P-\bar{P}')+Y=(P-\bar{P})'M^{-1}(P-\bar{P}) \tag{IIA2.7}$$
$$+[D-\bar{T}-G(P-\bar{P})]'V^{-1}[D-\bar{T}-G(P-\bar{P})]$$

where Y represents the normalization constant and is independent of P. Setting $P-\bar{P} = P-\bar{P}'+\bar{P}'-\bar{P}$ in Eq. (IIA2.7), and rearranging terms, we obtain

$$(P-\bar{P}')'(M')^{-1}(P-\bar{P}')+Y=(P-\bar{P}')'(M^{-1}+G'V^{-1}G)(P-\bar{P}') \qquad \text{(IIA2.8)}$$

$$+(P-\bar{P}')'[(M^{-1}+G'V^{-1}G)(\bar{P}'-\bar{P})-G'V^{-1}(D-\bar{T})]$$

$$+[(\bar{P}'-\bar{P})'(M^{-1}+G'V^{-1}G)-(D-\bar{T})'V^{-1}G](P-\bar{P}')$$

$$+(\bar{P}'-\bar{P})'M^{-1}(\bar{P}'-\bar{P})$$

$$+[D-\bar{T}-G(\bar{P}'-\bar{P})]'\ V^{-1}[D-\bar{T}-G(\bar{P}'-\bar{P})]\ .$$

Because Eq. (IIA2.8) must hold for all values of P, we may equate terms quadratic, linear, or constant in $(P-\bar{P}')$. From the quadratic we obtain Bayes' equation for updating the covariance matrix, and from the linear we obtain Bayes' equation for updating parameter values. The constant yields the invariant "Bayesian χ^2".

We begin with the covariance matrix; the coefficients of the quadratic $(P-\bar{P}')' \cdots (P-\bar{P}')$ in Eq. (IIA2.8) yield

$$(M')^{-1} = M^{-1} + G'\ V^{-1}\ G \qquad \text{(IIA2.9)}$$

Algebraic manipulation of this matrix equation gives

$$(M')^{-1}M = M^{-1}M + G'\ V^{-1}GM = I + G'V^{-1}GM$$

or

$$M'(M')^{-1}M = M' + M'G'V^{-1}GM$$

which reduces to

$$M = M'(I + G'V^{-1}GM) \qquad \text{(IIA2.10)}$$

where I represents the identity matrix. Thus we may define

$$Q = G'V^{-1}GM \qquad \text{(IIA2.11)}$$

as in Eq. (IIA1.13) and obtain from Eq. (IIA2.10) the result

$$M' = M(I + Q)^{-1} \qquad \text{(IIA2.12)}$$

which is exactly Bayes' equation for updating the covariance matrix, in the $(I + Q)$ inversion scheme, Eq. (IIA1.12).

To obtain the $(N + V)$ version of Bayes' equations for the covariance matrix, further algebraic manipulation is required. Using the identity

$$X^{-1} = Z(XZ)^{-1} \tag{IIA2.13}$$

with

$$X = I + G'V^{-1}GM = I + Q \tag{IIA2.14}$$

and

$$Z = G'(N + V)^{-1}G$$

gives, from Eq. (IIA2.12)

$$M' = MG'(N+V)^{-1}G \quad [(I + G'V^{-1}GM)G'(N+V)^{-1}G]^{-1}$$

$$= MG'(N+V)^{-1} \; G[G'(N+V)^{-1}G + G'V^{-1}GMG'(N+V)^{-1}G]^{-1} \tag{IIA2.16}$$

Setting

$$N = GMG' \tag{IIA2.17}$$

and rearranging give

$$M' = MG'(N+V)^{-1}G[G'\{(I+V^{-1}N)(N+V)^{-1}\}G]^{-1} \tag{IIA2.18}$$

The quantity in curly brackets in Eq. (IIA2.18) is equal to V^{-1}; making that substitution and introducing the identity $V^{-1}V = I$ into that equation give

$$M' = MG'(N+V)^{-1}VV^{-1}G[G'V^{-1}G]^{-1} \tag{IIA2.19}$$

Replacing V by $N + V - N$ then gives

$$M' = MG'(N+V)^{-1}\{N+V - N\}V^{-1}G[G'V^{-1}G]^{-1} \tag{IIA2.20}$$

or

$$M' = MG'V^{-1}G[G'V^{-1}G]^{-1} - MG'(N+V)^{-1}GMG'V^{-1}G[G'V^{-1}G]^{-1} \tag{IIA2.21}$$

in which we have replaced N by GMG'. This reduces immediately to

$$M' = M - MG'(N+V)^{-1}GM \quad . \tag{IIA2.22}$$

which is exactly Bayes' equation for updating the covariance matrix, Eq. (IIA1.9). Explicitly, this equation may be written

$$M'_{kl} = M_{kl} - \sum_{n=1}^{K} \sum_{i=1}^{L} \sum_{j=1}^{L} \sum_{m=1}^{K} M_{kn} G_{in} \left[(N+V)^{-1}\right]_{ij} G_{jm} M_{ml} \tag{IIA2.23}$$

where N is given by

$$N_{ij} = \sum_{k=1}^{K} \sum_{l=1}^{K} G_{ik} M_{kl} G_{jl} \quad . \tag{IIA2.24}$$

To obtain Bayes' equation for updating the parameter values, we equate the linear terms of Eq. (IIA2.8). Since the left-hand side of that equation has no terms linear in $(P-\bar{P}')$, the coefficient of $(P-\bar{P}')$ on the right-hand side must be zero. That is,

$$(M^{-1}+G'V^{-1}G)\,(\bar{P}'-\bar{P}) = G'V^{-1}(D-\bar{T}) \quad . \tag{IIA2.25}$$

From Eq. (IIA2.9), the first quantity on the left is just $(M')^{-1}$; we therefore have

$$\bar{P}' - \bar{P} = M'G'V^{-1}(D-\bar{T}) \tag{IIA2.26}$$

or, using Eq. (IIA2.12)

$$\bar{P}' = \bar{P} + M(I+Q)^{-1}G'V^{-1}(D-\bar{T}) \tag{IIA2.27}$$

which is exactly Bayes' equation for updating the parameter values using the $(I + Q)$ inversion scheme, Eq. (IIA1.11).

To obtain this equation in the $(N+V)$ inversion scheme, replace M' in Eq. (IIA2.26) by Eq. (IIA2.22) to give

$$\bar{P}'-\bar{P} = (M-MG'(N+V)^{-1}GM)G'V^{-1}(D-\bar{T}) \tag{IIA2.28}$$

which reduces to

$$\bar{P}' - \bar{P} = MG'(N+V)^{-1}(D-\bar{T}) \quad . \tag{IIA2.29}$$

Explicitly, this equation is

$$\bar{P}'_k = \bar{P}_k + \sum_{l=1}^{K} \sum_{i=1}^{L} \sum_{j=1}^{L} M_{kl} G_{il} \left[(N+V)^{-1}\right]_{ij} (D_j - \bar{T}_j) \tag{IIA2.30}$$

Finally, we note that the constant term in Eq. (IIA2.8) may be simplified using Eq. (IIA2.29) to give

$$Y=(D-\bar{T})'[(N+V)^{-1}GMG'(N+V)^{-1}+(I-(N+V)^{-1}N)V^{-1}(I-N(N+V)^{-1})](D-\bar{T}) \quad \text{(IIA2.31)}$$

which reduces to

$$Y=(D-\bar{T})'\ (N+V)^{-1}(D-\bar{T}) \quad \text{(IIA2.32)}$$

In SAMMY, this quantity is referred to as the "Bayesian χ^{2}". In the $(I + Q)$ inversion scheme, this quantity can be simplified to the form

$$Y = (D-\bar{T})'V^{-1}(D-\bar{T}) - (D-\bar{T})V^{-1}GM(I+Q)^{-1}G'V^{-1}(D-\bar{T}) \quad \text{(IIA2.33)}$$

in which the first term is the usual (least-squares) χ^2, and the second term can be viewed as a "correction" to χ^2.

II.A.3 Iteration Scheme

The linearity hypothesis, i.e., the assumption that the Taylor expansion of the theoretical values around the prior expectation value truncates after the linear term, is in general only approximately true. Therefore, the parameter values $\bar{P}'$ resulting from application of Bayes' equations are also only approximately correct. To obtain more accurate values, the Taylor expansion, Eq. (IIA2.4), may be performed not around $\bar{P}$ but around the new (intermediate) values $\bar{P}^{(n)}$, where n represents the nth iteration and $\bar{P}^{(0)} = \bar{P}$:

$$T \simeq \bar{T}^{(n)} + G^{(n)}(P - \bar{P}^{(n)}) \tag{IIA3.1}$$

Here the sensitivity matrix $G^{(n)}$ and the theoretical values $\bar{T}^{(n)}$ are evaluated at $P = \bar{P}^{(n)}$. With Eq. (IIA3.1) for T, the formula analogous to Eq. (IIA2.7) is

$$(P - \bar{P}^{(n+1)})^t (M^{(n+1)})^{-1} (P - \bar{P}^{(n+1)}) + Y = (P - \bar{P})^t M^{-1} (P - \bar{P})$$

$$+ [D - \bar{T}^{(n)} - G^{(n)}(P - \bar{P}^{(n)})]^t V^{-1} [D - \bar{T}^{(n)} - G^{(n)}(P - \bar{P}^{(n)})] \tag{IIA3.2}$$

Setting P equal to $P - \bar{P}^{(n+1)} + \bar{P}^{(n+1)}$ everywhere in the right-hand side of Eq. (IIA3.2) gives the formula analogous to Eq. (IIA2.8) with $\bar{T}$ in that expression replaced by $\bar{T}^{(n)} + G^{(n)}(\bar{P} - \bar{P}^{(n)})$, and G by $G^{(n)}$. The iterative forms of Bayes' equations follow immediately:

$$\bar{P}^{(n+1)} = \bar{P} + MG^{(n)t} (N^{(n)} + V)^{-1} [D - \bar{T}^{(n)} - G^{(n)}(\bar{P} - \bar{P}^{(n)})] \tag{IIA3.3}$$

$$M^{(n+1)} = M - MG^{(n)t} (N^{(n)} + V)^{-1} G^{(n)} M \tag{IIA3.4}$$

where

$$N^{(n)} = G^{(n)} M G^{(n)t} \tag{IIA3.5}$$

For the $(I + Q)$ inversion scheme, the iterative forms of Bayes' equations are

$$\bar{P}^{(n+1)} = \bar{P} + M(I + Q^{(n)})^{-1} G^{(n)t} V^{-1} [D - \bar{T}^{(n)} - G^{(n)}(\bar{P} - \bar{P}^{(n)})] \tag{IIA3.6}$$

$$M^{(n+1)} = M(I + Q^{(n)})^{-1} \tag{IIA3.7}$$

where

$$Q^{(n)} = G^{(n)t} V^{-1} G^{(n)} M \tag{IIA3.8}$$

II.B.1. Solving Bayes' Equations

The solution of Bayes' equations for the $(N+V)$ inversion scheme is described in Subsection II.B.1.a, and the solution for the $(I+Q)$ inversion scheme is in Subsection II.B.1.b.

II.B.1.a. Solving Bayes' equations: $(N+V)$ inversion scheme

SAMMY uses an early version of the code BAYES (NL82) to solve Bayes' equations in the $(N+V)$ inversion scheme. In matrix notation, the non-iterative form of Bayes' equations can be written

$$\bar{P}' = \bar{P} + MG^t(N+V)^{-1}(D-\bar{T}) \ , \qquad \text{(IIB1a.1)}$$

and

$$M' = M - MG^t\,(N+V)^{-1}\,GM \ , \qquad \text{(IIB1a.2)}$$

where

$$N = GMG^t \ . \qquad \text{(IIB1a.3)}$$

Solving these equations is equivalent to solving

$$AX = Y \qquad \text{(IIB1a.4)}$$

$K+1$ times (where K is the number of parameters for the problem), with A the $L \times L$ symmetric matrix $N+V$ (where L is the number of data points), and Y a column matrix equal to $(D-\bar{T})$ in Eq. (IIB1a.1) or equal to each of the K columns of the rectangular matrix GM in Eq. (IIB1a.2).

The inverse of matrix A is not evaluated directly. Rather, A is first factorized as

$$A = U\ B\ U^t \qquad \text{(IIB1a.5)}$$

where B is a block-diagonal matrix, and U is the product of elementary unit triangular and permutation matrices, so that inverses of U and B are immediately available. The solution X to Eq. (IIB1a.4) is then found from

$$X = (U^{-1})^t\ B^{-1}U^{-1}\ Y \qquad \text{(IIB1a.6)}$$

In SAMMY, the factorization of Eq. (IIB1a.5) is performed by LINPACK [JD79] subroutine SSPCO, and the $(K+1)$ solutions are obtained by LINPACK subroutine SSPSL. Subroutine NEWPAR oversees these operations.

It is necessary to modify this procedure slightly to account for the approximations built into Bayes' equations. As explained in Sect. IIA.3, an iteration scheme has been derived to correct for the non-linear relationship between parameters and theoretical values. The default in SAMMY is to perform two iterations, since (1) further iteration is expected to increased precision but not accuracy, and (2) test cases have shown this to yield consistent results. The interested reader may refer to example 4 of the original SAMMY manual [NL80], or, if he desires, make his own tests on his own data. Table VIA.1, card set 2, indicates the relevant parameter (ITMAX) to use. Note that k iterations (ITMAX $= k$) will yield the solution set $\bar{P}^{(k)}$ and $M^{(k)}$ from Eqs. (IIA3.3) and (IIA3.4).

[Note to users of earlier SAMMY versions: The meaning of ITMAX has been changed from that in use prior to April 1984, and now corresponds exactly to the total number of times the "THEORY-CROSS-BROADEN-SETV-(N+V)-FINAL" cycle appears between consecutive "DATA" segments in the LOG file. Caveat: Since ITMAX=2 is the default value, putting zero (or blank) in column 50 of card set 2 of the INPUT file will give ITMAX=2, not ITMAX=0. To obtain zero iterations (i.e., to evaluate cross sections but not update parameter values), the user must specify "DO NOT SOLVE BAYES Equations" in the INPut file.]

II.B.1.b. Solving Bayes' equations: $(I+Q)$ inversion scheme

In matrix form, the non-iterative form of Bayes' equations for the $(I + Q)$ inversion scheme can be written

$$\bar{P}' = \bar{P} + M(I+Q)^{-1} G'V^{-1}(D-\bar{T}) \qquad \text{(IIB1b.1)}$$

and

$$M' = M(I+Q)^{-1} \qquad \text{(IIB1b.2)}$$

where

$$Q = G'V^{-1} G M \qquad \text{(IIB1b.3)}$$

[Note that although Q (and thus $I+Q$) is not symmetric, nevertheless M' is symmetric. This can be shown by noting that

$$M' = M(I+Q)^{-1} = M(M + MG'V^{-1}GM)^{-1}M \ , \qquad \text{(IIB1b.4)}$$

provided that M^{-1} exists. In the form of Eq. (IIB1b.4), M' is clearly symmetric.]

The inverse of $(I+Q)$ is found using NAG [NAG] routine F01AAF. When M' is needed (i.e., for the final iteration), Eq. (IIB1b.2) is solved first and the array M' used in Eq. (IIB1b.1) to find $\bar{P}'$. When M' is not needed, the quantity $(I+Q)^{-1}G'V^{-1}(D-\bar{T})$ is first generated and then the multiplication by M is performed. Fewer computer operations and thus faster run time result from performing the multiplications in this order.

As with the $(N+V)$ inversion scheme, two iterations is the default in SAMMY.

The user has the ability to choose which inversion scheme to use, or SAMMY can make the choice automatically. Generally, the $(N+V)$ inversion scheme should be used unless the number of varied parameters in considerably smaller than the number of data points. If the data covariance matrix V is not diagonal, the $(N+V)$ inversion scheme must be used. When SAMMY is left to choose automatically, its choice will be the $(N+V)$ scheme unless both (1) V is diagonal and (2) less array storage space is require for the $(I+Q)$ scheme.

III. THEORETICAL CROSS SECTIONS

In this section are presented the formulae, as implemented in SAMMY, for generating theoretical values of cross sections from multilevel R-matrix theory. A summary of the formulae for the Reich-Moore approximation is given in Subsection III.A, and details are presented in Subsection III.B. The Multilevel Breit-Wigner approximation, as implemented in SAMMY, is described in Subsection III.C.

III.A. MULTILEVEL R-MATRIX THEORY: REICH-MOORE APPROXIMATION

Consider a neutron of energy E incident on a target of spin I. The combined system (neutron plus target) has resonances λ with spin and parity J^{π} at energies E. These resonances may decay through any of several particle channels c with spin s and orbital angular momentum l; the partial width for decay via channel c is $\Gamma_{\lambda c}$. In addition, gamma decay is allowed, with partial width $\Gamma_{\lambda}^{\gamma}$.

Cross-sections for the interaction described above may be calculated from multilevel R-matrix theory [AL58] in the Reich-Moore approximation [CR58]. An excellent review of R-matrix theory and its relationship to other resonance formalisms is presented in an article by Froehner [FF80]; the reader interested in either derivation or detail is referred to that article. Here we present only the relevant formulae.

III.A.1. Cross Section in Terms of R-Matrix

The angle-integrated cross sections from entrance channel c to exit channel c' with total angular momentum J is represented by $\sigma^J_{cc'}$. (The subscripts c and c' represent both the physical configuration and the quantum numbers; a detailed description of the channel, as used in SAMMY, is given in Subsection III.B.1.) This cross section is given in terms of the scattering matrix $U^J_{cc'}$ as

$$\sigma^J_{cc'} = \frac{\pi}{k_c^2} g_c \left| \delta_{cc'} - U^J_{cc'} \right|^2 \qquad \text{(IIIA1.1)}$$

where k_c^2 is the wave number associated with incident channel c (see Subsection III.B.4) and g_c is the spin statistical factor (see Subsection III.B.1).

Because the scattering matrix is unitary ($UU^+ = 1$), the total cross section (sum over all channels) may be expressed as

$$\sigma^{\text{total}} = \frac{2\pi}{k^2} \sum_J g_J \sum_{\substack{\text{incident} \\ \text{channels} \\ c}} \left(1 - Re(U^J_{cc}) \right) \qquad \text{(IIIA1.2)}$$

in which the spin statistical factor g_c is removed from the sum over c and renamed g_J since it depends only on the (conserved) total angular momentum J. The elastic (or scattering) cross section is

$$\sigma^{elastic} = \frac{\pi}{k^2} \sum_J g_J \sum_{\substack{\text{incident} \\ \text{channels} \\ c}} \left(1 - 2Re(U^J_{cc}) + \sum_{\substack{\text{incident} \\ \text{channels} \\ c'}} |U^J_{cc'}|^2 \right) \qquad \text{(IIIA1.3)}$$

Note that the innermost summation includes only those exit channels c' which are also incident channels.

Similarly, the reaction (or fission) cross section is

$$\sigma^{reaction} = \frac{\pi}{k^2} \sum_J g_J \sum_{\substack{\text{incident} \\ \text{channels} \\ c}} \sum_{\substack{\text{exit} \\ \text{channels} \\ c'}} |U^J_{cc'}|^2 \qquad \text{(IIIA1.4)}$$

and the capture cross section is

$$\sigma^{capture} = \frac{\pi}{k^2} \sum_J g_J \sum_{\substack{\text{incident} \\ \text{channels} \\ c}} \left(1 - \sum_{\substack{\text{all} \\ \text{channels} \\ c'}} |U^J_{cc'}|^2 \right) \qquad \text{(IIIA1.5)}$$

The absorption cross section is the sum of $\sigma^{reaction}$ and $\sigma^{capture}$.

Note that the total cross section is the sum of the other three:

$$\sigma^{total} = \sigma^{elastic} + \sigma^{reaction} + \sigma^{capture} \quad . \tag{IIIA1.6}$$

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

$$U^J_{cc'} = \Omega_l \; W^J_{cc'} \; \Omega_{l'} \tag{IIIA1.7}$$

where l represents the orbital angular momentum (see Subsection III.B.1), and Ω_l is given by

$$\Omega_l = \exp\{-i\phi_l\} \tag{IIIA1.8}$$

The potential scattering phase shifts ϕ_l are shown in Table IIIA1.1.

The matrix W in Eq. (IIIA1.7) is related to the R-matrix via (in matrix notation with indices suppressed)

$$W = P^{1/2}(I-RL)^{-1}\;(I-RL^*)P^{-1/2} \tag{IIIA1.9}$$

where the quantity L in Eq. (IIIA1.9) is given by

$$L = (S - B) + iP \tag{IIIA1.10}$$

with P the penetrability, S the shift factor and B the arbitrary boundary constant at the channel radius a_c, (see Table IIIA1.1). "I" in Eq. (IIIA1.9) represents the identity matrix.

SAMMY uses a modified form of Eq. (IIIA1.9) to evaluate W. Since S, B, and P are all real, L^* may be expressed as $L-2iP$, which gives

$$\begin{aligned} W &= P^{1/2}\;(I-RL)^{-1}\;(I-RL\;+\;2iRP)\;P^{-1/2} \qquad\qquad \text{(IIIA1.11)}\\ &= P^{1/2}\;(I-RL)^{-1}\;(I-RL)P^{-1/2}\;+\;(P)^{1/2}\;(I-RL)^{-1}\;2iRPP^{-1/2}\\ &= I\;+\;P^{1/2}\;(I-RL)^{-1}\;2i\;\{-(I-RL)L^{-1}\;+\;L^{-1}\}\;P^{1/2} \end{aligned}$$

where the quantity in curly brackets is equal to R. Further simplification gives

$$\begin{aligned} W &= I\;-\;2i\;P^{1/2}\;L^{-1}\;P^{1/2}\;+\;2iP^{1/2}\;(I-RL)^{-1}\;L^{-1}\;P^{1/2} \qquad\qquad \text{(IIIA1.12)}\\ &= I\;-\;2i\;P\;L^{-1}\;+\;2i\;P^{1/2}\;L^{-1}\;(L^{-1}-R)^{-1}\;L^{-1}\;P^{1/2} \end{aligned}$$

which is the form used directly in SAMMY. If subscripts are reinserted, this expression becomes

$$W_{cc'} = \delta_{cc'}(1-2iP_lL_l^{-1}) + 2i\sqrt{P_l}\;L_l^{-1}\left[(L^{-1}-R)^{-1}\right]_{cc'}L_{l'}^{-1}\sqrt{P_{l'}}$$

III.A.1.a. Logarithmic parameterization of external R-function

The "external R-function" is one particular choice for the contribution to the R-matrix within a specified region of energy due to those resonances or bound states external to that region. The parameterization of the external R-function used in SAMMY is

$$R_c^{ext}(E) = \bar{R}_{con,c} + \bar{R}_{lin,c}E + \bar{R}_{q,c}E^2 - s_{lin,c}(E_c^{up} - E_c^{down}) - (s_{con,c} + s_{lin,c}E)ln\left(\frac{E_c^{up} - E}{E - E_c^{down}}\right) \quad \text{(IIIA1a.1)}$$

Any or all of the seven free parameters may be varied during a SAMMY analysis (see Table VI.B.1, card set 3, and alternative to card set 3). Note that R^{ext} is strictly real in this parameterization.

The u-parameters (that is, the parameters on which Bayes' equations will operate; see Sect. II.B.2) associated with the external R-function are given by

$$\begin{aligned} u(E_c^{down}) &= E_c^{down} \\ u(E_c^{up}) &= E_c^{up} \\ u(\bar{R}_{con,c}) &= \bar{R}_{con,c} \\ u(\bar{R}_{lin,c}) &= \bar{R}_{lin,c} \\ u(\bar{R}_{q,c}) &= \bar{R}_{q,c} \\ u(s_{con,c}) &= \sqrt{s_{con,c}} \\ u(s_{lin,c}) &= s_{lin,c} \end{aligned} \quad \text{(IIIA1a.2)}$$

III.A.2.a.ii Resonance parameters

From Eq. (IIIA2.1), the derivative of R with respect to the reasonance u-parameters can be found:

$$\frac{\partial \mathrm{Re}R_{\mu\nu}}{\partial\sqrt{E_\lambda}} = \left[2\gamma_{\lambda\mu}\gamma_{\lambda\nu}\sqrt{E_\lambda}\right]\left[\left\{-(E_\lambda-E)^2+(\alpha_\lambda^2)^2\right\}/D_\lambda^2\right] \qquad \text{(IIIA2aii.1)}$$

$$\frac{\partial \mathrm{Im}R_{\mu\nu}}{\partial\sqrt{E_\lambda}} = \left[-4\gamma_{\lambda\mu}\gamma_{\lambda\nu}\sqrt{E_\lambda}\right]\left[(E_\lambda-E)\alpha_\lambda^2/D_\lambda^2\right] \qquad \text{(IIIA2aii.2)}$$

$$\frac{\partial \mathrm{Re}R_{\mu\nu}}{\partial\alpha_\lambda} = \left[-4\gamma_{\lambda\mu}\gamma_{\lambda\nu}\alpha_\lambda\right]\left[(E_\lambda-E)\alpha_\lambda^2/D_\lambda^2\right] \qquad \text{(IIIA2aii.3)}$$

$$\frac{\partial \mathrm{Im}R_{\mu\nu}}{\partial\alpha_\lambda} = \left[2\gamma_{\lambda\mu}\gamma_{\lambda\nu}\alpha_\lambda\right]\left[\left\{(E_\lambda-E)^2-(\alpha_\lambda^2)^2\right\}/D_\lambda^2\right] \qquad \text{(IIIA2aii.4)}$$

$$\frac{\partial ReR_{\mu\nu}}{\partial\gamma_{\lambda\mu}} = \left[\gamma_{\lambda\nu}(1+\delta_{\mu\nu})\right]\left[(E_\lambda-E)/D_\lambda\right] \qquad \text{(IIIA2aii.5)}$$

$$\frac{\partial \mathrm{Im}R_{\mu\nu}}{\partial\gamma_{\lambda\mu}} = \left[\gamma_{\lambda\nu}(1+\delta_{\mu\nu})\right]\left[\alpha_\lambda^2/D_\lambda\right] \qquad \text{(IIIA2aii.6)}$$

where

$$D_\lambda = (E_\lambda-E)^2 + \alpha_\lambda^4 \qquad \text{(IIIA2aii.7)}$$

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

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

$$|\, E-E_\lambda \,| > 20\left(\sum_c \Gamma_{\lambda c} + \Gamma_\lambda^\gamma\right) + 3(d+r), \qquad \text{(IIIA2aii.8)}$$

for resonances with $l>0$, where d represents the Doppler and r the resolution width. Moreover, the contribution to the imaginary part of R is set to zero whenever the distance from level λ is greater than 100 times that specified in Eq. (IIIA2aii.8). (The contribution to the *real* part of R is never assumed negligible).

For s-wave resonances ($l=0$) the user has the option of setting derivatives equal to zero beyond a certain distance, where the distance is twice that specified for non-s-waves. (See Table VIA.2 for details on invoking this option.)

III.B.2. Comparison of Reich-Moore Approximation to Multilevel Breit Wigner Approximation

Following Fröhner [FF80], we may write the exact equations for the scattering matrix U as

$$U_{cc'} = \Omega_l \left(\delta_{cc'} + i\sum_{\lambda,\mu} \Gamma^{1/2}_{\lambda c} A_{\lambda\mu} \Gamma^{1/2}_{\mu c'}\right) \Omega_{l'} \qquad \text{(IIIB2.1)}$$

where

$$(A^{-1})_{\lambda\mu} = (E_\lambda - E)\,\delta_{\lambda\mu} - \sum_c \gamma_{\lambda c} L_c \gamma_{\mu c} \qquad \text{(IIIB2.2)}$$

and all other quantities are as defined in Sect. III.A.

In the multilevel Breit Wigner (MLBW) approximation, all off-diagonal elements of A are neglected. That is,

$$(A^{-1})_{\lambda\mu} \simeq (E_\lambda - E - \sum_c \gamma^2_{\lambda c} L_c)\,\delta_{\lambda\mu} \qquad \text{(IIIB2.3)}$$

Using the definition of L_c from Eq. (IIIA.10), this may be rearranged as

$$(A^{-1})_{\lambda\mu} \simeq [E_\lambda - E - \sum_c (S_c - B_c)\,\gamma^2_{\lambda c} - i\sum_c P_c \gamma^2_{\lambda c}]\,\delta_{\lambda\mu} \qquad \text{(IIIB2.4)}$$

or

$$(A^{-1})_{\lambda\mu} \simeq (E_\lambda + \Delta^{MLBW}_\lambda - E - i\Gamma^{MLBW}_\lambda/2)\,\delta_{\lambda\mu} \qquad \text{(IIIB2.5)}$$

where the level shift Δ_λ is given by

$$\Delta^{MLBW}_\lambda = -\sum_c (S_c - B_c)\,\gamma^2_{\lambda c} \qquad \text{(IIIB2.6)}$$

and the total width Γ_λ by

$$\Gamma^{MLBW}_\lambda = \sum_c 2P_c\,\gamma^2_{\lambda c} = \sum_c \Gamma_{\lambda c} \qquad \text{(IIIB2.7)}$$

In the Reich-Moore (RM) approximation, only those off-diagonal elements arising from photon channels are neglected. That is,

$$(A^{-1})_{\lambda\mu} \simeq \left[E_\lambda - E - \sum_{c\in\gamma} (S_c - B_c)\ \gamma_{\lambda c}^2 - i \sum_{c\in\gamma} P_c \gamma_{\lambda c}^2\right] \delta_{\lambda\mu} - \sum_{c\notin\gamma} \gamma_{\lambda c}\ L_c\ \gamma_{\mu c} \qquad \text{(IIIB2.8)}$$

where by " $c\in\gamma$" we mean "c is a photon channel" and by " $c\notin\gamma$" we mean "c is a particle channel". Rearranging, we find

$$(A^{-1})_{\lambda\mu} \simeq (E_\lambda + \Delta_{\lambda\gamma}^{RM} - E - i\Gamma_\lambda^{RM\gamma}/2)\ \delta_{\lambda\mu} - \sum_{c\notin\gamma} \gamma_{\lambda c}\ L_c\ \gamma_{\mu c} \qquad \text{(IIIB2.9)}$$

where the level shift $\Delta_{\lambda\gamma}^{RM}$ is given by

$$\Delta_{\lambda\gamma}^{RM} = -\sum_{c\in\gamma} (S_c - B_c)\ \gamma_{\lambda c}^2 \qquad \text{(IIIB2.10)}$$

and the radiation width Γ_λ^γ by

$$\Gamma_\lambda^{RM\gamma} = \sum_{c\in\gamma} 2\ P_c\ \gamma_{\lambda c}^2 \qquad \text{(IIIB2.11)}$$

Data analysis using the RM approximation yields three (or more) parameters for each level: a resonance energy E_λ^{RM} equal to $E_\lambda + \Delta_{\lambda\gamma}^{RM}$, the radiation width $\Gamma_\lambda^{RM\gamma}$, and the particle channel widths $\Gamma_{\lambda c}$.

No direct comparison can be made of results obtained from data analysis using RM (e.g., via SAMMY) with those obtained from analysis using MLBW (e.g., via SIOB [GD78]), since the MLBW is a far more severe approximation. Nevertheless, the RM formulation can be further approximated to produce a form equivalent to MLBW, and the "analogous" MLBW parameters extracted from the RM parameters. (One cannot, of course, proceed in the opposite direction since the MLBW contains less information than RM.)

Making this comparison, we find, from Eqs. (IIIB2.6) and (IIIB2.10),

$$E_\lambda^{MLBW} = E_\lambda^{RM} - \sum_{c\notin\gamma} (S_c - B_c)\ \gamma_{\lambda c}^2 \qquad \text{(IIIB2.12)}$$

and, from Eqs. (IIIB2.7) and (IIIB2.11),

$$\Gamma_\lambda^{MLBW} = \Gamma_\lambda^{RM\gamma} + \sum_{c\notin\gamma} \Gamma_{\lambda c} \qquad \text{(IIIB2.13)}$$

CAUTION: Converting from RM parameters to MLBW parameters will not necessarily give the same values that an analysis using the MLBW formalism would yield. See Sect. III.C if you wish to perform such an analysis.

III.C. MULTILEVEL BREIT-WIGNER APPROXIMATION

In Sect. III.B.2 we discussed the relationship between the Reich-Moore resonance parameters and those which would be appropriate for multilevel Breit-Wigner (MLBW) resonances. We noted that it is possible for SAMMY, upon completion of a Reich-Moore R-matrix analysis, to derive the "analogous" MLBW parameters. The MLBW parameters thus derived are expected to be a reasonable approximation to those which would be obtained via analysis using MLBW cross sections directly.

In version O of SAMMY (and subsequent versions), it is possible to use MLBW cross sections directly for data analysis. This has the advantage that the calculation proceeds more rapidly since fewer computations are required, and the disadvantage that, since the scattering matrix for MLBW is not unitary, unphysical cross sections may be generated.

Formulae for MLBW cross sections are presented in Sect. III.C.1; these are identical to those used in ENDF files [ENDF-102]. Derivatives are given in Sect. III.C.2.

A note re broadening: Doppler- and resolution-broadening are accomplished in the same manner for MLBW cross sections as for Reich-Moore cross sections. See Sect. IV.

III.C.1. Multilevel Breit-Wigner Cross Sections

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

$$\sigma^{elastic} = \frac{\pi}{k^2} \sum_J g_J \sum_c \Bigg\{ (1 - \cos 2\phi)\left(2 - \sum_\lambda \Gamma_{\lambda c}\Gamma_\lambda / D_\lambda\right) + 2\sin 2\phi \sum_\lambda \Gamma_{\lambda c}(E - E_\lambda)/D_\lambda + \left[\sum_\lambda \frac{\Gamma_{\lambda c}(E-E_\lambda)}{D_\lambda}\right]^2 + \left[\sum_\lambda \frac{\Gamma_{\lambda c}\Gamma_\lambda/2}{D_\lambda}\right]^2 \Bigg\} \qquad \text{(IIIC1.1)}$$

in which the summation over c includes only incident (i.e., neutron) channels. The total width Γ_λ in Eq. (IIIC1.1) is given by

$$\Gamma_\lambda = \sum_c \Gamma_{\lambda c} + \Gamma_\lambda^\gamma \qquad \text{(IIIC1.2)}$$

in which the sum over c includes all channels. Partial widths $\Gamma_{\lambda c}$ and Γ_λ^γ are related to amplitudes $\gamma_{\lambda c}$ and α_λ, as in the Reich-Moore approximation, by

$$\Gamma_{\lambda c}^{neutron} = 2\gamma_{\lambda c}^2 P_c \qquad \text{(IIIC1.3)}$$

$$\Gamma_{\lambda c}^{fission} = 2\gamma_{\lambda c}^2$$

and

$$\Gamma_\lambda^\gamma = 2\alpha_\lambda^2$$

The denominator D_λ in Eq. (IIIC1.1) represents

$$D_\lambda = (E-E_\lambda)^2 + (\Gamma_\lambda/2)^2 \qquad \text{(IIIC1.4)}$$

Similarly, the fission (reaction) cross section is given by

$$\sigma^{fission} = \frac{\pi}{k^2} \sum_J g_J \sum_c \sum_{c'} \sum_\lambda \frac{\Gamma_{\lambda c}\Gamma_{\lambda c'}}{D_\lambda} \qquad \text{(IIIC1.5)}$$

in which the sum over c includes only incident (neutron) channels, the sum over c' includes only exit (fission) channels, and D_λ is again given by Eq. (IIIC1.4). The capture cross section is

$$\sigma^{capture} = \frac{\pi}{k^2} \sum_J g_J \sum_c \sum_\lambda \frac{\Gamma_{\lambda c}\Gamma_\lambda^\gamma}{D_\lambda} \qquad \text{(IIIC1.6)}$$

where, again, the sum over c includes only incident channels. Finally, total and absorption cross sections are given by the appropriate sums of the other three cross sections:

$$\sigma^{total} = \sigma^{elastic} + \sigma^{fission} + \sigma^{capture} \qquad \text{(IIIC1.7)}$$

$$\sigma^{absorption} = \sigma^{fission} + \sigma^{capture} \qquad \text{(IIIC1.8)}$$

The u-parameters (see Sect. II.B.2) associated with the MLBW resonances are defined similarly to those for Reich-Moore resonances:

$$u(E_\lambda) = \pm\sqrt{|E_\lambda|}, \qquad \text{(IIIC1.9)}$$

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

$$u(\Gamma_{\lambda c}) = \gamma_{\lambda c} \qquad \text{(IIIC1.10)}$$

and

$$u(\Gamma_\lambda^\gamma) = \alpha_\lambda \qquad \text{(IIIC1.11)}$$

where the reduced gamma width amplitude α_λ is given in terms of the gamma width Γ_λ^γ by

$$\Gamma_\lambda^\gamma = 2\alpha_\lambda^2 \quad . \qquad \text{(IIIC1.12)}$$

(Note that $\gamma_{\lambda c}$ and α_λ may be either positive or negative.) It is the u-parameters on which Bayes' equations operate.

The matching radius a may also be varied (i.e., treated as a u-parameter).

III.C.2. Derivatives of MLBW cross sections

From the form of the cross sections in Eqs. (IIIC1.1), (IIIC1.5), and (IIIC1.6), we note that there are only four expressions in which the resonance energies or widths occur. These expressions are denoted as follows:

$$A_{1c} = \sum_{\lambda} \Gamma_{\lambda c} \ (E-E_\lambda)/D_\lambda \tag{IIIC2.1}$$

$$A_{2c} = \sum_{\lambda} \Gamma_{\lambda c} \ \Gamma_\lambda^\gamma/D_\lambda \tag{IIIC2.2}$$

$$A_{3cc'} = \sum_{\lambda} \Gamma_{\lambda c} \ \Gamma_{\lambda c'}/D_\lambda \tag{IIIC2.3}$$

$$A_{4c} = \sum_{\lambda} \Gamma_{\lambda c} \ \Gamma_\lambda/D_\lambda \tag{IIIC2.4}$$

The fourth of these is actually redundant, since

$$A_{4c} = \sum_{c'} A_{3cc'} + A_{2c} \tag{IIIC2.5}$$

Thus we need only evaluate partial derivatives of A_{1c}, A_{2c}, and $A_{3cc'}$ with respect to the u-parameters. These derivatives may be written as follows:

$$\frac{\partial A_{1c}}{\partial \sqrt{E_\lambda}} = 2\sqrt{E_\lambda} \ \Gamma_{\lambda c} \left\{ -1 + 2(E-E_\lambda)^2/D_\lambda \right\} \ / \ D_\lambda \tag{IIIC2.6}$$

$$\frac{\partial A_{2c}}{\partial \sqrt{E_\lambda}} = 4\sqrt{E_\lambda} \ \Gamma_{\lambda c} \ \Gamma_\lambda^\gamma \ (E-E_\lambda) \ / \ D_\lambda^2 \tag{IIIC2.7}$$

$$\frac{\partial A_{3cc'}}{\partial \sqrt{E_\lambda}} = 4\sqrt{E_\lambda} \ \Gamma_{\lambda c} \ \Gamma_{\lambda c'} \ (E-E_\lambda) \ / \ D_\lambda^2 \tag{IIIC2.8}$$

$$\frac{\partial A_{1c}}{\partial \alpha_\lambda} = -2\alpha \ \Gamma_{\lambda c}(E-E_\lambda)\Gamma_\lambda \ / \ D_\lambda^2 \tag{IIIC2.9}$$

$$\frac{\partial A_{2c}}{\partial \alpha_\lambda} = 2\alpha \ \Gamma_{\lambda c}\left\{2 - \Gamma_\lambda^\gamma \ \Gamma_\lambda/D_\lambda\right\} \ / \ D_\lambda \tag{IIIC2.10}$$

$$\partial A_{3cc'}/\partial \alpha_\lambda = -2\alpha\ \Gamma_{\lambda c}\ \Gamma_{\lambda c'}\ \Gamma_\lambda\ /\ D_\lambda^2 \qquad \text{(IIIC2.11)}$$

$$\partial A_{1c}/\partial \gamma_{\lambda c''} = 2\ \Gamma_{\lambda c}\ (E - E_\lambda) \left\{\delta_{cc''} - \Gamma_\lambda\ \Gamma_{\lambda c''}/2D_\lambda\right\}\ /\ \left\{\gamma_{\lambda c''} D_\lambda\right\} \qquad \text{(IIIC2.12)}$$

$$\partial A_{2c}/\partial \gamma_{\lambda c''} = 2\ \Gamma_{\lambda c}\ \Gamma_\lambda^2 \left\{\delta_{cc''} - \Gamma_\lambda\ \Gamma_{\lambda c''}/2D_\lambda\right\}\ /\ \left\{\gamma_{\lambda c''} D_\lambda\right\} \qquad \text{(IIIC2.13)}$$

$$\partial A_{3cc'}/\partial \gamma_{\lambda c''} = 2\Gamma_{\lambda c}\ \Gamma_{\lambda c'} \left\{\delta_{cc''} + \delta_{c'c''} - \Gamma_\lambda\ \Gamma_{\lambda c''}/2D_\lambda\right\}\ /\ \left\{\gamma_{\lambda c''} D_\lambda\right\} \qquad \text{(IIIC2.14)}$$

IV.A.1. Doppler Broadening

Doppler-broadened cross sections [FF80, AF71] may be approximated by convoluting the unbroadened cross section with a Gaussian function, as

$$\sigma_D(E) = \frac{1}{\Delta_D\sqrt{\pi}} \int_{-\infty}^{\infty} \exp\left\{-\frac{(E-E')^2}{\Delta_D^2}\right\} \sigma(E')dE' \qquad \text{(IVA1.1)}$$

where the Doppler width Δ_D is given by

$$\Delta_D = \sqrt{\frac{4mEkT}{M}} \qquad \text{(IVA1.2)}$$

In this equation, m represents the reduced mass of the neutron, M is the target mass, k is Boltzman's constant, and T is the effective temperature of the sample material.

For most nuclei of interest (i.e., heavy nuclei), the reduced mass m may be replaced by the neutron mass, so that the ratio $m/M \simeq 1/A$, where A is the mass number of the target nucleus. Equation (IVA1.2) can then be expressed as

$$\Delta_D = \sqrt{4k\ T_o}\sqrt{\frac{ET}{AT_o}} \qquad \text{(IVA1.3)}$$

where T_o is room temperature, 293°K. If E is given in eV, and k is set to 8.617×10^{-5} eV/°K, then

$$\Delta_D = \sqrt{4\times 8.617\times 10^{-5}\times 293}\sqrt{\frac{ET}{293A}} = 0.3178\sqrt{\frac{ET}{293A}} \qquad \text{(IVA1.4)}$$

Equation (IVA1.4) will yield Δ_D in units of eV, as required in SAMMY or MULTI.

The infinite integration limits in Eq. (IV.A1.1) are approximated by $E \pm 3\Delta_D$.

Caveat: For very low energies the integration limits may fall below zero. SAMMY will not permit analysis of such low energy data.

Table VIA.1 Format of the INPut file

Note: All integer formats (e.g., I2, I5) require that the numbers be in the *right*-most columns.

Card set	Number of cards in this set	Which card is described here	Columns	Variable	Format	Meaning (units)	Range of values	Notes
1	1		1-80	TITLE	16A5	Title		
2	1		1-10	ELEMENT	A10	Sample element's name		
			11-20	AW	F10.1	Atomic weight (amu)		
			21-30	EMIN	F10.1	Minimum energy for this data set (eV)		EMIN and EMAX will be ignored here if they are given in the BATch file (see Table VIII.1)
			31-40	EMAX	F10.1	Maximum energy (eV)		
			41-45	NEPNTS	I5	Maximum number of data points to be analyzed at one time		NEPNTS is the number of data points to be included in each region, where "DIVIDE DATA INTO REGions" is specified in card set 3
			46-50	ITMAX	I5	Number of iterations (default = 2)		
3	as many as needed		1-20	WHAT	4A5	Alphanumeric information concerning program options	see Table VIA.2	
4	1		blank					
5	0 or 1		1-10	TEMP	F10.1	Effective temperature of the sample (K)	(0 for no Doppler broadening)	This card set is omitted if "BROADENING IS NOT WANTED" is specified in Card Set 3. If Card Set 4 appears in the PARameter file (see Table VIB.1), all values given here (in the INP file) in Card Set 5 will be ignored, except for DIST.
			11-20	DIST	F10.1	Flight path length (m)		Version O of SAMMY permits Doppler broadening without resolution broadening and vice versa.
			21-30	DELTAL	F10.1	Flight path uncertainty (m)		

Table VIA.1 Format of the INPut file (contd)

Card set	Number of cards in this set	Which card is described here	Columns	Variable	Format	Meaning (units)	Range of values	Notes
			31-40	DELTAE	F10.1	E-folding width of exponential resolution function (μs)	(0 for pure Gaussian resolution function)	
			41-50	DELTAG	F10.1	FWHM (μs) of Gaussian resolution function whose variance is equivalent to that of the square pulse	(0 for pure exponential resolution function)	
6	0 or 2	1	1-10	DELTAB	F10.1	Minimum channel width for interval from EMIN to EMAX (μs)		Omit this card set if "BROADENING IS NOT WANTED" in Card Set 3, or if DELTAG ≥ 0 in Card Set 5.
			11-15	NCF	I5	Number of crunch boundaries		
		2	1-10, 11-20, etc	(BCF(I), CF(I), I=1,NCF)	8F10.1	Crunch boundaries, read in increasing energy order (eV), Crunch factors (Integer units of DELTAB)		
7	1		1-10	CRFN	F10.1	Channel radius (F)	≥0	If CRFN is input as zero, its value is computed as $1.45*(1.009 + AWI)^{1/3}$ Values given here for both CRFN and THICK will be ignored if they also appear in Card Set 4 of the PARameter file (see Table VIB.1).
			11-20	THICK	F10.1	Sample thickness (at/b)		Needed only for TRANSmission or TOTAL cross section (see Card Set 8).
			21-30 31-40	DCOVA DCOVB	F10.1 F10.1	Constant term in data covariance Linear term		Data covariance matrix has additional term of the form (DCOVA+E, *DCOVB) *(DCOVA+E, *DCOVB). Usually these terms will be set to zero.
			41-50	VMIN	F10.1	Minimum uncertainty on data	≥0	If an experimental uncertainty in your DATa file is smaller than VMIN, SAMMY will increase the value to VMIN
			61-70	DATCR	F10.1	Data at the same energy have correlation DATCR	-1≤DATCR≤1	This applies only when a combination of data types are used (see Card Set 8 below).

Table VI.A.1. Format of the INPut file (contd)

Card set	Number of cards in this set	Which card is described here	Columns	Variable	Format	Meaning (units)	Range of values	Notes
8	1		1-80	CROSS	16A5	Type of cross section	TRANSmission TOTAL cross section - in CROSS section {ELASTic {SCATTering {FISSIon {REACTion CAPTUre ABSORption	Only those characters in capitals are required. Note that ABSORption is the sum of CAPTUre plus FISSIon.
Alterative to 8	At least 5	1	1-80	CROSS	16A5		COMBInation of TWO Types COMBInation of THREE types . . . COMBInation of SEVEN types	Columns 16 through 20 indicate how many types of data are to be included, to a maximum of SEVEN
WARNING. This alternative has never been used except for test cases. See N M.Larson when you start to use this option		2	1-80	$CROSS_i$	16A5	Type of cross section for data set 1		See the other version of Card Set 8.
		3	1-10	$EMIN_i$	F10.1	Minimum energy for data set 1 (eV)		These energies override those given in Card Set 2.
			11-20	$EMAX_i$	F10.1	Maximum energy for data set 1 (eV)		
		4	1-80	$CROSS_2$	16A5	Type of cross section for data set 2		
		5	1-10	$EMIN_2$	F10.1	Minimum energy for data set 2 (eV)		
			11-20	$EMAX_2$	F10.1	Maximum energy for data set 2 (eV)		
		etc.						Repeat cards 4 and 5 as many times as necessary, to a maximum of 7 data sets

Table VI.A.1 Format of the INPut file (contd)

Card set	Number of cards in this set	Which card is described here	Columns	Variable	Format	Meaning (units)	Range of values	Notes
9	1		1-10	SPINI	F10.1	Spin of sample nucleus	Integer or half-integer	Often set to zero
			11-20	ECHAN(1)	F10.1	Excitation energy of the residual nucleus for neutron channel number 1 in an inelastic channel (eV)		
			21-25	ISHIFT(1)	I5	Calculate shift for channel 1?	0=no 1=yes	
			26-30	LPENT(1)	I5	Calculate penetrabilities for channel 1?	0=no 1=yes	If 0, this is a fission channel. If 1, this is a reaction channel. If there is more than one channel, ECHAN(2) is in columns 31-40, ISHIFT(2) in 41-45, LPENT(2) in 46-50, ECHAN(3) in 51-60, etc.
10	As many as there are spin groups	1	1-10	SPINJ(1)	F10.1	(a) Spin for resonances in group 1	Integer or half-integer; positive for even parity and negative for odd parity	Use this option if the sample is pure
						(b) Spin factor g_j for resonances in group 1	not integer or half-integer	This option is often used when several isotopes or contaminants are present in the sample; the value which should be inserted here is the product of spin factor and isotopic abundance
			11-15	NENT(1)	I5	Number of entrance channels for resonances in group 1	≥1	If you wish to use more than three channels, please contact N. M. Larson first.
			16-20	NEXT(1)	I5	Number of exit channels, excluding the entrance channels	≥0	NENT + NEXT is the total number of channels for this spin group.
			21-25	LSPIN(1,1)	I5	Orbital angular momentum for channel 1 for resonances in group 1	Integer	

Table VIA.1 Format of the INPut file (contd)

Card set	Number of cards in this set	Which card is described here	Columns	Variable	Format	Meaning (units)	Range of values	Notes
			26-30	CHSPIN(1,1)	F5.1	Channel spin for channel 1, group 1	Integer or half-integer	If option (a) for SPINJ is chosen, consistency checks will be made to see whether the various angular momenta can add up properly. Inconsistencies will result in warning messages, but will not cause SAMMY to abort.
			31-40	ENBND(1,1)	F10.1	Boundary condition for channel 1, group 1 (eV)		
			41-45	LSPIN(2,1)	I5	Orbital angular momentum for channel 2 for resonances in group 1	Integer	Card is blank in columns 41-80 if there is only 1 channel (i.e., if NENT=1 and NEXT=0).
			46-50	CHSPIN(2,1)	F5.1	Channel spin for channel 2, group 1		
			51-60	ENBND(2,1)	F10.1	Boundary condition for channel 2, group 1 (eV)		
			61-65	LSPIN(3,1)	I5	Orbital angular momentum for channel 3, group 1		Card is blank in columns 61-80 if there are only 2 channels (i.e., if NENT+NEXT = 2).
			66-70	CHSPIN(3,1)	F5.1			
			71-80	ENBND(3,1)	F10.1			
		2, etc.						Same as card 1 in this card set, with the quantum numbers appropriate for group number 2.

Table VIA.1 Format of the INPut file (contd)

Card set	Number of cards in this set	Which card is described here	Columns	Variable	Format	Meaning (units)	Range of values	Notes
Alterative to Card Set 10	At least two for each spin group	1	1-3	J	I3	Spin group number	1,2,3...	See the author if you want more than 999
			10	NENT(J)	I1	Number of entrance channels	1,2,3	NENT + NEXT is the total number of channels for this spin group. See the author if you need more than 3 total.
			15	NEXT(J)	I1	Number of exit channels, excluding those which are also entrance channels	1,2	
			16-20	SPINJ(J)	F5.1	Spin for resonances in group J	Integer or half-integers, positive for even parity and negative for odd	
			21-30	ABNDNC(J)	F10.1	isotopic abundance for this spin group		

Table VI.A.1 Format of the INPut file (contd)

Card set	Number of cards in this set	Which card is described here	Columns	Variable	Format	Meaning (units)	Range of values	Notes
		2	5	N	I1	Channel number	1,2,3	
			10	LPENT(N,J)	I1	Calculate penetrability for channel N, spin group J?	0=no 1=yes	
			15	ISHIFT(N,J)	I1	Calculate shift?	0=no 1=yes	
			19-20	LSPIN(N,J)	I2	Orbital angular momentum	integer, ≥0	
			21-30	CHSPIN(N,J)	F10.1	Channel spin	integer or half integer	
			31-40	ENBND(N,J)	F10.1	Boundary condition (eV)	≥0	
			41-50	ECHAN(N,J)	F10.1	Excitation energy of residual nucleus in an inelastic channel (eV)	≥0	
		3 etc.	Repeat card number 2 for a total of (NENT + NEXT) cards.					
		4 etc.	Repeat (Card 1 and Card 2), once for every spin group.					
		last	blank					

Table VIA.2 Alphanumeric statements acceptable for use in the INPut file, card set 3

NOTE: Any of the valid statements listed here may be included in the INPut file, in any order. Usually only the first 20 characters of the statement are required; occasionally other information must be given in specific columns as indicated below. Characters shown here in lower case letters are optional in the INPut file, but are included here for clarity. In the event that contradictory statements are included, the last to appear is the instruction which SAMMY will honor. Default instructions need not be included explicitly. Options which are described "for debug purposes" should generally be avoided, since considerable output is generated thereby, especially on large jobs.

Category	Default	Statements	Notes
Input Control	X	DATA COVARIANCE IS Diagonal	
		DATA HAS OFF-DIAGONAL contribution to covariance matrix of the form $(a + b E_i)(a + b E_j)$	a and b are specified as DCOVA and DCOVB in the INP file, card set number 7 in Table VIA.1.
		DATA COVARIANCE FILE is named YYYYYY.YYY	Substitute your own file name for YYYYYY.YYY in columns 31-40. See Table VIC.2 for the format for this file.
	X	ADD CONSTANT TERM To data covariance DO NOT ADD CONSTANT term to data covariance USE DEFAULT FOR CONStant term to add to data covariance	These three statements refer to the option of adding a constant to the data covariance matrix, both on- and off-diagonal, over the energy region in which the effect of the (non s-wave) resonance is felt. Magnitude of this constant is specified in columns 68-80 in the parameter file, for each resonance. For the third option, the default value of this constant is set at 1.E-6 for every non s-wave resonance.
		DATA IS IN ODF FILE	The data file, whose name you specify either on-line or in your batch file, is in ORELA Data Format. Section 1 contains energy, 2 the data, and 3 the (absolute) uncertainty. See Sect. VI.C of this report for details.
		IGNORE INPUT BINARY covariance file	Your PARameter file specifies that the parameter covariance matrix is kept on a binary file. For this particular run, however, you wish to pretend that there were no previous runs generating such a file; instead you wish to use the large (ideally ∞) uncertainties that indicate no prior knowledge of parameter values.
	X	USE ORIGINAL SPIN GRoup format USE NEW SPIN GROUP Format	See Card Sets 9 and 10 in Table VIA.1

Table VIA.2 Alphanumeric statements acceptable for use in the INPut file, card set 3 (contd)

Category	Default	Statements	Notes
Output Control	X	DO NOT PRINT ANY INPut parameters PRINT ALL INPUT PARAmeters	
		PRINT VARIED INPUT Parameters	Resonances for which no parameters are flagged will not be printed. Use this option for direct comparison with output parameters, which are always printed in this mode.
	X	DO NOT PRINT INPUT Data PRINT INPUT DATA	
	X	DO NOT PRINT THEORETical values PRINT THEORETICAL VAlues	Often these are available in the ODF file (see Table VIIC.1) so they need not be printed in the LPT file.
	X	DO NOT PRINT PARTIAL derivatives PRINT PARTIAL DERIVAtives	Use this option only for debug purposes.
	X	DO NOT SUPPRESS INTErmediate printout	Updated parameter values and covariance matrix elements are printed after completion of each energy region.
		SUPPRESS INTERMEDIATe printout	Updated parameter values and c.m.e. are printed only upon completion of entire run.
		DO NOT SUPPRESS ANY intermediate printout	Updated parameter values are printed after each iteration of Bayes' equations (i.e., typically twice for each energy region). Updated covariance matrix elements are evaluated and printed only upon completion of an energy region. This option is generally used only for debug purposes.
	X	DO NOT PRINT DEBUG Information PRINT DEBUG INFORMATion	Use only for debug purposes.
	X	OUTPUT COVARIANCE MAtrix in binary form	The parameter covariance matrix is output in binary form in a separate file whose name is SAMMY.COV. (See Section VII.B.)
		DO NOT OUTPUT COVARIance matrix in binary form	This option is no longer available.
	X	DO NOT USE SHORT FORmat for output USE SHORT FORMAT FOR output	Resonance parameters are printed in the LPT file (Section VII.A), in F12.4 format rather than E format. While this may produce more legible output, often fewer significant digits will be printed.
	X	DO NOT PRINT REDUCED widths PRINT REDUCED WIDTHS	Reduced width amplitudes will be printed in the LPT file (Section VII.A), along with the square root of the resonance energies. That is, what is printed is the "γ-parameters" as described in Section III of this report.

Table VIA.2 Alphanumeric statements acceptable for use in the INPut file, card set 3 (contd)

Category	Default	Statements	Notes
Operation Control	X	SOLVE BAYES EQUATIONs	Update parameter values and covariances via Bayes' equations.
		DO NOT SOLVE BAYES Equations	Parameters are not updated, but remain fixed. Theoretical values of transmission or cross section are evaluated for each energy region specified, using these fixed parameter values.
	X	DO NOT DIVIDE DATA into regions - do entire energy range at once	
		DIVIDE DATA INTO REGions with a fixed number of data points per region	SAMMY will automatically choose energy regions of NEPNTS (see card set 2, Table VIA.1) data points each, for sequential analysis. Warning: SAMMY merely counts; it does not consider carefully whether the dividing point is located in a region where the theoretical values (σ or T) are nonlinear with respect to the parameters. Dividing in such a location (at or near a resonance) will invalidate the linearity assumption used in deriving Bayes' equations, and thus lead to spurious results. Users are urged to use this option only on the "zeroth pass," as an aid in deciding where to divide the data, and not for final runs.
	X	BROADENING IS WANTED BROADENING IS NOT WAnted	If you do not wish to have SAMMY Doppler- or resolution-broaden the theoretical values, be sure to remove card sets 5 and 6 (see Table VIA.1) from the INP file, as well as include this card.
	X	USE ORIGINAL GRID FOr broadening at end points USE EVEN GRID FOR BRoadening at end points	The original auxiliary grid, as used in MULTI, had eight points within a few resolution widths plus eight points within a few Doppler widths of both EMIN and EMAX, for use in broadening the cross section or transmission at the end points. (See Sect. IV.B.1.) The even grid uses datapoints outside [EMIN,EMAX] or, if your DATa file contains no such points, energy points chosen at the same relative spacing as in your data.
	X	USE NEW DEFAULT FOR uncertainty on resonance energies	Poor choice of words - "NEW" is as of April 1981! At any rate, the default initial uncertainty ΔE_λ on resonance energy E_λ is given by $\Delta E_\lambda = \tfrac{1}{2}\left[\lvert\Gamma_{\lambda\gamma}\rvert + \sum_c \lvert\Gamma_{\lambda c}\rvert + d + r\right]$ where d and r are the Doppler and resolution widths, respectively, evaluated at E_λ, and where the summation includes only particle channels. Caveat: For large s-wave resonances ($\Gamma_n \geq 1$ keV) this uncertainty will be too large and will cause SAMMY to give unreasonable results. Occasionally this may happen even for smaller resonances. To avoid this problem, input energy uncertainties explicitly via Table VIB.1, last card set, first alternative.
		USE ORIGINAL DEFAULT for uncertainty on resonance energies	The original default is $\Delta E_\lambda = 10\%\ E_\lambda$ or ΔE_λ = FUDGE*E_λ, if you choose to set a value other than 10% (see Table VIB.1, card set 2). It is highly recommended that you do not use this option.

Table VIA.2 Alphanumeric statements acceptable for use in the INPut file, card set 3 (contd)

Category	Default	Statements		Notes
Operation Control	X	DO NOT USE S-WAVE CUTOFF USE S-WAVE CUTOFF		Non s-wave resonances far away from the data being analyzed are omitted in parts of the calculation of the R-matrix. The definition of "far away" used in setting the partial derivatives to zero is $\lvert E - E_\lambda \rvert > 20 \left(\sum_c \Gamma_{\lambda c} + \Gamma_\lambda \right) + 3 (d + r)$ where d and r are Doppler and resolution widths, respectively. The definition of "far away" for the contribution to the imaginary part of r is 100 times that for the derivatives; contributions to the real part of r are always included. For s-wave resonances, the user may choose whether to use a similar cutoff. If a cutoff is desired, its value is twice that for non s-wave resonance. Caution: Though SAMMY will run faster with the cutoff option invoked, results may not be as accurate.
	X	DO NOT PERFORM SUMMAry analysis PERFORM SUMMARY ANALysis		Evaluate and print the summed strength function and the corresponding covariance matrix. Note: SAMMY stops upon completion of this task.
	X	LET SAMMY CHOOSE WHIch inversion scheme to use USE (N+V) INVERSION scheme USE (I+Q) INVERSION scheme		Original method. See Section II. See Section II.
	X	REICH-MOORE FORMALISm is wanted MLBW FORMALISM IS WAnted MULTILEVEL BREIT-WIGner formalism is wanted	Equivalent statements	See Section III.A. See Section III.C

Table VIA.2 Alphanumeric statements acceptable for use in the INPut file, card set 3 (contd)

Category	Default	Statements	Notes
ODF File control	X	DO NOT GENERATE ODF file automatically GENERATE ODF FILE AUtomatically } equivalent GENERATE PLOT FILE Automatically } statements	The output ODF file is described fully elsewhere (Table VIIC.1). To complete all sections of this file requires (1) initialization; (2) run SAMMY without solving Bayes' equations to obtain theoretical values determined by the input parameters; 3) solve Bayes' equations to obtain updated parameter values; and (4) obtain theoretical values determined by the updated parameters. That is, the ODF file requires an initialization plus three complete passes through SAMMY. The option to GENERATE ODF (or PLOT) FILE AUtomatically does all this busy-work for you. If you don't care to make any plots, by all means don't bother with this!
		ODF FILE IS WANTED--XXXXXX.XXX,ZERO-th order guess ODF FILE IS WANTED--XXXXXX.XXX,FINAl guess	These statements are all ignored if you choose to GENERATE ODF FILE automatically. To use these options, replace XXXXXX.XXX (columns 21-30) with the name of your ODF file. Be sure that file already contains energies and data (Sections 1, 2, 3, and possibly 6 and 7; see Table VIIC.1).
	X	DO NOT INCLUDE THEORetical uncertainties in plot file INCLUDE THEORETICAL uncertainties in plot file	The covariance matrix element connecting theory point T_i with point T_j is $$\sum_{k,n} \frac{\partial T_i}{\partial u_k} M_{kn} \frac{\partial T_j}{\partial u_n}$$ where M_{kn} is the covariance matrix element connecting parameter u_k with parameter u_n. The theoretical uncertainty on theory T_i is the square root of the diagonal element; that is, $$\Delta T_i^2 = \sum_{k,n} \frac{\partial T_i}{\partial u_k} M_{kn} \frac{\partial T_i}{\partial u_n}.$$ The values ΔT_i are reported in sections 10 and 11 of the ODF file.

Table VI.A.2 Alphanumeric statements acceptable for use in the INPut file, card set 3 (contd)

Category	Default	Statements	Notes
Requests for output that necessitate additional calculations		CHI SQUARED IS NOT Wanted } equivalent DO NOT PRINT LS CHI squared } statements	Remember that in Bayes' (as opposed to least-squares) χ^2 is an irrelevant quantity and is therefore not even calculated. If, however, you wish to know its value, you may request that it be generated. For each energy region,
	X	DO NOT PRINT BAYES Chi squared	$\chi^2_{LS}=\sum_i (D_i-T_i)(V^{-1})_i(D_i-T_i)$
	X X	CHI SQUARED IS WANTEd } equivalent PRINT LS CHI SQUARED } statements PRINT BAYES CHI SQUAred	is calculated, and χ^2 and χ^2/NDAT (where NDAT is the number of data points in that region) are reported. Note that we do *not* report χ^2/dof, where dof = degrees of freedom = NDAT-NPAR (where NPAR is the number of parameters), since with Bayes' method dof can be zero or negative. In addition to χ^2, the quantity we choose to call the Bayesian χ^2 may also be reported, where $\chi^2_B=\sum_{ij}(D_i-T_i)(N-V)^{-1}_{ij}(D_j-T_j)$. Caveat: Theoretical values T_i are generated using the values of the parameters *prior to* analysis of this energy region.
	X X	DO NOT PRINT WEIGHTEd residuals } equivalent DO NOT PRINT LS WEIGhted residuals } statements	Two types of weighted residuals may be printed. The least-squares weighted residual is defined as
	X	DO NOT PRINT BAYES Weighted residuals	$R_i^{LS}=(V^{-1})_{ii}(D_i-T_i)$
		PRINT WEIGHTED RESIDuals } equivalent PRINT LS WEIGHTED REsiduals } statements PRINT BAYES WEIGHTED residuals	where D is the experimental data, V its covariance matrix, and T the theoretical value evaluated at the *initial* values of the parameters. The Bayesian weighted residual is defined as $R_i^B=\sum_j (N+V)^{-1}_{ij}(D_j-T_j)$ where $N_{kn}=\sum_{ij}\frac{\partial T_k}{\partial u_i}M_{ij}\frac{\partial T_n}{\partial u_j}$ and M_{ij} is the initial covariance matrix element for parameters u_i and u_j.
	X	DO NOT PRINT ANALOGOus MLBW parameters PRINT ANALOGOUS MULTilevel Breit-Wigner parameters	Analogous multilevel Breit-Wigner (MLBW) parameters are defined as $E_\lambda^{MLBW}=E_\lambda^{RM}-\sum_{c=particle}\sum_{channels}(S_c-B_c)\gamma^2_{\lambda c}$ and $\Gamma_{MLBW}=\Gamma_\lambda^{RM}+\sum_c \Gamma_{\lambda c}^{RM}$ where "RM" refers to the Reich Moore parameters as determined by SAMMY. See Section III B 2.
	X	DO NOT PRINT PHASE shifts PRINT PHASE SHIFTS For input parameters	

Table VIB.1 Format of the PARameter file

Note: All integer formats (e.g., I2, I5) require that the numbers be in the right-most columns. Similarly, all exponents on E formats (e.g., 1.544E+05) need to be in right-most columns.

Card set	Must this set be present	Number of cards *in the* set	Which card *is* this	Column	Variable Name	Format	Meaning (Units)	Values	Notes
1	Yes	As many as you need (number of resonances, plus one)	Any of them except the last	1-11	ERES or E_λ	E11.4	Resonance energy E (eV)		
				12-22	Γ^γ	E11.4	Gamma width (milli-eV)		
				23-33	Γ_{c1}	E11.4	Particle width for channel 1 (milli-eV)		If any Γ is negative, SAMMY will use $\lvert\Gamma\rvert$ for the width and set the associated amplitude γ to be negative. That is, SAMMY will use $\gamma = -\chi\sqrt{\lvert\Gamma\rvert}$ where χ is the appropriate factor (see Sect. III.A.1.b).
				34-44	Γ_{c2}	E11.4	Particle width for channel 2 (milli-eV)		
				45-55	Γ_{c3}	E11.4	Particle width for channel 3 (milli-eV)		
				56-57	IS_{ERES}	I2	vary ERES?	0 = no, 1 = yes	
				58-59	IS_γ	I2	Vary Γ^γ?	0 = no, 1 = yes	
				60-61	IS_{c1}	I2	Vary Γ_{c1}?	0 = no, 1 = yes	
				62-63	IS_{c2}	I2	Vary Γ_{c2}?	0 = no, 1 = yes	
				64-65	IS_{c3}	I2	Vary Γ_{c3}?	0 = no, 1 = yes	
				66-67	IGROUP	I2	Quantum numbers for this resonance are those of group number IGROUP (see card set No. 10 in Table VIA.1)		
				68-80	DCOV	E13.4	Constant on-and-off diagonal data covariance to be used under this resonance		Usually these columns are blank, unless the option "ADD CONSTANT TERM To data covariance" is invoked. (See Table VIA.2). DCOV should be $\leq (\Delta d)^2$, where Δd is the (absolute) uncertainty on data near this resonance.
			last one	blank					It is OK to omit this card if this is the end of the file.

Table VIB.1 Format of the PARameter file (contd.)

Card set	Must this set be present	Number of cards in the set	Which card is this	Column	Variable Name	Format	Meaning (Units)	Values	Notes
2	Yes, if any additional card sets are present	1	1	1-11	FUDGE	E11.4	Initial uncertainty on varied parameters is FUDGE times the parameter value, for parameters not explicitly specified elsewhere.	>0. If =0, SAMMY uses FUDGE=0.1)	For resonance energy E_α, the initial uncertainty is set at 1/2 times the sum of all widths including Doppler and resolution widths). The value of FUDGE will not affect ΔE_α.
3	No	At least 3 At most (NGROUP × NCHAN) + 2	1	First Few	WHAT	A5	Alphanumeric indicator of what input follows	EXTERnal R-function parameters follow	Only the first five characters must be on the card, but the rest might as well be so that you know what's coming.
			2	1-3	IGROUP	I3	Spin group number	1,2,3, ..,NGROUP	
				4-5	ICHN	I2	Channel number	1,2, ..,NCHN	If ICHN=0 here, SAMMY assumes =1
				6-16	E_α^{down}	F	Logarithmic singularity below energy range (eV)		Parameters in the logarithmic parameterization of the external R-matrix for quantum numbers α (=IGROUP,ICHN), of the form
				17-27	E_α^{up}	F	Logarithmic singularity above energy range (eV)		
				28-38	$R_{const,\alpha}$	F	Constant term		$R_\alpha^{ext}(E)=R_{const,\alpha}+R_{lin,\alpha}\times E$
				39-49	$R_{lin,\alpha}$	F	Linear term		$-s_\alpha \ln\left[(E_\alpha^{up}-E)(E-E_\alpha^{down})\right]$
				50-60	s_α	F	Coefficient of logarithmic term	≥0	
				62	ISE_α^{down}	I1	Vary E_α^{down}?	0 = no, 1 = yes	
				64	ISE_α^{up}	I1	Vary E_α^{up}?	0 = no; 1 = yes	
				66	$ISR_{const,\alpha}$	I1	Vary $R_{const,\alpha}$?	0 = no; 1 = yes	
				68	$ISR_{lin,\alpha}$	I1	Vary $R_{lin,\alpha}$?	0 = no; 1 = yes	
				70	ISs_α	I1	Vary s_α?	0 = no, 1 = yes	
			3, etc	Just like 2					Include only those spin groups and channels for which you wish to parametize R^{ext} in this way.
			Last	blank					

Table VIB.1 Format of the PARameter file (contd.)

Card set	Must this set be present	Number of cards in the set	Which card is this	Column	Variable Name	Format	Meaning (Units)	Values	Notes
Alternative to 3	No	At least 3 At most (NGROUP × NCHAN) + 2	1	First Few	WHAT	A5	Alphanumeric indicator of what input follows	R-EXTernal parameters follow	Only the first five characters must be on the card, but the rest might as well be so that you know what s coming
			2	1-2	IGROUP	I2	Spin group number	1,2,3, . .,NGROUP	
				3	ICHN	I1	Channel number	1,2,...,NCHN	If ICHN=0 here, SAMMY assumes =1.
				4	ISE_c^{down}	I1	Vary E_c^{down}?	0 = no, 1 = yes	
				5	ISE_c^{up}	I1	Vary E_c^{up}?	0 = no, 1 = yes	
				6	$ISR_{con,c}$	I1	Vary $R_{con,c}$?	0 = no, 1 = yes	
				7	$ISR_{lin,c}$	I1	Vary $R_{lin,c}$?	0 = no 1 = yes	
				8	$ISs_{con,c}$	I1	Va $s_{con,c}$?	0 = no, 1 = yes	
				9	$ISs_{lin,c}$	I1	Vary $s_{lin,c}$?	0 = no, 1 = yes	
				10	$ISR_{q,c}$	I1	Vary $R_{q,c}$?	0 = no, 1 = yes	
				11-20	E_c^{down}	F	Logarithmic singularity below energy range (eV)		Parameters in the logarithmic parameterization of the external R-matrix for quantum numbers c (=IGROUP,ICHN), of the form
				21-30	E_c^{up}	F	Logarithmic singularity above energy range (eV)		
				31-40	$R_{con,c}$	F	Constant term		$R_c^{ext}(E)=R_{con,c}+R_{lin,c}\times E$
				41-50	$R_{lin,c}$	F	Linear term (eV^{-1})		$+R_{q,c}\times E^2$
				51-60	$s_{con,c}$	F	Constant coefficient of logarithmic term	≥0	$-s_{lin,c}(E_c^{up}-E_c^{down})$
				61-70	$s_{lin,c}$	F	Linear coefficient of logarithmic term (eV^{-1})		$-(s_{con,c}+s_{lin,c}\times E)\times$ $\ln\left[(E_c^{up}-E)/(E-E_c^{down})\right]$
				71-80	$R_{q,c}$	F	Quadratic term (eV^{-2})		
			3, etc.	Just like 2					Include only those spin groups and channels for which you wish to parameterize R^{ext} in this way.
			Last	blank					

Table VIB.1 Format of the PARameter file (contd.)

Card set	Must this set be present	Number of cards in the set	Which card is this	Column	Variable Name	Format	Meaning (Units)	Values	Notes
4	No	3	1	First few	WHAT	A5	alphanumeric indicator of what comes next	BROADening parameters (etc.) may be varied	only the first five characters are required
			2	1-10	CRFN	F	matching radius(F)	≥0	All six of these parameters appear in the INPut file, card sets 5 and 7 of Table VIA 1. However, if card set 4 appears in the PARamer file, values given in the INPut file will be ignored
				11-20	TEMP	F	effective temperature of the sample(K)		
				21-30	THICK	F	sample thickness(at/b)		
				31-40	DELTAL	F	flight path uncertainty(m)		
				41-50	DELTAG	F	FWHM(μs) of Gaussian resolution function whose variance is equivalent to that of the square pulse		
				51-60	DELTAE	F	e-folding width of exponential resolution function (μs)		
				62	IVBRD(1)	I	vary CRFN?	-1 or 0=no, 1=yes	A negative value here indicates that the value of this parameter is changed from earlier runs; only those parameters which are not varied may be changed in this fashion.
				64	IVBRD(2)	I	vary TEMP?	-1 or 0=no, 1=yes	
				66	IVBRD(3)	I	vary THICK?	-1 or 0=no, 1=yes	
				68	IVBRD(4)	I	vary DELTAL?	-1 or 0=no, 1=yes	
				70	IVBRD(5)	I	vary DELTAG?	-1 or 0=no, 1=yes	
				72	IVBRD(6)	I	vary DELTAE?	-1 or 0=no, 1=yes	
			3	(blank)					

Table VIB.1 Format of the PARameter file (contd.)

Card set	Must this set be present	Number of cards in the set	Which card is this	Column	Variable Name	Format	Meaning (Units)	Values	Notes
5	No	4	1	first few	WHAT	A5	alphanumeric indicator of what comes next	UNUSEd but correlated variables come next	At most eight unused variables are allowed. See the author if you need more.
			2	1-5	NUSED(1)	A5	name of first unused variable		Parameter files containing this card set are never generated directly by a user; rather, they result from using the code SAMADD or SAMMIX. See Section X for details.
				11-15	NUSED(2)	A5	name of second unused variable		
				71-75	NUSED(8)	A5	name of eighth unused variable		
			3	1-10	UNUSED(1)	F	value of first unused variable		
				11-20	UNUSED(2)	F	value of second unused variable		
				71-80	UNUSED(8)	F	value of eighth unused variable		
			4	(blank)					

Table VIB.1 Format of the PARameter file (contd.)

Card set	Must this set be present	Number of cards in the set	Which card is this	Column	Variable Name	Format	Meaning (Units)	Values	Notes
last (first alternative)	No	At least 2	1	First few	WHAT	A5	Alphanumeric indicator of what comes next	EXPLIcit uncertainties and correlations follow	First five characters must be present; the rest are optional.
			2	1-5	NN	I5	(a) To explicitly input the initial (or prior) uncertainty on resonance parameters, find the number of the resonance (i.e., count lines in card set #1 in this file). That number is "NN" and goes in column 1-5, right-adjusted. The value of MM for columns 6-10 is 1 if the parameter of interest is E_r, 2 if Γ_n, 3 if Γ_γ, 4 if Γ_α, etc. KK and LL are zero. VV then represents the absolute value of the uncertainty for this parameter, in the same units as the parameter itself		You will not include explicit uncertainties for every parameter, but only those for which you don't like the default value.
				6-10	MM	I5			
				11-15	KK	I5			
				16-20	LL	I5			
				21-30	VV	F			
							(b) To explicitly input the prior uncertainty on R-external parameters, set NN = (1000 plus IGROUP), where IGROUP is the group number. Let MM = 1 for E_c^{shift}, 2 for E_c^{sep}, 3 for $R_{ext,n}$, 4 for $R_{ext,\gamma}$, and 5 for s_c, all for channel 1. (For channel 2, MM = 6, 7, 8, 9, and 10 respectively; for larger channel numbers, just keep adding 5.) The absolute value of the uncertainty on that parameter is VV		
							(c) To explicitly input the prior uncertainty on broadening (etc) parameters, set NN=2000 + n, where n = 1 for radius, 2 for effective temperature, 3 for sample thickness, etc. (see card set #4. MM is irrelevant here.) The absolute uncertainty on that parameter is VV.		
							(d) To explicitly input correlations between the uncertainties on two parameters, let NN and MM indicate the first parameter, as in (a), (b), or (c) above. The second parameter is indicated by KK and LL (analogous to NN and MM, respectively). The correlation coefficient is then give by VV. Note that $-1 \leq VV \leq +1$		
			3,4, etc.				Repeat card #2 as many times as you want.		
			last	blank					this card may be omitted.

Table VIB.1 Format of the PARameter file (contd.)

Card set	Must this set be present	Number of cards in the set	Which card is this	Column	Variable Name	Format	Meaning (Units)	Values	Notes
last (second alternative)	No	At least 2	1	First few	WHAT	A5	Alphanumeric indicator of what comes next	RELATive uncertainties follow	
			2	1-11	RUNCS(1,1)	E11.4	Resonance energy, *exactly* as it appears in card set 1 above.		
				12-22	RUNCS(2,1)	E11.4	Relative uncertainty on resonance energy	≥0	
				23-33	RUNCS(3,1)	E11.4	Relative uncertainty on Γ_γ	≥0	
				34-44	RUNCS(4,1)	E11.4	Relative uncertainty on Γ_{n1}	≥0	
				45-55	RUNCS(5,1)	E11.4	Relative uncertainty on Γ_{n2}	≥0	
				56-66	RUNCS(6,1)	E11.4	Relative uncertainty on Γ_α	≥0	
				67-68	JUNCS(1,1)	I2	Flag specifying whether to use this uncertainty for ERES	=1 [use relative uncertainty given by RUNCS(2,1)] =0 (use SAMMY default)	
				69-70	JUNCS(2,1)	I2	Flag to use this uncertainty for Γ_γ	=1 [use RUNCS(3,1)] =0 (use default)	
				71-72	JUNCS(3,1)	I2	Flag for Γ_{n1}	=1 [use RUNSC(4,1)] =0 (use default)	
				73-74	JUNCS(4,1)	I2	Flag for Γ_{n2}	=1 [use RUNCS(5,1)] =0 (use default)	
				75-76	JUNCS(5,1)	I2	Flag for Γ_α	=1 [use RUNCS(6,1)] =0 (use default)	
			3,4, etc					Repeat card 2 as many times as needed	
			last	blank					this card may be omitted.
last (third alternative)	No	1	1	First few	WHAT	A5	Alphanumeric message	COVARiance matrix is in binary form in another file. (See Table VIIB.1).	The *output* parameter file makes use of this alternative.

VII. OUTPUT FROM SAMMY

Output from SAMMY consists of five files, itemized in Table VII.1.

Table VII.1 SAMMY output files

File Name	Contents
SAMMY.LPT	Descriptive output, to be queued to the lineprinter for examination.
SAMMY.IO	Lists only the initial and final values of physical parameters.
SAMMY.PAR	PARameter file with new values of varied parameters, in the same format as the input PARameter file. The third alternative is used for the last card set in the PAR file, Table VIB.1.
SAMMY.COV	New covariance matrix for the parameters, in binary form. Also new values for all varied parameters. See Table VIIB.1.
SAMMYA.ODF (optional)	ODF file from which plots can be produced. See Table VIIC.1.

X.B. PROCEDURES TO FOLLOW WHEN YOU HAVE PROBLEMS

1. If SAMMY Bombs

a. If possible, throw nothing away and modify nothing!

b. Bring the author a listing of the LOG file (or, if you ran interactively and do not have a hard copy, write down details of where and why SAMMY bombed, and the names of all input files and EMIN, EMAX). If you are working on the ORELA PDP-10 but via long-distance, give the author the name of the file and your PPN and she will obtain the listing.

c. If possible, describe how this case differs from cases you have run successfully in the past.

d. Feel free to call the author at home (690-3936), if she is not in her office.

2. If SAMMY Terminates Normally but you don't Believe the Results

a. Carefully check **all** of your input . . .

   i. Do you have the proper commands in the INP file?

   ii. Did you flag what you intended in the PAR file?

   iii. Did you slip a decimal point anywhere? (e.g., for EMIN and EMAX)

   iv. Is your data file messed up? (e.g., are some of the uncertainties unrealistically small?)

   v. Etc.; see Table XB.1.

b. List the LPT file. Look it over carefully to help locate possible input errors, for example. Be sure you look at this **before** you ask for help.

c. Did you use the "DIVIDE DATA INTO REGions of equal energy-range" option? If so, SAMMY may have chosen to divide the data very near a resonance. **Sometimes** this causes problems. To avoid this, resubmit the job, choosing energy-regions carefully (i.e., **do not** have SAMMY choose them for you).

d. If none of the above satisfy you, see the author. Please follow the steps in Part I! Also, bring a listing of the LPT file, please.

Table XB.1. Possible solutions to some common problems

Problems that may occur during a SAMMY run		Possible solutions
(1) SAMMY tells you that the the matrix is nearly singular.	(a)	Initial parameter uncertainties are too large. Modify by using "EXPLICit uncertainties or correlations" at the end of PAR file.
	(b)	Too many parameters are being varied.
	(c)	Too few data points are used.
	(d)	Sometimes this message can be ignored! But do so at your own risk.
(2) A "divide check" or "floating overflow" message appears.	(a)	Your INPut or PARameter or DAT file has a zero (or a number which SAMMY reads as zero) where none is permitted. List the LPT file and look it over carefully.
	(b)	SAMMY has a bug?!
(3) Cryptic messages occur before SAMMY bombs.	(a)	The PDP10 has had a bad day. Try again tomorrow.
	(b)	You are trying to analyze too many data points at one time. Use fewer points, or vary only the parameters of interest.
	(c)	You mistyped a file name.
(4) Results "run away" from your "reasonable" input.	(a)	Your input did not properly describe the background. Try adding more dummy reasonances, check if spin groups are properly assigned, etc.
	(b)	Data uncertainties are unrealistic. Zeros are never allowed and very small values should be increased.
	(c)	Total cross sections may look funny at large resonances, so increase the uncertainties. Better yet, use transmission, and increase uncertainties for low T.
	(d)	Systematic errors in data should be handled with off-diagonal data covariances.
	(e)	"DIVIDE DATA INTO REGions" landed in the middle of a resonance. Change the number of data points, or better yet, choose the regions yourself.
	(f)	The number of iterations is too small. (This is rarely true, experience has shown.)
	(g)	Your input contained errors such as misplaced decimal points.
	(h)	Try analyzing any "sensitive" energy regions first and/or last.
	(i)	Initial parameter uncertainties are too big. This is especially likely to be a problem for resonance energies.

XI.B USE OF TEMPORARY DATA FILES TO STORE INTERMEDIATE RESULTS

Output to and input from temporary files is a time-honored method of saving core space at the expense of runtime. Temporary files generated by SAMMY are listed in Table XIB.1, along with input and output files required by or produced by SAMMY. Upon successful completion of a run, SAMMY deletes the temporary files. An aborted run can sometimes be restarted if the user takes care not to destroy these files.

Table XIB.1 Files used by SAMMY

Unit Number	File Name	Segment (alternative unit number) Subroutines in which this file is written	Segment (alternative unit number, if different from the usual one) Subroutines in which this file is read	What is stored	Notes
5	teletype or batch (log) file	many places	MAS FILES, FIXNAM, FILE2X	see Table VID 1	
11	INPut file		MAS FINP,NEW	see Tables VIA.1 & VIA.2	
11	SAM22.DAT	MAS(22) NEW,SETT,SET	PAR,INP2,INPFIL,RDONE, HUH,RDBRD,COMBI,RDSPIN	copy of INPut file	see Unit Numbers 22,23, and 24 (second set thereof)
12	PARameter file		MAS FPAR PAR,FIRSTR,PARFIL,READRS,PREAD, READEX,BRDFIX,READDA,READUN, READRE,READAB	see Table VIB.1	
13	DATa file		MAS FDAT ODF CHCK13,READ13 DAT SECNDR,DATFIL	see Table VIC 1	
14	SAM14 DAT	MAS ODFDAT			if DATa file is in ODF, it is copied into SAM14.DAT in SAMMY-MASTER:ODFDAT
15	SAM15 DAT	MAS FIXFIL			for rewriting SAM16.DAT and SAM19.DAT in order to add additional information.
16	SAM16 DAT	MAS FILES,FILE2X	MAS FIXFIL PAR Main, FILES,FILESX, SRCH,ADDUP	equivalant of teletype input (see Table VID 1) for first and second passes through SAMMY	
17	SAM17 DAT	MAS Main END Main	END Main	Controls for which pass through SAMMY is to be made next	
18	SAM18 DAT	MAS FINP,FILES,FIXNAM, FILE2X ODF(16) CHCK16	ODF(16) Main,CHCK16, READ16	operation control for segment SAMMY-ODF	
19	SAM19 DAT	MAS FILES,FILE2X	see Unit number 16	equivalent of teletype input for third pass through SAMMY	renamed to SAM16.DAT in SAMMY-END
20	SAM20 DAT	PAR Main DAT Main THE Main CRO Main BRO Main FIN Main	DAT Main THE Main CRO Main BRO Main FIN Main	information from COMMON/ EXPAND/ and other COMMONs, dimensions for this problem	this file is the primary communications link between the various segments of SAMMY
21	SAMMY LPT	almost everywhere	never	line printer output	
22	SAMMYA ODF	ODF FIXODF	BRO THODF	see Table VIIC 1	
23	SAMMYB ODF	BRO THODF	FIN VODF		
24					
28	SAMMYG ODF				
28	SAM28 DAT	DAT Main,IDIMEN THE Main,IDIMEN CRO Main,IDIMEN MLB Main,IDIMEN BRO Main,IDIMEN SET Main,IDIMEN NPV Main,IDIMEN IPQ Main,IDIMEN FIN Main,IDIMEN	DAT Main THE Main CRO Main MLB Main BRO Main SET Main NPV Main IPQ Main FIN Main	array dimensions for automatically increasing storage	file is deleted after each use

Table XIB.1 Files used by SAMMY (contd)

Unit Number	File Name	Segment (alternative unit number) Subroutines in which this file is written	Segment (alternative unit number, if different from the usual one) Subroutines in which this file is read	What is stored	Notes
22 23 24	SAM22.DAT SAM22.DAT SAM22.DAT	MAS NEW.SETT.SET	PAR(11).INP2,INPFIL, RDONE,HUH,RDBRD, COMBI,RDSPIN, PREAD,READEX	a copy of INPut file, with changes appropriate for the first, second and third passes through SAMMY	SAMMY-END renames these files so that the one used in SAMMY-PAR is always called SAM22.DAT
24	SAMMY IO	PAR FILES,OUTPA2, OUTVS FIN Main,OUTPA2, OUTVS	nowhere	input and out values of parameters	
26	SAM26.DAT	PAR Main	FIN(16).FILE2X	[illegible] parts of SAM16.DAT	
26	SAM27.DAT	FIN FILE2X		copy of parts of SAM26.DAT	renamed to SAM26.DAT
32	SAMMY.PAR	FIN OLDORD		output PARameters (see Table VIB.1)	
41	SAM41.DAT	PAR SET41	FIN COMPAR	initial uncertainties on varied parameters	
42	SAM42.DAT	PAR RPARFL,BINALL FIN WRCOV,COMPAR	PAR.SET41,ADDUP,OUTVS FIN:OUTVS	parameter covariance matrix	
43	SAM43.DAT	DAT EORDER	THE.USET	data and raw covariance matrix	
44	SAM44.DAT	DAT EORDER	NPV RDATFL IPQ RDATF2	data and adjusted covariance matrix	
45	SAM45.DAT	NPV SETVDT	FIN.VODF	theoretical uncertainties	
46	SAM46.DAT	PAR ADDUP		covariance matrix for summed strengths	
46 47	SAM46.DAT SAM47.DAT	PAR.RPARFL,BINCOV NPV CHNGCV IPQ CHNGC2	PAR.OUTVR SET:Main NPV SETEMG,CHNGYY,CHNGCV IPQ:STQP1,CHISE2, CHNGX2,CHNGY2, CHNGC2,STPADD FIN:WRCOV,COMPAR, OUTVR	covariance matrix for u-parameters	these two files alternate, one holding the "old" matrix, the other the "new"
48	SAM48.DAT	BRO RESOLU or NORESO or NOBROA or TRANSX	BRO:OUTG NPV:SETG IPQ:RDATF2	partial derivatives	

Table XIB.1 Files used by SAMMY (contd)

Unit Number	File Name	Segment (alternative unit number): Subroutines in which this file is written	Segment (alternative unit number, if different from the usual one): Subroutines in which this file is read	What is stored	Notes
49	SAM49.DAT	PAR.BETSET,BINALL NPV:Main,WRITEU IPQ.Main,WRITEU	SET.Main BRO.Main,(FILCOPY) NPV.Main,READU IPQ:Main,READU FIN:Main,READU,WRCOV	Miscellaneous information needed in SAMMY-NPV or SAMMY-IPQ for solving Bayes' equations.	
49	SAM59.DAT	BRO.WR49			rename to SAM49.DAT
51	SAM51.DAT	BRO DOPPLR	BRO:TRANS or RESOLU or NORESO	intermediate steps during broadening	
52	SAM52.DAT	BRO TRANS	BRO:RESOLU(READGB) or NORESO or NOBROA	partly-broadened partial derivatives	
52	SAMMY.COV	FIN:WRCOV		output covariance matrix, etc.	See Table VIIB.1
53	DCV file		DAT:DATFIL	data covariance file	
54	SAM54.DAT	CRO:WORK MLB WRIT54	BRO.DOPPLR(READGB) or TRANS or RESOLU(READGB) or NORESO or NOBROA	unbroadened partial derivatives	
55	SAM55.DAT	BRO BROADN	BRO:BROADN,TRANSX	partly-broadened partial derivatives	
58	SAM58.DAT	NPV SETG,RDATFL IPQ.RDATF2	NPV:SETVDT IPQ.STQP1	partial derivatives	
59	SAM59.DAT	NPV:SETEMG	NPV:SETVDT	MG = large array	
62	COV file	during previous SAMMY run	PAR BINCOV,BINALL	initial values of parameter covariance matrix elements, etc.	See Table VIIB.1
62	SAM62.DAT	FIN:WRCOV	FIN.WRCOV	parts of covariance matrix	used only if radius is varied

XI.C DIVISION OF THE PROGRAM INTO STAND-ALONE SEGMENTS

The structure of program SAMMY makes it ideally suited for overlay, since each major operation is independent of the others. However, overlay is not particularly efficient on the PDP10 computer; instead, SAMMY makes use of the DECSystem-10 "CALL RUN" option which allows a FORTRAN program to initiate execution of another program. Thus SAMMY consists of 13 semi-autonomous programs, which pass information to each other via temporary files and which pass control to each other via the "CALL RUN" statement. Table XIC.1 describes the functions of each segment. Tree charts showing the subroutine structure of the segments are available from the author.

Table XI.C.1 Segments of the Code SAMMY

Segment	Abbreviation	Function	User Supplied Input (unit number)	Input from Temporary Files (unit number)	Output to Temporary Files (unit number)	Output to Permanent Files (unit number)	Control Passes to Which Segment	Control Comes from Which Segment
SAMMY MASTER (SAMMY)	MAS	read input commands from teletype (or batch file) and from INP file organize the manner in which SAMMY will run	teletype or batch file (5) INP file (11) PAR file (12) DAT file (13)	none	SAM14 DAT(14) SAM15 DAT(15) SAM16 DAT(16) SAM17 DAT(17) SAM18 DAT(18) SAM19 DAT(19) SAM22 DAT(22) SAM23 DAT(23) SAM DAT(24)	SAMMY LPT(21)	ODF or PAR	start
SAMMY ODF (SAMODF)	ODF	initialize ODF file by putting energies into S1 data and uncertainties in S2 and S3, S6 and S7	DAT file(13)	SAM18 DAT(18)		SAMMY LPT(21) SAMMYA ODF(22) SAMMYB ODF(23)	END	MAS
SAMMY PARAMETER (SAMPAR)	PAR	read input/output control statements, read physical parameters and covariance matrix, and generate u parameters	PAR file(12) COV file(62)	SAM22 DAT(22) SAM16 DAT(16)	SAM20 DAT(20) SAM26 DAT(26) SAM41 DAT(41) SAM42 DAT(42) SAM46 DAT(46) SAM49 DAT(49)	SAMMY LPT(21) SAMMY IO(24)	DAT	END or MAS
SAMMY DATA (SAMDAT)	DAT	read experimental data and covariance matrix, generate auxiliary energy grid	DATa file(13) Data CoVariance file(53)	SAM20 DAT(20)	SAM20 DAT(20) SAM43 DAT(43) SAM44 DAT(44)	SAMMY LPT(21)	THE	PAR or FIN
SAMMY THEORY (SAMTHE)	THE	housekeeping	none	SAM20 DAT(20) SAM43 DAT(43)	SAM20 DAT(20) SAM44 DAT(20)	SAMMY LPT(21)	CRO or MLB	DAT
SAMMY CROSS (SAMCRO)	CRO	generate cross sections and derivatives according to Reich Moore approximation or R matrix theory	none	SAM20 DAT(20)	SAM20 DAT(20) SAM54 DAT(54)	SAMMY LPT(21)	BRO	THE
SAMMY MLBW (SAMMLB)	MLB	generate cross sections and derivatives according to multilevel Breit Wigner approximation	none	SAM20 DAT(20)	SAM20 DAT(20) SAM54 DAT(54)	SAMMY LPT(21)	BRO	THE
SAMMY BROADEN (SAMBRO)	BRO	Doppler and/or resolution broaden the cross sections and partial derivatives convert to transmissions if necessary	none	SAM20 DAT(20) SAM54 DAT(54)	SAM20 DAT(20) SAM48 DAT(48) SAM49 DAT(49)	SAMMY LPT(21)	SET or NPV	CRO or MLB
SAMMY SETS (SAMSET)	SET	expand parameter covariance matrix from triangular to full form	none	SAM46 DAT(46) or SAM47 DAT(47) SAT49 DAT(49)	SAM46 DAT(46) or SAM47 DAT(47)		NPV or IPQ	BRO
SAMMY NPV (SAMNPV)	NPV	solve (S + F) form of Bayes equations	none	SAM44 DAT(44) SAM46 DAT(46) SAM47 DAT(47) SAM48 DAT(48) SAM49 DAT(49)	SAM45 DAT(45) SAM47 DAT(47) or SAM46 DAT(46)	SAMMY LPT(21)	FIN	BRO or SET
SAMMY IPQ (SAMIPQ)	IPQ	solve (F + Q) form of Bayes equations	none	SAM44 DAT(44) SAM46 DAT(46) or SAM47 DAT(47) SAM48 DAT(48)	SAM47 DAT(47) or SAM46 DAT(46) SAM49 DAT(49)	SAMMY LPT(21)	FIN	SET
SAMMY FINAL (SAMFIN)	FIN	convert from u parameters to physical parameters, output results	none	SAM20 DAT(20) SAM26 DAT(16) SAM41 DAT(41) SAM46 DAT(46) SAM47 DAT(47) SAM49 DAT(49)	SAM20 DAT(20) SAM27 DAT(26) SAM42 DAT(42)	SAMMY LPT(21) SAMMYA ODF(22) SAMMY IO(24) SAMMY PAR(32) SAMMY COV(52)	DAT or THE or END	NPV or IPQ
SAMMY END (SAMEND)	END	Decide what to do next, either run through the sequence PAR DAT-THE CRO-BRO SET NPY FIN (or an alternative sequence) again, or delete temporary file, and stop	none	SAM17 DAT(17)	SAM17 DAT(17)		PAR or STOP	FIN or ODF

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