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User's Guide for SAMMY: A Computer Model for Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations

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ABSTRACT

In this report we describe a method for determining the parameters of a model from experimental data based upon the utilization of Bayes' theorem. This method has several advantages over the least-squares method as it is commonly used; one important advantage is that the assumptions under which the parameter values have been determined are more clearly evident than in many results based upon least squares. Bayes' method has been used to develop a computer code which can be utilized to analyze neutron cross-section data by means of the R-matrix theory. The required formulae from the R-matrix theory are presented, and the computer implementation of both Bayes' equations and R-matrix theory is described. Results of our analysis of Ni^{60} transmission data from ORELA and of several artificial data sets, and a comparison of our results with those of an earlier multilevel R-matrix code, are also presented. Finally, details about the computer code and complete input/output information are given.

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I. INTRODUCTION

The nonlinear least-squares method is frequently used for obtaining estimates of parameters of a model by fitting experimental data. This procedure requires an initial estimate of the parameters of the model which are modified in an iterative fashion to minimize the value of χ^2. The method also provides an estimate of the errors in the parameters. Although the method of least-squares is widely used and has a well-understood theoretical foundation, in practice it is not totally free from problems. As the method is usually implemented and used, three difficulties often arise: i) the extent to which the final parameters are dependent upon the starting values is not known and is hard to assess; ii) when all parameters of the model are allowed to be adjusted, some of them frequently end up with values which are perceived to be unphysical; and iii) the estimate of the errors which the method provides are often perceived to be unreasonably small. How serious are these problems of course varies from case to case. The usefulness of the results obtained depends to some degree upon how serious these problems are in any given situation and what was done specifically to alleviate them. Consequently, this procedure which was expected to yield objective and well-understood answers, provides results which must be evaluated with great care. This is particularly true when we are interested in combining the information obtained from different experiments and the problems of fitting the data were not handled in a consistent fashion in the different experiments.

In Section II of this report we describe a method for determining the parameters of a model from experimental data based upon the utilization of Bayes' theorem. This method has several advantages over the least-squares method as it is commonly used; one important advantage is that the assumptions under which the parameter values have been determined are more clearly evident than in many results based upon least squares. The method has been used to develop a computer code (SAMMY) which can be utilized to analyze neutron cross-section data by means of the R-matrix theory. The required formulae from the R-matrix theory are presented in Section IV. Sections III and V describe the computer implementation of Bayes' equations and R-matrix theory, respectively. Results of our analysis of Ni^{60} transmission data from ORELA and of several artificial data sets, and a comparison of our results with those of an earlier multilevel R-matrix code, are given in Section VI. A brief summary appears in Section VII.

Five appendices complete this report: Miscellaneous algebraic details, too involved to be presented in the text, are given in Appendix A. A description of the computer code, including a detailed discussion of its space-saving features, is given in Appendix B. Appendix C explains input to and output from SAMMY, and input and output for a simple example are given in Appendix D. Finally, the code itself is listed in Appendix E.

II. BAYES' THEOREM

In this section we derive the formulae used in the code SAMMY to obtain the values of the parameters and their uncertainties using Bayes' theorem. We emphasize the conditions under which the formulae are applicable and the relationship of our results to the customary least-squares method. We adopt in this section the usual mode of description based on the theory of statistics since the reader is familiar with it. Derivation of our results from a different point of view will be presented elsewhere (PE79, PE80a).

Bayes' theorem is usually written:

$$p(A|B) \propto p(A)\, p(B|A) \qquad \text{(II.1)}$$

where:

A represents the parameters of the model and B the data.

$p(A|B)$ is the probability for the value of the parameters conditional upon the data B, and is what we seek. It is conventional to call $p(A|B)$ the posterior probability. When A represents several parameters, $p(A|B)$ is a joint probability density function (joint pdf). The expectation values of $p(A|B)$ are taken as the estimates for the parameters and its covariance matrix gives us a measure of how well the parameters are determined and of the parameters' interdependencies.

$p(B|A)$ is the probability for observing the data B given the parameters A. It is a function of the parameters A of the model and is known as the likelihood function of the data B.

$p(A)$ is the joint pdf for the value of the parameters A of the model, prior to consideration of the data B. It is known as the prior joint pdf. The expectation values of $p(A)$ are the prior estimates for

the values of the parameters and its covariance matrix gives a measure of how well the parameters are known before consideration of the data.

The constant of proportionality in Eq. (II.1) can be determined from the normalization condition.

The use of Eq. (II.1) as an estimator is considered controversial in many textbooks unless p(A) is an estimated joint pdf based upon some data or considered as an hypothesis. In order to avoid this problem, we will consider that the prior p(A) is based upon some data which we will denote by X, and rewrite Eq. (II.1) as:

$$p(A|BX) \propto p(A|X)\, p(B|AX) \quad . \tag{II.2}$$

In this form Bayes' theorem is always acceptable and has the meaning that p(A|BX) is the joint pdf based upon both data X and data B. It is often said that Eq. (II.2) is an "adjustment equation" where the estimates of the values of the parameters, from p(A|X), are adjusted on the basis of the data B to provide a new set of estimates. It should be noted at this stage that the form of Eq. (II.2) is valid only if the data B and X are independent. The extent to which the value of the parameters and their uncertainties are changed as a result of using Eq. (II.2) is a function of how accurate are the data B and how sensitive they are to the parameters. We postpone until later a discussion of the data X.

Let $A = \{P_k\}$ for $k = 1$ to K be the set of all parameters of the multilevel R-matrix theory. We use instead of A the letter P without an index to represent the K-dimensional column vector whose components are the P_k's, i.e.,

$$P = \{P_k\} \quad , \qquad k = 1,2,\ldots,K \tag{II.3}$$

We assume that the joint pdf $p(A|X)$ is a joint normal pdf having as an expectation value the vector $\bar{P}$ and a covariance matrix M. Under this assumption we have:

$$p(A|X) \propto \exp[\ -1/2\ (P-\bar{P})^t\ \ M^{-1}(P-\bar{P})]\ \ , \qquad (II.4)$$

where P is the "true" value of the parameters and the superscript t denotes the transpose.

The experimental data which we had symbolized by B and which is to be described by the R-matrix theory will now be represented by a data vector D whose components D^i are the L data points. We also assume that the experimental conditions are such that the data D, i.e. the D^i's, have a joint normal distribution about their "true" value T and the covariance matrix will be denoted by V. We therefore have the likelihood function,

$$p(B|AX) \propto \exp[\ -\ 1/2\ (D-T)^t\ V^{-1}(D-T)]\ \ . \qquad (II.5)$$

If, as we have just stated, T stands for the true value of the data, then the covariance matrix V represents the experimental "errors" of the data. The diagonal elements of V are the variances of the data points; and the off-diagonal elements, i.e. the covariances V^{ij}, represent the errors which jointly affect the data points D^i and D^j. It is conventional to state that the off-diagonal elements represent the correlated errors in the data. Although data are usually reduced in such a fashion that important correlations between data points are introduced, existing data analysis codes usually have no provisions for a nondiagonal covariance matrix V (PE80b). This is a major deficiency, which our code remedies. (Note that the inclusion of off-diagonal data covariances is not restricted to Bayes' method but could be done with

least-squares as well.) The importance of including correlations is illustrated by the examples in Section VI of the report.

We now need to relate the "true" value of the data T to the parameters P. Ideally T can be calculated exactly from the model, in our case the R-matrix theory. In practice it is not always so since the observed quantity often cannot be reduced to the form of cross sections because of various "experimental" problems such as Doppler broadening, multiple scattering, experimental resolution, etc. What is often done is to calculate the cross sections on the basis of the theory and then "fold into them" various effects to produce an estimate of the "true" values of the data D. In this process various approximations are used. In the likelihood function, Eq. (II.5), V must therefore be modified to include an estimate of the uncertainties in the theoretically calculated values T. These uncertainties are very often correlated over the range of the data being analyzed and contribute to the fact that the covariance matrix V is nondiagonal. In most data analysis codes used today, this problem is totally ignored and cannot be handled adequately since V is restricted to be diagonal. In what follows we will consider V to include all of the uncertainties: those from the data D and those from the theoretical estimates T based upon the R-matrix theory.

In the likelihood function, Eq. (II.5), we need to calculate T as a function of P, the true value of the parameters. This is done formally by considering T a function of P and performing a Taylor expansion about $\overline{P}$, the expectation value of $p(A|X)$, and keeping only the linear terms:

$$T(P) \simeq \overline{T} + G(P-\overline{P}) \quad , \tag{II.6}$$

where $\overline{T}$ is equal to $T(\overline{P})$.

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), the sensitivity matrix G is of dimension $L \times K$. The elements of G are the partial derivatives of T^n with respect to the parameters P_k evaluated at $P = \bar{P}$:

$$G^n_k = \left.\frac{\partial T^n}{\partial P_k}\right|_{P=\bar{P}} \qquad \text{for } n=1,2,\ldots,L \text{ and } k=1,2,\ldots,K \quad . \tag{II.7}$$

Substituting Eq. (II.6) into Eq. (II.5) and using Eq. (II.4) we obtain for the posterior joint pdf (Eq. (II.2)):

$$p(A|BX) \propto \exp[-1/2\,\{(P-\bar{P})^t\ M^{-1}(P-\bar{P}) + (D-\bar{T}-G(P-\bar{P}))^t\ V^{-1}(D-T-G(P-\bar{P}))\}]. \tag{II.8}$$

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,

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:

$$p(A|BX) \propto \exp[-1/2(P-\bar{P}')^t\ M'^{-1}\ (P-\bar{P}')] \quad . \tag{II.9}$$

As shown in Appendix A, equating the linear and quadratic terms of the exponents in Eqs. (II.8) and (II.9) yields our final results, hereafter referred to as Bayes' equations:

$$\bar{P}' - \bar{P} = M\, G^t\, (N+V)^{-1}\, (D-T) \quad , \tag{II.10}$$

$$M - M' = M\, G^t\, (N+V)^{-1}\, G\, M^t \quad , \tag{II.11}$$

where the L × L matrix N is defined as

$$N = G\, M\, G^t \quad . \tag{II.12}$$

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. As is clear from Eq. (II.8) and therefore reflected in Bayes' equations, the prior data X and the data B are treated on an equal footing. From Eq. (II.11) we see that it is the relative size of the elements of the matrix N and V which determines the extent to which the uncertainties in the parameters are changed. 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 are given in Appendix A.

The results, Eq. (II.10) and Eq. (II.11), are valid only if the three assumptions under which they were derived from Bayes' theorem are valid. In practice we use these equations when the assumptions are only approximately true; in the remainder of this section we discuss the consequences of this and the relationship of the results to the usual method of least-squares.

Instead of starting from Bayes' theorem we could have obtained our results (II.10) and (II.11) by postulating that we should minimize χ^2, given by:

$$\chi^2 = (P-\bar{P})^t M^{-1} (P-\bar{P}) + (D-T)^t V^{-1} (D-T). \qquad (II.13)$$

Data analysis codes which use the conventional least-squares method take as a starting point the fact that they want to minimize the second term of (II.13) to produce the result which we will call $\hat{P}$ and $\hat{M}$. The practical difficulties in that approach come from the nonlinearity of T with respect to the parameters P. The advantages and disadvantages of the method we are proposing derive solely from the inclusion of the first term in Eq. (II.13). It is clear from Eq. (II.13) that, if M is diagonal and its elements become very large, we recover the conventional least-squares results as already mentioned.

Bayes' equations were derived on the assumption that we could approximate T(P) by the first two terms of the Taylor expansion about $\bar{P}$. In the usual least-squares method this same linear approximation is made, but about $\hat{P}$ which minimizes the second term of Eq. (II.13). The value of $\hat{P}$ must be obtained by an iteration method; difficulties, when they occur, stem from the fact that the χ^2 surface does not exhibit a well-defined minima for some of the parameters P_k. This tends to occur for two classes of parameters P_k. The first class consists of those parameters for which the data D have very little sensitivity and the minimum is therefore very broad. The linearity approximation is not at fault here; rather, the parameters are not well determined by the data, and the "noise" in the data causes the maximum of the likelihood function to be far from what is perceived to be a physically reasonable

value. This often occurs because of some approximation in the theoretical calculation. The other class for which difficulties occur with the conventional least-squares method are those parameters for which the X^2 surface exhibits a "valley" in parameter space which extends beyond the domain of physically reasonable values, even though the partial derivatives of the theory with respect to these parameters may be large.

For both classes of parameters for which the conventional least-squares method has difficulties, the linear expansion of T(P) about $\bar{P}$ may not be a very good one and Bayes' method may also have difficulties. However, it is possible to improve upon formulae (II.10) and (II.11) by iterating in order to use an expansion of T(P) about $\bar{P}'$ instead of $\bar{P}$. The way in which this can be done is to estimate $\bar{P}'$ by first doing the expansion about $\bar{P}$; let us call this result ${}^{0}\bar{P}'$. Then, in Eq. (II.10) and (II.11) instead of calculating T and G at $P = \bar{P}$, we calculate them at $P = {}^{0}\bar{P}'$ and obtain a new estimate ${}^{1}\bar{P}'$. In principle one can iterate in this fashion until convergence is obtained. In practice it is seldom necessary to do so more than once since further iteration merely improves the precision of the P_k's beyond a limit justified by the accuracy with which they are determined. The presence of $\bar{P}$ and M in Eq. (II.10) and (II.11), unless the values of the diagonal elements of M are very large, prevents the solution from "running away" as it often does in the conventional least-squares method. We emphasize that in iterating Bayes' equations the values of $\bar{P}$ and M are left at their input values and it is only the quantities denoted by $\bar{T}$ and G which are recalculated at the previously estimated value of $\bar{P}'$. Algebraic details are given in Appendix A.

The "solution" to the problems we often encounter with the conventional method of least squares has been bought at the price that we must provide $\bar{P}$ and M . Even if the matrix V were diagonal, the matrix N will be nondiagonal and it is the matrix N+V which must be inverted. Therefore we no longer have any incentive to approximate V by a diagonal covariance matrix. The consequence of introducing $\bar{P}$ and M when they are known is that $\bar{P}'$ and M' are not independent of $\bar{P}$ and M. As we have emphasized in discussing Bayes' theorem, $\bar{P}$ and M must be based upon some data or be treated as an hypothesis, in which case we say that $\bar{P}'$ and M' are conditional upon the validity of our hypothesis.

We will first discuss the case where $\bar{P}$ and M are obtained from an analysis of some actual data X. (As pointed out earlier the data D must be independent of X; it is possible to modify Eq. (II.13) when the data D are not independent of $\bar{P}$ but we shall not consider this case here.) That is, the analysis of data X yielded an approximately normal joint pdf for the true value of P, at least in the neighborhood of $\bar{P}$; the central limit theorem ensures that this approximation is usually valid. Then the results $\bar{P}'$ and M' which we obtain using Bayes' equations will be identical to those obtained in the usual procedure where we first obtain $\hat{P}$ and $\hat{M}$ and then "combine" this value with $\bar{P}$ and M in the least-squares sense. If the model is nonlinear, the results of the two procedures will differ slightly since in one case the linear expansion is made about $\bar{P}'$ and in the other about $\hat{P}$.

Formula (II.13), although to our knowledge not used in current differential nuclear data analysis, is used in many codes to perform "data adjustment" where $\bar{P}$ and M are the "differential data" and D are some

"integral data". In our approach we take P to be the parameters of the theory and D to be the differential data. There is a practical problem with simultaneously evaluating and analyzing data as our formulae does: if two different sets of data ${}^1D$ and ${}^2D$ are analyzed separately but using the same values of $\bar{P}$ and M derived from data X, then it is a practical impossibility to combine the output of the two analyses, say ${}^1\bar{P}'$ and ${}^2\bar{P}'$, because they are correlated in some unknown fashion. This problem is of course to be contrasted with the one faced in the conventional least-squares approach, where we also cannot combine the analyses of data ${}^1D$ and ${}^2D$ if some of the physical parameters are fixed at different values or if different sets of the parameters are adjusted.

We now consider the situation when $\bar{P}$ and M do not come in their entirety from the analysis of some specific data X but may be considered an hypothesis. The results $\bar{P}'$ and M' of the analyses of data D are functions of $\bar{P}$ and M, and in the future will be of interest to us only if we are willing to continue to entertain this same hypothesis. We may in fact view the usual least-squares procedure (where some of the parameters are fixed at specific values and χ^2 is minimized by varying some other parameters) as producing an analysis of the data D which is valid conditional upon the hypothesis that all the fixed parameters have a true value equal to the value at which they were fixed. This may well be a very good hypothesis to consider at the time the data is analyzed or to answer some specific questions, but the utility of the results ceases the moment the hypothesis is no longer justified.

Our method based upon Bayes' theorem can be viewed as equivalent to what is usually done, if M is taken as diagonal, the M_{kk} corresponding

to fixed parameters are set infinitely small, and the M_{kk} corresponding to the adjusted parameters are set infinitely large. If we adopt this point of view, our procedure, where all of the elements M_{ij} are finite, becomes just a constrained least-squares method. Its great advantage is that it allows us to reduce the data D using a far less drastic hypothesis than we are often forced to use, and the results will more likely be considered useful much longer. Often data does exhibit very small sensitivity to some parameters, and large sensitivity to some other parameters, but there are many intermediate cases. Our method can be viewed as a way to obtain the joint pdf for the true value of the parameters P_k based upon the χ^2 surface in a specified region of parameter space defined by $\bar{P}$ and M. It can be argued that this method does not solve the problems we often encounter with the method of least-squares as much as it provides a way to cope with them in a more generally useful way. It is therefore very important when reporting the results $\bar{P}'$ and M' that we specify clearly the values of $\bar{P}$ and M upon which they are based. The extent to which $\bar{P}'$ differs from $\bar{P}$, but more importantly how the matrix elements of M' differ from those of M, tells us what we have learned about the parameters from the data D. The results $\bar{P}'$ and M' will continue to be useful as long as we consider $\bar{P}$ and M a reasonable hypothesis.

Finally the method we propose should provide a more realistic assessment of the uncertainties in the parameters. There are three major reasons why unrealistically small values for the uncertainties in the parameters are usually obtained in the conventional procedure. Two of the reasons are not related to our introduction of $\bar{P}$ and M in the

procedure but are related to the fact that the covariance matrix V is usually taken as diagonal. In most instances the data D to be analyzed results from manipulations and corrections made to experimentally observed quantities. Because these corrections and transformations in the data are not exact, properly propagated "errors" would yield a non-diagonal matrix V. The magnitudes of the elements of the matrix M' are very sensitive functions of the elements of V and are strongly affected by the nondiagonal elements of V. Secondly, in our calculations of the theoretical values of the data, which we have called T, we also make approximations; the matrix V should contain a contribution due to the uncertainties arising from these approximations. (The matrix N does not represent the uncertainties due to the approximations in the theoretical calculations.) The contributions to V due to the approximations in the theoretical calculation T are also highly nondiagonal. Until the effort is made to use realistic covariance matrices for V, the results of our analyses will not be reliable and in particular our estimates of the uncertainties in the parameters will not be reliable. Since the code described in this report does allow for a nondiagonal covariance matrix V and since no computer time is saved when V is diagonal, we urge users of the code to input more realistic covariance matrices for V. The burden of providing the "theoretical component" of the matrix V should normally be part of the code but has not yet been implemented in an automatic fashion in the code SAMMY. However, some options have been provided for generating some off-diagonal elements; these options should be used when appropriate to relieve the burden of preparing the input data.

The final reason why we often get too small uncertainties in the parameters is that, when we fix some parameters, the diagonal elements of the matrix M' are wrongly identified as the variance of the marginal pdf's of the parameters being varied. This, however, is true only if the joint pdf of <u>all</u> the parameters has a diagonal covariance matrix. Through the introduction of $\bar{P}$ and M we allow for the possibility of obtaining the full joint pdf of all the parameters. The diagonal elements of this full joint pdf are also the variances of the marginal pdf's of the parameters and do provide a realistic measure of how well we know each individual parameter. It is very important to report the full covariance matrix M' since it is essential for most applications to know the off-diagonal elements of M'. We recognize that this is a new burden on the user but we believe that, if a realistic covariance matrix V is used, the full covariance matrix M' is meaningfully produced by the code.

III. IMPLEMENTATION OF BAYES' EQUATIONS

1. Solving the Equations

Implementation of Bayes' equations is straightforward. In matrix form, these equations can be written

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

and

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

where

$$N = GMG^t. \tag{III.3}$$

Solving Eqs. (III.1) and (III.2) is equivalent to solving

$$AX = Y \tag{III.4}$$

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

Prudent numerical analysis procedure dictates that the inverse of a matrix never be evaluated directly. Rather, the matrix A is first factorized as

$$A = U\ B\ U^t \tag{III.5}$$

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 is then found from

$$X = (U^{-1})^t\ B^{-1} U^{-1}\ Y \quad . \tag{III.6}$$

In SAMMY, the factorization (III.5) is performed by LINPACK (D079) subroutine SSPCØ, and the (K+1) solutions are obtained by LINPACK subroutine SSPSL. Subroutine NEWPAR oversees these operations. Further details are given in the report on program BAYES (LA80).

2. Adjusting for Approximations

It is necessary to modify this procedure slightly to account for the approximations built into Bayes' equations. As explained in Appendix A, an iteration scheme has been derived to correct for the nonlinear relationship between parameters and theoretical values. In SAMMY, a single iteration is performed, since (1) further iteration is expected to increase precision but not accuracy, and (2) test cases have shown this to yield consistent results. (See, e.g., example 4 of Section VI).

3. Introduction of Off-Diagonal Data Covariances

Often $\ell > 0$ resonance parameters cannot be determined accurately because the underlying $\ell = 0$ structure is not well known. Introduction of a constant on- and off-diagonal data covariance in the neighborhood of the non-s-wave resonance permits effective decoupling of the s-wave from the non-s waves. This occurs because an additive constant covariance is mathematically equivalent to a constant, coherent correction term for either the data or the theory; algebraic details are presented in Appendix A. This type of off-diagonal data covariance matrix can be generated automatically by SAMMY, if the user so desires.

One other type of off-diagonal data covariance matrix which can be automatically generated by SAMMY is of the form

$$V^{ij} = \bar{V}^{ij} + (a+bE^i)(a+bE^j)$$

where $\bar{V}^{ij}$ is supplied by the user, E^i is the energy for data point i, and a and b are constants chosen by the user. This type of covariance is useful if there are energy-dependent coherent uncertainties in the data, for example, if a subtracted background is imperfectly known.

Other types of off-diagonal data covariances may be supplied directly by the user. Details for inputting all types of covariances are provided in Appendix C. Examples using off-diagonal data covariances are presented in Section VI.

IV. MULTILEVEL R-MATRIX THEORY

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_λ. These resonances may decay through any of several 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 Γ_λ^γ.

Cross-sections for the interaction described above may be calculated from multilevel R-matrix theory (LA58) in the Reich-Moore approximation (RE58). An excellent review of R-matrix theory and its relationship to other resonance formalisms is presented in the recent article by Froehner (FR80); the reader interested in both derivation and details is referred to that article. Here we present only the relevant formulae, beginning with the R-matrix itself:

$$R_{cc'}^{J^\pi} = \sum_\lambda \frac{\gamma_{\lambda c}\,\gamma_{\lambda c'}}{E_\lambda - E - i\alpha_\lambda^2}\,, \qquad \text{(IV.1)}$$

where all levels (resonances) with total spin and parity J^π are included in the sum. The channel width $\Gamma_{\lambda c}$ is given in terms of the reduced width $\gamma_{\lambda c}$ by

$$\Gamma_{\lambda c} = 2\gamma_{\lambda c}^{\,2}\, P_\ell\,, \qquad \text{(IV.2)}$$

where P_ℓ is the penetration factor, which depends only on the orbital angular momentum ℓ and the energy E; formulae for $P_\ell(E)$ are shown in Table IV.1. Similarly, the gamma width Γ_λ^γ is given in terms of the reduced

TABLE IV.1. PENETRATION FACTORS P_ℓ, LEVEL SHIFT FACTORS S_ℓ, AND POTENTIAL-SCATTERING PHASE SHIFTS ϕ_ℓ FOR ORBITAL ANGULAR MOMENTUM ℓ, CENTER OF MASS MOMENTUM k, AND CHANNEL RADIUS a_c, WITH $\rho = k a_c$

ℓ	P_ℓ	S_ℓ	ϕ_ℓ
0	ρ	0	ρ
1	$\rho^3/(1 + \rho^2)$	$-1/(1 + \rho^2)$	$\rho - \tan^{-1}\rho$
2	$\rho^5/(9 + 3\rho^2 + \rho^4)$	$-(18 + 3\rho^2)/(9 + 3\rho^2 + \rho^4)$	$\rho - \tan^{-1}(3\rho)/(3 - \rho^2)$
3	$\rho^7/(225 + 45\rho^2 + 6\rho^4 + \rho^6)$	$-(675 + 90\rho^2 + 6\rho^4)/(225 + 45\rho^2 + 6\rho^4 + \rho^6)$	$\rho - \tan^{-1}[\rho(15 - \rho^2)/(15 - 6\rho^2)]$
4	$\rho^9/(11\,025 + 1575\rho^2 + 135\rho^4 + 10\rho^6 + \rho^8)$	$-(44\,100 + 4725\rho^2 + 270\rho^4 + 10\rho^6)/(11\,025 + 1575\rho^2 + 135\rho^4 + 10\rho^6 + \rho^8)$	$\rho - \tan^{-1}[\rho(105 - 10\rho^2)/(105 - 45\rho^2 + \rho^4)]$

gamma width α_λ as

$$\Gamma_\lambda^\gamma = 2\alpha_\lambda^2 \quad . \tag{IV.3}$$

The R-matrix is related to physical observables via the W-matrix which, in matrix notation, is given by

$$W = P^{1/2}(I-RL)^{-1}(I-RL^*)P^{-1/2} \quad . \tag{IV.4}$$

SAMMY uses a different but equivalent form for W:

$$W = I - \frac{2iP}{L} + 2i\,\frac{\sqrt{P}}{L}\left(\frac{1}{L}-R\right)^{-1}\frac{\sqrt{P}}{L} \quad . \tag{IV.4a}$$

The quantity L_ℓ in Eq. (IV.4) is given by

$$L_\ell = (S_\ell - B_\ell) + iP_\ell \tag{IV.5}$$

with S_ℓ the shift factor, shown in Table IV.1, and B_ℓ the arbitrary boundary constant at the channel radius a_c. "I" in Eq. (IV.4) represents the identity matrix.

Integrated cross sections are then given in terms of W and the potential scattering phase shift ϕ, also shown in Table IV.1, as follows:

$$\sigma^{\text{total}} = \frac{2\pi}{k^2}\sum_J g_J \sum_{\substack{\text{incident}\\ \text{channels}\\ c}}\left(1 - \text{Re}\left(e^{-2i\phi_\ell}\, W_{cc}^J\right)\right) \tag{IV.6}$$

$$\sigma^{\text{elastic}} = \frac{\pi}{k^2}\sum_J g_J \sum_{\substack{\text{incident}\\ \text{channels}\\ c}}\left(1 - 2\text{Re}\left(e^{-2i\phi_\ell}\, W_{cc}^J\right) + \sum_{\substack{\text{incident}\\ \text{channels}\\ c'}}\left|W_{cc'}^J\right|^2\right) \tag{IV.7}$$

$$\sigma^{\text{reaction}} = \frac{\pi}{k^2} \sum_J g_J \sum_{\substack{\text{incident} \\ \text{channels} \\ c}} \sum_{\substack{\text{exit} \\ \text{channels} \\ c'}} \left| W_{cc'}^J \right|^2 \qquad \text{(IV.8)}$$

$$\sigma^{\text{capture}} = \frac{\pi}{k^2} \sum_J g_J \sum_{\substack{\text{incident} \\ \text{channels} \\ c}} \left(1 - \sum_{\substack{\text{all} \\ \text{channels} \\ c'}} \left| W_{cc'}^J \right|^2 \right) . \qquad \text{(IV.9)}$$

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

$$\sigma^{\text{total}} = \sigma^{\text{elastic}} + \sigma^{\text{reaction}} + \sigma^{\text{capture}} . \qquad \text{(IV.10)}$$

In Eq. (IV.6) through (IV.9), g_J is the spin statistical factor

$$g_J = \frac{2J+1}{2(2I+1)} \qquad \text{(IV.11)}$$

where I is the target spin. The quantity k is the neutron momentum in the center-of-mass system, related to laboratory kinetic energy E by

$$E = \frac{\hbar^2}{2Mc^2} k^2 \qquad \text{(IV.12)}$$

where M is given by

$$\frac{1}{M} = \frac{1}{M_{\text{neutron}}} \left(\frac{M_{\text{neutron}} + M_{\text{target}}}{M_{\text{target}}} \right)^2 . \qquad \text{(IV.13)}$$

Multiple-scattering corrections are not included in the capture cross sections; it is the authors' intention to introduce these corrections in the near future.

V. IMPLEMENTATION OF MULTILEVEL R-MATRIX THEORY

The implementation of multilevel R-matrix theory with Doppler- and resolution-broadening was borrowed from the least squares multilevel R-matrix code MULTI, developed by George Auchampaugh (AU74). The coding was extensively modified for clarity, for easier amendment and additions, and for greater compatibility with the PDP-10 computer system at ORELA. However, the basic design of this portion of the computer code SAMMY is exactly that which was first implemented in MULTI. (The code name SAMMY had its origin here: SAM = Severely Altered MULTI.)

Generation of theoretical cross sections and derivatives in SAMMY, as in MULTI, is accomplished as follows: The user specifies which of the physical parameters $E_\lambda, \Gamma_{\lambda c}, \Gamma_\lambda^\gamma$ are to be varied. These parameters are converted to "u-parameters" via

$$u(E_\lambda) = \pm\sqrt{|E_\lambda|}\ , \text{ where the negative sign is chosen if } E_\lambda < 0, \qquad (V.1)$$

$$u(\Gamma_{\lambda c}) = \gamma_{\lambda c} \text{ where } \Gamma_{\lambda c} = 2\gamma_{\lambda c}^2 P_\ell\ , \qquad (V.2)$$

$$u(\Gamma_\lambda^\gamma) = \alpha_\lambda \text{ where } \Gamma_\lambda^\gamma = 2\alpha_\lambda^2\ . \qquad (V.3)$$

(Note that γ_λ and α_λ may be either positive or negative.) It is the u-parameters on which Bayes' equations operate.

To solve Bayes' equations, it is necessary to know both the cross section and the derivative of the cross section with respect to each u-parameter, evaluated at every energy for which input data is available. The chain rule is used to evaluate partial derivatives:

$$\frac{\partial\sigma}{\partial u_i} = \sum_{\substack{\mu\le\nu \\ \omega\le\tau}} \frac{\partial R_{\mu\nu}}{\partial u_i} \frac{\partial W_{\omega\tau}}{\partial R_{\mu\nu}} \frac{\partial\sigma}{\partial W_{\omega\tau}} \qquad (V.4)$$

where the index J has been suppressed, since it is fixed for a given u. The restricted sums ($\mu \leq \nu$, $\omega \leq \tau$) result from the symmetry of R and W.

In Eq. (IV.1), the R-matrix is given as

$$R_{\mu\nu} = \sum_{\lambda} \frac{\gamma_{\lambda\mu}\gamma_{\lambda\nu}}{E_\lambda - E - i\alpha_\lambda^2} \tag{V.5}$$

from which the derivative of R with respect to the parameters can be found:

$$\frac{\partial \text{ Re } R_{\mu\nu}}{\partial \sqrt{E_\lambda}} = \left[2\ \gamma_{\lambda\mu}\ \gamma_{\lambda\nu}\ \sqrt{E_\lambda}\right]\left[\left\{-\left(E_\lambda - E\right)^2 + \left(\alpha_\lambda^2\right)^2\right\}/D_\lambda^2\right] \tag{V.6a}$$

$$\frac{\partial \text{ Im } R_{\mu\nu}}{\partial \sqrt{E_\lambda}} = \left[-4\ \gamma_{\lambda\mu}\ \gamma_{\lambda\nu}\ \sqrt{E_\lambda}\right]\left[\left(E_\lambda - E\right)\ \alpha_\lambda^2/D_\lambda^2\right] \tag{V.6b}$$

$$\frac{\partial \text{ Re } R_{\mu\nu}}{\partial \alpha_\lambda} = \left[-4\ \gamma_{\lambda\mu}\ \gamma_{\lambda\nu}\ \alpha_\lambda\right]\left[\left(E_\lambda - E\right)\ \alpha_\lambda^2/D_\lambda^2\right] \tag{V.7a}$$

$$\frac{\partial \text{ Im } R_{\mu\nu}}{\partial \alpha_\lambda} = \left[2\ \gamma_{\lambda\mu}\ \gamma_{\lambda\nu}\ \alpha_\lambda\right]\left[\left\{\left(E_\lambda - E\right)^2 - \left(\alpha_\lambda^2\right)^2\right\}/D_\lambda^2\right] \tag{V.7b}$$

$$\frac{\partial \text{ Re } R_{\mu\nu}}{\partial \gamma_{\lambda\mu}} = \left[\gamma_{\lambda\nu}\ \left(1 + \delta_{\mu\nu}\right)\right]\left[\left(E_\lambda - E\right)/D_\lambda\right] \tag{V.8a}$$

$$\frac{\partial \text{ Im } R_{\mu\nu}}{\partial \gamma_{\mu\nu}} = \left[\gamma_{\lambda\nu}\ \left(1 + \delta_{\mu\nu}\right)\right]\left[\alpha_\lambda^2/D_\lambda\right] \tag{V.8b}$$

where

$$D_\lambda = \left(E_\lambda - E\right)^2 + \alpha_\lambda^4 \quad . \tag{V.9}$$

In each of Eqs. (V.6) - (V.8), 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,μν) for the derivative of the real part of $R_{\mu\nu}$ with respect to the i^{th} parameter, and BI(i,μν) 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.

From Eq. (IV.4), W may be written in terms of R as

$$W_{\omega\tau} = \delta_{\omega\tau}\left(1-\frac{2iP_{\omega}}{L_{\omega}}\right) + 2i\frac{\sqrt{P_{\omega}}}{L_{\omega}}\,Y_{\omega\tau}\,\frac{\sqrt{P_{\tau}}}{L_{\tau}} \qquad (V.10)$$

where we have set

$$Y_{\omega\tau} = \left[\left(\frac{1}{L}-R\right)^{-1}\right]_{\omega\tau} \quad . \qquad (V.11)$$

In Appendix A, we show that the derivative of Y with respect to R is given by

$$\frac{\partial Y_{\omega\tau}}{\partial R_{\mu\nu}} = Y_{\omega\mu}\,Y_{\nu\tau} + Y_{\omega\nu}\,Y_{\mu\tau}\,(1-\delta_{\mu\nu}) \quad . \qquad (V.12)$$

Substitution of Eq. (V.12) into the derivative of Eq. (V.10) gives

$$\frac{\partial W_{\omega\tau}}{\partial R_{\mu\nu}} = 2i \frac{\sqrt{P_\omega}}{L_\omega} \left[Y_{\omega\mu} Y_{\nu\tau} + Y_{\omega\nu} Y_{\mu\tau} (1-\delta_{\mu\nu}) \right] \frac{\sqrt{P_\tau}}{L_\tau} \quad . \tag{V.13}$$

The derivative of the cross section with respect to W differs for each type of cross section. For total, it is

$$\frac{\partial \sigma^{\text{total}}}{\partial W^J_{\omega\tau}} = \begin{cases} \frac{-2\pi}{k^2} g_J e^{2i\phi_\ell} \delta_{\omega\tau} & \text{for } \omega \text{ an incident channel} \\ 0 & \text{otherwise.} \end{cases} \tag{V.14}$$

For elastic scattering, the derivative is

$$\frac{\partial \sigma^{\text{elastic}}}{\partial W^J_{\omega\tau}} = \begin{cases} \frac{2\pi}{k^2} g_J \left[-e^{2i\phi_\ell} \delta_{\omega\tau} + W^J_{\omega\tau} (2-\delta_{\omega\tau}) \right] & \text{for } \omega \text{ and } \tau \text{ incident channels} \\ 0 & \text{otherwise.} \end{cases} \tag{V.15}$$

For the reaction cross section, we must have $\omega \leq \tau$, which gives for the derivative

$$\frac{\partial \sigma^{\text{reaction}}}{\partial W^J_{\omega\tau}} = \begin{cases} \frac{2\pi}{k^2} g_J W^J_{\omega\tau} & \text{for } \omega \text{ an incident channel and } \tau \text{ an exit channel} \\ 0 & \text{otherwise.} \end{cases} \tag{V.16}$$

Finally, the derivative of the capture cross section is

$$\frac{\partial \sigma^{\text{capture}}}{\partial W^J_{\omega\tau}} = \begin{cases} \frac{-2\pi}{k^2} g_J W^J_{\omega\tau} & \text{for at least one of } \omega \text{ and } \tau \text{ an entrance channel} \\ 0 & \text{otherwise.} \end{cases} \tag{V.17}$$

The partial derivatives G^i_k, defined in Eq. (II.7) and required in Bayes' equations, are then found from Eq. (V.4), using Eqs. (V.6) through (V.9) for $\frac{\partial R}{\partial u}$, Eq. (V.13) for $\frac{\partial W}{\partial R}$, and Eqs. (V.14) through (V.17) for $\frac{\partial \sigma}{\partial W}$, all evaluated at energy E^i. Subroutine PARSH oversees the evaluation of the partial derivatives and the cross sections.

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 resonance. The working definition of "far away" is 20 times the sum of the partial widths for that resonance, i.e., far beyond the region where a resonance can produce any noticeable effect.

Doppler- and resolution-broadening of the cross sections in SAMMY is accomplished in precisely the same fashion as in MULTI; in addition, partial derivatives are broadened in SAMMY (but not in MULTI). An auxiliary energy array is set up in subroutine ESCALE, including all (primary) energies at which input data are provided plus enough additional points to ensure proper broadening (a minimum of nine points across the width of each resonance, and extra points at the beginning and end of the energy range). Cross sections and partial derivatives are generated at each auxiliary energy, as described above. Doppler-broadened cross sections and partial derivatives are calculated at each auxiliary energy by forming linear combinations of the unbroadened values, approximating a Gaussian convolution. Total cross sections are then converted to transmissions (with appropriate conversion of the partial derivatives), and resolution-broadened cross sections (or transmissions) and partial derivatives are formed at each primary energy from linear combinations of the Doppler-broadened values. The

resolution-broadening function can be either Gaussian, exponential, or a combination of the two. Finally, transmissions are converted to total cross-sections if input data are in that form. Subroutine BRØADN performs the broadening operations. For details regarding the precise form of the broadening functions, the reader is referred to the documentation of MULTI (AU74).

VI. CALCULATIONS AND COMPARISONS

The computer code SAMMY has been extensively fine-tuned and debugged via test calculations and via comparisons with the least-squares multilevel R-matrix code MULTI (AU74). Results of four such calculations are reported here. The first example is a repeat analysis of Ni^{60} transmission data, including direct comparison of MULTI and SAMMY results. The second and third examples use artificial data to demonstrate how off-diagonal data covariances can be used to decouple a p-wave resonance from an improperly fitted s-wave and to offset the effects of improper background subtraction. The final example illustrates the extent to which a sequential analysis of (uncorrelated) data sets is equivalent to a simultaneous analysis, in the extreme case where data from an s-wave resonance is divided near the resonance energy.

1. Ni^{60} Transmission Data

Preliminary results from C. Perey's (PE80c) MULTI analysis of Harvey's (HA80) Ni^{60} transmission data were used as starting values for a SAMMY analysis of that data. Data consisted of 2593 total cross sections and uncertainties in the energy range from 10 to 550 keV. Included were 212 resonances, of which 189 were within the data range (the others being dummies inserted in order to reproduce the backgrounds). Neutron widths (Γ_n) for each of these 189 resonances were varied; all resonance energies and gamma-ray widths (Γ_γ) were held fixed. Initial uncertainties on the neutron widths were arbitrarily set at 10% of the width.

A sampling of the results from this analysis is shown in Table VI.1. In general, SAMMY results (Column B) did not deviate far from the MULTI results (Column A) used as starting values for SAMMY. Theoretical curves generated from the two sets of parameters are rarely distinguishable.

A second SAMMY analysis of this same data was performed, using arbitrary starting values of Γ_n; these values were in the range 0.5 to 1.5 times the original starting values. Partial results from this analysis are also shown in Table VI.1. Results (Column C) are generally in closer agreement with both MULTI results (Column A) and previous SAMMY results (Column B) than with the starting values (Column D). One notable exception is parameter number 121; in this case, however, the output uncertainty is 10% of the value for Γ_n. Since 10% Γ_n was given as the starting value for the uncertainty, this result indicates that the parameter is unaffected by the data.

A modest attempt was made to use these same starting values (Column D in Table VI.1) as input to a MULTI analysis (five iterations only) of this data, though by no means was a complete analysis performed. Preliminary results are shown in Column E. From these partial results, it appears that MULTI has more difficulty than SAMMY in arriving at reasonable answers when starting values are far off. MULTI could, of course, do better were it allowed to iterate to convergence.

It should be noted that SAMMY results are obtained in a more straightforward fashion than MULTI results. With SAMMY, it is necessary to divide the almost 2600 data points into 24 data sets, analyzing each data set in turn but using output from one as input for the next. All 189 parameters are varied all the time, though of course most are virtually unaffected by

TABLE VI.1. COMPARISON OF MULTI AND SAMMY RESULTS FOR Ni^{60} TRANSMISSION DATA

Parameter Number	Energy of Resonance (keV)	A. MULTI Value of Γ_n (ev)	B. SAMMY Value of Γ_n Using Column A for Starting Value		C. SAMMY Results for Γ_n Using Arbitrary Starting Value		D. Starting Value for Col C and E	E. MULTI Partial Results for Γ_n Using Starting Values in Col D	
S 1/2			Value	Error	Value	Error		Value	Error
14	251.90	556.00	536.03	3.94	547.29	4.02	500.00	610.44	3.45
15	256.00	810.00	792.64	5.53	805.70	5.73	1000.00	982.00	3.65
16	257.60	1840.00	1800.20	6.54	1846.10	6.75	2000.00	2127.20	5.95
17	278.90	222.00	213.78	2.34	218.90	2.36	250.00	261.54	2.03
18	291.80	122.00	118.40	2.73	120.33	2.71	100.00	123.80	1.33
19	316.90	2840.00	2715.50	8.16	2794.50	8.22	2500.00	2960.20	8.13
20	325.38	6805.00	6924.80	13.64	6877.10	13.74	5000.00	6952.20	14.53
21	338.34	3370.00	3419.20	12.32	3402.60	12.53	2500.00	3291.90	12.03
P 1/2									
100	252.98	240.000	247.230	2.915	250.240	2.929	250.000	298.200	2.369
101	254.26	22.000	19.303	0.600	18.800	0.562	20.000	22.068	0.545
102	256.18	34.000	28.153	1.778	32.342	2.011	50.000	20.791	0.821
103	257.69	15.000	22.081	0.989	17.009	0.784	10.000	17.383	0.471
104	258.15	21.000	13.287	0.995	15.823	1.076	25.000	24.905	0.602
105	260.72	42.000	49.430	1.531	48.774	1.579	50.000	36.618	2.526
106	263.00	33.000	32.056	0.857	25.389	0.688	25.000	21.723	0.308
107	265.85	55.000	53.011	1.360	52.306	1.342	50.000	58.199	0.946
108	276.95	15.000	14.396	0.783	18.561	0.941	20.000	33.800	2.128
109	278.08	375.000	362.550	2.618	363.600	2.622	500.000	403.530	2.516
110	280.02	125.000	122.580	2.078	120.880	2.058	100.000	134.350	1.625
111	282.00	10.000	8.132	0.508	8.385	0.516	10.000	32.036	2.440
112	288.10	4.000	2.002	0.201	2.598	0.250	5.000	1 .298	3.715
113	290.50	32.000	22.013	1.124	26.920	1.277	50.000	43.403	1.246
114	292.50	129.000	134.710	2.664	133.400	2.615	100.000	157.070	1.466
115	294.20	10.000	8.432	0.478	7.411	0.412	8.000	14.254	5.236
116	294.70	15.000	10.493	0.653	8.870	0.548	10.000	15.491	3.309
117	295.40	133.000	115.650	1.871	119.290	1.880	100.000	151.440	1.942
118	302.00	10.000	6.830	0.472	7.782	0.476	12.000	3.166	5.093
119	306.50	385.000	351.580	3.430	357.210	3.495	250.000	422.260	2.762
120	311.30	20.000	15.311	0.901	17.267	1.093	25.000	13.433	1.738
121	313.40	7.000	7.000	0.700	5.000	0.500	5.000	1.601	3.123
122	321.40	17.000	17.481	0.820	18.273	0.854	20.000	16.247	2.403
123	328.90	37.500	37.119	1.614	40.721	1.650	50.000	40.152	1.414
124	335.93	145.000	146.050	2.186	132.460	2.211	100.000	137.480	1.427
125	339.75	10.000	6.705	0.729	11.596	1.291	20.000	2.231	8.166

TABLE VI.1. COMPARISON OF MULTI AND SAMMY RESULTS FOR Ni^{60} TRANSMISSION DATA (CONT'D)

Parameter Number	Energy of Resonance (keV)	A. MULTI Value of Γ_n (ev)	B. SAMMY Value of Γ_n Using Column A for Starting Value		C. SAMMY Results for Γ_n Using Arbitrary Starting Value		D. Starting Value for Col C and E	E. MULTI Partial Results for Γ_n Using Starting Values in Col D	
P 1/2 (Cont'd)			Value	Error	Value	Error		Value	Error
126	341.25	120.000	115.290	3.750	111.210	3.077	100.000	131.870	2.040
127	343.00	280.000	235.390	4.238	228.030	4.125	250.000	305.290	3.745
128	348.05	100.000	82.699	2.421	75.670	2.353	50.000	131.160	1.181
129	349.00	30.000	21.679	1.317	24.344	1.450	25.000	45.610	1.042
P 3/2									
157	334.01	115.000	116.930	1.394	104.940	1.409	100.000	122.520	1.810
158	342.40	33.000	29.912	1.185	36.500	1.277	50.000	43.446	0.565
D 3/2									
165	230.05	50.000	49.474	0.589	48.898	0.584	40.000	39.350	0.434
166	269.00	45.000	43.616	0.731	45.234	0.755	50.000	49.477	0.017
167	282.88	138.000	138.120	1.082	136.040	1.075	100.000	107.430	0.228
168	297.20	73.500	68.256	0.879	66.086	0.858	50.000	46.626	0.156
169	300.30	25.000	18.084	0.504	17.227	0.484	20.000	18.909	0.272
170	307.25	104.000	107.910	1.368	107.510	1.377	100.000	99.714	0.116
171	327.30	12.000	7.386	0.618	6.793	0.543	10.000	8.449	0.109

any given data set. Results thus obtained are valid and consistent over the entire energy region. Total time required for the SAMMY analysis was less than one week.

In contrast, the initial MULTI analysis required over six months of effort; this included searches on both energies and widths. Data were divided into seven data sets (more points per data set are allowed since MULTI need not store covariance matrices), each of which was analyzed independently. Frequent intervention and decision-making were required from the physicist doing the analysis, in order to ensure consistency between the various data sets. For our MULTI "analysis" (Column E in Table VI.1), the intention was to see how well MULTI could perform given only slightly more user-intervention than SAMMY requires. Only the Γ_n for resonances within the data set being analyzed could be varied, first because MULTI accepts a maximum of 150 search parameters, but more importantly because a search on "outside" parameters often yields drastic (and unrealistic) changes in the values of those parameters. Updated parameters from five iterations on one data set were used as input for the next data set, with the initial value being substituted when unphysical values were output. The "analysis" was discontinued after the fifth data set, since output values were too far afield to have any hope of reaching reasonable results from the two remaining data sets.

Parameter uncertainties presented in Table VI.1 may be viewed as unrealistically small. As discussed in Section II, this is because we have improperly assumed the data points to be independent, rather than included an off-diagonal covariance matrix to describe corrections made to the data and approximations made in generating the theoretical values. Correctly

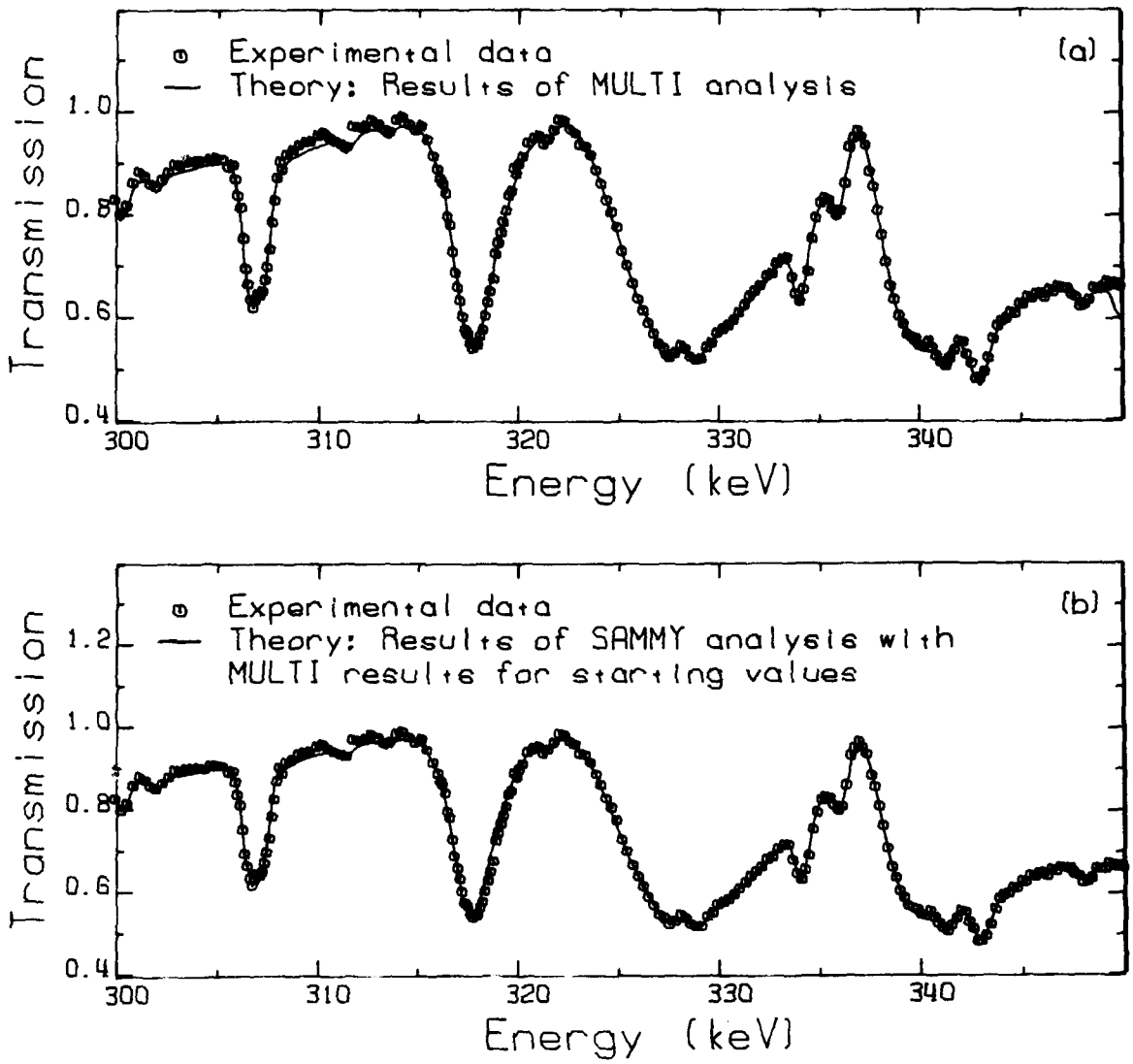

Fig. VI.1. Theoretical curves resulting from MULTI and SAMMY analyses of Ni^{60} data (HA80), corresponding to the five parameter sets listed in Table VI.1. Part *a* uses parameters generated by the MULTI analysis of Perey (PE80c) and part *b* those from the first SAMMY analysis. Curves shown in part *c* are from the second SAMMY analysis and part *e* from the second MULTI analysis, both of which used the arbitrary starting parameters whose curve is shown in part *d*.

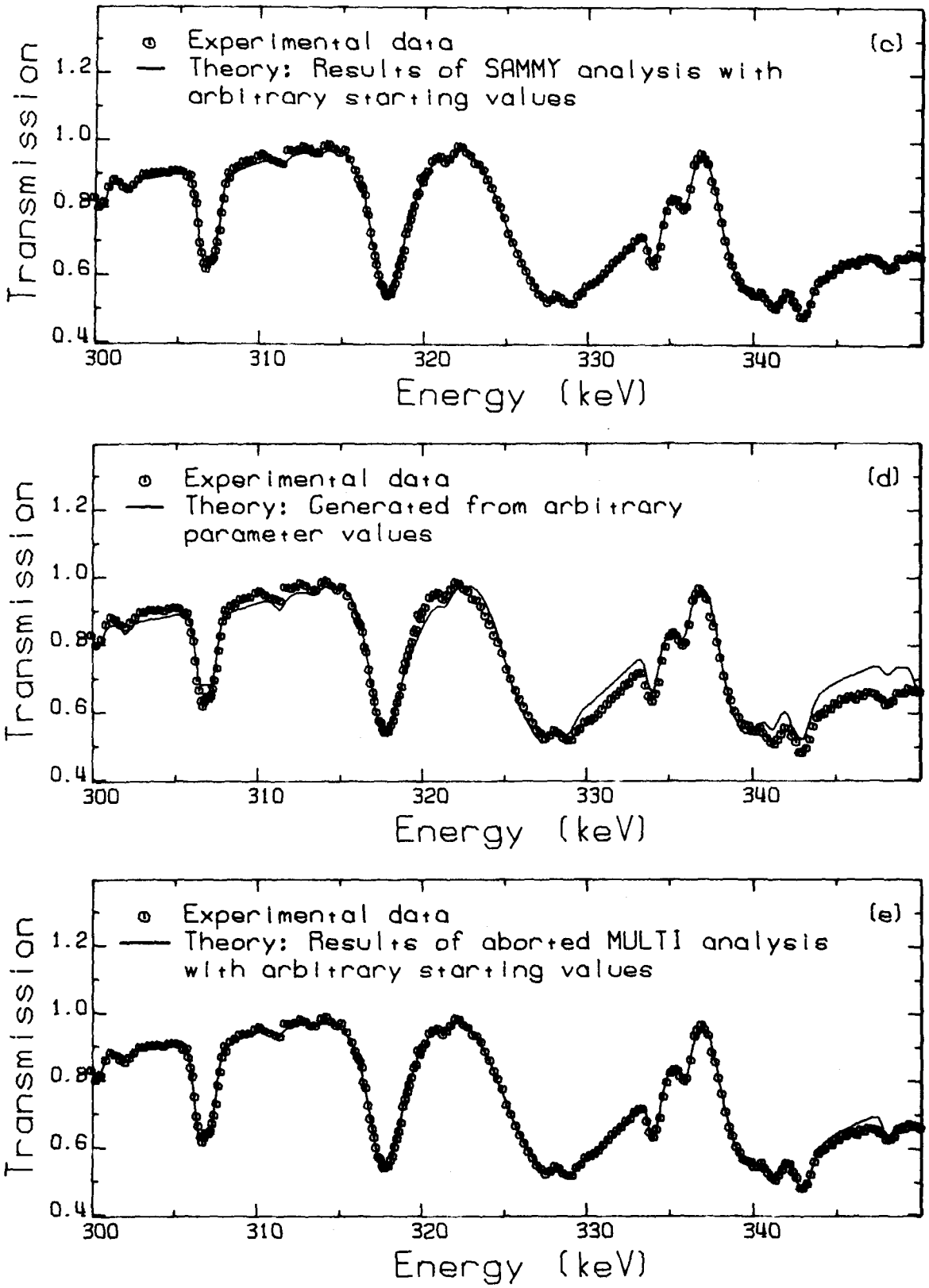

Fig. VI.1. (Cont'd).

including these effects would produce more reasonable values for data uncertainties.

One might naively expect the two SAMMY results (columns B and C of the table) to agree to within the quoted uncertainties. This does not happen for two reasons: First, the quoted uncertainties are unrealistically small, as discussed above. Secondly, the different starting values for the two runs do affect the resulting parameter values as can be seen directly from Bayes' equations. However, the different starting values produce only second-order effect on the uncertainties, especially when data uncertainties are much smaller than input parameter uncertainties, as they are in this example. Thus parameter values will differ slightly with different starting values, but parameter uncertainties will not.

Theoretical curves generated by using the five parameter sets corresponding to the columns A through E of Table VI.1 are given in Figure VI.1. For clarity, only a portion of the energy range is shown. Note that the complete MULTI analysis (part a) and both SAMMY analyses (parts b and c) provide reasonable fits to the experimental data, while the second MULTI analysis (part e) appears more strongly affected by its starting values (part d) than by the data.

2. The Effect of Improperly Fitted S-Wave on Neighboring P-Wave Resonance

Artificial data were generated in order to study the effect of off-diagonal data covariances in fitting a small p-wave located near the peak of a large s-wave resonance. Elastic scattering "data" for 123 energies were generated from the parameters shown in Column A of Table VI.2. No random noise was added to the data, so that these values are, in fact, exact. An arbitrary 1% uncertainty was assigned to each data point.

TABLE VI.2. PARAMETER VALUES FOR EXAMPLE NUMBER 2,
DECOUPLING P-WAVE RESONANCE FROM AN IMPROPERLY FITTED S-WAVE BACKGROUND

	A.	B.	C.	D.	E.
	Exact Values	Input Parameters	Results from MULTI	Results from SAMMY without Off-Diagonal Covariances	Results from SAMMY with Off-Diagonal Covariances
$E_{res}(S)$	156.00 keV	156.00 keV			
$\Gamma_n(S)$	3000.0 eV	3200.0 eV			
$E_{res}(P)$	160.00keV	160.00 keV	159.99 ± 0.0004	160.000 ± 0.003	160.000 ± 0.003
$\Gamma_n(P)$	50.000 eV	55.000eV	84.894 ± 0.832	42.954 ± 0.945	50.012 ± 1.149

It is assumed that the s-wave parameters are fixed (perhaps from earlier experiments) at the values shown in Column B of Table VI.2. The "known" value for Γ_n is noticeably different from the "exact" value, as shown by the discrepancy between "data" and the "theoretical" curve in Fig. VI.2, but is nevertheless fixed for this calculation. In other words, we have deliberately introduced a systematic error in the theoretical values. The purpose of this calculation is to obtain the hitherto "unknown" p-wave parameters, starting from arbitrary initial values, and thereby to illustrate how the effect of such systematic errors can be incorporated in SAMMY analyses.

Three distinct calculations were performed, each using all 123 data points. The first, using program MULTI, gives the erroneous results shown in Column C of Table VI.2. This is to be expected, since systematic errors must be handled external to MULTI and we have not done so. The second calculation, using SAMMY, treats each data point as independent, and leads to a value for the p-wave Γ_n (see Column D of the table) which does allow the theory to reproduce the data at the p-wave resonance. This value for Γ_n differs from the exact value, since the calculation attempts to fit both the p-wave peak and the s-wave background by adjusting only the one parameter. How well this is accomplished is illustrated in Fig. VI.2b, in which only the neighborhood of the p-wave resonance is shown.

The third calculation makes use of the "decoupling" procedure in SAMMY, described in Section III.3, to incorporate the effect of the systematic theoretical error. A constant on- and off-diagonal term is added to the original (diagonal) data covariance matrix in the neighborhood of the p-wave resonance; this allows the theoretical values to deviate from

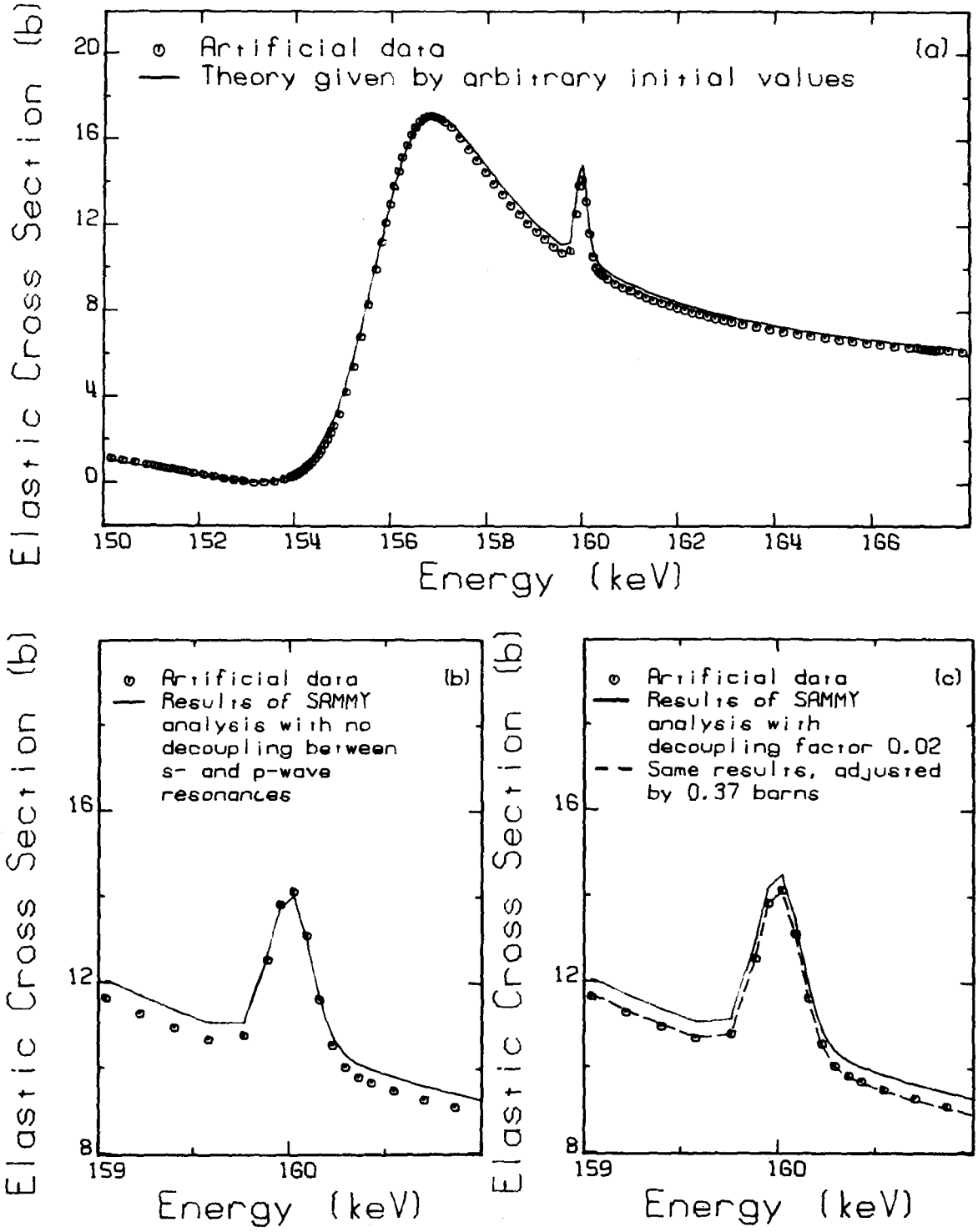

Fig. VI.2. Artificial data used to study the effect of an improperly fitted s-wave on a neighboring p-wave resonance. The theoretical curve in part *a* is generated from the input parameters. The theoretical curve in part *b* results from the SAMMY calculation with no decoupling between the s- and p-wave resonances; only the energy region near the p-wave is shown, though the entire range was used for the calculation. The solid curve shown in part *c* results from the SAMMY calculation with a decoupling parameter of 0.02; the dashed curve is the solid curve adjusted by 0.37 barns.

"experimental" values in a coherent fashion. Results of this calculation are in excellent agreement with the exact values, as shown by comparing Columns A and E of Table VI.2. Part c of Fig. VI.2 illustrates the degree to which these values reproduce this data: The upper curve was produced directly from the parameter values given by the calculation. The lower curve is the upper curve displaced by 0.37 barns, and falls directly on each data point.

It is interesting to note that the precise value chosen for the off-diagonal term is not critical, as long as it is big enough. The calculation reported here used the value 0.02, which is the same order of magnitude as the diagonal terms of the data covariance matrix. Values of 0.20 and 2.00 yielded equivalent results; the value 0.002 yielded Γ_n smaller than the exact result but still larger than that obtained with no off-diagonal covariances. Thus, it appears that one should take care to accurately estimate the decoupling term.

3. Errors in Background Subtraction

Other artificial data were generated to consider the problem of background subtraction. Elastic cross sections from two s-wave and three p-wave resonances were evaluated at 123 data points; the maximum cross section was approximately 16 barns. To these values was added a constant background of $2.00 \pm .02$ barns, with the error normally distributed. Poisson-type noise was then added, and the results were taken as the raw "experimental" data. Data uncertainties ranged from 0.2 to 0.6, so that diagonal members of the covariance matrix were in the range from 0.04 to 0.40. To simulate improper background subtraction, no background was subtracted from the raw data.

Three separate analyses were again performed; results are tabulated in Table VI.3. Although many codes handle this kind of problem by adjusting a background (see, e.g., SIØB, (DE78)), neither MULTI nor SAMMY is equipped to do so. Thus the MULTI analysis (Column C of the table) strayed far from the "exact" values (Column A), as did the first SAMMY analysis which used a diagonal data covariance matrix (Column D). However, when a constant value of 0.04 was added to the data covariance matrix in SAMMY, results (Column E) are in good agreement with the exact values. Thus SAMMY can be used to obtain reasonable values for resonance parameters when the background level is not well determined and it is so communicated to the code.

Fig. VI.3a shows the curve generated from the results of the first SAMMY analysis. Note that the shape of the theoretical curve is considerably distorted from the shape of the data. Part b of the figure shows the curve generated from the results of the SAMMY analysis with off-diagonal data covariances; the solid curve is exactly as generated, and the dashed curve is displaced by 2.00 barns.

4. Simultaneous vs. Sequential Analysis of S-Wave

The ability to perform a sequential analysis of independent data sets, and obtain results which are equivalent to a simultaneous analysis of that same data, is a major strength of Bayes' method and represents a significant improvement over the sequential (and therefore separate) analyses performed with conventional least-squares methods. Because the derivation of Bayes' equations from Bayes' theorem involves several approximations (Gaussian distributions and linearity), the asserted equivalence of simultaneous vs. sequential analysis is also approximate. To examine the validity of this equivalence, the artificial data of example 2 were analyzed three

TABLE VI.3. PARAMETER VALUES FOR EXAMPLE NUMBER 3
USING CONSTANT DATA COVARIANCE TO OFFSET IMPROPER BACKGROUND SUBTRACTION

	A. Exact Values	B. Input Values	C. Results from MULTI	D. Results from SAMMY with no Correlations in Data Set	E. Results from SAMMY with Additive Constant Data Covariance
E_{res}(S)	156.31 keV	156.50	156.29±.01	156.32±.01	156.31±.01
Γ_n(S)	480.00 eV	500.00	730.18±10.72	654.28±11.46	486.85±9.75
E_{res}(S)	161.69 keV	162.00	161.62±.01	161.71±.01	161.69±.01
Γ_n(S)	1330.0 eV	1300.0	1350.6±21.69	1204.9±21.0	1326.3±22.07
E_{res}(P)	151.36 keV	151.40	151.21±.01	151.41±.01	151.37±.01
Γ_n(P)	17.000 eV	18.000	59.908±2.094	29.295±1.675	18.229±1.801
E_{res}(P)	154.30 keV	154.40	154.30±.01	154.31±.01	154.30±.01
Γ_n(P)	166.00 eV	170.00	349.09±5.20	310.67±.5.92	170.77±4.95
E_{res}(P)	160.16 keV	160.20	160.19±.01	160.21±.01	160.17±.01
Γ_n(P)	18.000 eV	17.500	65.117±1.504	33.888±1.663	17.272±1.616

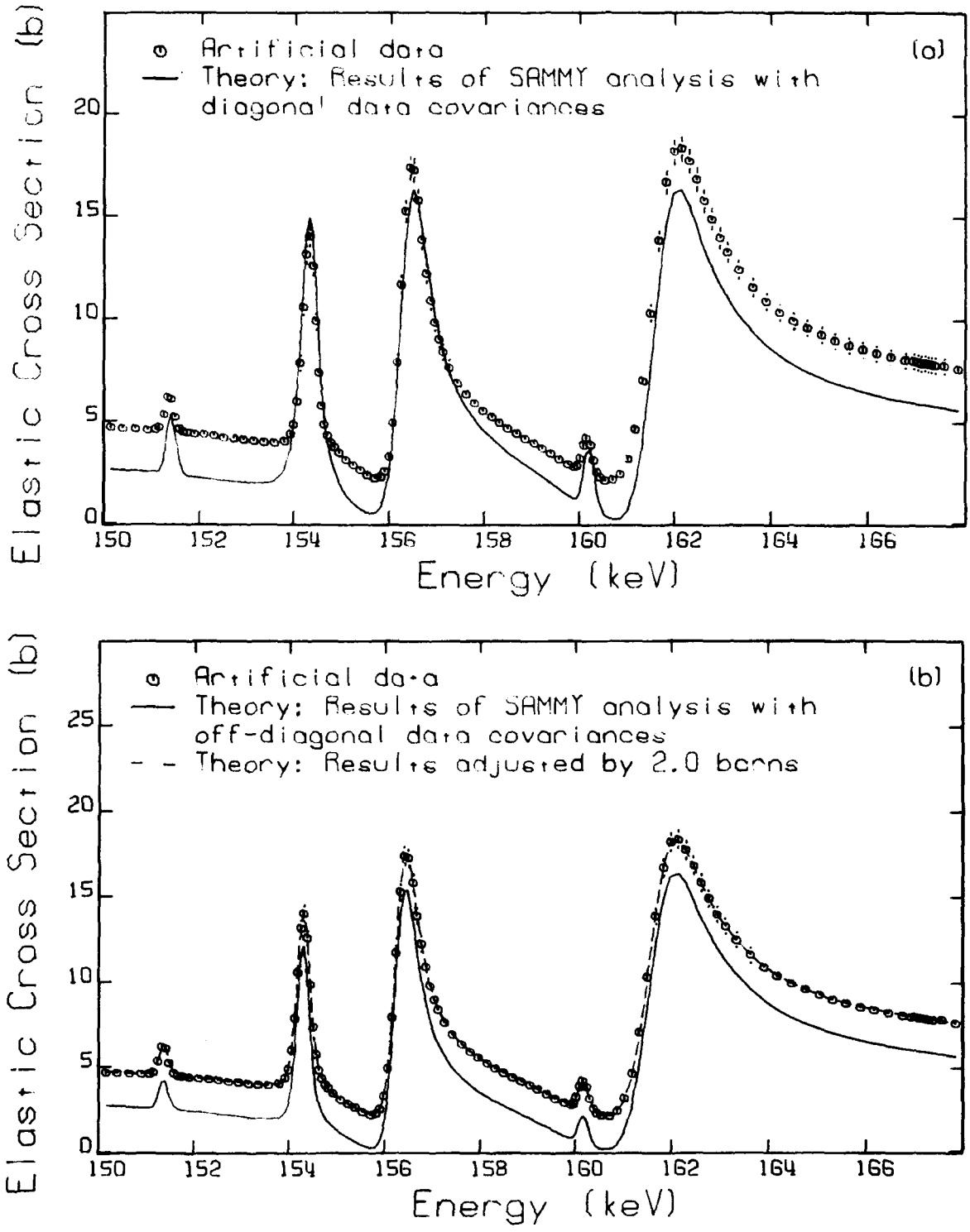

Fig. VI.3. Artificial data used to study the effect of improperly subtracted background. The theoretical curve in part *a* shows the results of the SAMMY analysis with diagonal data covariance matrix, in part *b* with off-diagonal covariance matrix. The dashed curve in part *b* is the solid curve adjusted by 2.0 barns, which is the value of the unsubtracted background.

different ways: First, all 123 data points were included simultaneously; results are given in Column C of Table VI.4, part a. Secondly, a low-energy piece (65 data points, from 150 keV to 158 keV) was analyzed first, followed by the remaining data (58 data points, 158 to 168 keV); results are in Column D of the table. Finally, the order of the two segments was reversed, and the analysis repeated; results are in Column E. In all cases, the resonance energies were held fixed and neutron widths varied; only diagonal data covariances were included. Agreement among the three calculations is well within the quoted uncertainties.

In part b of Table VI.4, the calculations are repeated with more accurate values as input. Again agreement among the three calculations is within the quoted uncertainties. (It is interesting to note that the output values are only weakly dependent on input values; this is to be expected when input uncertainties are large.)

TABLE VI.4. SIMULTANEOUS VS. SEQUENTIAL ANALYSIS OF AN S-WAVE RESONANCE FOR TWO SETS OF STARTING VALUES

	A.	B.	C.	D. Results from Sequential Analysis		E. Results from Sequential Analysis	
	Exact Values of	Input Values	Results from Simultaneous Analysis	(after only 150 to 158 keV)	(Final Results)	(after only 158 to 168 keV)	(Final Results)
part a							
	3.0000 keV	3.2000±.3200	3.0003±.0009	(3.0007±.0009)	3.0007±.0009	(2.9994±.0093)	3.0000±.0009
	50.000 eV	55.000±5.500	50.021±.971	(55.000±5.500)	50.000±.963	(50.050±1.025)	50.026±.964
part b							
	3.0000 keV	3.1000±.3100	3.0000±.0009	(3.0000±.0009)	3.0000±.0009	(3.0001±.0092)	3.0000±.0009
	50.000 eV	51.000±5.100	49.535±.962	(51.000±5.100)	49.534±.960	(49.532±1.020)	49.535±.960

VII. SUMMARY AND CONCLUSIONS

This report is intended as a users' guide to the Bayesian multilevel R-matrix code SAMMY. Bayes' theorem and our reasons for preferring its use to the customary least-squares approach are discussed in some detail, as are the assumptions required for the derivation of Bayes' equations from Bayes' theorem. A summary of multilevel R-matrix theory, as implemented in SAMMY, is presented. Four examples of data analyses are presented, illustrating both the strengths of Bayes' method and the necessity of including data correlations (off-diagonal data covariances). Thus in this report, we have attempted not only to explain how to use SAMMY, but also to indicate some of its advantages over MULTI, a code incorporating the same R-matrix theory formulations but using conventional least squares.

The code SAMMY is available from the Radiation Shielding Information Center (RA80). The authors would appreciate any comments on all aspects of SAMMY, including suggestions for refinements.

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APPENDIX A. ALGEBRAIC DETAILS

In this appendix are presented those algebraic details which, though important for complete understanding of the theory manifested in SAMMY, are sufficiently complex so as to obscure the broad understanding of our method were they to be presented in the text. Included here are the derivation of Bayes' equations from Bayes' theorem, development of an appropriate iteration scheme for Bayes' theorem, a derivation of least-squares equations from Bayes' equations, a proof that a constant covariance matrix is equivalent to a coherent data correction, and evaluation of the derivatives of X^{-1}.

1. Deriving Bayes' Equations

In Section II, a detailed discussion of Bayes' theorem and its application to neutron physics is presented. It is stated there that Bayes' equations may be derived directly from Bayes' theorem,

$$p(A|BX) \propto p(A|X)p(B|AX) \ , \tag{A1}$$

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 B, is

$$p(A|X) \propto \exp\left\{-\frac{1}{2}\,(P-\bar{P})^t M^{-1}(P-\bar{P})\right\} \tag{A2}$$

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

$$p(B|AX) \propto \exp\left\{-\frac{1}{2}\,(D-T)^t V^{-1}(D-T)\right\} \tag{A3}$$

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:

$$T = \bar{T} + G(P-\bar{P}) \tag{A4}$$

where the sensitivity matrix G is defined by

$$G^{i}_{k} = \left.\frac{\partial T^{i}}{\partial P_{k}}\right|_{P=\bar{P}} \tag{A5}$$

and the theoretical value $\bar{T}^{i}$ is also evaluated at $P = \bar{P}$.

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

$$p(A|BX) \propto \exp\left\{-\frac{1}{2}\,(P-\bar{P}')^{t}\,(M')^{-1}(P-\bar{P}')\right\} \quad . \tag{A6}$$

Substitution of Eq. (A2) through (A6) into Eq. (A1) and equating the exponents yields, in matrix form,

$$\begin{aligned}(P - \bar{P}')^{t}(M')^{-1}(P - \bar{P}') + Y = (P - \bar{P})^{t}M^{-1}(P - \bar{P}) \\ + [D - \bar{T} - G(P - \bar{P})]^{t}\, V^{-1}\, [D - \bar{T} - G\,(P - \bar{P})]\end{aligned} \tag{A7}$$

where Y represents the normalization constant and is independent of P.

Setting $P - \bar{P} = P - \bar{P}' + \bar{P}' - \bar{P}$ in Eq. (A7), and rearranging terms, we obtain

$$(P-\bar{P}')^t (M')^{-1}(P-\bar{P}')+Y = (P-\bar{P}')^t (M^{-1}+G^t V^{-1}G)(P-\bar{P}') \tag{A8}$$

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

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

$$+ (\bar{P}'-\bar{P})^t M^{-1}(\bar{P}'-\bar{P})$$

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

Because Eq. (A8) must hold for all values of P, we may equate terms quadratic, linear, or constant in $(P - \bar{P}')$. Equating the quadratic terms gives Bayes' equation for updating the covariance matrix:

$$(M')^{-1} = M^{-1} + G^t V^{-1} G \tag{A9}$$

Multiplication of both sides by M on the left and M' on the right yields

$$M' = [1+MG^t V^{-1}G]^{-1}M \tag{A10}$$

Using the identity $X^{-1} = (YX)^{-1}Y$ with $Y = G^t(N+V)^{-1}G$, substituting N for GMG^t, and rearranging give

$$M' = [G^t\{(N+V)^{-1}(1+NV^{-1})\}G]^{-1}G^t(N+V)^{-1}GM \quad . \tag{A11}$$

The quantity in curly brackets in Eq. (A11) is equal to V^{-1}; introducing the identity $V^{-1}V = I$ into that equation gives

$$M' = [G^t V^{-1}G]^{-1}G^t V^{-1}V(N+V)^{-1}GM \quad . \tag{A12}$$

Algebraic manipulation then yields

$$M' = [G^t V^{-1} G]^{-1} G^t V^{-1} GM - [G^t V^{-1} G]^{-1} G^t V^{-1} GMG(N+V)^{-1} GM \qquad (A13)$$

which reduces to

$$M' = M - MG^t(N+V)^{-1}GM \quad . \qquad (A14)$$

This is exactly Bayes' equation for updating the covariance matrix, Eq. (II.11) or (III.2). Explicitly, this equation may be written

$$M'_{k\ell} = M_{k\ell} - \sum_{n=1}^{K} \sum_{i=1}^{L} \sum_{j=1}^{L} \sum_{m=1}^{K} M_{kn} G^i{}_n \left((N+V)^{-1}\right)^{ij} G^j{}_m M_{m\ell} \qquad (A15)$$

where N is given by

$$N^{ij} = \sum_{k=1}^{K} \sum_{\ell=1}^{K} G^i{}_k M_{k\ell} G^j{}_\ell \quad . \qquad (A16)$$

To obtain Bayes' equation for updating the parameter values, we equate the linear terms of Eq. (A8). 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,

$$(M^{-1}+G^tV^{-1}G)(\bar{P}'-\bar{P}) = G^tV^{-1}(D-\bar{T}) \quad . \qquad (A17)$$

From Eq. (A9), the first quantity on the left is just $(M')^{-1}$; we therefore multiply both sides of Eq. (A17) by M', using Eq. (A14), and obtain

$$\bar{P}'-\bar{P} = (M-MG^t(N+V)^{-1}GM)G^tV^{-1}(D-\bar{T}) \qquad (A18)$$

which reduces to

$$\bar{P}'-\bar{P} = MG^t(N+V)^{-1}(D-\bar{T}) \quad . \qquad (A19)$$

Explicitly, this equation is

$$\bar{P}'_k = \bar{P}_k + \sum_{\ell=1}^{K} \sum_{i=1}^{L} \sum_{j=1}^{L} M_{k\ell} G^i{}_\ell \left((N+V)^{-1}\right)^{ij} (D^j - \bar{T}^j) \quad . \tag{A20}$$

Finally, we note that the constant term in Eq. (A8) may be simplified using Eq. (A19) to give

$$Y = (D-\bar{T})^t \left[(N+V)^{-1} G M G^t (N+V)^{-1} + \left(1-(N+V)^{-1}N\right)V^{-1}\left(1-N(N+V)^{-1}\right)\right](D-\bar{T}) \tag{A21}$$

which reduces to

$$Y = (D-\bar{T})^t (N+V)^{-1} (D-\bar{T}) \quad . \tag{A22}$$

2. 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 fact 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. (A4), may be performed not around $\bar{P}$ but around the new (intermediate) values $\bar{P}^{(n)}$, where n represents the nth iteration and $\bar{P}^{(0)} \equiv \bar{P}$:

$$T \simeq \bar{T}^{(n)} + G^{(n)}\left(P-\bar{P}^{(n)}\right) \quad . \tag{A23}$$

Here the sensitivity matrix $G^{(n)}$ and the theoretical values $\bar{T}^{(n)}$ are evaluated at $P = \bar{P}^{(n)}$. With Eq. (A23) for T, the formula analogous to Eq. (A7) is

$$\left(P-\bar{P}^{(n+1)}\right)^t\left(M^{(n+1)}\right)^{-1}\left(P-\bar{P}^{(n+1)}\right) + Y = (P-\bar{P})^t M(P-\bar{P})$$
$$+ \left[D-\bar{T}^{(n)}-G^{(n)}\left(P-\bar{P}^{(n)}\right)\right]^t V^{-1}\left[D-\bar{T}^{(n)}-G^{(n)}\left(P-\bar{P}^{(n)}\right)\right] \quad . \tag{A24}$$

Setting P equal to $P - \bar{P}^{(n+1)} + \bar{P}^{(n+1)}$ everywhere in the right-hand side of Eq. (A24) gives the formula analogous to Eq. (A8), 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 Bayes' equations follow immediately:

$$\bar{P}^{(n+1)} = \bar{P} + MG^{(n)t}\left(N^{(n)}+V\right)^{-1}\left(D-\bar{T}^{(n)}-G^{(n)}\left(\bar{P}-\bar{P}^{(n)}\right)\right) \tag{A25}$$

$$M^{(n+1)} = M - MG^{(n)t}\left(N^{(n)}+V\right)^{-1} G^{(n)}M \tag{A26}$$

where

$$N^{(n)} = G^{(n)}M\,G^{(n)t} \quad . \tag{A27}$$

3. Derivation of Least Squares from Bayes' Equations

The equivalence of the least-squares method with Bayes' equations in the limit of large M (i.e., in the extreme case where there is no prior knowledge of the values of the parameters) is best demonstrated by considering Eq. (A17):

$$\left(M^{-1}+G^t V^{-1} G\right)\left(\bar{P}'-\bar{P}\right) = G^t V^{-1}\left(D-\bar{T}\right) \tag{A28}$$

or, in the iterative form,

$$\left(M^{-1} + G^{(n)t}\, V^{-1}\, G^{(n)}\right)\left(\bar{P}^{(n+1)} - \bar{P}\right)$$

$$= G^{(n)t}\, V^{-1}\left(D - \bar{T}^{(n)} - G^{(n)}\left(\bar{P} - \bar{P}^{(n)}\right)\right) \quad . \tag{A29}$$

For large M, the term $G^{t}V^{-1}G$ overwhelms M^{-1}, and this equation reduces immediately to

$$\bar{P}^{(n+1)} = \bar{P}^{(n)} + \left(G^{(n)t}\, V^{-1}\, G^{(n)}\right)^{-1}\, G^{(n)t}\, V^{-1}\left(D - \bar{T}^{(n)}\right) \tag{A30}$$

which is the well-known least-squares formula.

Similarly, parameter uncertainties and covariances can be found from the iterative form of Eq. (A9):

$$\left(M^{(n+1)}\right)^{-1} = M^{-1} + G^{(n)t}V^{-1}G^{(n)} \tag{A31}$$

which reduces to

$$M^{(n+1)} = \left(G^{(n)t}V^{-1}G^{(n)}\right)^{-1} \tag{A32}$$

in the limit of large M. In least-squares applications, the quoted covariance matrix is usually the value given in Eq. (A32), multiplied by χ^2, where

$$\chi^2 = \frac{1}{d}\left(D - \bar{T}^{(n)t}\right)V^{-1}\left(D - \bar{T}^{(n)}\right) \tag{A33}$$

d being the number of degrees of freedom in the problem (d = number of data points minus number of parameters).

4. Use of Data Covariances to Indicate Coherent Data Corrections

In Section III.3, we indicated that a constant term added to the data covariance matrix is mathematically equivalent to a constant, coherent correction to either the data or the theory. To see that this is so, write the covariance matrix in the form

$$V = \bar{V} + AA^t \tag{A34}$$

where $\bar{V}$ is the original covariance matrix, and A is a column matrix whose elements are zero outside the range where the correction is to be applied, and constant inside the range. Bayes' equations require the inverse of $N + \bar{V} + AA^t$, which is equivalent to

$$\left(N+\bar{V}+AA^t\right)^{-1} = \left(N+\bar{V}\right)^{-1}\left[1 - \frac{1}{1+A^t\left(N+\bar{V}\right)^{-1}A}\,AA^t\left(N+\bar{V}\right)^{-1}\right] \tag{A35}$$

as can be verified by multiplying the right-hand side by $(N + \bar{V} + AA^t)$. Substitution of this expression into the first of Bayes' equations (Eq. III.1) gives

$$\bar{P}' = \bar{P} + MG\left(N+\bar{V}\right)^{-1}\left(D-\Delta D-\bar{T}\right) \tag{A36}$$

where the correction term D is given by

$$\Delta D = \frac{1}{1+A^t\left(N+\bar{V}\right)^{-1}A}\,AA^t\left(N+\bar{V}\right)^{-1}\left(D-\bar{T}\right) \quad . \tag{A37}$$

Thus, the presence of an additive constant term (AA^t) in the data covariance matrix is equivalent to a coherent correction to the data or to the theory. Also, note that if the elements of column matrix A are not zero or constant, Eqs. (A36) and (A37) remain valid, but the correction term ΔD varies from point to point.

5. Derivative of X^{-1} with Respect to R

In Section V, we require the derivative of $Y = X^{-1}$ with respect to R, where the matrix X is given by

$$X_{\mu\nu} = \frac{\delta_{\mu\nu}}{L_\mu} - R_{\mu\nu} \quad . \tag{A38}$$

To determine the derivative of Y with respect to X, note that the derivative of

$$\sum_\beta X_{\varepsilon\beta} Y_{\beta\alpha} = \delta_{\varepsilon\alpha} \tag{A39}$$

with respect to $X_{\mu\nu}$ is

$$\sum_\beta \left[\delta_{\varepsilon\mu} \delta_{\beta\nu} + \delta_{\varepsilon\nu} \delta_{\beta\mu} \left(1-\delta_{\mu\nu}\right)\right] Y_{\beta\alpha} + \sum_\beta X_{\varepsilon\beta} \frac{\partial Y_{\beta\alpha}}{\partial X_{\mu\nu}} = 0 \quad . \tag{A40}$$

Multiplication by $Y_{\omega\varepsilon}$ and summation over ε give

$$Y_{\omega\mu} Y_{\nu\alpha} + Y_{\omega\nu} Y_{\mu\alpha} \left(1-\delta_{\mu\nu}\right) + \frac{\partial Y_{\omega\alpha}}{\partial X_{\mu\nu}} = 0 \tag{A41}$$

where we have used the fact that Y is the inverse of X. Finally, we note that the derivative with respect to R is the negative of the derivative with respect to X; this gives

$$\frac{\partial Y_{\omega\alpha}}{\partial R_{\mu\nu}} = Y_{\omega\mu} Y_{\nu\alpha} + Y_{\omega\nu} Y_{\mu\alpha} \left(1-\delta_{\mu\nu}\right) \tag{A42}$$

for the required derivative (Eq. (V.12) in the text).

APPENDIX B. DESCRIPTION OF THE COMPUTER CODE SAMMY

The computer code SAMMY was developed for ease and efficiency of running on the DECsystem-10 (PDP-10) at ORELA. (Conversion to other machines should nevertheless be straightforward; helpful suggestions are given at the end of this appendix.) Because core storage rather than CPU time is the limiting factor on the PDP-10, a number of techniques have been used to preserve core, occasionally at the expense of runtime. These techniques include dynamic allocation of array storage, use of temporary data files to store intermediate results, and division of the program into four substationally independent segments.

1. Dynamic Allocation of Array Storage

All arrays required by the computer program are stored in one location in CØMMØN/EXPAND/A(n) where n is a large number. Allocation of space in this common block is accomplished via a call to FUNCTIØN IDIMEN, which remembers the last location allocated, and appends the new array to that position. When an array is no longer needed, its space is released for future use via another call to IDIMEN. IDIMEN issues a warning if more than n words are required in CØMMØN/EXPAND/, and also indicates the maximum size actually used in each segment of the program.

Dynamic allocation of array storage is best illustrated with a simple example. Let us suppose that two vectors V1 and V2, both of length N, are to be initialized, added, and stored in V1, after which V2 is no longer required. A program to perform these operations is given in Table B.1. Notice that mnemonic names can be used in the usual manner in all subroutines, provided arrays are input to the subroutines through argument listings.

TABLE B.1. ILLUSTRATION OF DYNAMIC ALLOCATION OF ARRAY STORAGE

```
   PRØGRAM MAIN
   CØMMØN/EXPAND/A(10000)
   CØMMØN/ØVER/NSIZE
   NSIZE = 10000
   .
   .
   .
   N=50
   IV1=IDIMEN(N)                 allocate storage for V1
   IV2=IDIMEN(N)                 allocate storage for V2
   CALL SET(A(IV1),A(IV2),N)     initialize V1 and V2
   CALL ADD(A(IV1),A(IV2),N)     add V1 = V1 + V2
   I=IDIMEN(-IV2)                release storage for V2
   .
   .
   .
   I=IDIMEN(0)                   request that IDIMEN print out the maximum
                                 length used
   STØP
   END



   SUBRØUTINE SET(V1,V2,N)
   DIMENSIØN V1(N),V2(N)
   READ (11) V1
   READ (11) V2
   RETURN
   END



   SUBRØUTINE ADD(V1,V2,N)
   DIMENSIØN V1(N),V2(N)
   DØ 10 I=1,N
10 V1(I)=V1(I)+V2(I)
   RETURN
   END
```

There are several advantages to using dynamic allocation of array storage: First, core requirements are kept to a minimum, since only the array length actually needed is allocated and temporary arrays are released when no longer needed. Secondly, because allocation is made during the execution of a program, substantial changes in the dimensions for a specific case do not always require recompilation of the program. Finally, when recompilation is required (when the maximum array space requirement is larger than n), only the main routine need be recompiled; other routines using CØMMØN/EXPAND/A(1) will have array A dimensioned 1, since the loader allocates CØMMØN storage space according to the first subroutine loaded.

2. 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 B.2. Upon successful completion of a run, SAMMY deletes these files. An aborted run can sometimes be restarted if the user takes care not to destroy these files.

3. Division of the Program into Four 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 PDP-10 computer; instead, SAMMY makes use of the DECsystem-10 "CALL RUN" option, which allows a FØRTRAN program to initiate execution of another program. Thus SAMMY consists of four 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 B.3 describes the functions of the four segments. Tree charts showing the subroutine structure of each segment are given in Figs. B.1-B.4.

TABLE B.2. TEMPORARY FILES USED BY SAMMY

File Name	Use
SAM42.DAT	store covariance matrix for physical parameters
SAM43.DAT	store data and covariance matrix for the data
SAM44.DAT	store data and modified covariance matrix
SAM46.DAT	store covariance matrix for u-parameters
SAM47.DAT	store covariance matrix for updated u-parameters
SAM48.DAT	store partial derivatives
SAM49.DAT	pass minimal information from THEORY segment to RESULTS segment
SAM20.DAT	pass complete information between any two program segments

TABLE B.3. SEGMENTS OF THE CODE SAMMY

Segment	Function	User-Supplied Input	Input from Temporary Files	Output to Temporary File	Control Passes to Which Segment	Control Comes from Which Segment	Reasonable Estimates for Length of Array in CØMMØN/EXPAND (in words)	Core Requirement with that Size Array (in words)
SAMMY-PARAMETER	read input/output control statements, read physical parameters and covariance matrix, and generate u-parameters	"INPut file" "PARameter file" "CØVARIANCE file"	none	SAM20.DAT SAM42.DAT SAM46.DAT SAM49.DAT	SAMMY-DATA	(initial segment)	5000	18K
SAMMY-DATA	read experimental data and covariance matrix	"DATa file"	SAM20.DAT	SAM20.DAT SAM43.DAT	SAMMY-THEØRY	(1)SAMMY-PARAMETER (2)SAMMY-RESULTS	15000	21K
SAMMY-THEØRY	generate theoretical values and partial derivatives	none	SAM20.DAT SAM43.DAT SAM46.DAT	SAM20.DAT SAM44.DAT SAM49.DAT	SAMMY-RESULTS	(1)SAMMY DATA (2)SAMMY-RESULTS	20000	37K
SAMMY-RESULTS	find solution of Bayes' equations to give new values of parameters and covariance matrix	none	SAM20.DAT SAM44.DAT SAM46.DAT SAM48.DAT SAM49.DAT	SAM20.DAT SAM42.DAT SAM47.DAT	(1)SAMMY-DATA if more data needed (2)SAMMY-RESULTS if cycle needed (see Section III) (3)Stop if end of run	SAMMY-THEØRY	40000	53K

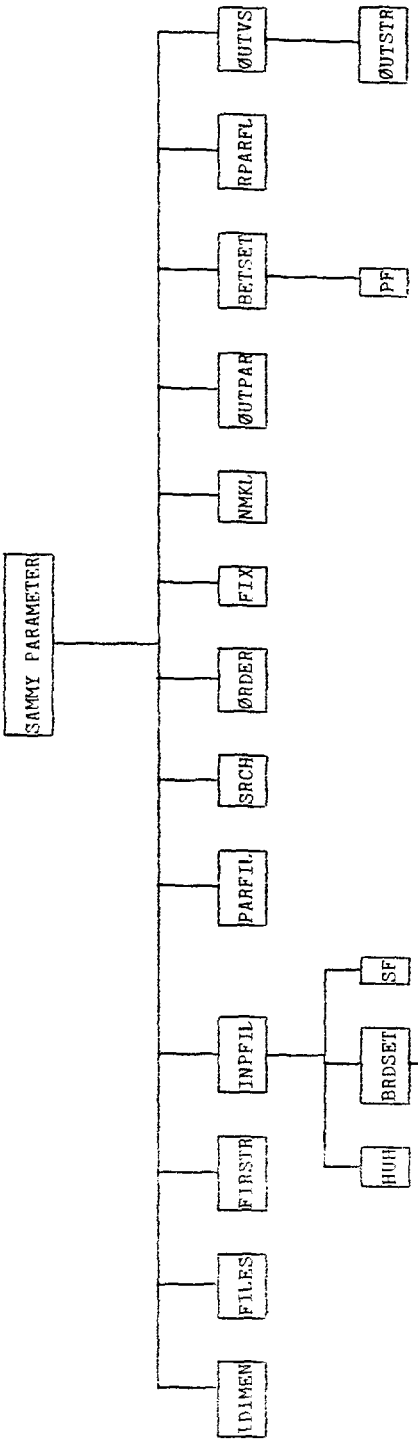

Figure B.1. Tree charts showing the subroutine structure of segment SAMMY-PARAMETER. A subroutine is called by the routine above it in the chart.

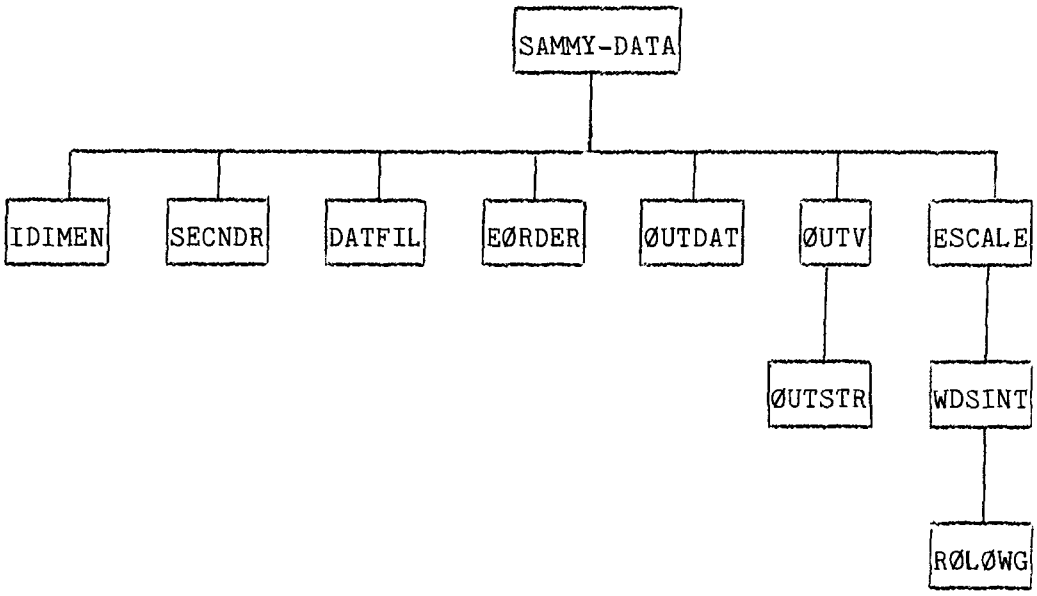

Figure B.2. Tree charts showing the subroutine structure of segment SAMMY-DATA. A subroutine is called by the routine above it in the chart.

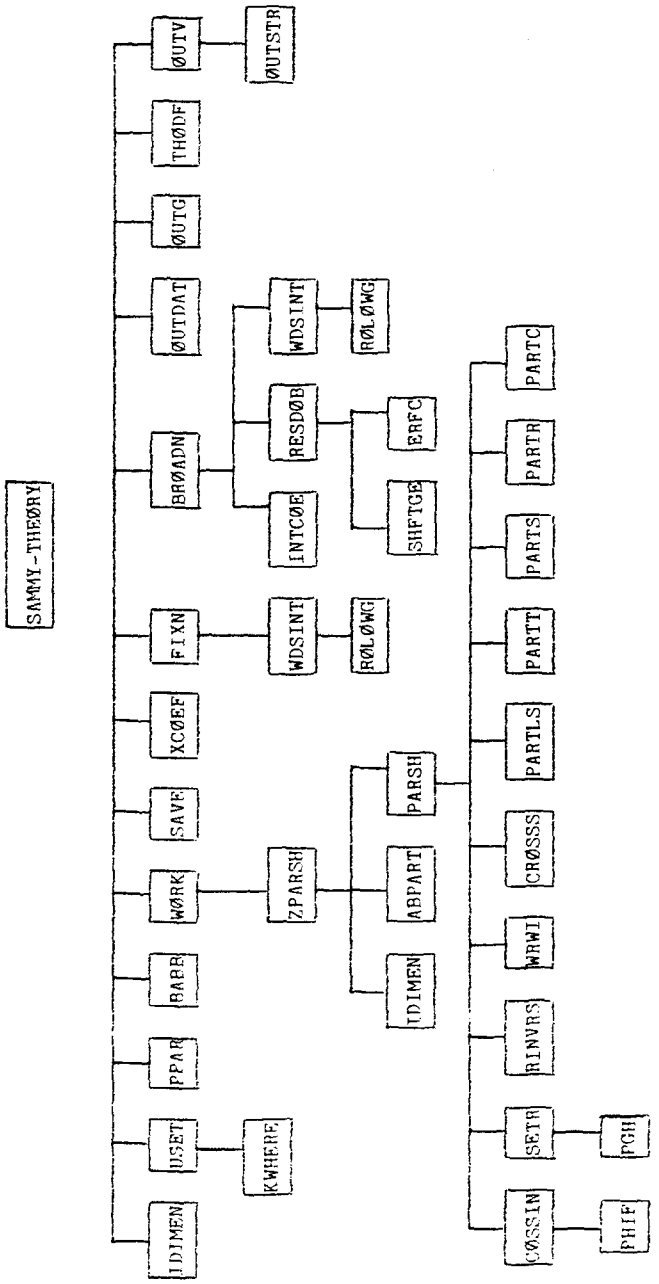

Figure B.3. Tree Charts showing the subroutine structure of segment SAMMY-THEØRY. A subroutine is called by the routine above it in the chart.

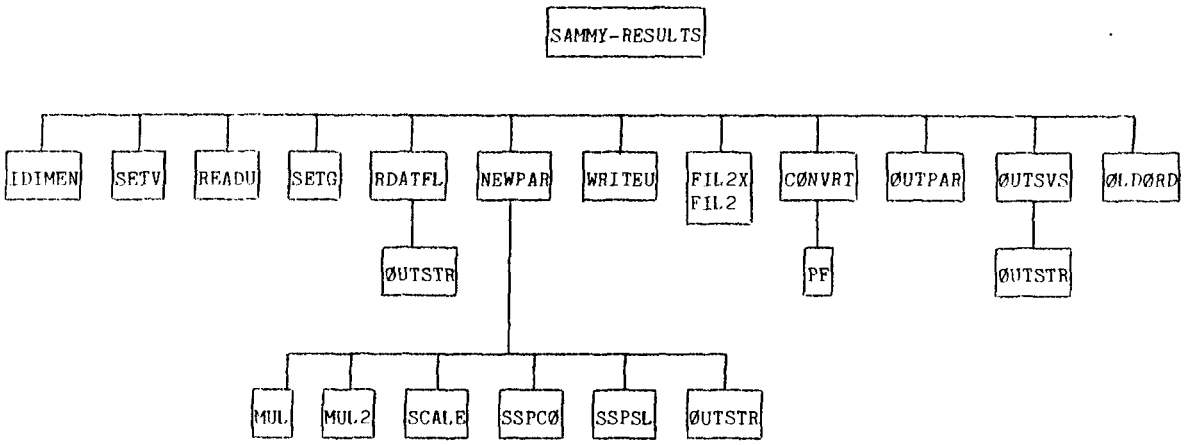

Figure B.4. Tree charts showing the subroutine structure of segment SAMMY-RESULTS. A subroutine is called by the routine above it in the chart.

4. Conversion to Other Computer Systems

Most of the programming in SAMMY is standard FØRTRAN IV, with relatively few operations specific to the PDP-10 for which SAMMY was designed. For this reason, conversion to another computer should proceed without major difficulties.

No plotting options are available within SAMMY. Instead, an ØDF (ØRELA Data Format) file may be generated, from which plots are produced using the in-house data-manipulating and plotting package ØPRØDF (CR78). Persons converting SAMMY to other systems should simply drop all references to ØDF files, including subroutine THØDF in segment SAMMY-THEØRY, and the auxiliary program SAMØDF. Plotting routines suitable for the particular computer system can then be substituted.

File naming, opening, closing, deleting, and renaming are all done with FØRTRAN statements in SAMMY on the PDP-10 computer. Other computers may require JCL (job control language) to accomplish these functions.

Some computer systems may not allow one FØRTRAN program to call another; in this case, JCL can perhaps be used to couple SAMMY's four segments. Alternatively, the four segments could be reunited (thus probably eliminating the SAM20.DAT temporary file) and, to save core, overlaid if possible.

The authors would appreciate feedback concerning the ease or difficulty of implementing SAMMY on other computers.

APPENDIX C. INPUT TO SAMMY

A minimum of three user-supplied input files are required to run SAMMY. The first, or "INPut" file, contains general information about the interaction being studied, quantum numbers for nucleus and resonances, and output control information. The second, or "PARameter" file, gives initial estimates for resonance parameters and (perhaps) initial estimates for correlations between parameters. The third, or "DATa" file, provides the experimental energies, data, and uncertainties. An optional fourth, or "CØVariance" file, contains the covariance matrix for the parameters in binary form, as generated by a previous SAMMY run. An optional fifth, or "DCV" (data covariance) file, provides off-diagonal data covariances.

The PAR and DAT files are identical to the analogous files required by program MULTI, except that the PAR file may have information about parameter uncertainties appended to it. The DAT file is not restricted to those data points needed for a particular calculation; SAMMY will search through the file to find only those points within the desired energy range. SAMMY's INP file contains much of the same information as does MULTI's INP file, but formats have been changed and controls are now written in English rather than as numbers in certain columns. These changes were designed to eliminate input errors as much as possible. Details and formats for the INP file are given in Tables C.1 and C.2, for PAR in Table C.3, for DAT in Table C.4, and for DCV in Table C.5. Note that this format for the PAR file permits a maximum of three neutron + fission channels, though there is no such limitation inherent in SAMMY; modifications of input and output formats to permit more than three channels will be made as they are needed.

TABLE C.1. FORMAT OF THE INPUT FILE

Card Number	Columns	Variable	Format	Meaning (Units)	Range of Values
1	1-80	TITLE	16A5	title	
2	1-10	ELEMENT	A10	sample element	
	11-20	AW	F10.1	atomic weight	
	21-30	EMIN	F10.1	minimum energy for this data set (eV)	
	31-40	EMAX	F10.1	maximum energy (eV)	
	41-45	NEPNTS	I5	max number of data points to be analyzed at one time	$\lesssim$ 130
3,4, etc.	1-20	WHAT	4A5	alphanumeric information concerning program options	see Table C.2
5*	1-10	TEMP	F10.1	effective temperature of the sample (K)	
	11-20	DIST	F10.1	flight path (M)	
	21-30	DELTAL	F10.1	flight path uncertainty (M) (full width of equivalent square pulse)	
	31-40	DELTAE	F10.1	E-folding width of exponential resolution function (μS)	
	41-50	DELTAG	F10.1	FWHM of Gaussian resolution function (μS)	
6+	1-10	DELTAB	F10.1	minimum channel width for interval from EMIN to EMAX (μS)	
	11-15	NCF	I5	number of crunch boundaries	

*This card is omitted if broadening is not wanted.

+These cards are omitted if broadening is not wanted, or if DELTAG $\gtrsim$ 0.

TABLE C.1. FORMAT OF THE INPUT FILE (CONT'D)

Card Number	Columns	Variable	Format	Meaning (Units)	Range of Values
7+	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)	
8	1-10	CRFN	F10.1	channel radius (eV) or, if input as zero, computed as 1.45* (1.009 + AW)**0.333	≥ 0
	11-20	THICK	F10.1	sample thickness (AT/B)	
	21-30	DCØVA	F10.1	data covariance matrix has	
	31-40	DCØVB	F10.1	additional term of the form (DCØVA+E_i*DCØVB)*(DCØVA+E_j*DCØVB)	
9	1-80	CRØSS	16A5	type of cross-section (only the first five characters are relevant)	TØTAL {ELASTic {SCATTering {FISSIon {REACTion CAPTUre NOTE: If TØTAL cross section, transmission data is assumed unless the letters "CRØSS" appear in columns 26-30
10	1-10 11-20	SPINI ECHAN(1)	F10.1 F10.1	SPIN of target nucleus energy of R-matrix channel 1 relative to neutron binding energy (eV)	half integer

TABLE C.1. FORMAT OF THE INPUT FILE (CONT'D)

Card Number	Columns	Variable	Format	Meaning (Units)	Range of Values
	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
	31-40	ECHAN(2)	F10.1	energy for channel 2	
	etc.				
11, 12, etc.	1-10	SPINJ(1)	F10.1	spin for resonances in group 1	half-integer
(one card	11-15	NENT(1)	I5	number of entrance channels for resonances in group 1	≥ 1
for each spin group)	16-20	NEXT(1)	I5	number of exit channels	≥ 0
	21-25	LSPIN(1,1)	I5	orbital angular momentum for channel 1 for resonances in group 1	integer
	26-30	CHSPIN (1,1)	F5.1	channel spin	half-integer
	31-40	ENBND(1,1)	F10.1	boundary condition (eV)	
	41-45	LSPIN(2,1)	I5	orbital angular momentum for channel 2 for resonances in group 1	integer
	etc.				

TABLE C.2. ACCEPTABLE "ALPHANUMERIC INFORMATION CONCERNING PROGRAM OPTIONS", FOR CARDS 3, 4, ... IN THE INPUT FILE. Any of the listed statements may be used, in any order, terminating with a blank line. Only the first twenty characters and occasional others (capitalized below) need be exactly as shown here. Defaults are indicated in the first column.

Default?	Statement
X	DØ NØT PRINT INPUT Data
	PRINT INPUT DATA
X	DØ NØT PRINT ANY INPut parameters
	PRINT ALL INPUT PARAmeters
	PRINT VARIED INPUT Parameters
X	DØ NØT PRINT PARTIAL derivatives
	PRINT PARTIAL DERIVAtives
X	DØ NØT PRINT THEØRETical values
	PRINT THEØRETICAL VAlues from input parameters
	PRINT THEØRETICAL CRoss sections
X	DØ NØT PRINT WEIGHTEd residuals
	PRINT WEIGHTED RESIDuals from input parameters
	DØ NØT SUPPRESS INTErmediate printout
X	SUPPRESS INTERMEDIATe printout
X	BRØADENING IS WANTED
	BRØADENING IS NØT WAnted
	ØDF FILE IS WANTED--XXXXXX.XXX,ZERØ-th order guess*
	ØDF FILE IS WANTED--XXXXXX.XXX,FINAl guess*
X	ØDF FILE IS NOT WANTed
X	CHI SQUARED IS WANTEd
	CHI SQUARED IS NØT Wanted
X	DØ NØT DIVIDE DATA Into regions - do entire energy range at once
	DIVIDE DATA INTØ REGions with a fixed number of data points per region
	DØ NØT SØLVE BAYES Equations - just generate chi squared
X	SØLVE BAYES EQUATIØNs
	DØ NØT ØUTPUT CØVARIance matrix in binary form
X	ØUTPUT CØVARIANCE MAtrix in binary form
X	DATA CØVARIANCE IS Diagonal
	DATA HAS ØFF-DIAGØNAl contribution to covariance matrix of the form $(a + bE)^2$
	DATA CØVARIANCE FILE is named YYYYYY.YYY+
	PRINT DEBUG INFØRMATion
X	DØ NØT PRINT DEBUG Information
	DECØUPLE S-WAVES FRØm other resonances
X	DØ NØT DECØUPLE S-WAves from other resonances

*Before using this option, execute program SAMØDF to initialize file XXXXXX.XXX. Substitute your own file for XXXXXX.XXX.

+Substitute your own file name for YYYYYY.YYY.

TABLE C.3. FORMAT OF THE PARAMETER FILE

Card	Column	Variable Name	Format	Meaning (Units)	Values
1,2, etc.	1-11	ERES	E11.4	Resonance Energy (eV)	
	12-22	Γ^{γ}	E11.4	Gamma-width (Milli-eV)	
	23-33	Γ_{c1}	E11.4	width for channel 1 (Milli-eV)	
	34-44	Γ_{c2}	E11.4	width for channel 2 (Milli-eV)	
	45-55	Γ_{c3}	E11.4	width for channel 3 (Milli-eV)	
	56-57	IS_{ERES}	I2	vary ERES?	0 = no 1 = yes
	58-59	IS	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	IGRØUP	I2	quantum numbers for this resonance are those of group number IGRØUP (See cards 11, 12, etc. in Table C.1.)	

TABLE C.3. FORMAT OF THE PARAMETER FILE (CONT'D)

Card	Column	Variable Name	Format	Meaning (Units)	Values
	68-80	DCØV	E13.4	constant off-diagonal data covariance to be used under this resonance	
3					blank
4	1-11	FUDGE	E11.4	prior parameter uncertainty is FUDGE times parameter value	0. < FUDGE (0.1 is default)
5,6, etc.	1-5	NN(1)	I5	If KK and LL are zero, the prior uncertainty in resonance NN, parameter MM (ERES, Γ^{γ}, Γ_{c1}, Γ_{c2}, Γ_{c3} for MM = 1,2,3,4,5, respectively) is VV.	NN and KK ≤ the number of resonances;
	6-10	MM(1)	I5		
	11-15	KK(1)	I5		
	16-20	LL(1)	I5		MM and LL ≤ the number of channels +2.
	21-30	VV(1)	F		
				For KK and LL not equal to zero, the prior correlation coefficient between resonance NN, parameter MM and resonance KK, parameter LL is VV. Here $\|VV\| \leq 1$.	
				If NN is negative, parameter uncertainties are stored in a binary covariance file generated by a previous SAMMY run.	

TABLE C.4. FORMAT OF THE DATA FILE

Energies are assumed order from high to low, with three data points per line.

Card	Column	Variable	Format	Meaning (Units)
1,2,etc.	1-15	$ENERGY_1$	E15.8	energy (eV)
	16-30	$DATA_1$	E15.8	experimental cross section (barns) or transmission
	31-17	$FRACT_1$	F7.5	fractional uncertainty in $DATA_1$
	38-52	$ENERGY_2$	E15.8	
	53-67	$DATA_2$	E15.8	
	68-74	$FRACT_2$	F7.5	
	75-89	$ENERGY_3$	E15.8	
	90-104	$DATA_3$	E15.8	
	105-111	$FRACT_3$	F7.5	

TABLE C.5. FORMAT OF THE DCV FILE

Card	Columns	Variable	Format	Meaning
1	1-10	VARDAT(1,1)	F10.1	Variance for data point 1
2	1-10	VARDAT(2,1)	F10.1	Covariance between data points 1 and 2
	11-20	VARDAT(2,2)	F10.1	Variance for data point 2
3	1-10	VARDAT(3,1)	F10.1	Covariance between data points 1 and 3
	11-20	VARDAT(3,2)	F10.1	Covariance between data points 2 and 3
	21-30	VARDAT(3,3)	F10.1	Variance for data point 3
4	1-10	VARDAT(4,1)	F10.1	Covariance between data points 4 and 1
	etc.			

Note that the ordering of data points is low energy to high, and only those data points to be used in the calculation can be referenced in the DCV file. A more convenient format for input of off-diagonal data covariances will be implemented as it is required.

Execution of SAMMY can proceed interactively, with the user responding to teletype prompts from SAMMY, or in the BATCH mode with responses given as part of the input stream. Teletype prompts and appropriate responses are described in Table C.6.

Output from SAMMY consists of two (or three) files, described in Table C.7.

Conversion of a MULTI-type INP file to a SAMMY-type INP file may be accomplished by running Program SAMSWI; teletype prompts and appropriate responses for SAMSWI are given in Table C.8. The user is urged to compare the SAMMY INP file to Table C.2, to be sure the appropriate options are chosen.

Plotting routines are not an integral part of the code SAMMY. Rather, SAMMY writes theoretical values for cross sections or transmissions on an ØDF (ØRELA data format) file, from which plots may be produced using ØPRØDF (CR78). Because of the sequential nature of data analysis in SAMMY, it is necessary to initialize the OØF file prior to running SAMMY. To accomplish this, program SAMØDF generates a five- (or nine-) section ØDF file and inserts energies and experimental data in the appropriate sections. Details are given in Tables C.9 and C.10.

TABLE C.6. TELETYPE INPUT FOR SAMMY

SAMMY Prompt	User Response
1. What is the name of the input file?	Input file name plus extension, e.g., AAAAAA.INP*
2. What is the name of the parameter file?	PARameter file name, e.g., AAAAAA.PAR*
3. What is the first data file name? EMIN? EMAX?	DATa file name, e.g., AAAAAA.DAT*, followed by the minimum and maximum energies (in eV) for this step in F format, separated by commas. EMIN and EMAX need not be repeated here if they are correct in the INP file, card 2. Caution: Be sure EMIN does not start prior to Column (or Space) 11.
4. What is the name of the covariance file? (Optional question, asked only if parameter file indicates there is a covariance file.)	Binary file from a previous SAMMY run, e.g., AAAAAA.CØV*
5. What is new EMIN? EMAX? Data set name?	Energy range (in eV) for the next step, in F format, separated by commas. If EMIN = 0., program will terminate. If the data set name is blank, the previous DATa file is assumed.
Repeat Step 5 as needed	

*File names may be chosen for convenience; extensions need not be INP, PAR, DAT, and CØV.

TABLE C.7. SAMMY OUTPUT FILES

File Name	Contents
SAMMY.LPT	Descriptive output, to be queued to the line printer for examination.
SAMMY.PAR	New resonance parameters, in the same format as the input PARameter file. For binary output of the covariance matrix, "-1" will occur in columns 4 and 5 on the last card of SAMMY.PAR.
SAMMY.CØV (optional)	New covariance matrix for the parameters, in binary form.

TABLE C.8. TELETYPE INPUT FOR SAMSWI

SAMSWI Prompt	User Response
1. What's the name of the MULTI "INP" file?	file name and extension
2. What would you like the new SAMMY "INP" file to be called?	file name and extension
3. What's title?	alphanumerical title for the problem

TABLE C.9. TELETYPE INPUT FOR SAMØDF

SAMØDF Prompt	User Response
1. What's name for output ØDF file	filename and extension, e.g., AAAAAA.ØDF
2. Is data total or other cross section? T = total	T if data is total cross section or transmission; blank otherwise
3. Is data transmission or cross section? T = trans. (Optional Question)	T if transmission; blank otherwise
4. What's thickness? (Optional Question)	thickness of target in atoms/barn
5. What's name of the first data file (lowest energy)?	file name plus extension for the lowest-energy data, e.g., AAAAAA.DAT*
6. What's EMIN and EMAX for this data set? (in eV)	energy range in eV*
7. What's name of next data file (next lowest energy)?	filename plus extension, or blank if there are no more files

Repeat steps 6 and 7 as needed.

*In SAMØDF, the entire energy range for a given file may be included simultaneously; it is not necessary to divide into small pieces as is done in SAMMY.

TABLE C.10. SECTIONS OF ØDF FILE GENERATED BY SAMØDF

Section Number	Contents
1	energy (keV)
2	experimental cross section (barns)
3	uncertainty in experimental cross section (barns)
4	zeroth order theoretical cross section as evaluated by SAMMY
5	final theoretical cross section as evaluated by SAMMY
6*	experimental transmission
7*	uncertainty in experimental transmission (absolute)
8*	zeroth order theoretical transmission as evaluated by SAMMY
9*	final theoretical transmission as evaluated by SAMMY

*These sections are omitted for the partial cross sections, included for total cross sections or transmissions.

APPENDIX D. SAMPLE INPUT AND OUTPUT

Input and output for example number 3 in Section VI are presented in the microfiche inside the back cover of this report. SAMTRY.BAT is the file which should be submitted to the PDP-10 to run SAMMY in the batch mode; equivalently, one could run SAMMY in the interactive mode (via the R SAMMY command) and respond to SAMMY's questions with the answers given in that file.

The file SAMTRY.INP is the INPut file for this example, SAMTRY.PAR the PARameter file, and SAMTRY.DAT the DATa file. The two output files are SAMMY.PAR and SAMMY.LPT.

APPENDIX E. FØRTRAN LISTINGS

FØRTRAN listings of all the SAMMY programs are shown on the microfiche inside the back cover of this report. File SAMPAR.F4 contains the listing of the program SAMMY-PARAMETER, SAMDAT.F4 contains SAMMY-DATA, SAMTHE.F4 contains SAMMY-THEØRY, and SAMRES.F4 contains SAMMY-RESULTS. The LINPACK subroutines required by SAMMY-RESULTS are listed in file LINPACK.F4. Program SAMØDF is in file SAMØDF.F4, and SAMSWITCH in SAMSWI.F4.

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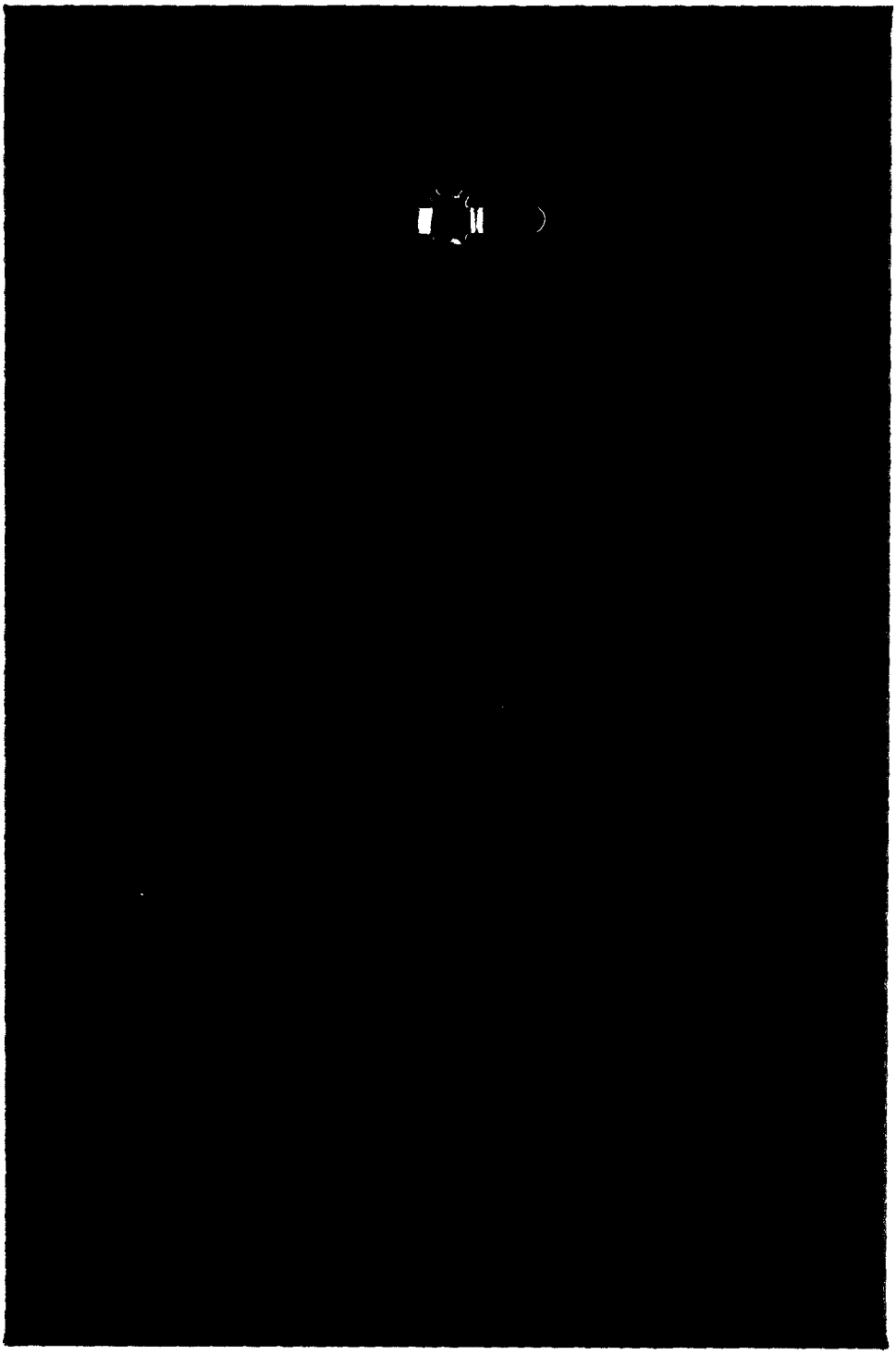

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