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**MULTILEVEL EXPANSION AND ITS APPLICATION
TO NEUTRON RESONANCE ANALYSIS**

Final Report

By
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July 1972

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MULTILEVEL EXPANSION AND ITS APPLICATION TO NEUTRON RESONANCE ANALYSIS

Final Report
Contract AT(11-1)-2022-1

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July 1972

USAEC, Technical Information Center
Oak Ridge, Tennessee

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TABLE OF CONTENTS

	Page
Summary	1
(1) Correlated Analysis of the ^{239}Pu fission, capture, and total cross sections	1
(2) Computer Program Development	1
(3) Exploratory Work	1
Task (1)	2
Task (2a)	2
Task (2b)	3
Task (2c)	3
Task (3a)	3
List of Publications and Technical Reports supported in part by Contract AT(11-1)-2022 and 2022-1.....	4
 I. Introduction	 7
II. Multilevel description of low energy neutron reactions in fissile elements	11
III. Ambiguities in the R-matrix representation	14
IV. Development of computer programs	15
V. References	21

APPENDICES

A. Multilevel description of neutron resonance reactions in fissile elements. ^{a) c)}	
B. Ambiguities in R-matrix representations of fissile element cross sections with two fission channels. ^{b) c)}	
C. Program CODILLI-2	24
D. Program LEMA-CHAMA	54
E. Program TRIPLE	106
F. Interactive Use of Program CODILLI 2 with SCORE III-A: Least Squares Data Fitting of ^{239}Pu Using Program CODILLI with SCORE	155
G. Multilevel analysis of ^{239}Pu cross sections in the low energy region	176

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- (a) This manuscript has been submitted for publication to Nuclear Physics,
and is being revised.
- (b) This report will be published in Physical Review C, 1972.
- (c) In view of the fact that this report will be published in a journal, a copy
of it is not appended here. Copies may be obtained upon request from the
Department of Physics of the University of Illinois, Urbana, Ill. 61801.

Summary

The scope of the work under this contract consisted of a continuation of the work supported under contract AT(11-1)-2022, and it included the following specific tasks:

(1) Correlated Analysis of the ^{239}Pu fission, capture, and total cross sections, to be reported in the ENDF-B format, with the aim of obtaining consistent generalized Kapur-Peierls and R-matrix parameters in the context of operational testing of Program TRIPLE.

(2) Computer Program Development

(a) Operational checks of Program TRIPLE, and deposition of the Program, with suitable test cases at the ANL code center.

(b) Development of Program GAMPLEX, to include three modes of deriving R-matrix parameters from the generalized Kapur-Peierls parameters obtainable from Programs CODILLI and TRIPLE, using a least-squares procedure, (GAMPLEX I), a perturbative method for the few channel case (GAMPLEX II), and a method permitting at least in principle the direct calculation of level matrix parameters from the generalized Kapur-Peierls parameters. (GAMPLEX III).

(c) To make Program CODILLI a part of the SCORE package, and to analyze and prepare Program TRIPLE for eventual inclusion in the SCORE package.

(3) Exploratory Work

(a) To investigate the usefulness of programs CODILLI and TRIPLE for the analysis of fertile and other non-fissile elements, and the necessary computer implementation of these programs for such purposes.

(b) To make a preliminary investigation aiming towards the adaptation of parts of the SCORE package for use on interactive devices now becoming available at the University of Illinois in order to facilitate the implementation of Task (2c).

Task (1) has been completed, resulting in a correlated evaluation of the capture, fission, and total cross sections of ^{239}Pu in the 6 to 70 eV region, reported in Appendix G. The results will be reported to the National Cross Section Center for eventual inclusion in the ENDF-B file; as pointed out in Appendix G, the format of ENDF-B for multilevel parameters appears not to be consistent with the type of results obtained in this analysis.

Completion of this task, and thus of the whole work of this contract was greatly delayed by circumstances beyond control of this contractor. While CODILLI-2 was delivered for use with SCORE on January 15, 1971, it was possible to make test runs on SCORE only during the second half of September 1971. For technical reasons discussed in Appendix F, practically the whole ^{239}Pu analysis had to be performed using the batch mode version of CODILLI-2 and TRIPE at Illinois after that time, thus naturally delaying completion of the tasks of the contract.

Task (2a) has been completed; the Programs TRIPE and CODILLI-2 will be deposited with the ANL data center during coming academic year, when University of Illinois funds will permit the necessary final computer runs to provide the material required by the ANL Code center. Code listings will be available as University of Illinois Technical Reports.

Task (2b) could be completed only in part; investigation of the ^{239}Pu has shown that the perturbative approach envisaged for GAMPLEX II is adequate, and more suitable than the method provided for GAMPLEX I. GAMPLEX was implemented after the termination of the contract through the Routines QUARTETT and PERLA (supported by University of Illinois funds). The work on GAMPLEX III led to the result that there exist intrinsic ambiguities in the R-matrix theory representation of fissile element cross sections, reported in Appendix B. Computer implementation of this approach appears at present as a complex task of interest only for fissile elements other than ^{239}Pu which exceeded the resources of this contract.

Task (2c) has been completed, and a version of Program CODILLI-2 is now operational as part of the SCORE package, as reported in Appendix F.

Task (3a) has been implemented in the new version of Program CODILLI, as reported in Appendix C. Program TRIPLE, discussed in Appendix E, has not been adapted for this purpose.

The investigation envisaged under Task (3b) led to a negative result, that is, no part of the original SCORE package could be adapted effectively to the University of Illinois 360/75 computer. After termination of this contract this work was continued and resulted in demonstrating the feasibility of an iterative-interactive system for data analysis, based on the use of Program CODILLI and on the combined use of the University of Illinois IBM 360/75 and PDP-8 computers. The first results of this work were presented at the ANS meeting in June 1972. (Informal Session on Reactor Physics).

A list of publications and reports, not including progress reports, supported in part by this contract, is attached.

List of Publications and Technical Reports supported in part
by Contract AT(11-1)-2022 and 2022-1.

- COO-2022-1. F. T. Adler and D. B. Adler. Threefold analysis of low energy neutron cross sections with the multilevel expansion. Trans. Am. Nuclear Soc. 12, 287-289 (1969).
- COO-2022-2. F. T. Adler and D. B. Adler. Use of the complex partial widths of the Kapur-Peierls formalism in cross section analysis and approximate derivation of R-matrix parameters. Trans. Am. Nuclear Soc. 12, 287 (1969).
- COO-2022-3. F. T. Adler and D. B. Adler. Derivation of R-matrix parameters from Kapur-Peierls type parameters. Bull. Am. P. S. 1969 (Boulder Meeting).
- COO-2022-4. D. B. Adler and F. T. Adler. Multilevel description of low energy neutron reactions in fissile elements. University of Illinois Technical Report # 185. (October 1969). Technical Report # 1.
- COO-2022-5. D. B. Adler. LEMA-CHAMA: A FORTRAN IV program to calculate neutron cross sections with either level matrix or channel matrix formalisms and with the complex pole expansion of the collision matrix. University of Illinois Technical Report # 184. (1969). Technical Report # 2.

List of Publications (continued)

- C00-2022-7 D. B. Adler and F. T. Adler. CODILLI II: A FORTRAN IV program for the analysis of neutron resonances with Program SCORE. Technical Report No. 3. University of Illinois Technical Report # 186.
- C00-2022-10 D. B. Adler and F. T. Adler. Multilevel analysis of U^{235} scattering data. Trans. Am. Nuclear Soc. 14, 804, 1971.
- C00-2022-11 D. B. Adler and F. T. Adler. Ambiguities in R-matrix parameters for interfering resonances with two fission channels. Trans. Am. Nuclear Soc. 14, 803, 1971.
- C00-2022-12 F. T. Adler and D. B. Adler. Correlated analysis of fissile element cross sections and interpretation in terms of R-matrix parameters. 2nd International Conference on Nuclear Data for Reactors, Proceedings Vol. II, 777-788 (1970), IAEA, Vienna.
- C00-2022-13 D. B. Adler, P. F. Rose, N. H. Marshall, F. T. Adler, Multilevel data analysis with the SCORE III A version of CODILLI 2, presented at ANS Reactor Physics Informal Session, Miami, October 1971.
- C00-2022-14 D. B. Adler. TRIPLE: A Fortran IV program for the threefold analysis of neutron cross section data with the multilevel formalism, December 19
- C00-2022-15 D. B. Adler and F. T. Adler. Uniqueness of R-matrix parameters in the analysis of low energy neutron cross section in fissile nuclei. . To appear in Physical Review C, August 1972.

- COO-2022-16. F. T. Adler. Operational experience with Program SCORE III: least squares data fitting of ^{239}Pu using Program CODILLJ with SCORE, October 1971.
- COO-2022-17. D. B. Adler and F. T. Adler. A multilevel analysis of ^{239}Pu cross sections in the 6-70 eV region, July 1972.

I. Introduction

The Wigner-Eisenbud¹⁾ dispersion theory of nuclear reactions is generally used as the basis for the analysis of low energy neutron cross sections of fissile elements in the resolved resonance region. In the determination of resonance energies, partial reaction width and fission widths amplitudes, two approaches were used originally: (1) the direct inversion of the energy-dependent Wigner level matrix suited for the treatment of a few levels and an arbitrary number of fission channels, applied to the investigation of neutron resonances in fissile elements first by Vogt^{2,3)} and then by other authors.^{4,5)} (2) A specialization of R-matrix theory developed by Reich and Moore,^{6,7,8)} based on the partitioning of the channel matrix and the elimination of the radiative capture channels, thus side-stepping the problem of inverting the level matrix. This method is particularly well suited to treat an unspecified number of levels for a small number of fission channels, where the channel matrix can be inverted more readily.

These two approaches are in practice complementary, and are in form equivalent as it is always possible to associate a level matrix to the partitioned channel matrix of the Reich-Moore formulation.

An alternative approach, the multilevel expansion,^{9,10)} has also proved useful in this context. This approach is based on the diagonalization of the truncated Wigner level matrix, leading to cross section expansions in terms of the complex poles of the Wigner level matrix, as reported in Appendix A.

Cross section expansions for one-body resonances using complex resonance energies were considered in the thirties by Breit,^{11,12)} and

by Kapur and Peierls,¹³⁾ and in a more general manner by Siegert.¹⁴⁾

The early literature has been reviewed and discussed by Breit.^{15,16)} The general formalism for such expansions has been introduced in terms of R-matrix theory by Wigner,¹⁷⁾ and Thomas.¹⁸⁾ For many nuclear reactions, the usefulness of the complex pole expansion is open to doubt because of the energy dependence of the complex eigenvalues and because of the complicated conditions these eigenvalues and the expansion coefficients have to satisfy in order to assure that the related R-matrix elements are real, as required by the basic theory.

This consideration led to criticism of the use of the multilevel expansion for the analysis of neutron resonances, and to questions regarding the physical meaning of the resonance parameters thus obtained.⁸⁾ For the specific problem of neutron resonance analysis of fissile elements in the resolved resonance range where $\Gamma_f \gg \Gamma_n$ the multilevel expansion can however be justified because the neutron widths Γ_n are slowly varying functions of the neutron momentum, so that complex eigenvalues and residues are energy independent to a very good approximation, as discussed briefly in Section II.

This circumstance justifies the use of the multilevel expansion in data analysis, where it has proved very useful. As shown in Appendix A, the line shape parameters enter the cross sections in a linear form, and the related least squares analysis is greatly simplified, as compared to the other R-matrix approaches which lead necessarily to a larger number^{6,7,19)} of parameters entering the cross section expansions in a non-linear manner.

In the multilevel expansion, only the parameters μ and γ related to resonance energy and half-width enter non-linearly; it is therefore an attractive tool for interactive data analysis, as discussed in Section III.

A general problem, shared by the multilevel expansion and the other methods of resonance analysis, pertains to the uniqueness of parametrization. This problem, as already noted by Breit,¹¹⁻¹³⁾ arises from the flexibility of nuclear cross section representations by dispersion formulac. Such representations are definitely non-unique if one starts from a given set of experimental data with their inherent uncertainties. In the case of the fissile isotopes it is moreover essential to perform a correlated analysis^{20,21)} of fission, capture, and total cross sections to achieve a meaningful result for the parameters so that they may be applied in practical reactor calculations, and for the purpose of general theoretical studies, such as those on the statistical distribution of levels and resonance energies.

The uniqueness of the representation of experimental data has been investigated from various angles: Michaudon²²⁾ has considered the effect of missed small levels in a resonance analysis; the possible occurrence of quasi-resonances²³⁻²⁶⁾ has been studied extensively by Lynn. It may be of interest to note that Moore⁸⁾ indicates that the multilevel expansion is a particularly useful tool to investigate such effects, which are more likely to occur in the fissile uranium isotopes than in Pu^{239} . In fact Lynn surmises²⁶⁾ that it may be a practical possibility to describe the Pu^{239} cross section in detail in terms of a full set of "individual resonance parameters,"

notwithstanding the possibility of occurrence of quasi-resonances. In the region below 50 eV no evidence for such quasi-resonances has been found, but it should be noted that Lynn suggests the region between 80 and 86 eV may contain an actual experimental example of a quasi-resonance.

A related, and perhaps more basic problem is to determine theoretically whether more than one set of R-matrix parameters can be found that describes the same set of fission, total, and capture cross sections. This problem is particularly relevant with reference to the problem of deriving R-matrix parameters from those obtained by data analysis performed with the multilevel expansion. As shown in Section III and Appendix B, one can obtain more than one set of R-matrix parameters to describe a given mathematically defined set of cross section data (that is of idealized cross sections corresponding to a single spin-parity state of the compound nucleus and having no inherent errors). The most important conclusion of this study has been that while fission widths amplitudes are subject to degeneracy, partial widths and resonance spacings, basic for statistical studies, are not affected as long as the levels are relatively well spaced.

Section II summarizes the derivation of the multilevel formalism from R-matrix theory; effects of the energy dependence of the parameters and of the distant resonances are presented in Appendix A, and summarized in Section II.

The ambiguities of the R-matrix representation for fissile element cross sections with two fission channels, and the evidence of the existence of such a degeneracy are presented in Appendix B, and summarized in Section III.

The computer programs developed during this work are considered in Section IV; the programs are collected in Appendices C to E. The interactive use of Program CODILLI-2²⁷⁾ with the SCORE III package is discussed in Appendix F.

Finally, results of the analysis of the correlated analysis of Pu²³⁹ cross sections using the multilevel expansion and the program developed under this contract are described in Appendix G.

II. Multilevel description of low energy neutron reactions in fissile elements

A cross section expansion for low energy neutron reactions is obtained by diagonalizing the truncated Wigner level matrix with inclusion of the effects of the distant resonances. The energy dependency of poles and residues is found to be negligible in this energy region. The cross section expansions thus obtained are given in terms of energy-independent poles and resonance parameters, while the remaining energy dependence is accounted for in explicitly formulated background functions which vary slowly with energy. At the same time the formal relation to the R-matrix theory is given explicitly, so that the parameters relevant to the expansion are related directly to the corresponding R-matrix parameters. This approach makes the unitarity of the multilevel expansion evident.

In analyzing cross section data it becomes necessary to consider only a finite energy interval containing a finite number of resonances. Within the R-matrix theory the level matrix is then truncated, and a certain energy dependence is introduced, which is reflected in the elements of the level matrix, as if the reduced widths were energy dependent.²⁸⁾ A background matrix²⁸⁾

is then introduced in the definition of the collision matrix to compensate for the effects of the infinitely many resonances which are not included in the finite level matrix, and are defined as distant from those included in the energy interval of interest. Thomas¹⁸⁾ and Vogt²⁸⁾ have shown that in the absence of interferences between "local" and distant levels this separation amounts to a redefinition of the potential scattering phase shifts and of the boundary value matrix $L^{(0)}$ of the Wigner-Eisenbud theory.

Starting from the same R-matrix formulation an approach which can be closely related to a "generalized Kapur-Feierls formalism," in which the energy dependence of the parameters is made explicit, is derived and presented in Appendix A.^{*}

^{*}As the underlying idea of the approach (i.e., choice of boundary condition for the external wave function) was first introduced by Kapur and Peierls¹³⁾ for the case of one body resonances, it has become customary, following the terminology of Lane and Thomas²⁹⁾ to refer to the multilevel expansion as to a "generalized Kapur-Feierls approach."

If the energy dependence of the poles and residues of the collision matrix is fully negligible, the multilevel expansion appears formally equivalent to the Humblet-Rosenfeld expansion,^{30,31,32)} the essential difference being that in the multilevel expansion poles and residues, as well as background contributions are expressed explicitly, although sometimes in a complicated manner in terms of the parameters of R-matrix theory.

In Appendix A it is shown that the energy dependence of the level matrix, arising from the distant resonances may be more relevant than the one arising from the $\sqrt{E}$ dependence of the penetration factor. It can be seen, in fact, that for s-waves neutron cross sections in fissile elements, the latter effect remains very small as long as $\Gamma_n \ll \Gamma_f$ and can be included by introducing background contributions having a smooth dependence on $\sqrt{E}$.

The energy dependence arising from the distant resonances becomes small (but not necessarily negligible) if the group of the resonances related to the energy interval of interest is appropriately chosen. The distant resonance effects are explicitly separated into two types of contributions given as slowly varying functions of E : (a) in the form of background terms (b) in the form of additional interference terms between local and distant levels which affect mostly the valleys between the cross section maxima. These effects may be relevant,²⁰⁾ even if the spacing of the resonances is relatively large, as for example for Pu^{239} , where strong fission channels interferences may occur between pairs of levels of which one (e.g., negative energy level) is external to the energy interval of interest. For a given energy interval, background terms of well defined energy dependence are added, to compensate for the distant resonances and momentum dependence.

The expansions derived here can be utilized advantageously with least squares fitting techniques,^{21, 33, 34)} as most of the parameters describing the resonance lines appear linearly in the cross section formulae, in contrast with the Reich-Moore and with the Vogt approaches. While there is no restriction for the number of resonances and (or) for the number of interfering fission

channels, constraints can be imposed, which reflect the unitarity of the R-matrix theory, and which are utilized particularly when analyzing simultaneously fission, capture, and total cross section data.

The numerical evaluation of multilevel parameters from known R-matrix parameters is obtainable from Program LEMA-CHAMA³⁵⁾ described in Appendix D. The reciprocal problem, of determining R-matrix parameters from known multilevel parameters, has been presented elsewhere.^{36,37,38)} Relevant computational approaches are discussed in Appendix F.

III. Ambiguities in R-matrix representation

Mathematically defined cross section sets (fission, total, and capture) and associated multilevel parameters, have been generated from prescribed R-matrix parameter sets, using the program LEMA-CHAMA (described in Appendix D.) These "idealized" data sets can be used to investigate the problem of uniqueness of R-matrix representations. The particular sets chosen were so chosen that a perturbation approach can be used to simplify the formalism, when deriving R-matrix parameters from the multilevel parameters, (well spaced resonances). Two interfering fission channels were chosen for this purpose, as lowest number for which ambiguities may occur.

In the case of three interfering resonances two different sets of fission channel widths amplitudes have been obtained, while for the case of four interfering resonances four different sets of widths amplitudes have been obtained. The methods used, together with the numerical results, are described in Appendix B.

The possibility has been noted, but not investigated in detail, that in the case of more closely spaced resonances other ambiguities may arise.

The observed ambiguities indicate that special care has to be taken in the derivation of R-matrix parameters from multilevel parameters obtained by the fitting of experimental data. These results have been reported in a preliminary form;^{39,40)} a detailed presentation of this work, as given in Appendix B, will appear in Physical Review C.

IV. Development of computer programs

(a) Outline of the work done

The computer programs developed under Contract AT(11-1)-2022-1 form an interrelated family of FORTRAN IV programs intended primarily for data analysis of resonance neutron cross sections in the resolved resonance energy region, with the multilevel expansion.

Two complementary tasks have been considered in the preparation of these programs:

1. Least squares analysis of resonance data, with implementation of interactive computer use, and simultaneous treatment of three data sets (such as total, fission, and capture cross sections) in the batch mode.

- 1a. Program CODILLI-2 (batch-mode version), and
SCORE III-A version.

- 1b. Program TRIPLE (simultaneous analysis of three data sets).

2. Extraction of R-matrix parameters from multilevel parameters.
 - 2a. For this task, the program LEMA-CHAMA generating multilevel parameters and cross section curves from R-matrix parameters was generalized from the existing program LEMA,⁴¹⁾ and used to obtain test cases.
 - 2b. Program COMPLEX has been subsequently implemented to derive R-matrix parameters from multilevel parameters for three and four interfering resonances.
 - 2c. Based on perturbation approximations, the routines PERLA and QUARTET, have also been developed, and used in the context of the problem of ambiguity of the R-matrix parameters.
3. Auxiliary routines were necessary to facilitate the preparation of the work on SCORE III-A:
 - 3a. Transformation of single level resonance parameters to multilevel parameters, in order to construct a library useful in SCORE III-A for treatment of impurities.
 - 3b. Perturbation approximation (ROUTINE MINI-BWSIG) to evaluate multilevel parameters from R-matrix parameters as to construct an initializing set of values for the SCORE III-A Library, by processing existing R-matrix compilations.

- 3c. SCATT - a routine calculating resonance scattering multilevel parameters from those of the total cross section.

These three routines have been transmitted to AI for preparatory work on SCORE III.

4. The first step in the collaboration with SCORE dealt with the preparation and adaptation of the routine SIGPLOT, designed to calculate and display cross section curves from given multilevel parameters, without least squares analysis of data.

(b) Summary of code descriptions.

CODILLI-2, reported in Appendix C, is a modification of the original program CODILLI,²⁷⁾ for use on SCORE III-A, and for independent batch-mode operation. It can include six different nuclear species, which may in particular be pairs of spin states of the same nuclide, and 20 interfering resonances. It can as well handle non-fissile elements, as the resonance lines by option can be treated as symmetrical. A special option permits using the program side-stepping the least squares analysis, performing the function of the original independent routine CURVEPLOT²⁷⁾ (later adjusted for SCORE as SIGPLOT).

The batch-mode version contains further options. One of the options provides for the analysis of scattering data.⁴²⁾ A second option provides for the possibility of subtracting the contribution of the impurities from the analyzed data, and to generate a data deck, free of impurities, useable on Program TRIPLE. A third option is the possibility of mixing contributions

of different nuclides and to generate fictitious "data with impurities" which can be used as test cases. The six "data" sets used in code checking of CODILLI-2 for SCORE and transmitted to AI for debugging purposes were constructed in this manner.

The batch-mode version contains also the plotting (CALCOMP) option of the fitted data and trial function.

TRIPLE, described in Appendix E, can treat simultaneously three data sets for the same nuclide, according to four different combinations:

- 1) total, fission, capture (2 modes, see below)
- 2) two independently measured fission sets and one total cross section data set
- 3) two fissions, one capture data sets.
- 4) two total cross sections, one fission cross section data sets.

The two modes for case 1 represent different treatment of the scattering, as difference between total and absorption cross sections.²¹⁾

The purpose is to obtain simultaneously multilevel parameters satisfying the unitarity conditions, and values of resonance energies and half widths compatible with the three data sets. The energy scales, often not matching, when determined by independent measurements, are made compatible by an internal evaluation of the relative calibration error. Resolution effects and Doppler effects are taken into account independently for each data set.

The program also evaluates first order perturbation estimates of the partial reaction widths, for the case 1.

Treatment of impurities is not possible, because of the large memory requirements, so that it is necessary to process the data, before the use of

TRIPLE, using for example the available options in CODILLI-2.

At present, two versions are available, one including 20 interfering resonances, the other (faster version) with a reduced number of 10 interfering resonances. The maximum number of data points is 2000 per data set. The fitted data and the trial function by option can be plotted (CALCOMP).

LEMA-CHAMA, described in Appendix D, includes two branches for the evaluation of cross section values: LEMA, using the level matrix inversion, and CHAMA, using the channel matrix inversion. Each branch produces the corresponding multilevel parameters obtained through diagonalization of the level matrix.

GAMPLEX derives R-matrix parameters from multilevel parameters, for two, three, and four interfering resonances. The mathematical approach has been presented elsewhere.³⁷⁾

PERLA contains as a special branch the second order perturbation calculation of multilevel parameters from R-matrix parameters. This branch of PERLA was utilized to provide AI with the routine MINI-BWSIG. A second branch of PERLA contains the calculation of a two channels, three levels case, giving the possible different fission vectors which reproduce the same multilevel parameters. This branch can be initialized either from R-matrix parameters, or from multilevel parameters.

QUARTET, similarly based on perturbation approximation, is a searching routine for the angles in channel space, which reproduce the same multilevel parameters for four resonances with two fission channels.

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APPENDIX C

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CODILLI II: A FORTRAN IV Program for the Analysis of
Neutron Resonances with Program SCORE^{*}

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TABLE OF CONTENTS

	Page
Abstract	25
I. Introduction	26
II. Trial Function	30
Multilevel expansion with Doppler broadening	30
III. The Trial Function with Resolution Effects	35
(1) Reaction Cross Sections	35
(2) Total Cross Section	37
IV. Trial Function with Constants	41
(1) Constraints obtainable from unitarity	41
(2) Constraints introduced by assuming symmetrical lines	42
V. Least Squares Fit and Estimate of the Quality of the Fit	43
VI. The Resolution Width for Time-Of-Flight Measurements	46
VII. Interface with SCORE: Routines PREAMB and EDIT	46
VIII. Comments	51
References	53

ABSTRACT

This FORTRAN IV version of Program CODILLI has been made compatible with Program SCORE so that it can be used in the interactive analysis of neutron resonance data with Program SCORE. The batch-mode version of CODILLI II can be used independently. CODILLI II utilizes the multilevel expansion in a form which is applicable to the analysis of neutron resonance data of fissile as well as of non-fissile nuclides. Options are included which permit to treat selected resonances as symmetrical, so that non-fissile nuclides can readily be analyzed. The program allows either to use a least-squares data fitting procedure, or to calculate cross section curves from prescribed resonance parameters. In either case, the cross section curve may include contributions of several (at present four) nuclides. Different spin states may also be treated as separate isotopes. Tests have been implemented which allow to display the quality of fit of individual lines or of the entire cross section curve.

Provisions are made to treat experimental resolution effects in a flexible manner, with particular attention to the use of the program in analyzing LINAC data.

The option of calculating with CODILLI II cross section curves from prescribed parameters is of particular relevance for the anticipated use with Program SCORE. The "conversational mode" of this program will allow for a rapid adjustment of parameters which enter the trial function in a non-linear form, and thus eliminate the need for non-linear fitting procedures which were contained in the older version of CODILLI.

I. INTRODUCTION

This FORTRAN IV version of Program CODILLI⁽¹⁾, for the multilevel analysis of low-energy neutron cross sections, is intended for two applications:

(I) To be utilized as a subprogram of Program SCORE.⁽²⁾

(II) To be used independently, as a least-squares fitting program, similarly to the original version.⁽¹⁾

The aim of making this new version of CODILLI useful as a subprogram of SCORE, has affected many choices in the modification of the original version:

(a) SCORE provides the possibility of interactively changing input parameters and of rapidly displaying the calculated cross section curve for comparison with the fitted data. This feature of SCORE becomes particularly attractive in relation to a least squares analysis, as the parameters occurring non-linearly in the trial function can be modified interactively, rather than evaluated through cumbersome iterative calculations.

This potential of SCORE is of special relevance for the use of Program CODILLI, where the multilevel trial function contains as nonlinear parameters only the values of the poles of the collision matrix (resonance energy μ and half width ν), in contrast with other approaches based on the R-matrix formalism.^{(3) (4)} The least squares branch of CODILLI therefore has been compacted to the linear fitting (providing the line shape parameters), with the assumption that the "conversational mode" between evaluator and SCORE will supply a rapidly convergent definition of

the nonlinear parameters. The goal, of obtaining a high degree of accuracy in the data fitting, is however a partial answer to the general problem, as only by simultaneous analysis of total, fission, and capture data, sets of parameters mutually compatible (and physically meaningful) are derivable. ⁽⁵⁾

(b) A multipurpose option, of by-passing the least-squares procedure of CODILLI, has been inserted. The cross section curve can be calculated directly from parameters which are either present in the library of SCORE, or have been modified interactively or calculated by previous use of the least-squares fit in CODILLI.

This branch is equivalent to the routine SIGPLOT, obtained in turn from the original graphic routine CURVEPLOT, ⁽¹⁾ and it can be used for different purposes:

(1) Prior to the fitting it might be desirable to test the quality of existing parameters, so as to gauge interactively the initial values of μ and ν , as well as to reduce the number of the unknown, by choosing to subtract from the trial function the contributions of well-fitted resonances.

(2) After the fitting, minor interactive input changes permit to switch to this branch and to evaluate and display the unbroadened cross section, for a test of its positiveness.

(3) This branch of CODILLI can also be used for trial-and-error fitting which can be particularly useful for the case of transmission data, and as such can provide rapid inspection of the fitted curve. For the batch-mode of

CODILLI it can also be used to produce "synthetic data."

This branch supercedes the existing SCORE subroutine ADLER⁽⁶⁾ which constitutes a more specialized version of SIGPLOT.

(c) To facilitate the use of the program CODILLI with SCORE, the existing subroutine TEST⁽⁷⁾, previously used in the transition from linear to nonlinear fits, has been compacted to calculate only the "goodness of fit" value around each resonance peak, and to test the positiveness of the unbroadened cross section curve, at each energy value. Failure to reproduce positive values is recognized by an error flag. The partial goodness of fit values are returned to SCORE for display, or output in printing in the batch-mode version.

For the batch-mode operation, a more comprehensive subroutine TEST is provided which is similar to the version published earlier,⁽⁷⁾ and contains additional features beyond those discussed above.

(d) The program CODILLI has been amplified to contain additional physical aspects, underlying the data analysis, which could not be included in the original IBM-7094 version:

(1) The trial function is generalized to include several isotopes. This permits the treatment of impurities within the data fitting, thus avoiding the cumbersome procedure of subtracting impurity effects from the data, prior to the fitting.

(2) The two spin states of a fissile nuclide can thus be introduced as if they were two distinct "isotopes." This separation offers the choice of using the condition

$$\sum_j R_j = 0, \quad (1)$$

valid for the group of interfering resonances of the same spin state,⁽⁸⁾ as a constraint

(3) A method has been implemented⁽⁵⁾ to treat, by option, individual levels as purely symmetrical. This procedure is useful for capture data, and necessary for non-fissile elements. In this manner the Program is generalized to the analysis of any type of cross section data in the resonance region.

(4) Effects of resonances far from the energy interval being fitted can be calculated by option using asymptotic expansions,⁽⁹⁾ to provide contributions for each individual isotope. These contributions, which depend intrinsically on the energy interval, do not preclude the possibility of fitting the background constants, as defined previously.^{(1)(*)}

(e) In preparation for a future compaction of the program to fit into a graphics package, two branches of the original CODILLI have been reduced:

(1) The treatment of the statistical errors has been limited to three options, inclusive of "equal weights," experimentally given errors, and calculated inverse weights.

(2) The analysis of experimental data requires in each case the availability of an appropriate calculation for the resolution function. In this regard, the original version of CODILLI was designed to accommodate in a flexible form the requirements for any possible case. In the

(*)

The type of constants introduced in either case correspond to the prescriptions of the ENDF/B Format Modification No. 10. (See reference 10).

present version provisions are made for Gaussian resolution functions and for a generalized WIDTH subroutine which should be particularly adapted for the analysis of LINAC data.

(f) The utilization of Program CODILLI within the Program SCORE will require a special routine PREAMB from which CODILLI will be called as a subroutine. The routine PREAMB casts the input information from SCORE into a form useable within CODILLI. An EDIT routine returns the results obtained in CODILLI through PREAMB in a form suitable for display on the interactive panels generated by SCORE, and thus to the SCORE library.

(g) Various computational changes have also been introduced. In view of the shorter word length of the IBM 360, as compared to the IBM 7094, for which the original program was written, the new version is entirely in double precision arithmetic. The matrix inversion is now performed using the Cholesky decomposition. (11)

The trial function and the constraints are described in Sections II, III, and IV of this report. Special aspects of the least-squares procedure are outlined in Section V. The special problem of the calculation of the resolution width is summarized in Section VI. Section VII outlines the content of the routines PREAMB and EDIT which serve the purpose of transferring information from SCORE to CODILLI and vice-versa.

The FORTRAN listing of CODILLI II will be presented in a separate report, together with a description of the subroutines and of the input used in the batch-mode version of CODILLI II. This report will also consider operating aspects and the results of numerical experiments with test problems.

II. TRIAL FUNCTION:

Multilevel Expansion with Doppler Broadening

The Doppler broadened cross section, in presence of a number NISO of distinct nuclides, is written in the form

$$\begin{aligned}
\frac{\sqrt{E} \sigma^{(DB)}(E)}{cc} = & \sum_{I=1}^{NISO} \left\{ \sum_{k=1}^{NR(I)} \left[GR_k^{(I)} \phi_k^{(I)}(E) + GI_k^{(I)} \phi_{NR(I)+k}^{(I)}(E) \right] \right. \\
& + \sum_{k=1}^{NOUT(I)} \left[DGR_k^{(I)} \Omega_k^{(I)}(E) + DGI_k^{(I)} \Omega_{NOUT(I)+k}^{(I)}(E) \right] \\
& + 2g^{(I)} \frac{(1 - \cos \omega^{(I)})}{\sqrt{E}} + b_1^{(I)} + b_2^{(I)}/E + b_3^{(I)}/E^2 + b_4^{(I)}/E^3 \\
& \left. + b_5^{(I)}E + b_6^{(I)}E^2 \right\} C(I) \\
& + \sum_{j=1}^{KNEG} A_j/E^{j-1} + \sum_{j=1}^{KPOS} P_j E^j
\end{aligned} \tag{2}$$

where:

$cc = 6.52 \cdot 10^5$ barns $\times$ eV is a conversion constant,

$\omega^{(I)} = 2\sqrt{E} WN(I)$ is the potential scattering phase-shift and

$WN(I)$ is the "hard sphere" nuclear radius in $eV^{-1/2}$

$(WN(I) = \sqrt{\frac{\pi}{cc}} a(I) \text{ where } a(I) \text{ is in } (\text{barns})^{1/2}).$

$NISO$ represents the number of isotopes present,

$NR(I)$ the number of fitted resonances, $NOUT(I)$ the number of known resonances for the I -th isotope, and $g^{(I)}$ is the corresponding statistical g -factor. The factor $C(I)$ is the relative concentration. Using the requirement of SCORE, that the separated spin states be treated as independent nuclides, one has

$$\sum_I g^{(I)} C(I) = 1. \quad (3)$$

This condition is controlled only by input.

The constants $b_j^{(I)}$ are calculated from known parameters, arising from resonances, the energy of which, μ_k , is either $\gg E$, or $\ll E^{(9)}$. Omitting the index I , one has, for each isotope

$$\begin{aligned} b_1 &= \sum_k (GI_k + GR_k v_k/\mu_k) (v_k/\mu_k) \\ b_2 &= - \sum_k GI_k v_k \\ b_3 &= \sum_k v_k \mu_k (GI_k + GR_k v_k/\mu_k) \\ b_4 &= \sum_k \mu_k^2 v_k (2 GR_k v_k/\mu_k - GI_k) \\ b_5 &= \sum_k (2GR_k v_k/\mu_k + GI_k) (v_k/\mu_k^2) \\ b_6 &= \sum_k (3GR_k v_k/\mu_k + GI_k) (v_k/\mu_k^3). \end{aligned} \quad (4)$$

The background constants A_i , B_i are instead to be fitted, and $KNEG \leq 4$, $KPOS \leq 2$.

As described previously⁽¹⁾ the vectors $\Phi_k(E)$ are given by: (omitting the index I):

$$\begin{aligned} \Phi_k &= \cos w \psi_k - \sin w \chi_k \\ \Phi_{NR+k} &= \cos w \chi_k + \sin w \psi_k \end{aligned} \quad (5)$$

where ψ_k and χ_k are the symmetrical and asymmetrical line shape functions used conventionally in the Doppler broadening,⁽¹⁾ with an average effective kinetic energy related to the experimental conditions. Finer effects requiring more complicated treatment of the temperature broadening can be implemented, if needed, by generalizing the subroutine SHAPE.⁽¹⁾

The vectors $\Omega_k(E)$ are similarly defined as in (5), in terms of the resonance energies of the resonances belonging to the group NOUT (I).

Because the NOUT(I) group does not necessarily contain only resonances external to the energy interval to be fitted, but also contain prefitted impurities, resonances assumed to belong to one of the two spin states, etc. the broadening effects are necessary.

The group NR(I), of the fitted resonances, may include resonances which are neighboring, labelled as NEIGH(I), besides those which are actually internal to the energy interval, labelled NOR(I):

$$NR(I) = NOR(I) + NEIGH(I). \quad (6)$$

The neighboring resonances, contributing only with the "tail" of the resonance line and necessary only when negative energy levels are postulated, can be included without broadening effects, thus

$$\begin{aligned} \Phi_k &= [v_k^2 \cos w - v_k(\mu_k - E) \sin w] / [(\mu_k - E)^2 + v_k^2] \\ \Phi_{NR+k} &= [v_k(\mu_k - E) \cos w + v_k^2 \sin w] / [(\mu_k - E)^2 + v_k^2] \end{aligned} \quad (7)$$

for $k = NOR(I) + 1, \dots, NR(I)$.

In actual fitting, initial values of the unknown parameters may be provided by input, so that the unknowns are calculated as differences. The expansion (2) can thus be written as sum of a known term, $y_o(E)$, and of a trial function, $y_t(E)$, so that

$$\frac{\sqrt{E} \sigma^{DB}(E)}{cc} = y_t(E) + y_o(E) \quad (8)$$

where

$$y_o(E) = \sum_{I=1}^{NISO} \left\{ \sum_{k=1}^{NR(I)} [GR_k^{(o)(J)} \phi_k(E) + GI_k^{(o)(I)} \phi_{NR+k}(E)] \right. \\ \left. + \sum_{k=1}^{NOUT(I)} [DGR_k^{(I)} \Omega_k(E) + DGI_k^{(I)} \Omega_{NR+k}(E)] \right. \\ \left. + 2g^{(I)} \frac{(1 - \cos u)}{\sqrt{E}} + b_1^{(I)} + \dots + b_6^{(I)} E^2 \right\} C(I) \quad (9)$$

$$y_t(E) = \sum_{I=1}^{NISO} \left\{ \sum_{k=1}^{NR(I)} [X_k^{(I)} \phi_k(E) + X_{NR+k}^{(I)} \phi_{NR+k}(E)] \right\} \\ + \sum_{j=1}^{KNEG} A_j E^{1-j} + \sum_{j=1}^{KPOS} B_j E^j \quad (10)$$

where the factor $C(I)$ is included in the unknowns

$X, A, B,$

and the broadening effects on the backgrounds are considered negligible.

III. THE TRIAL FUNCTION WITH RESOLUTION EFFECTS

The effects of the experimental resolution are introduced by convoluting the expression of the theoretically prescribed cross section with an appropriate resolution kernel. (12,13,14)

(1) Reaction Cross Sections

For a reaction cross section, $\sigma(x)$, the resolution effects are calculated for the reaction rate⁽¹⁾ to give

$$\frac{\sqrt{E} \sigma^{(x)}(E)}{cc} = \int R(E, E') \sqrt{E'} \frac{1}{cc} \sigma^{(DB)}(E') dE' \quad (11)$$

where $R(E, E')$ is the resolution function, and $\sqrt{E} \sigma^{(D.B.)}/cc$ represents the Doppler broadened cross section given in the previous section. Using the notations of eq.(8), one can write

$$\frac{\sqrt{E} \sigma^{(x)}(E)}{cc} = Y_O(E) + Y_T(E) \quad (12)$$

where the known term is:

$$Y_O(E) = \int R(E, E') Y_O(E') dE' \quad (13)$$

and the trial function accordingly is given by:.

$$\begin{aligned} Y_T(E) &= \int R(E, E') Y_T(E') dE' \\ &= \sum_{l=1}^{NISO} \sum_{k=1}^{NR(l)} \left[X_k^{(l)} \phi_k(E) + X_{NR(l)}^{(l)} + k \phi_{NR(l)} + k(E) \right] \\ &\quad + \sum_{j=1}^{KNEG} A_j E^{1-j} + \sum_{j=1}^{KPOS} B_j E^j. \end{aligned} \quad (14)$$

The functions y_o , y_e are those of equations (9) and (10), and the vector $\bar{\Phi}$ is defined by

$$\bar{\Phi}_k(E) = \int R(E, E') \Phi_k(E') dE' \quad (15)$$

while the broadening effects on background terms and NEIGH type resonances are considered negligible.

For each different type of measurement, the resolution kernel $R(E, E')$ may be prescribed as a given function of $(E-E')$, with an associated energy dependent width^(13,14,15) or purely represented by a point-wise curve.⁽¹⁶⁾

In the actual numerical treatment, four subcases can be distinguished:

(1-a) For a gaussian type of resolution function, when the data are analyzed for energy intervals which are small, compared with the changes with energy of the resolution width, the latter can be approximated by a constant, and included into the effective temperature.

(1-b) For a more general treatment of a gaussian resolution function, the energy dependent resolution width can be combined, at each energy point, with the Doppler width.

In either case, the vector $\bar{\Phi}$ of eq. (15) and the function Y_o of eq. (13) can be calculated as in equations (5) and (9), combining in the line shape functions ψ and χ the Doppler and resolution effects.

(1-c) For a non-gaussian resolution function which is prescribed analytically, the broadening effects are calculated by a straight-forward numerical integration, as in eq. (13) and (15).

(1-d) The case in which the resolution kernel is not defined analytically requires another type of numerical treatment, to be introduced in the program case by case.

The first three subcases are taken into account in the programs CODILLI,⁽¹⁾ CURVEPLOT⁽¹⁾ and SIGPLOT, in the same subroutine (SCRAMB) and distinguished by the value of an index, JS (respectively JS = 1, 4, 2).

In the original versions of these programs, the calculation of the resolution width was introduced case-by-case, by implementing the program with an ad hoc subroutine WIDTH. The larger memory availability of the IBM-360 allows to include a more general subroutine WIDTH, encompassing a number of known gaussian resolution widths, selected internally case-by-case.

The case (1-d), which has been encountered for the analysis of the Petrel data⁽¹⁶⁾ is implemented in the current versions of CODILLI, CURVEPLOT, SIGPLOT, and TRIPLE, but has been eliminated from the SCORE version, in order to compact the program.

In these cases, which apply to fission and capture cross sections, the unknowns appear linearly in the trial function. As discussed below, the same type of calculation may be used for the analysis of total cross section data obtained from thin sample transmission measurements, or to obtain a zero-order set of parameter values for a subsequent fit of a transmission curve. To a certain approximation, scattering data can also be fitted in this manner.

2. Total Cross Section

For the total cross section, the resolution function is convoluted with the theoretically calculated transmission curve^(12,13,15) to give

$$e^{-n\sigma^{(t)}(E)} = \int R(E,E') e^{-n\sigma^{(D.B.)}(E')} dE' \quad (16)$$

where n represents the sample thickness in atom/barn, $\sigma^{(D.B.)}$ the Doppler

broadened total cross section, as defined in eq.(8), and $\sigma^{(t)}(E)$ the trial function for the measured total cross section data.

(The unknowns, in this case, occur nonlinearly in the trial function.

Three approaches are possible, depending on the availability of prefitted parameters.

(2-a) If prefitted total parameters are given, or a set of fission and capture parameters, the curve can be fitted by trial-and-error, using the option (b) of section I. SCORE allows in this case interactive changes in the parameters, which may well converge to an improved description of the data.

(2-b) For thin sample measurements, equation (16) can be approximated to the form^(*)

$$\sigma^{(t)}(E) \approx \int R(E,E') \sigma^{(D.B.)}(E') dE' \quad (17)$$

and the calculation falls in the cases described under (1).

If no initial parameter values are available, the approximation (17) is often useful in providing initial parameter values, even for large values of n , and usually more effective than using, for instance, fission parameters as zero order values.

(2-c) When a set of prefitted total parameters is available, the relation given in eq.(16) can be approximated to the form:

(*) By definition $\int R(E,E') dE' = 1$.

$$e^{-n\sigma^{(t)}(E)} \approx \int R(E, E') e^{-n\sigma^{(o)}(E')} [1 - n\delta\sigma(E')] dE' \quad (18)$$

where

$$\sigma^{(o)}(E) = \frac{cc}{\sqrt{E}} y_o(E) \quad (19)$$

$$\delta\sigma(E) = \frac{cc}{\sqrt{E}} y_t(E) \quad (20)$$

and y_o and y_t are given by eq. (9) and (10).

Defining:

$$Y_o(E) = \int R(E, E') e^{-n\sigma^{(o)}(E')} dE' \quad (21)$$

$$Y_T(E) = \int R(E, E') e^{-n\sigma^{(o)}(E')} n\delta\sigma(E')$$

$$\begin{aligned} &= \sum_{I=1}^{NISO} \sum_{k=1}^{NR(I)} [X_k^{(I)} \bar{\Phi}_k(E) + X_{NR(I)+k}^{(I)} \bar{\Phi}_{NR(I)+k}(E)] \\ &+ \sum_{j=1}^{KNEG} \bar{A}_j \bar{\Phi}_j^{(-)} + \sum_{j=1}^{KPOS} \bar{B}_j \bar{\Phi}_j^{(+)} \end{aligned} \quad (22)$$

the trial function acquires the form

$$e^{-n\sigma^{(t)}(E)} = Y_o(E) + Y_T(E) \quad (23)$$

where the unknowns appear now linearly in Y_T . In particular one has:

$$\bar{\Phi}_k(E) = \int R(E, E') e^{-n\sigma^{(o)}(E')} \Phi_k(E') \frac{1}{\sqrt{E'}} dE' \quad (24)$$

$$\bar{\Phi}_j^{(-)}(E) = \int R(E, E') e^{-n\sigma^{(o)}(E')} \frac{dE'}{\sqrt{E'}(E')^{j-1}} \quad (25)$$

$$\bar{\Phi}_j^{(+)}(E) = \int R(E, E') e^{-n\sigma^{(o)}(E')} \frac{dE'(E')^j}{\sqrt{E'}} \quad (26)$$

and:

$$\left. \begin{aligned} X_k^{(I)} &= -n \text{ cc } \delta GR_k^{(I)} C(I) \\ X_{NR(I)+k}^{(I)} &= -n \text{ cc } \delta GL_k^{(I)} C(I) \end{aligned} \right\} \quad (27)$$

$$\bar{A}_j = -n \text{ cc } A_j C(I) \quad , \quad \bar{B}_j = -n \text{ cc } B_j C(I) \quad (28)$$

where the vector Φ_k is defined in equations (5) and (7), and $C(I)$ is the relative concentration of the I -th isotope or impurity.

This type of calculation is treated in CODILLI with the option JS = 3, by straightforward numerical integration, for all cases of resolution kernels which are defined as analytical functions of $(E-E')$, through the subroutines SCRAMB and WIDTH. ⁽¹⁾

IV. TRIAL FUNCTION WITH CONSTRAINTS

This version of CODILLI provides for options (through the index IFIT (I)) which introduce two different types of constraints for the asymmetrical parameters. Each case has the consequence of reducing the number of the free parameters in the fitting.

(1) Constraints obtainable from unitarity

For the totality of interfering resonances of the same spin states asymmetrical line-shape parameters, (for any cross section type)

$$H_k = G I_k v_k \quad (29)$$

satisfy the condition^(8,17) (which follows from the unitarity of the formalism)

$$\sum_k H_k = 0. \quad (30)$$

Each parameter H_k contains in turn the superposition of effects of all other resonances of the same group, with "resonance-denominators" of the form

$$\frac{1}{(\mu'_k - \mu_k)^2 + (v'_k + v_k)^2} \quad (31)$$

which become large when the resonance pair, k, k' is widely separated.

If therefore, the data analysis is initiated utilizing a large set of NOUY resonances, the condition (30) may be assumed to be well approximated, provided the resonance energies μ_k and half-widths v_k are defined to a good degree of confidence.

In this case, one of the asymmetrical parameters, e.g., $GI_{NR(I)}^{(I)}$ can be eliminated from the unknowns, and calculated after the fitting as

$$GI_{NR(I)}^{(I)} = - \frac{1}{v_{NR(I)}} \left\{ \sum_{k=1}^{NR(I)-1} GI_k^{(I)} v_k + \sum_{k=1}^{NOUT(I)} DGI_k^{(I)} v_k \right\} \quad (32)$$

The error of $GI_{NR(I)}^{(I)}$ is calculated accordingly as the combined error of the other fitted parameters. This option is taken setting $IFIT(I) = 1$. The constraint is ignored for $IFIT(I) = 0$.

2. Constraints introduced by assuming symmetrical lines

Capture cross section resonances⁽⁴⁾ frequently appear less strongly affected by the interference effects than total or fission do, and thus, may be represented by symmetrical line shape functions.⁽⁵⁾ Impurities from non-fissile nuclides also require only symmetrical lines.

This version of CODILLI contains the option of treating each individual resonance with or without asymmetry, by selecting the value of an index,

$$MS(K, I)$$

to be 1 or 0 respectively, where K is the resonance index and I the nuclide index. The number of unknowns is thus reduced for each "symmetrical" case.

In this manner the program CODILLI can readily be utilized to analyse cross sections of non-fissile elements. The parameters obtained in this case are directly interpretable in terms of R-matrix partial widths; as

$$v_k = (\Gamma_{kn} + \Gamma_{ky})/2 \quad (33)$$

$$GR_k^{(x)} = \Gamma_{kn}^0 \Gamma_{kx} / 2v_k^2 \quad (34)$$

where (x) represents capture or scattering.

For capture cross section lines of fissile elements, treated symmetrically, the relation (34) is however not rigorously verified, as in this case the condition

$$GI_k^{(\gamma)} = 0 \quad (35)$$

represents only an approximation. (4) (17)

The combination of the choices, that all levels are symmetrical and the constraint given by (30) be imposed is obviously inconsistent, and is recognized in CODILLI by an error flag. In this case the calculation proceeds, ignoring the constraint (30).

V. LEAST SQUARES FIT AND ESTIMATE OF THE QUALITY OF THE FIT

The linear least squares calculation included in this version of CODILLI does not differ from the original⁽¹⁾, except for the matrix inversion method.

The normal equations are:⁽¹⁾

$$\sum_k Q_{jk} X_k = R_j \quad (36)$$

where

$$R_j = \sum_{i=1}^{NP} w_i \left(Y_{\text{exp}}(i) - Y_o(i) \right) \bar{\Phi}_j(i) \quad (37)$$

$$Q_{jk} = \sum_{i=1}^{NP} w_i \bar{\Phi}_j(i) \bar{\Phi}_k(i) \quad (38)$$

where NP is the total number of data points, and w_i are the statistical weights.

The matrix of the normal equations is symmetrical, and can be inverted by methods requiring only storage of the $N(N+1)/2$ different elements of Q , rather than N^2 elements.

The method selected is the Cholesky⁽¹¹⁾ method of decomposition of a symmetrical, positive definite matrix. With respect to the original inversion algorithm of Gauss-Seidel, the Cholesky method implies a saving of $N(N-1)/2$ storage locations, thus favoring the final aim of containing the program in a graphics package.

Another aspect of this method has been utilized: the inversion is achieved only if the matrix to be inverted is (positive definite and) well-posed. Although Q satisfies the condition:

$$\begin{aligned} \sum_{j,k} Q_{jk} X_j X_k &\equiv \sum_{i=1}^{NP} w_i \sum_j X_j \bar{\Phi}_j(i) \sum_k X_k \bar{\Phi}_k(i) \\ &= \sum_{i=1}^{NP} w_i \left[\sum_j X_j \bar{\Phi}_j(i) \right]^2 > 0, \end{aligned} \quad (39)$$

the instance can occur (of poorly defined values of μ_j and ν_j) in which by round-off errors Q becomes nonpositive-definite. The subroutine employed in CODILLI returns in this case an error flag, indicating that the trial function is ill defined, and the calculation terminates, or reverts to the SCORE display panels.

After the unknowns have been determined, the goodness of fit around each resonance peak is being calculated, as

$$\chi_k^2 = \sum_i w_i \left(Y_{\text{exp}}(i) - Y_T(i) - Y_O(i) \right)^2 / N_k \quad (40)$$

for the number N_k of data points in the interval $\mu_k - 5\nu_k$, $\mu_k + 5\nu_k$. The quantity χ_k^2 is returned to SCORE for display, and printed as output in the batch-mode version of CODILLI.

This calculation, which is a part of the subroutine TEST^(*) will provide a quantitative guide in evaluating visually the adequacy of the results for each individual fitted resonance. At this point the evaluator should be able to either "reguess" the values of μ_k and ν_k as input to a new fit, or to judge that the level, as well fitted, can be shifted to the array NOUT. The latter part of this process is incorporated in the batch-mode version of TEST, by testing the values of χ_k^2 for a wanted accuracy.

Finally, a test on the positiveness of the theoretical (unbroadened) cross section is given, displaying an error flag when values occur which are less or equal zero. The failure to reproduce positive cross section values, which in principle represents a violation of unitarity, can occur either from input errors, or from the wrong selection of values of μ and ν , as well as from wrong assignments to the constraint indices. (e.g., imposing the condition of being symmetrical to a pair of closely spaced resonances selected to belong to the same spin state). For the batch-mode version of CODILLI, this part of TEST is preliminary to an optional nonlinear fit.

*Adapted from the existing subroutine TEST(J)⁽⁷⁾ where N_k is however defined in the interval $\mu_k - 3\nu_k$ to $\mu_k + 3\nu_k$.

VI. THE RESOLUTION WIDTH FOR TIME-OF-FLIGHT MEASUREMENTS

At each energy value, the gaussian (total) width at $1/e$ of the height of the gaussian resolution function, is calculated from the relation⁽¹⁴⁾

$$HR(E) = \frac{1}{\mu L} \sqrt{B_1^{(N)} E^2 + (B_2^{(N)} + B_3^{(N)}) E^3} \quad (\text{in eV}) \quad (41)$$

where L is the flight-path in meters, the constant $\mu = 72.3 \text{ eV}^{1/2} \mu \text{ sec/meter}$, $B_1^{(N)}$ is a constant related to the slowing down of the moderator [here in $(\mu \text{ sec})^2 \text{ eV}$] and $B_2^{(N)}$, $B_3^{(N)}$ are parameters related to burst and (variable) channel width [here in $(\mu \text{ sec})^2$.] The upper index N refers to the cross section type.

In the present version of CODILLI values of HR are provided for the following representative cases: for U^{235} , capture and fission of the RPI-ORNL measurements,⁽¹⁴⁾ total of the Saclay⁽¹³⁾ measurement; for Pu^{239} , capture and fission of the RPI-ORNL measurements,⁽¹⁸⁾ total of the Saclay data.⁽¹⁹⁾

A more general WIDTH subroutine will be implemented, for use with SCORE, to obtain the gaussian resolution width HR from any time-of-flight measurement, by interactive input of the experimental parameters,⁽¹⁴⁾ such as moderator thickness, sample thickness, neutron burst and channel width, etc.

The subroutine reported here, and included at present in CODILLI, was used in the same form in test problems with program TRIPLE.⁽⁵⁾

VII. INTERFACE WITH SCORE: ROUTINES PREAMB AND EDIT

In its use with SCORE, program CODILLI will have the function of a sub-program, called from the routine PREAMB, which translates the input information acquired interactively in SCORE, into the format used in CODILLI.

The input information can be classified in two types:

(1) information selectively retrieved from the SCORE library (e.g., experimental data points, existing values of the poles of the collision matrix and line shape parameters).

(2) information input interactively through the SCORE panels which control the course of the calculation (e.g., experimental sample temperature, indices selecting resolution and Doppler broadening, options related to the constraints, etc.)

The information, either retrieved or selected interactively, will appear in a sequence of SCORE display panels which in their general structure have been described previously.⁽²⁰⁾ It is assumed* that the relevant indices and parameters determining the flow of the calculation will appear in the following order:

(1) choice of nuclides, of cross section type, of data, and of the energy interval to be fitted;

(2) index IDOP^(**): for IDOP = 1 experimental sample temperature
DOPPAR(1) = 0
IDOP = 2 experimental sample temperature
DOPPAR(2) ≠ 0 in °K

(3) index IRES^(**): for IRES = 1 resolution width RESPAR(1) = 0
IRES = 2 constant resolution width RESPAR(1) ≠ 0 in
IRES = 3 calculated gaussian width;

(4) values of the atomic mass number, ATWT(I) of each selected nuclide present in the data in addition to the nuclide being analyzed.

* The proposed panels are outlined in Memorandum #3, "Phase 2 of adaptation of CODILLI to Program SCORE," December 9, 1970 by F. T. Adler, which summarizes the relevant conversations with C. L. Dunford of A.I. The definitions of the arrays ISEL and A are those currently used for SCORE.

** This index is not used in CODILLI although included in the COMMON BLOCK.

(5) selection of arrays A, and CONS, containing at the start of the calculation for each isotope the assumed values of μ , ν , and of the line shape parameters of each cross section type, and of the background constants (for each isotope and cross section type).

(6) selection of the weighting option:

JWE = 1 equal weight

JWE = 2 weight calculated from experimental statistical errors

JWE = 3 weight calculated as $1/y_{exp}$,

where JWE is the index controlling the subroutine WEIGHT.

(7) selection of the index JS controlling the mode of folding the resolution function. For JS = 2,3, the choice of NI = number of integration steps in the Simpson integration, should be selected. NI by default is set = 32.

(8) choice of KNEG and KPOS, for background constants.

(9) choice of the constraint index IFIT (I).

(10) For each resonance of the array A, a logical index, ISEL (3,K) is selected to establish the role of the K-th resonance in the calculation.

The array A (250,8) transmits from the SCORE library through a COMMON BLOCK the values of μ , ν , and of the line shape parameters in the following sequence:

A(250,1) resonance energies μ

A(250,2) resonance half widths ν

A(250, 2ITP + 1) GR^(ITP)

A(250, 2ITP + 2) GI^(ITP)

where

ITP = 1 represents total cross section

ITP = 2 represents fission cross section

ITP = 3 represents capture cross section

and where 250 is the maximum total number of the resonance involved in the calculation (for all isotopes selected). Similarly the array CONS (6, 3, 10) contains precalculated background constants, 6 for each cross section type and nuclide, in the ENDF/B format.

An array, NORR(11) is also supplied interactively, to be used as a pointer in retrieving from the array A the parameters related to each isotope. By definition

NORR(1) = 1, and, using now the CODILLI notations,

NORR (I + 1) = NORR(I) + NR(I) + NOUT(I).

The logical array ISEL (3, 250) (three indices for each resonance), establishes the role of the k-th resonance with the following convention:

	TRUE	FALSE
ISEL(1,K)	included	discarded
ISEL(2,K)	fitted	used as background
ISEL(3,K)	fitted with asymmetry	fitted symmetrically

Through the arrays NORR and ISEL, the routine PREAMB rearranges the parameters provided by the array A into the arrays required by CODILLI. In particular, for ISEL (1, K) = T(True) the K-th resonance is tested to determine whether ISEL (2,K) is T or F. In the first case the K-th resonance

belongs to the NR(I) array, in the second to the NOUT(I) array. At the same time, the pair of parameters, contained in A(K, 2ITP + 1), A(K, 2ITP + 2) are stored either in GR(K,I) and GI(K,I), or in DGR (K,J) and DGI(K,I). For those of the NR(I) array, ISEL (3,K) = T merges into MS(K,I) = 1 and ISEL (3,K) = F into MS(K,I) = 0.

Discarded resonances (ISEL (1,K) = F) can be used, if the index IBK (I) > 0, to construct asymptotic expansions of 6 background constants for each isotope.

COBILLI is finally called as a subroutine from PREAMB.

After completion of a linear fit, the calculated line shape parameters and background constants are returned into the appropriate SCORE arrays A, and CONS through the routine EDIT, to be displayed by SCORE panels.

VIII. COMMENTS

The current CODILLI II version will be further compacted for the final goal of including it into a self-contained graphics package.

The specifications of the current version are outlined below:

The maximum number of data points available from SCORE being 500, the upper limit to the number of resonances to be fitted (NR), for each nuclide, has been tentatively set equal to 20. At present, the program can accommodate four different nuclides, and 20 NOUT resonances per nuclide. These figures can be modified readily, to include if needed a larger number of nuclides, while the maximum number of resonances per nuclide can be finalized only after sufficient experience is gained with the use of CODILLI II on SCORE.

In order to obtain, for a given measurement, a final set of parameters, ranging over large energy intervals, thus requiring the simultaneous treatment of numbers of data points larger than SCORE's limit (500), it might be necessary to complement the calculation on SCORE with batch-mode calculations utilizing a larger part of the computer memory than that conventionally assigned to graphics packages.

With the multilevel formalism, the statistical g factor is incorporated in the line shape parameters GR, GI, for total, fission and capture, so that the spin state separation is not necessary in order to fit the data. In this manner, the present program can be used to accommodate three nuclides in addition to the principal nuclide being analyzed.

The role of the spin assignment can however be investigated, by separating the assumed spin states and treating them as if they belonged to different nuclides.

The branch for the scattering cross section has not been made operational for the SCORE version. This branch, requiring the correct spin state separation, and the treatment of non-linearities in the line shape parameters is being implemented in the batch-mode version of CODILLI II, and will be reported separately.

In Part 2 of this report, the listing of CODILLI II will be presented, together with a description of the subroutines, of the input for the batch mode version, and illustrative numerical examples.

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LEMA-CHAMA: A FORTRAN IV Program to Calculate Neutron Cross
Sections with Either Level Matrix or Channel Matrix Formalisms
and with the Complex Pole Expansion of the Collision Matrix.*

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TABLE OF CONTENTS

	Page
Abstract	55
1. Introduction	56
2. Remarks on the level matrix formalism	58
3. Remarks on the Reich-Moore formalism	62
4. Methods of calculation	65
5. Eigenvalues and eigenvectors of the level matrix	66
6. Cross section calculations	73
References	75
Appendix A-Input and Output	77
Appendix B-Program LEMA-CHAMA	81

ABSTRACT

The program LEMA-CHAMA calculates low energy neutron cross sections in fissile elements with two optional branches.

1) LEMA: starting from the Wigner level matrix; 2) CHAMA: starting from the Reich Moore channel matrix and in either case with the alternate Kapur-Peierls multilevel expansion, based on the complex poles of the collision matrix.

The parameters for the multilevel expansion are generated through the eigenvalues and eigenvectors of the Wigner level matrix. Other quantities of physical interest in either statistical investigations, or in the study of the reverse problem (extraction of R-matrix parameters from given multilevel parameters) are provided by the code.

This FORTRAN IV program is a generalization of the program LEMA previously reported.

Introduction

The purpose of this work is to unify the methods of calculation for low energy neutron cross sections in fissile elements, using either of the existing R-matrix approaches^{(1),(2),(3)} and their relations to the "generalized Kapur Peierls" expansion.⁽⁴⁾

The computer program reported here (LEMA-CHAMA) is a straightforward generalization of a previous program (LEMA)⁽⁵⁾ prepared to convert the level matrix parameters of Vogt's approach⁽³⁾ into multilevel parameters of the Kapur-Peierls type. This newer version contains as an alternative the inclusion of the Reich-Moore⁽²⁾ approach and the pertinent cross section calculation using the partitioned channel matrix inversion.

The algorithm is based on the derivation of eigenvalues and eigenvectors of the level matrix, as in program LEMA⁽⁵⁾. This is possible, as it is readily seen that one can always associate a level matrix to the partitioned channel matrix of the Reich-Moore formalism.⁽⁶⁾

This algorithm is necessary when, along with the multilevel parameters describing the cross section shape, information is needed on other quantities of physical interest, such as the complex partial width of the theory.⁽¹⁾⁽⁴⁾ More important, the parameter conversion in terms of the complex orthogonal matrix of the level matrix eigenvectors⁽⁵⁾ ensures step-by-step validity of the unitarity of the formalism. As a by-product, sum rules derived from unitarity can be obtained for the multilevel parameters and for the complex partial widths, providing relations among R-matrix and Kapur-Peierls parameters, which become useful for statistical investigations.

Finally, the role of the distant resonances, relevant in statistical studies, is best introduced into the formalism through a level matrix approach.⁽¹⁾ Although this version of LEMA-CHAMA does not include the treatment of the background matrix,⁽¹⁾ it contains the preparatory algorithm for a generalization in this direction.

Recently a program for generating statistical distributions of the Kapur-Peierls parameters starting from R-matrix parameters distributions, and employing a similar treatment of the level matrix eigenvalues, has been reported by Moldauer and Hwang.⁽⁷⁾

The program LEMA-CHAMA presented here differs in the possibility of deriving Kapur-Peierls parameters from either Reich-Moore⁽²⁾ or Level matrix⁽³⁾ approaches.

As it is well known the cross section calculation with the Reich-Moore formalism offers many practical advantages with respect to the one based on the level matrix inversion, as in presence of many levels the matrix inversion technique is time consuming. This remark does not apply, however, to the process of diagonalization, for which the use of efficient eigenvalue-search subroutines is made once and for all through the program, allowing the inclusion of large numbers of resonances.⁽⁵⁾⁽⁷⁾

Because of the completeness of the information obtainable with the level matrix diagonalization, this algorithm appears preferable (and only moderately longer in computer time) to the one recently proposed by de Saussure,⁽⁸⁾ which, by side-stepping the role of the level matrix, provides in part only the information required for a statistical investigation.

The FORTRAN IV program LEMA-CHAMA provides for 33 interfering resonances for each spin state, and for additional 33 single level resonances for the same spin state. These numbers may be increased, as the program does not occupy the entire

fast memory of the IBM-360-75 of the University of Illinois. An example of running time: 4 minutes for 50 resonances, with 500 energy points, where, at each energy value, the cross section curves are evaluated in double precision arithmetic by both Reich-Moore and multilevel expansions.

In Appendix A are described the input and output operations.

In Appendix B is given the listing of the program and of the associated subroutines.

2. Remarks on the level matrix formalism

For a given spin-parity state the inverse level matrix is defined by⁽¹⁾

$$A_{\lambda\lambda'}^{-1} = (E_{\lambda} - E) \delta_{\lambda\lambda'} - \xi_{\lambda\lambda'}, \quad (1)$$

where

$$\xi_{\lambda\lambda'} = -\Delta_{\lambda\lambda'} + i\Gamma_{\lambda\lambda'} = (L' \gamma_{\lambda} \cdot \gamma_{\lambda'}) \quad (2)$$

and where λ, λ' range over the finite level set relevant to the energy region ΔE . The shift matrix Δ and the width matrix Γ include, through

$$L' = L(1 - R^0 L)^{-1}, \quad (3)$$

the effects of the distant resonances (R^0), and the channel boundary condition (L). The matrix L is defined by

$$L_c = S_c + iP_c - B_c \quad (4)$$

where S_c is the shift function, P_c the channel penetrability and B_c the channel boundary value.⁽⁹⁾ For s-wave neutrons $S_c = 0$ and B_c can be assumed to be zero. For the particular case of the fissile elements the neutron widths are usually smaller than the reaction widths, so that the momentum dependence of the neutron penetration factor can be ignored.⁽³⁾⁽⁵⁾ Thus the elements of the inverse level matrix, defined in (1), contain the explicit energy dependence of the diagonal part and the implicit energy dependence of R^0 .

Correspondingly the collision matrix is given by:

$$U_{cc'} = e^{i\Omega_c + i\Omega_{c'}} \left[\left((1 - R^0 L)^{-1} R^0 \right)_{cc'} + \sum_{\lambda\lambda'} A_{\lambda\lambda'} \alpha_{\lambda c} \alpha_{\lambda' c'} \right] \quad (5)$$

where

$$\alpha_{\lambda c} = \sum_{c'} (1 - R^0 L)^{-1}_{cc'} \gamma_{\lambda c'} \quad (6)$$

where $\gamma_{\lambda c}$ is the reduced width amplitude for the c channel.⁽¹⁾

If the background matrix

$$(1 - R^0 L)^{-1} R^0 \quad (7)$$

can be taken as diagonal⁽¹⁾⁽⁹⁾ its effects can be included in the potential scattering phase shift, thus regarded as slowly varying with the energy. This assumption however depends on the choice of the distant resonances. For the specific case of the fissile elements R^0 may include not only resonance energies E_λ lying outside the energy interval ΔE , but also levels which are unresolved within ΔE , such as "hidden levels",⁽¹⁰⁾ or undetected "quasi-resonances".⁽¹¹⁾ In these cases the energy dependence of R^0 and $\alpha_{\lambda c}$ cannot be ignored, as it produces partial width amplitudes having resonance shape,⁽⁶⁾

which in turn affects the shift matrix and in the width matrix. Even when levels lying within ΔE are excluded from R^0 , fission channel interferences may still occur between local and distant levels, so that R^0 cannot always be taken as diagonal.

This circumstance arises in any type of numerical application of the level matrix formalism, where it is unavoidable to deal with a finite number of resonances. As a consequence the parameters thus derived remain related to the specific energy region ΔE ^{(9),(6)}. Unless independent physical reasons permit to isolate group of interfering levels in a finite number, so that $R^0 = 0$, the truncated level matrix contains in principle the energy dependence of R^0 . It is possible, however, to specify R^0 in a manner that the closest resonances to ΔE are included in A^{-1} .

In this case, for the resonances not included in A^{-1} , and for which

$$|E_\lambda - E| \gg 1$$

one can approximate

$$(1 - R^0 L)^{-1} \approx 1 + R^0 L \quad (8)$$

and

$$a_{\lambda c} \approx v_{\lambda c} + i \sum_{\lambda'}^{(o)} \frac{v_{\lambda' c} \Gamma_{\lambda \lambda'}}{E_{\lambda'} - E} \quad (6')$$

where (o) refers to the level set of R^0 . It can be shown that in this manner the shift matrix contributes only to the diagonal elements of A^{-1} and the width matrix is energy independent, except for the momentum dependence of the neutron

width. In this case the distant resonances introduce only smoothly varying background terms, while the relevant resonance parameters are still energy-independent. ⁽⁶⁾

In the transition from the level matrix formalism to the generalized Kapur-Peierls expansion these considerations are necessary in order to ascertain the energy independence of the poles of the collision matrix and of the related resonance parameters. ⁽⁶⁾ These considerations also apply to the Humblet formalism ⁽¹²⁾ in which the complex poles are defined in momentum space, as roots of the determinantal equation

$$|1 - RL| = 0 \quad . \quad (9)$$

In the Humblet formalism the momentum dependence of the penetration factor is taken into account rigorously, but the poles inherently contain the effects of R^0 , whenever calculated in a finite number.

In the complex pole expansion of the collision matrix the effects of "hidden" interfering resonances within ΔE are readily introduced by adding poles, ⁽⁶⁾ thus introducing a number of resonance terms larger than the number of the originally postulated levels. Additional resonances external to ΔE , which may be in an unlimited number if R^0 is chosen by statistical law can be described by appropriate background terms, utilizing the approximation given in (8), provided the resonances which are closer to ΔE are included in A^{-1} . With these precautions it is legitimate to define energy independent eigenvalues within the interval ΔE . ⁽⁶⁾

These considerations become meaningful mostly in the attempt of deriving statistical properties of the generalized Kapur-Peierls parameters, as effects of overlap and interferences may affect the parameter values. A version of LEMA-CHAMA with inclusion of the background matrix will be reported separately.

The present version of LEMA-CHAMA does not include the calculation of the background matrix, and is a straightforward generalization of the program LEMA previously reported.⁽⁵⁾ Through the calculation, the inverse level matrix is defined by

$$A_{\lambda\lambda}^{-1} = (E_{\lambda} - E) \delta_{\lambda\lambda} - i\Gamma_{\lambda\lambda}, \quad (10)$$

and the collision matrix is obtained from (5) by putting $R^0 = 0$. The width matrix is considered constant, and $\Gamma_{\lambda n}$ is evaluated at the resonance energy E_{λ} .

3. Remarks on the Reich-Moore formalism

In the Reich-Moore formulation of the R-matrix theory, the level matrix is not explicitly defined, as the approach is based on the partitioned R matrix⁽²⁾

$$\bar{R}_{cc'} = \sum_k \frac{\beta_{kc} \beta_{kc'}}{E_k - E - i\frac{\Gamma_k}{2}} \quad (11)$$

where c, c' range over the channel space defined by neutron and fission channels, and where

$$2\beta_{\lambda n}^2 = \Gamma_{\lambda n} \quad (12)$$

$$2 \sum_{c(fis)} \beta_{\lambda c}^2 = \Gamma_{\lambda f}. \quad (13)$$

The collision matrix is thus obtained:

$$U_{cc'}^J = e^{i\Omega_c + i\Omega_{c'}} \sum_{c''} (1 + i\bar{R})_{cc''} (1 - i\bar{R})_{c''c}^{-1}, \quad (14)$$

where J refers to a given spin-parity state. From (14) total, scattering, and fission cross sections are calculated, from the basic definitions.

One has

$$\sigma_T^J(E) \sqrt{E} = \frac{C}{\sqrt{E}} g_J \operatorname{Re}(1 - U_{nn}^J) \quad (15)$$

$$\sigma_n^J(E) \sqrt{E} = \frac{C}{\sqrt{E}} g_J |1 - U_{nn}^J|^2 \quad (16)$$

$$\sigma_f^J(E) \sqrt{E} = \frac{C}{\sqrt{E}} g_J \sum_{c(fis)} |U_{nc}^J|^2 \quad (17)$$

where C is a conversion constant from barns to eV and g_J is the statistical factor. The capture cross section can be evaluated by difference.

As discussed repeatedly⁽¹³⁾⁽⁸⁾ the partitioning of the channel matrix, sidestepping the level matrix calculation, has many practical advantages when compared to the corresponding level matrix approach, as the rank of $\bar{R}$, appearing in (14) is always small, while the rank of A, appearing in (5) equals the number of the resonances and can become large. One can, moreover, in $\bar{R}$, include large number of resonances, without markedly affecting the over-all computer time.

In the transition to the multilevel formulation, however, it is necessary to define the eigenvalues of the level matrix, as⁽⁴⁾ real and imaginary part of it are interpreted respectively as resonance energy and half-width of the resonance line.

As the time consuming aspect of the level matrix approach is purely the inversion of the level matrix at each energy step when evaluating the cross section curves through the formulas (15), (16), and (17), and not the diagonalization process, the extraction of the level matrix eigenvalues from a given "Reich-Moore" or "level matrix" compilation, does not appear forbidding.

It is always possible, in fact, to associate a well-defined level matrix to the partitioned channel matrix $\bar{R}$ given in eq.(11).

Following the general formalism⁽¹⁾ one has

$$(1 - i\bar{R})^{-1} = 1 + i \sum_{\lambda\mu} A_{\lambda\mu} (\beta_\lambda \times \beta_\mu) \quad (18)$$

where

$$A_{\lambda\mu}^{-1} = (E_\lambda - E - i\frac{\Gamma_{\lambda\gamma}}{2}) \delta_{\lambda\mu} - i(\beta_\lambda \times \beta_\mu) \quad (19)$$

and where

$$(\beta_\lambda \times \beta_\mu) \equiv \xi_{\lambda\mu}^{RM} = \sum_{c(fiss)} (\beta_{\lambda c} \beta_{\mu c}) + \frac{1}{2} \sqrt{\Gamma_{\lambda n} \Gamma_{\mu n}} \quad (20)$$

It should be noted that the "Reich-Moore" level matrix differs from the level matrix used by Vogt⁽³⁾ only in the treatment of the neutron channel contributions to the off-diagonal elements of A^{-1} . In the latter case the off-diagonal element, $\xi_{\lambda\mu}$, of eq.(1) is defined by

$$\xi_{\lambda\mu}^{Vogt} = \frac{1}{2} \sqrt{\Gamma_{\lambda f} \Gamma_{\mu f}} \cos(\theta_\lambda - \theta_\mu) \quad (21)$$

thus introducing the momentum dependence of the neutron penetration factor only in the diagonal elements of A^{-1} . As for low-energy neutron cross sections in fissile elements this contribution is small, the difference between (20) and (21) is negligible.⁽³⁾⁽⁵⁾ In numerical examples, the Vogt approach seems to favor the wings of the cross section lines, while the Reich-Moore approach seems to reproduce the peaks more exactly. On the other hand, through (21), the

fission channel interference effects can be described with more latitude than with equation (20). This aspect of the formalism becomes of relevance in the reverse process, of reducing multilevel parameters to R-matrix parameters.

In the present calculation, the neutron channel contributions have been included, however, in either level matrix definition so that by posing:

$$\xi_{\lambda\mu}^{(Vogt)} = \frac{1}{2} \sqrt{\Gamma_{\lambda f} \Gamma_{\mu f}} \cos(\theta_{\lambda} - \theta_{\mu}) + \frac{1}{2} \sqrt{\Gamma_{\lambda n} \Gamma_{\mu n}} + \delta_{\lambda\mu} \Gamma_{\lambda\gamma}/2 \quad (21')$$

complete equivalence between the two approaches is obtained.

4. Methods of calculation

The program LEMA-CHAMA contains two main branches:

1) LEMA: The initial R-matrix parameter set is given in terms of level matrix parameters, according to Vogt⁽³⁾ formulation. The cross section curves are calculated, from equations (15), (16), and (17), by inversion of the E-dependent level matrix, given in (10). This branch of the calculation has been kept in its original form⁽⁵⁾.

2) CHAMA: The initial R-matrix parameters are given in terms of the Reich-Moore formalism (channel matrix).⁽²⁾ The cross section curves are calculated according to equations (15), (16), and (17), by inversion of the partitioned channel matrix, given in (11).

Both branches flow into the general calculation of eigenvalues and eigenvectors of the level matrix, as described below.

In either case, the generalized Kapur-Peierls parameters defining the cross section shape are derived. The energy dependent cross section values are tabulated, in each case, as calculated from either LEMA branch (level

matrix inversion) or CHAMA branch (channel matrix inversion) and, in parallel, from the multilevel parameters related to the Kapur-Peierls expansion.

For both branches a set of single level parameters can be added, useful for the analysis of hidden resonance effects.⁽¹⁰⁾

5. Eigenvalues and eigenvectors of the level matrix

In the present version of LEMA-CHAMA the complex eigenvalues calculation is obtained from the Subroutine FRANCI,⁽¹⁴⁾ as more precise and efficient than the one utilized in LEMA.⁽⁵⁾

Denoting with

$$c_k = u_k - i v_k \quad (22)$$

the k-th eigenvalues of A^{-1} , the complex orthogonal transformation, S ,⁽⁴⁾⁽⁵⁾ diagonalizing A^{-1} , satisfies the system of equations

$$\sum_{\lambda=1}^N A_{\lambda\lambda}^{-1} S_{\lambda'k} = (c_k - E) S_{\lambda k} \quad (23)$$

where $k = 1, \lambda = 1, N$ and where N is the total number of resonances included in A^{-1} .

As discussed previously,⁽⁵⁾ the matrix S is obtained from (23) by solving the N times the system of $N-1$ equations provided by (23) for $\lambda \neq k$. For each fixed value of k one obtains the $N-1$ components

$$\frac{S_{\lambda k}}{S_{kk}} \quad (\lambda \neq k) \quad (24)$$

as solutions. The orthogonality of S provides the normalization condition

$$\sum_{\lambda=1}^N S_{\lambda k}^2 = 1 \quad (25)$$

thus determining fully the eigenvector matrix S . The matrix inversion is here performed through the subroutine `MATINV` in the manner described previously as used in `LEMA`.⁽⁵⁾

This procedure is straightforward, except for the choice of the ordering of the eigenvalue sequence. The order of the eigenvectors, S , depends on the ordering sequence of the eigenvalues c_k with respect to the original R -matrix eigenvalues E_λ . Permutations in the order of the index k correspond to different matrices S , related to each other by a real orthogonal (involutory) transformation. It appears natural to choose the order of the eigenvalues c_k following the increasing magnitude of the real part, μ_k ,

$$\mu_1 < \mu_2 < \mu_3 \dots \quad (26)$$

which is the order chosen for the original R -matrix values E_λ :

$$E_1 < E_2 < E_3 \dots \quad (27)$$

Once the eigenvalue array is obtained from `FRANCI`, the appropriate permutation is obtained through the subroutine `REARR`, so that S is uniquely determined.

Complex widths amplitudes and complex partial widths are thus derived according to the definitions⁽⁴⁾⁽⁵⁾

$$\tilde{\gamma}_{kc} = \sum_{\lambda=1} S_{\lambda k} \sqrt{\Gamma_{\lambda c}} \quad (28)$$

$$\tilde{\Gamma}_{k(x)} = \sum_{c(x)} \tilde{\gamma}_{kc}^2 \quad (29)$$

Through the orthogonality of S , which reflects the unitarity of U , one verifies also that

$$\sum_k \tilde{Y}_{kc} \tilde{Y}_{kc'} = \sum_{\lambda} \sqrt{\Gamma_{\lambda c} \Gamma_{\lambda c'}} \quad (30)$$

From (30) one has also

$$\sum_k \sum_{c(x)} \tilde{Y}_{kc}^2 = \sum_{\lambda} \tilde{\Gamma}_{\lambda(x)} = \sum_{\lambda} \Gamma_{\lambda(x)} \quad (31)$$

for each reaction process (x) . Thus the sum of the complex partial widths over the array of the interfering levels is real and equals the corresponding sum of the R-matrix partial widths.

For fission, capture, and scattering cross sections, the auxiliary complex hermitean matrix^{(6) (15)}

$$X_{kk'}^{(x)} = \sum_{c(x)} \tilde{Y}_{kc} \tilde{Y}_{k'c}^* \quad (32)$$

is formed, where (x) stands for either fission or capture and $\sum_{c(x)}$ refers to all the channels intervening into the reaction (x) . In particular for capture one has

$$X_{kk'}^{(\gamma)} = \sum_l S_{\lambda k} S_{\lambda k'}^* \Gamma_{\lambda \gamma} \quad (33)$$

and for scattering

$$X_{kk'}^{(n)} = \tilde{Y}_{kn} \tilde{Y}_{k'n}^* \quad (34)$$

In absence of interferences these matrices become real diagonal (S is unity) and from (32) and (29) one has:

$$X_{kk'}^{(x)} = \delta_{kk'}, \quad \Gamma_{k(x)} = \tilde{\Gamma}_{k(x)} \quad (35)$$

From the unitarity of the collision matrix⁽⁶⁾ one has also

$$\sum_{(x)} X_{kk'}^{(x)} = X_{kk'} = \frac{c_{k'}^* - c_k}{i} Y_{kk'} \quad (36)$$

where

$$Y_{kk'} = \sum_{\lambda} S_{\lambda k} S_{\lambda k'}^* \quad (37)$$

is a complex orthogonal hermitean matrix satisfying the relations

$$\sum_{k'} Y_{kk'} Y_{k''k'} = \delta_{kk''} \quad (38)$$

and transforming $\tilde{Y}$ into its complex conjugate:

$$\sum_{k'} Y_{kk'} \tilde{Y}_{k'c}^* = \tilde{Y}_{kc} \quad (39)$$

From (36) one has in particular

$$X_{kk} = 2\Omega_k Y_{kk} \quad (40)$$

where

$$Y_{kk} > 1. \quad (41)$$

For non-interfering levels (S unity)

$$Y_{kk'} = \delta_{kk'}. \quad (42)$$

From the complex orthogonality of S one also obtains the relations⁽⁴⁾

$$\sum_k (\mu_k - i\nu_k) = \sum_\lambda (E_\lambda - i\Gamma_{\lambda\lambda}) \quad (43)$$

$$\sum_k \tilde{\Gamma}_k = \sum_k 2\nu_k = \sum_\lambda 2\Gamma_{\lambda\lambda} \quad (44)$$

where

$$\tilde{\Gamma}_k = \sum_{(x)} \tilde{\Gamma}_{k(x)} \quad (45)$$

represents the total complex width, which only in absence of interferences is real and equals the line width:

$$\tilde{\Gamma}_k \approx 2\nu_k = 2\Gamma_{kk} \quad (46)$$

With the auxiliary matrices defined in eqs (32) to (34) the line shape parameters utilized in the cross section expansion are constructed⁽⁴⁾

$$G_k^{(x)} + i H_k^{(x)} = \frac{2ig_J}{\sqrt{E}} \sum_{k'=1}^N \frac{\tilde{X}_{kk'}^n \lambda_{kk'}^{(x)}}{c_{k'}^* - c_k} \quad (47)$$

where g_J represents the statistical factor for the spin state J and k' ranges over the number of the interfering levels (of the same spin state).

Two sets of sum rules can be verified directly from the properties of the matrix $X^{(x)}$:

- 1) Sum over reaction channels (utilizing (36) and (39)):

$$\sum_{(x)} \left(G_k^{(x)} + i H_k^{(x)} \right) = \frac{2ig_J}{\sqrt{E}} \tilde{\gamma}_{kq}^2 \equiv \tilde{\Gamma}_{kn}^0 \quad (48)$$

so that, defining real and imaginary parts of the complex reduced neutron width Γ_{kn}^o as

$$\tilde{\Gamma}_{kn}^o = \alpha_k^o + i\beta_k^o \quad (49)$$

one can write

$$\sum_{(x)} G_k^{(x)} = \alpha_k^o \quad (50)$$

$$\sum_{(x)} H_k^{(x)} = \beta_k^o. \quad (51)$$

2) Sum over the totality of the interfering levels (utilizing the hermiticity of $X^{(x)}$):

$$\sum_k (G_k^{(x)} + iH_k^{(x)}) = \sum_k G_k^{(x)} \quad (52)$$

and, utilizing the orthogonality of S:

$$\sum_k (\alpha_k^{(o)} + i\beta_k^{(o)}) = \sum_k \alpha_k^o = \sum_{\lambda} \Gamma_{\lambda n}^o \quad (53)$$

where $\Gamma_{\lambda n}^o$ represents the reduced neutron width of the R-matrix theory.

Thus the sums, over the levels, of the "asymmetrical" parameters vanishes^{(5) (16)}

$$\sum_k H_k^{(x)} = \sum_k \beta_k^o = 0. \quad (54)$$

It can be noted that for non-interfering levels

$$\alpha_k^0 \rightarrow \Gamma_{kn}^0 \quad \beta_k^0 \rightarrow 0 \quad (55)$$

$$G_k^{(x)} \rightarrow \frac{\Gamma_{kn}^0 \Gamma_{k(x)}}{\Gamma_k} \quad H_k^{(x)} \rightarrow 0 \quad (56)$$

Thus, only in absence of interferences (and neglecting overlap effects) the "symmetrical" parameters $G_k^{(x)}$ are proportional to the corresponding reaction widths.

Whenever $\Gamma_{\lambda\lambda} \ll |E_\lambda - E_\lambda|$, the level matrix inversion can be performed by perturbation methods^{(4) (17)} giving the results (55) and (56) as zero-order values. By perturbation it is apparent that interference effects enter linearly (first order) in the asymmetrical parameters and only to the second order in the symmetrical parameters. Thus to a first order also

$$\alpha_k^0 \approx \Gamma_{kn}^0, \quad G_k^{(x)} \approx \frac{\Gamma_{nn}^0 \Gamma_{k(x)}}{2\nu_k} \quad (57)$$

For well separated levels these results can be utilized to obtain estimates of the R-matrix widths from α^0 and $G^{(x)}$.

The cross section expansions are given in terms of the line shape parameters^{(15) (16)} where background terms, arising from distant resonances, are omitted:

$$\sigma_n^T(E) \sqrt{E} = C \sum_{k=1}^{N_{\text{tot}}} \frac{\nu_k (\alpha_k^0 \cos 2\Omega - \beta_k^0 \sin 2\Omega) + (\mu_k - E) (\alpha_k^0 \sin 2\Omega + \beta_k^0 \cos 2\Omega)}{(\mu_k - E)^2 + \nu_k^2} + 2C \frac{(1 - \cos 2\Omega)}{\sqrt{E}} \quad (58)$$

where η represents the potential scattering phase shift, C is a conversion constant from barns to eV, and where the sum over k includes the total number of resonances, that is, for s-wave neutrons, two spin states J .

For reaction cross sections one has similarly

$$\sigma_n^{(x)}(E) \sqrt{E} = C \sum_{k=1}^{N_{\text{tot}}} \frac{\nu_k G_k^{(x)} + (\mu_k - E) H_k^{(x)}}{(\mu_k - E)^2 + \nu_k^2} \quad (59)$$

It can be seen readily from (58) and (59) that the asymmetries of the cross section curves do not affect the area under the curve, while the symmetrical parameters G_k can be interpreted as a measure of the same area.

In the calculation described here, the line shape parameters G_k , H_k , α_k^0 , β_k^0 , are given in units of $(\text{eV})^{1/2}$ (as the reduced neutron width Γ_n^0) while the complex partial widths $\tilde{\Gamma}_{k(x)}$, the level matrix eigenvalues (μ_k, ν_k) and the X-matrices are in eV. The matrices S and Y are thus dimensionless, while the values of $\sigma(E)$ are in barns.

6. Cross section calculations

For either branch of the program (LEMA, or CHAMA) the eigenvalues of the level matrix, the complex partial widths, and the matrices $X^{(x)}$ and Y are obtained as output. As in the original version⁽⁵⁾ the line shape parameters are also punched on cards, to be used with associated computer programs (CODILLI,⁽¹⁶⁾ CURVEPLOT, TRIPLE, and GAMPLEX⁽¹⁵⁾). Because in the practical use of equations (58) and (59) Doppler and resolution broadening are generally included, the values punched on cards are:

$$GR_k^{(x)} = \frac{G_k^{(x)}}{v_k} \quad , \quad GI_k^{(x)} = \frac{H_k^{(x)}}{v_k} \quad (60)$$

$$GR_k^{(T)} = \frac{G_k^o}{v_k} \quad GI_k^{(T)} = \frac{\beta_k^o}{v_k} \quad (61)$$

(in $[eV]^{-1/2}$), so that the Doppler broadened cross section expansion is given for example by

$$\sigma_n^{(x)}(E) \sqrt{E} = C \sum_k (GR_k^{(x)} \psi_k + GI_k^{(x)} \chi_k) \quad (62)$$

where ψ_k and χ_k are the customary symmetrical and asymmetrical line shape functions. (16)

The cross section values calculated from the R-matrix parameters can be optionally punched on cards. This option is useful in three ways:

- (a) to provide synthetic data in the code checking process of large programs such as TRIPLE;
- (b) to compare by graphical display the calculation from either level matrix or channel matrix inversion (used as "data") with the values obtained from the poles expansions (58) and (59);
- (c) and finally to study effects of hidden resonances and of quasi-resonances. (5)

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Appendix A - Input and Output

A-1 Indices controlling input and output operations.

ISW = index for three possible input format for the fission channels interferences. For ISW = 1 the angle θ_λ for the λ -th level fission vector is input (Vogt approach). For ISW = 2 the matrix $\cos(\theta_\lambda - \theta_{\lambda'})$, is given (Vogt approach). Then two choices have been made necessary to accomodate parameters obtained by different authors within Vogt's formulation of the level matrix. For ISW = 3 the input is in the Reich-Moore format.

IPUNCH if = 1 the calculate cross sections are to be punched on cards and printed.
if = 0 the calculate cross sections are only printed.

J Spin state index.
J = 1,2 correspond to the two possible s-wave spin states for the two groups of interfering levels.
J = 3,4 correspond to the two possible spin states for the two groups of non-interfering (single level) resonances.

NO (J) = number of resonances belonging to the same spin state J. Precisely, NO(1) refers to the interfering set of the first spin state, NO(3) to the non interfering set of the same spin state, and similarly NO(2), NO(4) correspond to the second spin state ($NO(J) \leq 33$)

NCHA(J) = number of open fission channels for the case ISW = 3 (≤ 2)

A-2 Floating point constants

ATM = atomic mass number

WN = "nuclear radius" in $\text{eV}^{-\frac{1}{2}}$, so that the potential scattering phase shift is given by $\Omega = WN \sqrt{E}$

CC = conversion constant $C = 6.52 \times 10^5$ barns x eV

EMIN= lowest energy value

EMAX= largest energy value

DELE= energy increment, in eV, defining the points at which the cross sections are calculated.

} defining the energy interval ΔE (in eV)

A-3 Resonance parameters

For each spin state $J = 1, 4$ and for each level K of the set $NO(J)$

ER (K,J) = resonance energy, E_k (eV)

GON(K,J) = reduced neutron width, $\Gamma_{kn}^o = \frac{2g_J}{\sqrt{E}} \Gamma_{kn}$ ($\text{eV}^{\frac{1}{2}}$)

GG (K,J) = radiative capture width, Γ_{ky} (eV)

GF (K,J) = fission width Γ_{kf} (of channel 1 for ISW = 3) (eV)

GN (K,J) = neutron width Γ_{kn} (eV)

For spin states $J = 1, 2$, and for each level of the set $NO(J)$

TETA (K,J) = θ_k angle for the fission vector Γ_{nf} for ISW = 1

= Γ_{kf} (of channel 2) for ISW = 3 (in eV)

GO (K,L,J) = $\cos(\theta_{\lambda} - \theta_{\lambda})$ for ISW = 2

GFACT(J) = value of the statistical factor g_j

A-4 Input format of LEMA-CHAMA

Format

Card 1 ISW, IPUNCH, IDNUM* (215,A4)

2 ATM, WN, CC, EMIN, EMAX, DELE (6E12.3)

These cards are followed by four sets of cards for each spin state:

Set J = 1 R matrix parameters for the resonances of the first spin
state, in the mode corresponding to ISW

Set J = 2 As above, for the second spin state

Set J = 3 Single level parameters for the non interfering levels
of the first spin state

Set J = 4 As above, for the second spin state.

Each of the 4 sets contains:

Format

Card 1 GFACT(J), NO(J), NGHA(J)** (5E12.3,215)

followed by NO(J) cards, one per resonance

for ISW=2: ER(K,J)***, GON(K,J), GG(K,J), GF(K,J), GN(K,J) (5E12.3)

for J = 1,2,3,4

for ISW=3: ER(K,J)***, GON(K,J), GG(K,J), GF(K,J), GN(K,J), TETA(K,J) (5E12.

for J = 1,2

for ISW=2 and J = 1,2 additional cards are needed with GO(K,L,J) stored as a
triangular matrix:

GO(K,L,J) for each K, 5 to a card (5E12.3)

K = 1, NO(J) -1, L = K + 1, NO(J)

thus for NO(J) ≤ 6 there are 5 cards

First card GO(1,2,J), GO(1,3,J), GO(1,NO,J) (5E12.3)

Second card GO(2,3,J), GO(2,NO,J)

Last card GO(NO-1, NO,J)

For NO(J) = 7 the first row of the matrix GO will need 2 cards, the
second row 1 card, etc.

* identification of the calculation, which may be blank

** blank or zero for ISW < 3

*** in increasing order of ER

1. Printed output

The input parameters.

The eigenvalues of the level matrix, μ_k , ν_k .

Complex partial widths $\tilde{\gamma}_{k(x)}$ in the order $\tilde{\gamma}_{kn}^{(1)}$, $\tilde{\gamma}_{ky}^{(1)}$, $\tilde{\gamma}_{kf1}^{(1)}$, $\tilde{\gamma}_{kf2}^{(1)}$

Complex partial widths $\tilde{\Gamma}_{kx}$ in the order $\tilde{\Gamma}_{kn}$, $\tilde{\Gamma}_{ky}$, $\tilde{\Gamma}_{kf}$

and $\sum_k \tilde{\Gamma}_{kn}$, $\sum_k \tilde{\Gamma}_{ky}$, $\sum_k \tilde{\Gamma}_{kf}$

Matrices X^{Fis} , X^{cap} , Y for the levels internal to ΔE .

Resonance parameters α_k^O , β_k^O , G_k^F , H_k^F , G_k^Y , H_k^Y .

Tabulation of

E $\sigma_T^{(1)}$, $\sigma_T^{(2)}$, $\sigma_f^{(1)}$, $\sigma_f^{(2)}$, $\sigma_Y^{(1)}$, $\sigma_Y^{(2)}$, $\sigma_n^{(1)}$, $\sigma_n^{(2)}$

where (1) refers to either level matrix or channel matrix calculation, and
(2) to multilevel expansion.

2. Punched output

If $IPUNCH > 0$, E , $\sigma_T^{(1)}$, $\sigma_f^{(1)}$, $\sigma_Y^{(1)}$, $\sigma_n^{(1)}$ are punched out.

In all cases the input card 2 and the multilevel parameters are
punched out in the form:

```
level K   $\mu_k$ ,  $\nu_k$ ,  $GRT_k$ ,  $GLT_k$ , IDNUM      (4E15.8, 12x, A4)
           $\mu_k$ ,  $\nu_k$ ,  $GRF_k$ ,  $GIF_k$ , IDNUM
           $\mu_k$ ,  $\nu_k$ ,  $GRG_k$ ,  $GIG_k$ , IDNUM
```

APPENDIX B

```

C      PROGRAM LEMA-CHAMA
C
C      L E M A - C H A M A
C      CALCULATION OF S-WAVE NEUTRON CROSS SECTIONS FROM R-MATRIX --
C      PARAMETERS THROUGH THE WIGNER LEVEL MATRIX, AND (OR) THROUGH
C      THE REDUCED CHANNEL MATRIX INVERSION (REICH-MOORE METHOD)--
C      DOUBLE PRECISION FORTRAN IV VERSION OF LEMA II--SEE REPORT
C      COO-1546-3--(1967)--- WITH ALTERNATE CALCULATION THROUGH THE
C      CHANNEL MATRIX INVERSION, FOR TWO FISSION CHANNELS---1968--
C      BY OPTION (INDEX ISW) THE CALCULATION BRANCHES TO
C      A) LEMA--CALCULATION OF CROSS SECTION VALUES BY INVERSION
C      OF THE WIGNER LEVEL MATRIX, UTILIZING THE SUBROUTINE MATINV
C      AS DESCRIBED IN LEMA II--
C      B) CHAMA--CALCULATION OF CROSS SECTION VALUES BY INVERSION
C      OF THE REDUCED CHANNEL MATRIX, USING THE REICH-MOORE METHOD FOR
C      TWO FISSION CHANNELS (SUBROUTINE REVERT)---
C      FOR EITHER OPTION, THE EIGENVALUES OF THE WIGNER LEVEL
C      MATRIX ARE EVALUATED (SUBROUTINE FRANCI AND SATELLITES), AS WELL
C      AS THE PERTAINING 'KAPUR-PEIERLS' MULTILEVEL PARAMETERS
C      PROVIDING THE CROSS SECTION EXPANSION IN TERMS OF THE POLES ---
C      OF THE COLLISION MATRIX-- AT EACH ENERGY STEP CROSS SECTION
C      VALUES OBTAINED FROM EITHER A) OR B) ARE OUTPUT, IN PARALLEL
C      WITH THE VALUES CALCULATED FROM THE POLE EXPANSION--
C      THIS VERSION WILL TREAT 33 INTERFERING RESONANCES AND
C      ADDITIONAL 33 NON-INTERFERING RESONANCES PER SPIN STATE--
C      ORIGINAL VERSION OF LEMA -- JULY 1965--
C      ORIGINAL LEMA II ADAPTED TO FORTRAN IV, DOUBLE PRECISION, IN
C      JULY 1968-- ADDITION OF CHAMA BRANCH, NOVEMBER 1968-----
C
C      WARNING-----THROUGH THE CALCULATION THE REDUCED NEUTRON WIDTH
C      GON(K,J) IS DEFINED AS 2*GFACT(J)*GN(K,J)/SQRT(E)--IF THE DATA
C      CHOSEN FOR THE CALCULATION ENTAIL A DIFFERENT DEFINITION OF THE
C      REDUCED NEUTRON WIDTH, E.G. GON(K,J) = GN(K,J)/SQRT(E)
C      THE PERTINENT SCALING SHOULD BE INTRODUCED BY THE USER
C      WITHIN LOOPS 32,35,36,42, AS INDICATED BY COMMENT CARD--
C
C
C      IMPLICIT REAL*8 (A-H,O-Z)
C      DIMENSION ALFA(33), AINV(33,33), ALG(33,4), B(33,1), BEG(33,4),
1      BETA(33), CAPG(33,4), CAPHT(33,4), D(33,33), DET(33,4),
2      DW(33,4), ER(33,4), FISG(33,4), FISH(33,4), FU(33),
3      G(33,33), GAT(33,33), GFS(33), GGAT(33), GF(33,4), GU(33),
4      GG(33,4), GN(33,4), GON(33,4), GFACT(4), GO(33,33,2),
5      HGA(33), HFS(33), OTINV(33,33), OT(33,33), OI(4), O2(4),
6      NO(4), NCHA(2), TETA(33,4), VIM(33,4), VRE(33,4)
C      COMPLEX*16 AT(33,33), ANRM, CAN(33,33), CAPVE(33,33), CJEIG,
1      EIGVAL(33), FACT, FIN(33,33), FISVE(33,33), SCAVE(33,33)
2      , SWA,SWC, SWG, WA(33), WC(33), WG(33), WS(33),
3      TWA(33), TWC(33), TWG(33), ZZ, ZZZ
C      COMMON      CAN,FIN
C      DATA T1/'      GO(K,')
C      REAL*4 T2,PUNCH(6),GRT,GIT,GRF,GIF,GRC,GIC,IONUM
C      DATA T2/','J) '/'
C
C
1000  READ(5,102) ISW,IPUNCH ,IONUM
      READ(5,100 ) ATM,WN,CC,EMIN,EMAX,DELE

```

```

      IF(I PUNCH) 2443, 2443, 2442
2442 PUNCH(1)=ATM
      PUNCH(2)=WN
      PUNCH(3)=CC
      PUNCH(4)=EMIN
      PUNCH(5)=EMAX
      PUNCH(6)=DELE
      WRITE(7,100) PUNCH
2443 IF(1SW=3) 2445, 2444, 2445
2444 WRITE(6,2352)
      GO TO 2446
2445 WRITE(6,70)
2446 WRITE (6,71)  ATM, WN, CC, EMIN, EMAX, DELE ,IONUM
      LINES = 11
      ISW=1SW
      J=1
2400 READ(5,103 ) GFACT(J),NO(J),NCHA(J)
      NR=NO(J)
      IF(J-2) 2449,2447,2447
2447 IF(LINES+NR+4-56) 2449,2448,2448
2448 WRITE(6,89)
      LINES=5
2449 WRITE (6,72) J, J, GFACT(J), J, NO(J)
      LINES = LINES + 4
      IF(J-2) 2500,2500,2501
2501 ISW=4
2500 IF(NR) 2401,2401,50
      50 GO TO (51,52,53,54), ISW
      51 WRITE(6,75)
      GO TO 2050
      52 WRITE(6,77)
      GO TO 2050
      53 WRITE(6,2350) NCHA(J)
      GO TO 2050
      54 WRITE(6,74)
2050 LINES=LINES+4
      GO TO (2051,2052,2053,2054), ISW
2051 DO 42 K = 1,NR
      READ(5,100 ) ER(K,J),GON(K,J),GG(K,J),GF(K,J),GN(K,J),TETA(K,J)
CCC      SEE WARNING --- INSERT HERE MODIFICATION OF 'GON' IF NEEDED
      GN(K,J)= GON(K,J)*DSORT(DABS(ER(K,J)))/(2.00*GFACT(J))
      LINES = LINES + 1
      42 WRITE (6,76) K,ER(K,J),GON(K,J),GG(K,J),GF(K,J),GN(K,J),TETA(K,J)
      GO TO 2401
2052 DO 36 K=1,NR
      READ(5,101 ) ER(K,J),GON(K,J),GG(K,J),GF(K,J),GN(K,J)
CCC      SEE WARNING --- INSERT HERE MODIFICATION OF 'GON' IF NEEDED
      GN(K,J)= GON(K,J)*DSORT(DABSTER(K,J)))/(2.00*GFACT(J))
      LINES = LINES + 1
      36 WRITE (6,73) K,ER(K,J),GON(K,J),GG(K,J),GF(K,J),GN(K,J)
      KMAX=NR-1
      DO 37 K=1,KMAX
      KMJN=K+1
237 READ(5,101) (GOK,L,J),L=KMJN,NR)
      DO 7037 K=1,NR
      GOK(K,J)=1.00
      KMJN=K+1

```

```

      DO 7037 L=KMIN,NR
7037 GO(L,K,J)=GO(K,L,J)
      NROWS = 1 + (NR-1)/5
      DO 1 NROW = 1,NROWS
      NCOLS = 5 + NR - 5*NROW
      IF (NCOLS - 5) 78,78,79
79   NCOLS = 5
78   K1 = 5*(NROW-1) + 1
      K2 = 5*(NROW-1) + NCOLS
      GO TO (80,81,81,81,81), NROW
80   IF (56 - LINES - NR) 82,83,83
82   WRITE (6,89)
      LINES = 5
83   WRITE (6,84) (I1,I,I2, I = K1,K2)
      WRITE (6,85)
      LINES = LINES + 4
      GO TO 86
81   IF (57 - LINES - NR) 87,88,88
87   WRITE (6,89)
      WRITE (6,84) (I1,I,I2, I = K1,K2)
      WRITE (6,85)
      LINES = 9
      GO TO 86
88   WRITE (6,90) (I1, I, I2, I = K1,K2)
      WRITE (6,85)
      LINES = LINES + 3
86   DO 91 K = 1,NR
      LINES = LINES + 1
91   WRITE (6,92) K, (GO(K,L,J), L = K1,K2)
1    CONTINUE
      GO TO 2401
2053 DO 32 K=1,NR
      READ(5,100 ) ER(K,J),GON(K,J),GG(K,J),GF(K,J),GN(K,J),TETA(K,J)
CCC   SEE WARNING --- INSERT HERE MODIFICATION OF 'GON' IF NEEDED
      GN(K,J)= GON(K,J)*DSQRT(DABS(ER(K,J)))/ (2.DO*GFACT(J))
      LINES = LINES + 1
32   WRITE(6,2351)K,ER(K,J),GON(K,J),GG(K,J),GF(K,J),TETA(K,J),GN(K,J)
      GO TO 2401
2054 DO 35 K=1,NR
      READ (5,101 ) ER(K,J),GON(K,J),GG(K,J),GF(K,J),GN(K,J)
CCC   SEE WARNING --- INSERT HERE MODIFICATION OF 'GON' IF NEEDED
      GN(K,J)= GON(K,J)*DSQRT(DABS(ER(K,J)))/ (2.DO*GFACT(J))
      LINES = LINES + 1
35   WRITE (6,731) K,ER(K,J),GON(K,J),GG(K,J),GF(K,J),GN(K,J)
2401 J=J+1
      IF (J-4) 2400,2400,2402
C
C FORM OFF-DIAGONAL ELEMENTS OF THE LEVEL MATRIX
2402 ISW=ISTW
      J=1
62   NR=ND(J)
      IF (NR) 61,61,2
2   DO 4 L =1,NR
      DO 4 LL=1,NR
      Y=GF(L,J)*GF(LL,J)
      GO TO (2061,2062,2063,61),ISW
2061 YY=DSQRT(Y)

```

```

      GO(L,LL,J)=YY*DCOS(TETA(L,J)- TETA(LL,J))/2.0
      GO TO 2072
2062 YY=DSQRT(Y)
      GO(L,LL,J)=YY*GO(L,LL,J)/2.0
      GO TO 2072
2063 IF(Y) 2064,2071,2065
2064 BIN=-1.0
      GO TO 2066
2065 BIN=1.0
2066 YY=DSQRT(BIN*Y)
      GO(L,LL,J)= BIN*YY/2.0
2067 Y=TETA(L,J)*TETA(LL,J)
      IF(Y) 2068,2072,2069
2068 BIN=-1.0
      GO TO 2070
2069 BIN=1.0
2070 YY=DSQRT(BIN*Y)
      GO(L,LL,J)=GO(L,LL,J)+ BIN*YY/2.0
      GO TO 2072
2071 GO(L,LL,J)=0.0
      GO TO 2067
2072 IF(L=LL) 4, 5,4
      5 GO(L,L,J)=GO(L,L,J)+GG(L,J)/2.0
      4 CONTINUE
      61 J=J+1
      IF(J-2) 62,62,63
C
CALCULATION OF EIGENVALUES IN DOUBLE PRECISION
C
      63 J=1
      163 NR=NO(J)
      EAV =0.0
      PUNCH(1)=GFACT(J)
      WRITE(7,103)PUNCH(1),NR(J),PUNCH(1)
      IF(NR) 165,165,164
      164 DO 166 K=1,NR
      DO 166 KK=1,NR
      XX=GON(K,J)*GON(KK,J)
      IF(XX) 167,1665,167
      167 SKK=DSQRT(DABS(ER(K,J)))
      SK =DSQRT(DABS(ER(K,K)))
      SQKKK=DSQRT(XX*SK*SKK)
      GO TO 166
      1665 SQKKK=0.0
      166 GA(K,KK) =GO(K,KK,J)+SQKKK/14.0*GFACT(J)
      WRITE(6,89)
      LINES=5
      DO 168 K=1,NR
      EAV=EAV+ER(K,J)
      DO 168 KK=1,NR
      168 D(K,KK)=0.0
      EAV=EAV/DFLOAT(NR)
      DO 169 K=1,NR
      169 D(K,K)= ER(K,J)
      DO 170 K=1,NR
      DO 170 KK=1,NR
      XZ=-GA(K,KK)

```

```

      A(K, KK)=DCMPLX(D(K, KK), XZ)
      FACT=DCMPLX(TEAV, 0.000)
170  A(K, KK)=A(K, KK)/FACT
      N=NR
      DO 600 K=1, NR
      DO 600 KK=1, NR
      600  CAN(K, KK)=A(K, KK)
      CALL FRACNT(A, EIGVAL, N, ANDRM, 33)
      DO 601 K=1, NR
      DO 601 KK=1, NR
      601  A(K, KK)=CAN(K, KK)
      CALL REARRR(NR, EIGVAL)
      IF (54 - LINES - NR) 502, 503, 503
      502  WRITE (6, 89)
      LINES = 5
      503  WRITE(6, 500) J
      LINES = LINES + 6
      DO 172 K=1, NR
      EIGVAL(K)=EIGVAL(K)*FACT
      LINES = LINES + 1
      CJEIG=DCONJG(EIGVAL(K))
      172  WRITE (6, 501) K, CJEIG
      WRITE(6, 85)
      LINES=LINES+2
C
C  OBTAIN EIGENVECTOR FOR K-TH EIGENVALUE.
C
      K=1
      460  MK=0
      L=1
      400  IF(L-K) 402, 411, 402
      411  IF(K-NR) 401, 409, 401
      401  L=L+1
      GO TO 400
      402  MK=MK+1
      NR=0
      LL=1
      403  IF(LL-K) 405, 414, 405
      414  IF(K-NR) 404, 408, 404
      404  LL=LL+1
      GO TO 403
      405  NK=NK+1
      G(MK, NK)=GA(LL, LL)
      IF(MK-NK) 407, 406, 407
      406  G(MK, NK) =G(MK, MK)+DAIMAG(EIGVAL(K))
      D(MK, NK)=ER(L, JT=DREAL(EIGVAL(K)))
      WG(MK)=DCMPLX(0.000, GA(L, K))
      407  IF(LL-NR) 404, 408, 408
      408  IF(L-NR) 401, 409, 409
C
C  SOLVE FOR VECTOR Y
C
      409  NMAX=NR-1
      DO 410 LK=1, NMAX
      DO 410 LLK=1, NMAX
      410  Q(LK, LLK) =G(LK, LK)

```

C INVERT Q

C

```

      DO 421 I=2,NMAX
421  B(I,1)=0.0
      B(1,1)=1.0
      CALL MATINV(Q,NMAX,B,0,DETERM)
      DO 420 LK=1,NMAX
      DO 420 LK=1,NMAX
420  DINV(LK,LLK)=G(LK,LLK) + Q(LK,LLK)*D(LK, LK)*D(LLK,LLK)

```

C

C INVERT OINV

C

```

      DO 422 I=2,NMAX
422  B(I,1)=0.0
      B(1,1)=1.0
      CALL MATINV(OINV,NMAX,B,0,DETERM)
      DO 440 LK=1,NMAX
      DO 440 LK=1,NMAX
440  AINV(LK,LLK)=0.0
      DO 442 LK=1,NMAX
      DO 442 LK=1,NMAX
      DO 441 MK=1,NMAX
441  AINV(LK,LLK)=AINV(LK,LLK) + OINV(LK,MK)*D(MK,MK)*Q(MK,LLK)
442  A(LK,LLK)=DCNPLX(AINV(LK,LLK),OINV(LK,LLK))
      DO 443 LK=1,NMAX
443  WA(LK)=10.0,0.0,0.0
      DO 444 LK=1,NMAX
      DO 444 LK=1,NMAX
444  WA(LK) = WA(LK) + A(LK,LLK)*WG(LLK)
      FACT=(1.0,0.0,0.0)
      DO 445 LK=1,NMAX
445  FACT = FACT + RA(LK)*WA(LK)
      ZZ=(1.0,0.0,0.0)
      ZZZ=ZZ/FACT
      SCAVE(K,K) =CDSQRT(ZZZ)
      LK=1
      L=1
451  IF(L-K) 452,450,452
450  L=L+1
452  IF(L-NR) 453,453,454
453  SCAVE(L,K)=SCAVE(K,K)*WA(LK)
      L=L+1
      LK=LK+1
      IF(LK=NMAX) 451,451,454
454  K=K+1
      IF(K-NR) 460,460,461
461  DO 462 K=1,NR
      DO 462 KK=1,NR
462  A(K,KK)=SCAVE(K,KK)

```

C

CALCULATE COMPLEX PARTIAL WIDTHS

C

```

      DO 180 K=1,NR
      WC(K)=(10.0,0.0,0.0)
      WG(K)=(10.0,0.0,0.0)
      WS(K)=(0.0,0.0,0.0)
180  WA(K)=(0.0,0.0,0.0)

```

```

      SWA=(0.0,0.0)
      SWG=(0.0,0.0)
      SWC=(0.0,0.0)
      TF148=LINES-2*NR-5) 506,507,507
506 WRITE (6,89)
      LINES = 5
507 WRITE(6,85)
      WRITE(6,504)
      LINES=LINES+8
      DO 182 K=1,NR
      DO 181 L=1,NR
        IF(GON(L,J)) 1182,1182,1181
1181 WG(K)= WG(K) +DSQRT(GON(L,J))*A(L,K)
1182 WC(K)= WC(K) +DSQRT(GG(L,J))*A(L,K)
        IF(GF(L,J)) 1183,1184,1183
1183 XY=DABS(GF(L,J))
        XX=DSQRT(XY)
        WAKT= WAKT+ XX*A(L,K)*GF(L,J)/XY
1184 IF(JSW-3) 181,1185,181
1185 IF(TETAT(L,J)) 1186,181,1186
1186 XY=DABS(TETA(L,J))
        XX=DSQRT(XY)
        WS(K)= WS(K)+ XX*A(L,K)*TETA(L,J)/XY
181 CONTINUE
      LINES=LINES+1
      WRITE(6,505) K,WG(K),WC(K),WAKT,WS(K)
182 CONTINUE
      WRITE(6,85)
      LINES=LINES+4
      WRITE(6,560)
      DO 183 K=1,NR
        FUK=DREAL(EIGVAL(K))
        GU(K) = -DAIMAG(EIGVAL(K))
        YE=DSQRT(DABSTFUK)
        ZZZ=DCMPLX(XE/(2.00*GFACT(J)),0.00)
        TWA(K)=(0.00,0.00)
        TWC(K)=(0.00,0.00)
        DO 2183 L=1,NR
        DO 2183 LL=1,NR
          IF(L-LL) 2182,2181,2182
2182 TWA(K)= TWA(K)+2.00*GO(L,LL,J)*A(L,K)*A(LL,K)
          GO TO 2183
2181 TWC(K)= TWC(K)+ GG(L,J)*A(L,K)*A(LL,K)
          TWA(K)= TWA(K)+(2.00*GOTE(L,L,J)-GG(L,J))*A(L,K)*A(LL,K)
          TWG(K)= ZZZ*WG(K)*WG(K)
2183 CONTINUE
        SWA= SWA + TWA(K)
        SWC= SWC + TWC(K)
        SWG= SWG + TWG(K)
        LINES=LINES+1
183 WRITE(6, 505) K,TWG(K),TWC(K),TWA(K)
      DO 3183 K=1,NR
      DO 3183 KK=1,NR
        FISVE(K,KK)=(0.0, 0.0)
        CAPVE(K,KK)=(0.0, 0.0)
        SCAVE(K,KK)=(0.0, 0.0)
3183 CONTINUE

```



```

WRITE(6,85)
WRITE(6,518) SWG,SWC,SWA
LINES=LINES+8
KCT=0
K=1
KMA=1
7000 IF(FU(K)-EMIN) 7003,7002,7001
7001 IF(FU(K)-EMAX) 7002,7002,7005
7002 KCT=KCT+1
7003 K=K+1
      KMA=K
      IF(K=NR) 7000,7000,7005
7005 CONTINUE
C
CALCULATE KAPUR-PEIERLS TYPE PARAMETERS
C
      IF(LINES-56+(KCT*KCT)) 1190,1190,1189
1189 WRITE(6,89)
      LINES=5
1190 CONTINUE
      LINES=LINES+2
      DO 184 K=1,NR
      DO 184 KK=1,NR
      DO 186 L=1,NR
      DO 186 LL=1,NR
      ZZ=DCONJG(TWGL,LL,KK)
      IF(L=LL) 188, 187, 188
188 FISVE(K,KK)=FISVE(K,KK)+2.0*GGIL,LL,J)*A(L,K)*ZZ
      GO TO 186
187 CAPVE(K,KK)=CAPVE(K,KK)+GGIL,J)*A(L,K)*ZZ
      FISVE(K,KK)=FISVE(K,KK)+ZZ*A(L,K)*DABS(GF(L,J))
      IF(IJW-3) 186,1188,186
1188 FISVE(K,KK)=FISVE(K,KK)+A(L,K)*ZZ*DABS(TETA(L,J))
186 CONTINUE
      ZZ=DCONJG(CDSORT(TWG(KK)))
      FACT=ZZ*CDSORT(TWG(K))
      ZZZ=(FISVE(K,KK)+CAPVE(K,KK)+FACT)/(DCONJG(EIGVAL(KK))-
1EIGVAL(K))
      XXR=DREAL(ZZZ)
      XXI=DAIMAG(ZZZ)
      SCAVE(K,KK)=DCMPLX(-XXI,XXR)
      FIN(K,KK)=FISVE(K,KK)*WG(K)*DCONJG(TWG(KK))
184 CAN(K,KK)=CAPVE(K,KK)*WG(K)*DCONJG(WG(KK))
      IF(KCT) 7007,7007,7004
7004 KMIN=KMA-KCT
      KMAX=KMA+1
      WRITE(6,550)
      DO 7006 K=KMIN,KMAX
      DO 7006 KK=KMIN,KMAX
      WRITE(6,551) K,KK,FISVE(K,KK),CAPVE(K,KK),SCAVE(K,KK)
7006 LINES=LINES+1
7007 DO 185 K=1,NR
      TWG(K)=WG(K)**2
      ALFA(K)=DREAL(TWG(K))
      BETA(K)=DAIMAG(TWG(K))
      TWA(K)=(0.00,0.00)
      TWC(K)=(0.00,0.00)

```

```

      DO 189 KK=1,NR
      FACT=DCONJG(EIGVAL(KK))-EIGVAL(K)
      TWA(K)=FIN(K,KK)/FACT+TWA(K)
189   TWC(K)=CAN(K,KK)/FACT+TWC(K)
      GFS(K)=-DAIMAG(TWA(K))
      GGA(K)=-DAIMAG(TWC(K))
      HFS(K)=DREAL(TWA(K))
185   HGA(K)=DREAL(TWC(K))
      GO TO 200

```

```

C
C SINGLE LEVEL EIGENVALUES
C

```

```

      174 NR=NO(J)
      PUNCH(1)=GFACT(J)
      WRITE(7,103)PUNCH(1),NO(J)
      IF(NR) 185,185,176
176   IF (154 - LINES - NR) 520,521,521
520   WRITE(6,89)
      LINES = 5
521   WRITE(6,500) J
      LINES = LINES + 6
      DO 178 K=1,NR
      S=DSQRT(ER(K,J))
      GA(K,K)=GF(K,J) +GON(K,J)*S/(GFACT(J)*4.0) +GG(K,J)
      XZ=-GA(K,K)/2.0
      EIGVAL(K)=DCMPLX(ER(K,J),XZ)
      XXG=-XZ
      LINES = LINES + 1
178   WRITE(6,501) K,ER(K,J),XXG
      WRITE(6,85)
      LINES=LINES+2

```

```

C
C SINGLE LEVEL PARAMETERS
C

```

```

      DO 191 K=1,NR
      FU(K)=ER(K,J)
      GU(K)=GA(K,K)/2.0
      BETA(K)=0.0
      HGA(K)=0.0
      HFS(K)=0.0
      GGA(K)=GON(K,J)*GG(K,J)/(2.0*GU(K))
      GFS(K)=GON(K,J)*GF(K,J)/(2.0*GU(K))
191   ALFA(K)=GON(K,J)

```

```

C
C STORE PARAMETERS
C

```

```

      200 IF (148 - LINES - NR) 509,510,510
509   WRITE(6,89)
      LINES = 5
510   WRITE(6,85)
      WRITE(6,508)
      LINES=LINES+6
      DO 190 K=1,NR
      DF(K,J)=FU(K)
      DW(K,J)=GU(K)
      BEG(K,J)=BETA(K)
      ALG(K,J)=ALFA(K)

```

```

CAPG(K,J)=GGA(K)
CAPH(K,J)=HGA(K)
FISG(K,J)=GFS(K)
FISH(K,J)=HFS(K)
LINES = LINES + 1
PUNCH(1)=FU(K)
PUNCH(2)=GU(K)
GRY=ALFA(K)/GU(K)
GIT=BETA(K)/GU(K)
GRF=GFS(K)/GU(K)
GIF=HFS(K)/GU(K)
GRC=GGA(K)/GU(K)
GIC=HGA(K)/GU(K)
WRITE(7,898)PUNCH(1),PUNCH(2),GRY,GIT,IONUM,
1      PUNCH(1),PUNCH(2),GRF,GIF,IONUM,
2      PUNCH(1),PUNCH(2),GRC,GIC,IONUM
190 WRITE(6,505) K,ALFA(K),BETA(K),GFS(K),HFS(K),GGA(K),HGA(K)
WRITE(6,85)
LINES=LINES+1
165 J=J+1
IF(J-2) 163,163,173
173 IF(J-4) 174,174,175
C
C BEGIN ENERGY DEPENDENT CALCULATION OF LEVEL MATRIX
175 IF(1SW-3) 524,525,524
524 WRITE(6,511)
GO TO 526
525 WRITE(6,531)
526 LINES=8
C
3 E=EMIN
30 ^=DSORT(E)
IF(1SW-3) 2003,2030,2003
2003 DO 60 J=1,4
6 NR=ND(J)
IF(NR) 60,60,55
55 DO 17 L=1,NR
VRE(L,J)=0.0
17 VIM(L,J)=0.0
Q1(J)=0.0
Q2(J)=0.0
GO TO (57,57,58,58),J
57 DO 7 L=1,NR
DO 7 LL=1,NR
Y=GON(L,J)*GON(LL,J)
IF(Y) 1157,1157,8
1157 SL=0.0
GO TO 1158
8 SL=DSORT(Y)
1158 G(L,LL)=G(L,LL,J)+ SL*S/14.0*GFACT(J)
7 CONTINUE
DO 111 K=2,NR
111 B(K,1)=0.0
BIT(1)=1.0
DO 11 L=1,NR
DO 11 LL=1,NR
11 A(INV(L,LL))=G(L,LL)

```

```

      CALL MATINV(AINV,NR,B,0,DETERM)
      DO 12 L=1,NR
      DO 12 LL=1,NR
      Q(L,LL)=AINV(L,LL)
12  QINV(L,LL)=G(L,LL)+Q(L,LL)*(ER(L,J)-E)*(ER(LL,J)-E)
      DO 112 K=2,NR
112  B(K,1)=0.0
      B(1,1)=1.0
      DO 120 L=1,NR
      DO 120 LL=1,NR
120  AINV(L,LL)=QINV(L,LL)
      CALL MATINV(AINV,NR,B,0,DETERM)
      DO 121 L=1,NR
      DO 121 LL=1,NR
121  QINV(L,LL)=AINV(L,LL)
      DO 14 L=1,NR
      DO 14 LL=1,NR
14  D(L,LL)=0.0
      DO 15 L=1,NR
      DO 15 LL=1,NR
      DO 15 M=1,NR
15  D(L,LL)=D(L,LL)+QINV(L,M)*(ER(M,J)-E)*Q(M,LL)
      DO 20 L=1,NR
      DO 20 LL=1,NR
      Y=DSQRT(GON(LL,J))
      VRE(L,J)=VRE(L,J)+D(L,LL)*Y
20  VIM(L,J)=VIM(L,J)+QINV(L,LL)*Y
      DO 21 L=1,NR
      Y=DSQRT(GON(L,J))
      Q1(J)=Q1(J)+VRE(L,J)*Y
      Q2(J)=Q2(J)+VIM(L,J)*Y
      GO TO 60
58  DO 59 L=1,NR
      GAM=GG(L,J)+GFL(L,J)+GDN(L,J)*S/(2.0*GFACT(J))
      GAM=GAM/2.0
      W=TER(L,J)-E)**2+GAM*GAM
      Y=DSQRT(GON(L,J))
      VRE(L,J)=Y*(TER(L,J)-E)/W
      Q1(J)=Q1(J)+Y*VRE(L,J)
      VIM(L,J)=Y*GAM/W
59  Q2(J)=Q2(J)+Y*VIM(L,J)
60  CONTINUE
C
C      CALCULATE UNBROADENED CROSS SECTIONS
C
19  SIGG=0.0
      SIGA=0.0
      SIGS=0.0
      ARG=2.0*WN*5
      SIGT=(1.0-DCOS(ARG))/S*2.0
      DO 22 J=1,4
      NR=ND(J)
      IF(NR) 22,22,66
66  DO 23 L=1,NR
      SIGG=SIGG+GG(L,J)*(VRE(L,J)**2+VIM(L,J)**2)
      GN(L,J)=GON(L,J)*S/(2.0*GFACT(J))
23  SIGS=SIGS+GN(L,J)*(VRE(L,J)**2+VIM(L,J)**2)

```

```

      SIGA=SIGA+Q21J1
      SIGT=SIGT-Q1T(J)*DSIN(ARG)*Q21J)*UCUS(ARG)
22  CONTINUE
      TOT=SIGT*CC/S
      CAP=SIGG*CC/(2.0*S)
      SIGS=SIGS*CC/(2.0*S)
      FIS=SIGA*CC/S-SIGS-CAP
      SCAT=TOT-FIS-CAP
      IF(1PUNCH) 1100,1100,1101

```

C
C ENERGY DEPENDENT CROSS SECTION CALCULATION A LA REICH-MOORE--
C NOVEMBER 1968--

```

2030 J=1
      SCAT=0.0
      FIS=0.0
      TOT=0.0
20 1 NR=ND(J)
      IF(NR) 2145,2145,2045
2045 NCH=NCHA(J)
      NM=NCH+1
      DO 2032 L=1,NM
      DO 2032LL=1,NM
      CAN(L,LL)=(0.0,0.0)
2032 ATL(LL)=(0.0,0.0)
      DO 2033 L=1,NM
      CAN(L,L)=(1.0,0.0)
2033 A(L,L)=(1.0,0.0)
      ARG=2.0*WN*S
      DO 2043 K=1,NR
      IF(GON(K,J)) 2034,2035,2034
2034 XX=S*GON(K,J)/(4.0*GFACT(J))
      XY=DSORT(XX)
      FISVE(K,1)=DCMPLX(XY,0.000)
      GO TO 2036
2035 FISVE(K,1)=(0.0,0.0)
2036 IF(GF(K,J)) 2037,2038,2037
2037 XX=DSORT(DABS(GF(K,J))/2.0)
      XX=XX*GF(K,J)/(DABS(GF(K,J)))
      FISVE(K,2)=DCMPLX(XX,0.000)
      GO TO 2039
2038 FISVE(K,2)=(0.0,0.0)
2039 IF(NCH=2) 2043,2040,2043
2040 IF(TETA(K,J)) 2041,2042,2041
2041 XX=DSORT(DABS(TETA(K,J))/2.0)
      XX=(TETA(K,J)/(DABS(TETA(K,J))))*XX
      FISVE(K,3)=DCMPLX(XX,0.000)
      GO TO 2043
2042 FISVE(K,3)=(0.0,0.0)
2043 CONTINUE
      DO 2131 K=1,NR
      XR=FR(K,J)-E
      XI=-GG(K,J)/2.0
      ZZZ=DCMPLX(XR,XI)
      DO 2130 L=1,NM
      DO 2130LL=1,NM
      ZZ=(0.0,1.0)
      A(L,LL)=A(L,LL)+ZZ*FISVE(K,L)*FISVE(K,LL)/ZZZ

```

```

2130 CAN(L,LL)=CAN(L,LL)- ZZ*FISVE(K,L)*FISVE(K,LL)/ZZZ
2131 CONTINUE
      CALL REVERT(NM)
      DO 2133 L=1,NM
      DO 2133 LL=1, NM
      SCAVE(L,LL)=(0.0,0.0)
      DO 2132 IL=1,NM
2132 SCAVE(L,CLT)=SCAVE(L,LL)+ATC,ILT)*FTN(ITL,CLT)
2133 CONTINUE
      SIGA=0.0
      DO 2134 L=2,NM
      ZZ=DCONJG(SCAVE(1,L))
      XX=DREAL(ZZ*SCAVE(1,L))
2134 SIGA=SIGA+XX
      ZZ=DCMPLX(0.000,-ARG)
      ZZZ=CDEXP(ZZ)
      ZT=ZZZ*SCAVE(1,1)
      ST=1.0-DREAL(ZZZ)
      ZZZ=SCAVE(1,1)*OCONJG(SCAVE(1,1))
      SIGS=1.0+DREAL(ZZZ)-2.0*DREAL(ZZ)
      SIGA=SIGA*GFACT(J)
      SIGS=SIGS*GFACT(J)
      SIGT=SIGT*GFACT(J)*2.0
      TOT=TOT+SIGT
      FIS=FIS+SIGA
      SCAT=SCAT+SIGS
      GO TO 2146
2145 TOT=TOT+2.0*GFACT(J)*1.0-DCOS(ARGT)
      SCAT=SCAT+2.0*GFACT(J)*(1.0-DCOS(ARG))
2146 J=J+1
      IF(J-2) 2031,2031,2140
C      ADDING SINGLE LEVEL CONTRIBUTIONS TO REICH-MOORE CASE--
2140 IF(J-4) 2151,2151,2150
2151 NR=NOIJ)
      IF(NR) 2146,2146,2152
2152 PART1=0.0
      PART2=0.0
      PARTA=0.0
      PARTC=0.0
      DO 2153 K=1,NR
      X=(DE(K,J)-E)
      BW=X**2 + DW(K,J)**2
      SEV=DW(K,J)/BW
      SOD=X/BW
      PART2=PART2+SEV*ALG(K,J)+SOD*BEG(K,J)
      PART1=PART1+SOD*ALG(K,J)-SEV*BEG(K,J)
      PARTA=PARTA+SEV*FISG(K,J)+SOD*FISH(K,J)
2153 PARTC=PARTC+SEV*CAPG(K,J)+SOD*CAPH(K,J)
      PARTS=PART2*DCOS(ARG)-PART1*DSIN(ARG)
      TOT=TOT+PARTS*S
      PARTS=PARTS-PARTA-PARTC
      SCAT=SCAT+PARTS*S
      FIS=FIS+PARTA*S
      GO TO 2146
2150 TOT=TOT*CC/E
      FIS=FIS*CC/E
      SCAT=SCAT*CC/E

```

```

CAP=TOT-FIS-SCAT
IF (IPUNCH) 1100,1100,1101
C
C PUNCHES DATA ON CARDS IF INDEX IPUNCH IS A POSITIVE INTEGER
1101 PUNCH 522, E, TOT, FIS, CAP, SCAT
C
C CALCULATE UNBROADENED CROSS SECTIONS FROM PARAMETERS-- FOR BOTH
C TYPE OF CALCULATION, I.E. VOGT AND REICH-MOORE---
C
1100 TOT2=TOT
FIS2=FIS
CAP2=CAP
SCAT2=SCAT
J=1
TOT=0.0
CAP=0.0
FIS=0.0
201 NR=ND(J)
IF (NR) 205,205,202
202 DO 203 K=1,NR
FU(K)=OE(K,J)
GUT(K)=DW(K,J)
ALFA(K)=ALG(K,J)
BETA(K)=BEG(K,J)
GFS(K)=FISG(K,J)
HFS(K)=FISH(K,J)
GGA(K)=CAPG(K,J)
203 HGA(K)=CAPH(K,J)
C
S=DSORT(E)
ARG=2.0*WN*S
CD=DCOS(ARG)
SI=DSIN(ARG)
PART1=0.0
PART2=0.0
DO 204 K=1,NR
X=FU(K)-E
BW=X*X+GUT(K)*GUT(K)
SEV=GUT(K)/BW
SOD=X/BW
PART1=PART1+ SOD*ALFA(K)-SEV*BETA(K)
PART2=PART2+ SOD*BETA(K)+SEV*ALFA(K)
FIS=FIS+SEV*GFS(K)+SOD*HFS(K)
204 CAP =CAP+SEV*GGA(K)+SOD*HGA(K)
TOT=TOT+CD*PART2-SI*PART1
205 J=J+1
IF (J-4) 201,201,206
206 CAP=CAP*CC/S
FIS=FIS*CC/S
TOT=TOT*CC/S + 2.0*CC*(1.0-CD)/E
SCAT=TOT - FIS - CAP
WRITE(6, 517) E,TOT2,TOT,FIS2,FIS,CAP2,CAP,SCAT2,SCAT
LINES=LINES+1
IF (LINES - 56) 207,512,512
512 IF (ISW-3) 519,529,519
519 WRITE(6,513)
WRITE(6,511)

```

```

      GO TO 530
529 WRITE(6,523)
      WRITE(6,531)
530 LINES=8
207 E=E+DELE
      IF(E=EMAX) 30,30,24
24 IF(LINES=8) 540,30, 515
515 DO 542 KL=LINES,53,3
542 WRITE(6,85)
      IF(ISW=3) 527,528,527
527 WRITE(6,513)
      GO TO 540
528 WRITE(6,523)
540 WRITE(6,2354)
      GO TO 1000

C
70 FORMAT (1H1, 55X,23HP R O G R A M L E M A//38X, 57HCALCULATION O
2F RESONANCE CROSS SECTIONS WITH LEVEL MATRIX/38X, 58BINVERSION AND
3 WITH COMPLEX EIGENVALUES OF THE LEVEL MATRIX//)
71 FORMAT (7H'ATM' = F7.2,10X, 5HWN = 1PE10.4,10X, 5HCC = 1PE10.4,10X,
27HEMIN = 0PF6.3,10X,7HEMAX = F6.3, 8X, 7HDELE = F5.4/55X,'R U N',
25X,A4//)
72 FORMAT (3H-J=11, 8X, 6HGFAC(11, 3H) =E10.4, 6X,3HND(11,3H) =12/)
73 FORMAT (1H 48X, 12, 5E15.6)
74 FORMAT(1H0/5X,'SINGLE LEVEL PARAMETERS',
1 20X, 1HX, 10X, 2HER,14X, 3HGON, 13X, 2HGG, 14X, 2HGF,
2 14X, 2HGN/)
75 FORMAT (1H-, 29X, 5HISW=1, 7X, 1HX, 8X, 2HER, 13X, 3HGON, 12X,
2 2HGG, 13X, 2HGF, 13X, 2HGN, 12X, 4HTETA/)
76 FORMAT (1H 40X, 12, 6E15.6)
77 FORMAT (1H-, 29X, 5HISW=2, 15X, 1HX, 9X, 2HER, 14X, 3HGON, 13X,
2 2HGG, 14X, 2HGF, 14X, 2HGN/)
84 FORMAT (1H-,29X,16HMATRIX GO(K,L,J),4X,1HX,5(3X,A8,12,A4))
85 FORMAT(1H0/)
89 FORMAT (1H1, 43X, ' P R O G R A M L E M A --C H A M A ---
177)
90. FORMAT (1H0, 50X, 5(3X, A8, 12, A4))
92 FORMAT (1H 48X, 12, 5E15.6)
100 FORMAT(6E12.3)
101 FORMAT(5F12.3)
102 FORMAT(215,A4)
103 FORMAT(1E12.3,215)
898 FORMAT(4E15.8,12X,'TOT ',A4 /4E15.8,12X,'FIS ',A4 /4E15.8,12X,'CAP
1 ',A4)
500 FORMAT(10X,'EIGENVALUES OF THE LEVEL MATRIX FOR THE DATA SET
1 J =', 13, // 32X,'K ', 16X,'MU',14X,'NO')
501 FORMAT (31X, 12, F21.5, F15.5)
504 FORMAT(1H,10X,' COMPLEX PARTIAL WIDTHS TO 1/2 POWER FOR TWO FISS
1STON CHANNELS--IN VOGT S CASE GAMF2 IS SET =0'//1H,22X,'GAMN',
223X,'GAMG',23X,'GAMF1',22X,'GAMF2',77X,1HX,7X,'REAL',8X,'IMAGINARY',
3,7X,'REAL',8X,'IMAGINARY',7X,'REAL',8X,'IMAGINARY',7X,'REAL',8X,'
4IMAGINARY'//)
505 FORMAT(6X,12,4(3X,E12.6,2X,E12.6))
508 FORMAT( 15X,'RESONANCE PARAMETERS IN UNITS OF EV TO 1/2 POWER--')
1 7X, 1HX 7X, 5HALPHA 10X, 4H
2BETA 11X, 4HGFIS 10X, 4HMFIS 11X, 4HGCAP 10X, 4H
511 FORMAT(1H1,54X, 'PROGRAM L E M A ' /

```



```

1          50X, 30H--UNBROADENED CROSS SECTIONS--///7H ENERGY, 1
20X, 5HTOTAL, 9X, 5HTOTAL, 11X, 7HFSSION, 7X, 7HFSSION, 10X, 7HCA
3PTURE, 7X, 7HCAPTURE, 8X, 10HSCATTERING, 4X, 10HSCATTERING/ 17X, 6
4H(LMA)* 7X, 8H(P.E.)* 10X, 5H(CMA), 9X, 6H(P.E.), 11X, 5H(CMA), 9X
5, 6H(P.E.), 11X, 5H(LMA), 8X, 6H(P.E.))//)
513  FORMAT (1H= 1X, 59H* (LMA) --- EVALUATED FROM INVERSION OF WIGNER C
2FVEL MATRIX/44H ** (P.E.) -- EVALUATED FROM POLES EXPANSION)
517  FORMAT (1H, F6.3, 3(F17.5, F14.5), F16.6, F14.6)
518  FORMAT(1H//1H, 10X, ' SUM OVER LEVELS OF THE COMPLEX PARTIAL WIDTHS'
1//1H, 10X, ' SUMGAMN= ', 2E12.4, 15X, ' SUMGAMG= ', 2E12.4//1H, 10X, '
2 SUM(GAMF1+GAMF2)= ', 2E12.4//)
522  FORMAT (5E15.8)
523  FORMAT (1H= 1X, 59H* (CMA)-EVALUATED WITH REICH-MOORE CHANNEL MATRI
1X INVERSION/44H ** (P.E.) -- EVALUATED FROM POLES EXPANSION)
541  FORMAT(1H1, 54X, 'PROGRAM C H A M A '//
1          50X, 30H--UNBROADENED CROSS SECTIONS--///7H ENERGY, 1
20X, 5HTOTAL, 9X, 5HTOTAL, 11X, 7HFSSION, 7X, 7HFSSION, 10X, 7HCA
3PTURE, 7X, 7HCAPTURE, 8X, 10HSCATTERING, 4X, 10HSCATTERING/ 17X, 6
4H(CMA)* 7X, 8H(P.E.)* 10X, 5H(CMA), 9X, 6H(P.E.), 11X, 5H(CMA), 9X
5, 6H(P.E.), 11X, 5H(CMA), 8X, 6H(P.E.))//)
550  FORMAT( ' INTERMEDIATE OUTPUT FOR MATRICES X FOR FISSION AND
1CAPTURE AND MATRIX Y FOR THE LEVELS BETWEEN EMIN AND EMAX'//
2          13X, 'K', 3X, 'KK', 4X, 'XFISS(K, KK)', 24X, 'XCAPT(K, KK)',
324X, 'Y-MATRIX'//)
551  FORMAT (10X, 2I4, 2E15.4, 4X, 2E15.4, 4X, 2E15.4)
560  FORMAT(1H, 10X, ' COMPLEX PARTIAL WIDTHS' //22X, 'GAMN IN EV ',
1 10X, 'GAMG IN EV', 16X, 'GAMF IN EV'//
2          7X, 1RK, 7X, 'REAL', 8X, 'IMAGINARY'
2, 7X, 'REAL', 8X, 'IMAGINARY', 7X, 'REAL', 8X, 'IMAGINARY'//)
2350 FORMAT(1H//, ' ISW=3--REICH-MOORE PARAMETERS WITH ', 17, ' OPEN
1FISSION CHANNELS'//7X, 1HK, 9X, 2HER, 12X, 3HGON, 13X, 2HGG, 12X, 3HGF1, 12
2X, 3HGF2, 13X, 2HGN//)
2351 FORMAT(6X, 12, 6E15.4)
2352 FORMAT (1H1, 55X, 25HP R O G R A M ' C H A M A '//38X, 'CALCULATION OF
2 RESONANCE CROSS SECTIONS WITH CHANNEL MATRIX INVERSION'/38X, 'AND
2 WITH COMPLEX EIGENVALUES OF THE LEVEL MATRIX'//)
2354 FORMAT(1H1/)
END

```

```

SUBROUTINE MATINV(A,N,B,M,DETERM)
C   MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS
REAL*8 A(33,33),B(33,1),PIVOT(33),AMAX,T,SWAP,DETERM
DIMENSION IPIVOT(33),INDEX(33,2)

C   INITIALIZATION
C
DETERM=1.0
DO 20 J=1,N
20 IPIVOT(J)=0
DO 550 I=1,N

C   SEARCH FOR PIVOT ELEMENT
C
AMAX=0.0
DO 105 J=1,N
IF (IPIVOT(J)-1) 60, 105, 60
60 DO 100 K=1,N
IF (IPIVOT(K)-1) 80, 100, 740
80 IF (DABS(AMAX)-DABS(A(J,K))) 85, 85, 100
85 IROW=J
ICOLUMN=K
AMAX=A(J,K)
100 CONTINUE
105 CONTINUE
IPIVOT(ICOLUMN)=IPIVOT(ICOLUMN)+1

C   INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL
C
IF (IROW-ICOLUMN) 140, 260, 140
140 DETERM=-DETERM
DO 200 L=1,N
SWAP=A(IROW,L)
A(IROW,L)=A(ICOLUMN,L)
200 A(ICOLUMN,L)=SWAP
IF(M) 260, 260, 210
210 DO 250 L=1, M
SWAP=B(IROW,L)
B(IROW,L)=B(ICOLUMN,L)
250 B(ICOLUMN,L)=SWAP
260 INDEX(I,1)=IROW
INDEX(I,2)=ICOLUMN
PIVOT(I)=A(ICOLUMN,ICOLUMN)
CC   INSTRUCTION ERASED TO AVOID UNDER OR OVERFLOW*****
C**** DETERM=DETERM*PIVOT(I)
IF(PIVOT(I)) 330,720,330

C   DIVIDE PIVOT ROW BY PIVOT ELEMENT
C
330 A(ICOLUMN,ICOLUMN)=1.0
DO 350 L=1,N
350 A(ICOLUMN,L)=A(ICOLUMN,L)/PIVOT(I)
IF(M) 380, 380, 360
360 DO 370 L=1,M
370 B(ICOLUMN,L)=B(ICOLUMN,L)/PIVOT(I)

C   REDUCE NON-PIVOT ROWS

```

C

```
380 DO 550 L=1,N
    IF (L1-ICOLUM) 400, 550, 400
400 T=A(L1,ICOLUM)
    A(L1,ICOLUM)=0.0
```

```
DO 450 L=1,N
450 A(L1,L)=A(L1,L)-A(ICOLUM,L)*T
    IF (M) 550, 550, 460
460 DO 500 L=1,M
500 B(L1,L)=B(L1,L)-B(ICOLUM,L)*T
550 CONTINUE
```

C INTERCHANGE COLUMNS

C

C

```
DO 710 I=1,N
    L=N+1-I
    IF (INDEX(L,1)-INDEX(L,2)) 630, 710, 630
630 JROW=INDEX(L,1)
    JCOLUM=INDEX(L,2)
    DO 705 K=1,N
        SWAP=A(K,JROW)
        A(K,JROW)=A(K,JCOLUM)
        A(K,JCOLUM)=SWAP
```

705 CONTINUE

710 CONTINUE

RETURN

720 WRITE(6,730)

730 FORMAT(20H 'MATRIX IS SINGULAR')

740 RETURN

END

```

SUBROUTINE REVERT(NM)
  REAL*8  RET
  COMPLEX*16 CAN(33,33),FIN(33,33),DET
  COMMON CAN,FIN
  GO TO (1,100,200),NM
1  SET=CAN(1,1)*DCONJG(CAN(1,1))
  IF(BFT) 2,3,2
2  FIN(1,1)=1.0/CAN(1,1)
  GO TO 4
3  WRITE(6,1000) NM
4  RETURN
1000 FORMAT(' THE CHANNEL MATRIX, OF RANK',I2,' IS SINGULAR'/'
100  DET=CAN(1,1)*CAN(2,2)-CAN(1,2)*CAN(1,2)
  RET=DET*DCONJG(DET)
  IF(RET) 101,3,101
101  FIN(1,1)=CAN(2,2)/DET
  FIN(2,2)=CAN(1,1)/DET
  FIN(1,2)=-CAN(1,2)/DET
  FIN(2,1)=FIN(1,2)
  RETURN
200  DET=CAN(1,1)*CAN(2,2)*CAN(3,3)+2.0*CAN(1,2)*CAN(2,3)*CAN(1,3)-
  1CAN(2,2)*CAN(1,3)*CAN(1,3)-CAN(1,1)*CAN(2,3)*CAN(2,3)-CAN(3,3)*
  2CAN(1,2)*CAN(1,2)
  RET=DET*DCONJG(DET)
  IF(BFT) 210,3,210
210  L=1
  L1=2
  L2=3
  GO TO 201
202  L1=1
  GO TO 201
203  L2=2
  GO TO 201
201  FIN(L,L1)=(CAN(L1,L1)*CAN(L2,L2)-CAN(L1,L2)*CAN(L1,L2))/DET
  L=L+1
  IF(L-3) 202,203,204
204  L=1
  LL=2
  LK=3
  GO TO 205
205  FIN(L,LL)=(CAN(L,LL)*CAN(LL,LK)-CAN(L,LL)*CAN(LK,LK))/RET
  FIN(LL,L1)=FIN(L,LL)
  L=L+1
  IF(L-3) 206,207,208
206  L1=3
  LK=1
  GO TO 205
207  L1=1
  LK=2
  GO TO 205
208  RETURN
END

```

```

SUBROUTINE REARR(NR,EIGVAL)
C      SUBROUTINE TO REARRANGE THE EIGENVALUE VECTOR IN ORDER
C      OF INCREASING VALUE.      ---JULY 1968-----
REAL*8 FU(33),STR2,DREAL
COMPLEX*16 EIGVAL(33),STR1
IF(NR=1) 30,30,10
10 DO 12 K=1,NR
12 FU(K)=DREAL(EIGVAL(K))
DO 25 K=1,NR
KSMAL=K
DO 20 J=K,NR
IF(FU(J)-FU(KSMAL)) 15,15,20
15 KSMAL=J
20 CONTINUE
IF(KSMAL-K) 21,25,21
21 STR1=EIGVAL(K)
EIGVAL(K)=EIGVAL(KSMAL)
EIGVAL(KSMAL)=STR1
STR2=FU(K)
FU(K)=FU(KSMAL)
FU(KSMAL)=STR2
25 CONTINUE ----
30 RETURN
END

```

```

SUBROUTINE FRANCI (A,VALU,NSUB,ANORM,NMAX)
C
C   DIMENSION A(NMAX,NSUB), VALU(NMAX)
C*** REMOVE OR MODIFY NEXT FOUR STATEMENTS IN SINGLE PRECISION VERSION
COMMON /QR/ ITER(200), DUMMY(500)
C*** NEXT STATEMENT ADDED OR REWRITTEN TO BYPASS BUG IN COMPILER
COMPLEX*16 A,VALU,ANN,DIF,DISCSQ,DISC,E,G
REAL*8 DEL,ANORM2,ANORM,EPS,DUMMY
DATA EPS/2338000000000000000/
C
C   KITER=0
C   N=NSUB
C
C   REDUCE MATRIX TO UPPER HESSENBERG FORM (WITH REAL SUBDIAGONAL)
C
C   CALL SUBDIA(A,N,NMAX)
C
C   COMPUTE MATRIX NORM
C
C   ANORM2=0.00
C   DO 40 I=1,N
C     I1=I-1+1/I
C   DO 40 J=I1,N
C**** CHANGE FUNCTION NAME IN NEXT STATEMENT IN SINGLE PRECISION
C   ANORM2=ANORM2+A(I,J)*DCONJG(A(I,J))
C   40 CONTINUE
C   ANORM2=DABS(ANORM2)
C**** CHANGE FUNCTION NAME IN NEXT STATEMENT IN SINGLE PRECISION
C   ANORM=DSQRT(ANORM2)
C
C   DEL=ANORM*EPS
C
C   BEGINNING OF LOOP FOR ITERATIVE DETERMINATION OF EIGENVALUES
C   (ARRAY ITER HAS EFFECTIVELY BEEN CLEARED TO ZERO BY SUBDIA)
C
C   50 K=NSUB+1-N
C
C   FIND ROOTS OF LOWER 2X2 MINOR
C
C   60 ANN=A(N,N)
C   IF (N-1) 250, 220, 70
C   70 IF( ABS( REAL(A(N,N-1))) .LE. DEL) GO TO 220
C**** NEXT TWO STATEMENTS ADDED OR REWRITTEN TO BYPASS BUG IN COMPILER
C   HALF=(0.500,0.000)
C   DIF=(A(N-1,N-1)-ANN)*HALF
C   DISCSQ=DIF**2+A(N-1,N)*A(N,N-1)
C**** CHANGE FUNCTION NAME IN NEXT STATEMENT IN SINGLE PRECISION
C   DISC=DSQRT(DISCSQ)
C   F=DISC+DIF+ANN
C   G=F-DISC-DISC
C   IF (N.F0.2) GO TO 230
C   IF( ABS( REAL(A(N,N-1))) .LE. DEL) GO TO 230
C
C   CHOOSE SHIFT TOWARD ACCELERATING CONVERGENCE
C   (ROOT OF LOWER 2X2 MINOR CLOSEST TO LAST DIAGONAL ELEMENT)
C

```

```

C**** CHANGE FUNCTION NAMES IN NEXT TWO STATEMENTS IN SINGLE PRECISION
Z1=(E-ANN)*DCONJG(E-ANN)
Z2=(G-ANN)*DCONJG(G-ANN)
IF (Z2.LT.Z1) E=G
KITER=KITER+1
IF(KITER.GT.100) GO TO 249
C
C   PERFORM QR ITERATION
C
C   CALL QR1(A,N,DEL,E,NMAX)
C
ITER(K)=ITER(K)+1
GO TO 60
C
C   SINGLE EIGENVALUE CONVERGED
C
220 VALU(K)=ANN
N=N-1
GO TO 50
C
C   PAIR OF EIGENVALUES CONVERGED
C
230 VALU(K)=E
VALU(K+1)=G
N=N-2
GO TO 50
C
249 WRITE(6,1)
1   FORMAT(1H,'THE NUMBER OF ITERATIONS EXCEEDS 100,EXECUTION OF FRAN
CCT IS TERMINATED')
250 RETURN
END
SUBROUTINE QR1(A,N,DEL,ZET,NMAX)
C
C   SINGLE COMPLEX QR ITERATION
C
C
C   DIMENSION A(NMAX,N)
COMMON /QR/ DUMMY(100), NU(100), MU(100), CMU(100)
C**** REMOVE OR MODIFY NEXT TWO STATEMENTS IN SINGLE PRECISION VERSION
COMPLEX*16 A,ZET,MU,CMU,DIAG,W
REAL*8 DEL,KAP,NU,SUPERD,TEMPI,DUMMY
INTEGER Q
C**** NEXT STATEMENT ADDED OR REWRITTEN TO BYPASS BUG IN COMPILER
COMPLEX*16 X,Y,Z
C
N1=N-1
N2=N1-1
C
C   FIND Q
C
DO 50 I1=1,N2
I=N1-11
IF ( ABS( REAL(A(I+1,1))) .LE. DEL) GO TO 60
50 Q=I
C
C   SHIFT ORIGIN
C

```

```

      AD DD 100 I=Q,N
100 A(I,I)=A(I,I)-ZET
C
C      REDUCE TO TRIANGLE (ROWS)
C
      DD 200 I=Q,N
      DIAG=A(I,I)
      SUPERD=0.00
      IF (I.EQ.N) GO TO 150
      SUPERD=A(I+1,I)
      A(I+1,I)=(0.00,0.00)
C**** CHANGE FUNCTION NAMES IN NEXT TWO STATEMENTS IN SINGLE PRECISION
150 TEMP1=DIAG*DCONJG(DIAG)
      KAP=DSQRT(0.000001+TEMP1*TEMP1+SUPERD**2)
      MU(I)=DIAG/KAP
C**** CHANGE FUNCTION NAME IN NEXT STATEMENT IN SINGLE PRECISION
      CMU(I)=DCONJG(MU(I))
      NUT(I)=SUPERD/KAP
      A(I,I)=KAP
      IF (I.EQ.N) GO TO 200
      I=I+1
      DD 199 J=I,N
      W=A(I,J)
C**** NEXT FIVE STATEMENTS ADDED OR REWRITTEN TO BYPASS BUG IN COMPILER
      X=DCMPLX(MU(I),0.00)
      Y=MU(I)
      Z=CMU(I)
      A(I,J)=W*Z+X*A(I+1,J)
199 A(I+1,J)=Y*A(I+1,J)-X*W
200 CONTINUE
C
C      INVERSE OPERATION (COLUMNS)
C
      DD 300 J=Q,N1
      J1=J+1
      DD 300 I=Q,J1
      W=A(I,J)
C**** NEXT FIVE STATEMENTS ADDED OR REWRITTEN TO BYPASS BUG IN COMPILER
      X=DCMPLX(MU(J),0.00)
      Y=MU(J)
      Z=CMU(J)
      A(I,J)=W*Y+X*A(I,J+1)
      A(I,J+1)=Z*A(I,J+1)-X*W
300 CONTINUE
      J=N
C**** NEXT STATEMENT ADDED OR REWRITTEN TO BYPASS BUG IN COMPILER
      Y=MU(J)
      DD 400 I=Q,N
C**** NEXT STATEMENT ADDED OR REWRITTEN TO BYPASS BUG IN COMPILER
      A(I,J)=Y*A(I,J)
400 A(I,I)=A(I,I)+ZET
      RETURN
      END
      SUBROUTINE STURDAT(A,N,NMAX)
C
C      HOUSEHOLDER REDUCTION OF COMPLEX MATRIX TO UPPER HESSENBERG FORM
C

```



```

        DIMENSION A(NMAX,N), WVEC(100), PVEC(100), QVEC(100), CWVEC(100)
        COMMON /QR/ WVEC, PVEC, CWVEC
        EQUIVALENCE (PVEC,QVEC)
C**** REMOVE OR MODIFY NEXT TWO STATEMENTS IN SINGLE PRECISION VERSION
        COMPLEX*16 A,WVEC,PVEC,QVEC,DIV,SCALAR,CWVEC
C**** NEXT STATEMENT ADDED OR REWRITTEN TO BYPASS BUG IN COMPILER
        COMPLEX*16 TWO
        REAL*8 TEMP,SUM,TEMP1
C
        DO 200 I=1,N
C
C      REDUCE COLUMN OF MATRIX
C
        WVEC(I)=(0.00,0.00)
        IF (I.EQ.N) GO TO 200
        I1=I+1
        I2=I1+1
C
C      SIMILARITY TRANSFORMATION TO PRODUCE REAL SUBDIAGONAL ELEMENT
C
        J=I1
C**** CHANGE FUNCTION NAME IN NEXT STATEMENT IN SINGLE PRECISION
        TEMP1=COABS(A(J,I))
        IF (TEMP1.EQ.0.0) GO TO 60
        DIV=A(J,I)/TEMP1
        DO 30 K=1,N
        30 A(K,J)=DIV*A(K,J)
        DO 40 K=I,N
        40 A(J,K)=A(J,K)/DIV
C
        60 IF (I2.GT.N) GO TO 200
        SUM=0.00
        DO 70 J=I2,N
C**** CHANGE FUNCTION NAME IN NEXT STATEMENT IN SINGLE PRECISION
        70 SUM=SUM+A(J,I)*DCONJG(A(J,I))
        SUM=DABST(SUM)
        IF (SUM.EQ.0.0) GO TO 200
        J=I1
        TEMP=A(J,I)
C**** CHANGE FUNCTION NAMES IN NEXT THREE STATEMENTS IN SINGLE PRECISION
        SUM=DSQRT(DABS(SUM+TEMP**2))
        ATJ,I)=DCMPLX(1,DSIGN(SUM,TEMP),0.000)
        TEMP1=DSQRT(1.00+DABS(TEMP)/SUM)
        WVEC(I)=TEMP1
        CWVEC(J)=WVEC(I)
C**** CHANGE FUNCTION NAME IN NEXT STATEMENT IN SINGLE PRECISION
        DIV=DSIGN(TEMP1*SUM,TEMP)
        DO 85 J=I2,N
        WVEC(J)=A(J,I)/DIV
C**** CHANGE FUNCTION NAME IN NEXT STATEMENT IN SINGLE PRECISION
        CWVEC(J)=DCONJG(WVEC(J))
        85 CONTINUE
        SCALAR=(0.00,0.00)
        DO 95 J=I1,N
        PVEC(J)=(0.00,0.00)
        DO 90 K=I1,N
        90 PVEC(J)=PVEC(J)+A(K,J)*CWVEC(K)

```

```

        SCALAR=SCALAR+PVEC(J)*WVEC(J)
95 CONTINUE
C+** NEXT TWO STATEMENTS ADDED OR REWRITTEN TO BYPASS BUG IN COMPILER
        TWO=(2.000,0.000)
        SCALAR=SCALAR/TWO
        DO 120 J=11,N
            QVEC(J)=PVEC(J)-SCALAR*CWVEC(J)
            DO 120 K=11,N
                A(K,J)=A(K,J)-WVEC(K)*QVEC(J)
120 CONTINUE
            DO 180 K=1,N
                QVEC(K)=-SCALAR*WVEC(K)
            DO 170 J=11,N
170 QVEC(K)=QVEC(K)+A(K,J)*WVEC(J)
            DO 180 J=11,N
                A(K,J)=A(K,J)-QVEC(K)*CWVEC(J)
180 CONTINUE
C
200 CONTINUE
C
        RETURN
        END

```

APPENDIX E

TRIPLE: A Fortran IV program for the threefold least-squares analysis of neutron cross section data with the multilevel formalism.[†]

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TABLE OF CONTENTS

	Page
Summary	107
I. Introduction	107
II. Method of Analysis	112
A. Basic problems related to the triple fit	112
B. Multilevel expansions	115
III. Least Squares Equations for the Simultaneous Fitting of Three Cross Section Sets	117
IV. Definition of the Trial Functions	120
A. Multilevel Expansion with Doppler Broadening	120
B. Resolution Effects on Reaction Cross Sections	122
C. Total Cross Section	123
V. Constraints for the Triple Fit	127
A. Simultaneous Analysis of Total Fission and Capture Data (IFIT = 1, and IFIT = 5)	127
B. Simultaneous Analysis of Three Data Sets for Two Cross Section Types	129
VI. Preliminary Calculations: Energy scale, statistical errors, and resolution functions. Subroutines ALIGN, WEIGHT, SIGRES, WIDTH..	131
VII. Calculations of the Trial Function for Single Data Sets: Subroutines YPHI, PHID0, SIGAP, SIGIN, SIGOUT.....	135
VIII. Solution of the Normal Equations: Subroutines SIGTRE, INVERT, TEST, SIGPLT, GRAPH	139
IX. Editorial Subroutines: Subroutines LEGE and SCRIBE	144
X. Auxiliary Subroutines: Subroutines WRITE And SKIP	146
Tables I through V	147-151
References	152

Summary

A flexible program for the correlated analysis of three neutron cross section sets in the low energy region, using the multilevel formalism, is described. The program TRIPLE simultaneously analyzes by least-squares fission capture and total cross section data, or three data sets of which two are independent measurements of the same reaction type. The Program, which can be adapted readily to interactive systems, as SCORE III-A, includes also a Calcomp plotter routine displaying data, trial function, and deviations for each of the cross sections analyzed. The results can readily be used either for cross section evaluations in reactor physics applications, or as input for the derivation of compatible R-matrix parameters.

I. INTRODUCTION

Low energy neutron cross sections of fissile elements have been analyzed by a least-squares procedure employing a multilevel expansion which is derived from the Wigner-Eisenbud theory of nuclear reactions.^{1,2/} To each resonance level, a pair of parameters μ and ν , describing the resonance energy and the half-width, is assigned. For a given type of cross section (total, fission, capture or scattering) each level is also characterized by two line-shape parameters, G and H , which are the coefficients of the symmetrical and asymmetrical line shape functions respectively.^{3/} In order to take into account properly the channel-level interferences it is essential to include in the least squares analysis effects of neighboring and distant levels. A finite number of close levels, or of levels having known parameters is thus introduced in the analysis, while the distant resonances are described by their asymptotic cumulative contributions, expressed as slowly varying background terms. In fitting a finite energy region, these background terms remain related to the region itself, and cannot be used in

general to express the same type of contribution for different energy intervals, in contrast to the line shape parameters G and H which continue to have the same meaning beyond the fitted region.

The level parameters μ and ν enter non-linearly in the trial functions, so that a convergence towards the best fitting set of values can be attained either by utilizing "non-linear" least squares procedures,^{4/} or by repetitive linear fits, among which a best fitting set is selected with the aid of graphic displays and of appropriate numerical tests, or by interactive modes.^{5/}

One of the goals of the analysis of measured data is the derivation of parameter sets describing in a compatible manner all the cross sections of the same nuclide, to be of use in reactor physics calculations. Thus, in analyzing total and fission cross sections separately, it is necessary to verify, a posteriori, that the two data sets are well fitted by the same set of values of μ and ν , and that the scattering and capture curves evaluated from the fitted parameters of total and fission give a realistic result. For example, in the analysis of total and fission data of ²³⁹Pu the available measured η values^{6/} have been used as a guide line to determine parameters compatible with total, fission and η data, although the latter could not be included in the fit. Auxiliary routines were used for this purpose, as reported earlier.^{7/}

The less cumbersome procedure, of analyzing simultaneously fission and capture data, simultaneously measured, offers advantages, but it is not sufficient to determine accurately the total cross section parameters.^{8/}

By simultaneous analysis of three data sets, such as total, fission, and capture, the compatibility of the parameters describing the resonance lines is introduced as a condition, that the values of μ and ν be shared by the three data sets, and that unitarity be satisfied as relations of sums among the line shape parameters, of total, fission, and capture resonances.

Program TRIPLE is a Fortran IV program for the least squares analysis of three cross section sets of the same nuclide, with the multilevel expansion. The program includes also the possibility of fitting simultaneously data sets of which two represent the same type of cross section, measured in different experiments. The question, often raised,^{9/} about the uniqueness of multilevel parameters in the context of least squares analysis, may be more exactly defined by comparing in the fitting procedures different data sets for the same type of cross section.

The earlier version of TRIPLE^{10/} contains non-linear searching routines for the "best values" of μ and ν . These routines cannot be entirely automated,^{3/} and require often repetitive runs.

The experience made with interactive systems^{11/} has shown that, for the same amount of human judgment applied to the problem, the careful use of an interactive system, such as SCORE III A,^{12/} substitutes efficiently the non-linear iteration scheme.

For this reason, the version of TRIPLE described here is limited to the part providing only linear fits. This program is a complement to Program CODILLI II,^{5/} and should be used after a preliminary analysis of the individual data sets with CODILLI II.

The reasons for this recommendation are as follows:

(1) Measured data contain impurities, the concentrations of which are not always exactly specified. It is possible to fit impurities, and to subtract their contributions, in analyzing data with CODILLI II. Data sets from which the impurities have been eliminated can then be treated in TRIPLE, in which the introduction of impurities (often different from a set of data to another) would represent a sizeable increase in storage locations, and complications in its use.

(2) Transmission data can properly be treated only if preliminary parameter values of the total cross section are known from start. These can be obtained from preliminary test runs with CODILLI II.

(3) One of the two branches of TRIPLE for the analysis of total, fission, and capture cross sections requires preliminary information on the values of the scattering parameters. These are obtainable from data fitting of total and of scattering data from CODILLI II.^{13/}

(4) Finally, the choice of the resonance energies μ and ν , for a given data set, can be readily made using CODILLI II, either interactively, or in the batch mode, which includes the possibility of rapid iterations on selected values of μ and ν .^{14/} The accurate definition of at least two values of μ within a given energy interval is essential, when it becomes necessary to compare the energy scales of different data sets. As discussed in Section II, this problem is treated in TRIPLE, within a special subroutine, so that, for all these data sets, the energy scale used in the fitting procedure is unified. In contrast to other approaches,^{15/} the individual data arrays, for each data set, are kept separate through the fitting, while the energy scales are made to be the same for the three sets. Similarly, resolution and temperature effects are calculated independently for each data set.

The final output of the Program consists of sets of resonance parameters μ , ν , $G^{(\ell)}$, $H^{(\ell)}$, where $\ell = 1, 2, 3$ for total fission and capture analysis, or $\ell = 1, 2$ for the case of two identical cross sections. These parameters, which are also given as punched output, can be further used as follows:

- (1) for calculations of Doppler broadened cross section values,
- (2) for subsequent least squares fits in different energy ranges
- (3) as "input" for programs designed to extract R-matrix parameters from the multilevel parameters.^{16,17/}

Anticipating the possibility of interpreting the multilevel parameters in terms of R-matrix parameters, for the case in which total, fission, and capture data are fitted, program TRIPLE also provides zero order values of the partial reaction widths, obtainable from perturbation calculations.^{18/}

The program is described in the following sections. In Section II the general physical problems connected with the fitting are summarized together with the basic notations used in the text. Section III describes the structure of the least squares equations for the triple fit.

In Section IV are discussed the general properties of the trial functions, and in Section V the types of constraints encountered.

Sections VI to X contain a description of the interrelated mathematical aspects of the Program, and of the subroutines necessary for the calculation.

A summary of the test problem used in the code checks, the program listing, and detailed description of input and output formats are given separately in Part 2 of this report.

II. METHOD OF ANALYSIS

A. Basic problems related to the triple fit

The method of analysis used in the Program TRIPLE is based on the multilevel expansions which have been employed in the Program CODILLI,^{4,5/} with some modification in the treatment of the background terms. Three independently measured data sets, for the same nuclide, can be fitted simultaneously with TRIPLE by least squares techniques. The three data sets may arise from different measurements, and be characterized by different sets of data points and different experimental conditions. These different conditions imply often not only different sample temperatures, different resolution functions and different energy scales, but also different types of impurities or different concentrations. All these aspects have to be taken into account in order to obtain meaningful results.

The purpose is to derive compatible multilevel parameters fitting the data, and, possibly, closely fitting other data sets; uniqueness of results with least squares analysis cannot be a goal, by repeatedly stated by numerous investigators. Compatibility can be, to some extent, introduced by constraints among the multilevel parameters describing the data. The basic constraint is the "natural" one, that resonance energies and half-widths be shared by the three sets, as representative of the fissile element.

Others, equally straightforward when treating fission capture and total cross sections, will reflect the unitarity of the formalism, that, for each resonance:

$$\left. \begin{aligned} \sum_{(x)} G^{(x)} &= \alpha^0 \\ \sum_{(x)} H^{(x)} &= \beta^0 \end{aligned} \right\} \quad (1)$$

where (x) represents a "reaction" (as scattering, fission, and capture), and α^0, β^0 are the line shape parameters of the total cross section. When treating two sets of the same type (e.g., two sets of fission data and one capture) the parameters of the double set (e.g. fission) will be made to be compatible with both cross section data.

From this version of TRIPLE non-linear iterations on the values of μ, ν (resonance energy and half width) have been excluded as opposed to the original version. The elimination of this branch was made after the testing of CODILLI II with SCORE III-A.^{11/} The experience with the interactive mode of CODILLI II with SCORE III-A has shown that the interactive selection of resonance energies and half width is, in principle, more effective than non-linear searching routines incorporated in the Program.

This version of TRIPLE should be used, therefore, as a complementary tool, after initial sets of parameters were derived from CODILLI II.

This requirement also applies to the treatment of the impurities, the introduction of which would enlarge anomalously the storage locations of TRIPLE. In CODILLI II^{5/} impurities can be fitted, or treated as known contributions, depending on how well defined are the values of the relative concentrations. An ad hoc branch has been introduced in CODILLI II so as to subtract the contributions of the impurities, and to generate data sets suited for use with TRIPLE.^{14/} The elimination of these problems has permitted to assemble a version of TRIPLE which is relatively compact, and in which all other problems tied to the simultaneous analysis of three data sets can be treated efficiently. These aspects of the analysis are listed below and described in detail in Section VI.

Energy scale Different data sets, except when derived from simultaneous measurements,^{19,20/} are defined generally at different points, and frequently present slight shifts in the energy scales. These are most evident in comparing for example the symmetrical lines of those impurities which may occur in both data sets (e.g., ^{240}Pu in the ^{239}Pu measurements of the total cross section at Saclay,^{21/} and in the ^{239}Pu capture data of ORNL-RPI ^{20/}), or in comparing large peaks of narrow resonances.

As discussed by G. de Saussure^{19/} these calibration errors arise from uncertainties in the measurements of the parameters defining the energy values. Often this difference is "small," but it results in apparently poor fits, if the values of the resonance energies fitting one data set are forced to describe the other set.

This difficulty can be overcome by selecting, within a given energy interval, two resonances as "bench-marks," and calculating the relative shift from one set to another. The entire array of energy points of one set can thus be shifted, to overlap the energy points of the other. In this manner TRIPLE aligns internally all data sets on a "unified scale," in reference to one of the three data sets. This calculation, preliminary to the fitting, is handled in the Subroutine ALIGN (Section VI).

Statistical errors. Different data sets have different errors. These are usually given either as listed values,^{21/} or in terms of algebraic relations permitting to calculate them from the data.^{20/} The first case offers no problem (but one of storage locations). In the second case, preliminary calculations are needed to generate the error values, along with the data, for each data point. The statistical weights are accordingly evaluated in the Subroutine WEIGHT (Section VI).

Resolution effects. For each data set a separate resolution broadening prescription is given, defining the type of resolution function. Program TRIPLE contains provisions for a variety of possibilities, through the Subroutine SIGRES (Section VI).

For Gaussian resolution function the subroutine WIDTH (Section VI) provides the energy dependent values of the resolution width, which is given as a prescribed function of the energy with parameters which depend on the specific experimental conditions of the measurement. This subroutine therefore may need to be replaced by others, depending on the data used.

For resolution functions other than Gaussian the subroutine SIGRES should be adapted case by case, according to the data.

B. Multilevel expansions

The multilevel expansion used in TRIPLE have been described previously,^{4/} and are summarized here. For a reaction cross section $\sigma^{(x)}$ the theoretical expansion is given by

$$\sigma_t^{(x)}(E) \sqrt{E} = C \left\{ \sum_{k=1}^N \frac{G_k^{(x)} v_k + H_k^{(x)} (\mu_k - E)}{(\mu_k - E)^2 + v_k^2} + \sum_{j=1}^{KNEG} A_j^{(x)} \sqrt{E}^{1-j} + \sum_{j=1}^{KPOS} B_j \sqrt{E}^j \right\} \quad (2)$$

where N represents the number of resonances related to a given energy interval, μ_k is the resonance energy, v_k the half-width, $G_k^{(x)}$, $H_k^{(x)}$ the symmetrical and asymmetrical line shape parameters for the k-th level. The terms of the second and third summation represent the background effects of the distant resonances.^{3/}

For the total cross section one has similarly:

$$\sigma_t^{\text{tot}}(E) = \frac{C}{\sqrt{E}} \left\{ \frac{2(1-\cos\omega)}{\sqrt{E}} + \sum_{k=1}^N \frac{(\alpha_k^0 \cos\omega + \beta_k^0 \sin\omega) v_k + (\beta_k^0 \cos\omega - \alpha_k^0 \sin\omega) (\mu_k - E)}{(\mu_k - E)^2 + v_k^2} \right. \\ \left. + \sum_{j=1}^{\text{KNEG}} A_j^T \sqrt{E}^{1-j} + \sum_{j=1}^{\text{KPOS}} B_j^T \sqrt{E}^{-j} \right\} \quad (3)$$

where ω represents the potential scattering phase shift, and α_k^0, β_k^0 are the symmetrical and asymmetrical parameters for the k -th level in the total cross section. In Eq. (2) and (3) $C = 6.52 \times 10^5$ barns eV, $\sigma^{(x)}, \sigma^{\text{tot}}$ are in barns; E, μ_k , and v_k in eV, $G^{(x)}, H^{(x)}, \alpha^0, \beta^0$ in $(\text{eV})^{\frac{1}{2}}$. The summation over N is understood over all the resonances related to a given energy interval, without spin states separation.

The background constants A, B describe the cumulative effect of distant resonances, combined with effects of the energy dependence of the neutron width.^{22/} While the asymptotic contributions of the distant resonances give terms in positive and negative powers of E ,^{3/} the energy variation of the neutron width introduces corrections in terms of $\sqrt{E}$.^(*) These corrections are in general small for fissile elements ($\Gamma_n < \Gamma_f$). On the other hand, the distant resonance effects tend to vanish if in N are included many resonances external to the energy interval of interest, and, in an ideal situation in which "all resonances" were known, the background terms would reduce purely to the corrections arising from Γ_n .

It should be emphasized that these background terms, whether in the approximation used in CODILLI II, or in the expansion inclusive of momentum dependent terms, are tied to the energy interval examined, and cannot be used to extrapolate the cross section curves beyond it.

(*) This modification was not introduced in CODILLI II, because of the strict requirement of adjusting the calculation to the ENDF-B Format.^{23/}

III. LEAST SQUARES EQUATIONS FOR THE SIMULTANEOUS FITTING OF THREE CROSS SECTION SETS.

The least squares sum for the analysis of an experiment which is a combination of several experiments can be written as sum of partial least squares sums whenever a common set of parameters can represent jointly the various experiments.

Using this general property, and generalizing a procedure used for the analysis of two data sets ^{8/} one can write the least squares sum S for the triple fit as

$$S = \sum_{l=1}^3 \lambda_l S_l \quad (4)$$

where S_l is the partial least squares sum (for the l -th data set)

$$S_l = \sum_{i=1}^{NP_l} [Y_x^{(l)}(E_i) - Y_t^{(l)}(E_i)]^2 w_i^{(l)} \quad (5)$$

and λ_l is a weighting factor,

$$0 < \lambda_l \leq 1 \quad (6)$$

introduced to express the relative importance of each data set. The choice $\lambda_l = 1$ for all values of l means that each data set is taken as equally important. Cases of "poor data" can be treated with a $\lambda_l < 1$ aiming to de-emphasize their effect in the fitting procedure, thus bringing the likelihood function

$$e^{-\lambda_l S_l}$$

of the "poor" set to the same order of magnitude as one of the "better" sets.

This decision can be made if the data have been separately pretreated, for example with CODILLI II.

In Eq. (6) $Y_x^{(\ell)}(E_i)$ represents the experimental value at the energy point E_i , for the set (ℓ) , $Y_t^{(\ell)}(E_i)$ the corresponding trial function, NP_ℓ the number of points of the set (ℓ) , and $w_i^{(\ell)}$ the statistical weight at the i -th point.

Representing the set of parameters to be fitted as a vector X , with NX components, the trial function for the set (ℓ) can be written in the form

$$Y_t^{(\ell)} = \sum_{j=1}^{NX} X_j M_{\ell j} + Y_0^{(\ell)} \quad (7)$$

where $Y_0^{(\ell)}$ is the known part of the trial function, and $M_{\ell j}$ are known functions of the energy. Although not all the unknowns X_j will appear in the expansion for a given set (ℓ) , these notations are useful to derive the appropriate normal equations.

Minimizing S one has

$$\frac{\partial S}{\partial X_m} = \sum_{\ell=1}^3 \lambda_\ell \sum_{i=1}^{NP_\ell} [Y_x^{(\ell)}(i) - Y_t^{(\ell)}(i)] w_i^{(\ell)} \sum_{\ell'=1}^3 M_{\ell'm}(i) = 0. \quad (8)$$

Because for $\ell' \neq \ell$ there are no points in common, the double sum reduces to a single sum, giving the system of normal equations:

$$R_m = \sum_k Q_{mk} X_k \quad (9)$$

where

$$R_m = \sum_{\ell=1}^3 \lambda_\ell \sum_{i=1}^{NP_\ell} w_i^{(\ell)} [Y_x^{(\ell)}(i) - Y_0^{(\ell)}(i)] M_{\ell m}(i) \quad (10)$$

$$Q_{mk} = Q_{km} = \sum_{\ell=1}^3 \lambda_\ell \sum_{i=1}^{NP_\ell} w_i^{(\ell)} M_{\ell k}(i) M_{\ell m}(i) \quad (11)$$

For indices, k, m , corresponding to components of X which are not shared by different data sets, Q reduces to block diagonal submatrices. For indices k, m , corresponding to parameters common to two, or three data sets, the block diagonal form is bordered by elements representing the correlation between the parameters shared by the different sets.

This structure is, of course, also the structure of the error matrix (reciprocal of Q) so that this procedure provides also the errors of the parameters and their correlation.

Because Q is symmetric and positive definite, its inversion can readily be obtained using the method of Cholesky which has the advantage of reducing to $n(n+1)/2$ the storage locations required for a matrix of rank n .

IV. DEFINITION OF THE TRIAL FUNCTIONS

In forming the trial functions for the least squares analysis from the theoretical cross section formulae given in Eqs. (2) and (3), Doppler and resolution effects need to be taken into account.^{19,24/}

A. Multilevel Expansion with Doppler Broadening

The temperature effects, introduced in the expansions (2) and (3), give the Doppler broadened σ_{DB} in the form

$$\sigma_{DB}^{(x)}(E) \sqrt{E/C} = \sum_{k=1}^N (GR_k^{(x)} \phi_k^{(s)} + GI_k^{(x)} \phi_k^{(a)}) + 2(1 - \cos\omega)/\sqrt{E} \\ + \sum_{j=1}^{KNEG} A_j \sqrt{E}^{1-j} + \sum_{j=1}^{KPOS} B_j^{(x)} \sqrt{E}^j \quad (12)$$

In Eq. (12) (x) may denote fission, capture, or total, and

$$\phi_k^{(s)} = \cos\omega \psi_k - \sin\omega \chi_k \quad (13)$$

$$\phi_k^{(a)} = \cos\omega \chi_k + \sin\omega \psi_k \quad (14)$$

The line shape parameters of Eqs. (2) and (3) are here scaled to give

$$GR_k^{(x)} = G_k^{(x)} / v_k \quad \text{for reaction cross section} \\ = \alpha_k^{(o)} / v_k \quad \text{for total cross sections} \quad (15)$$

$$GI_k^{(x)} = H_k^{(x)} / v_k \quad \text{for reaction cross section} \\ = \beta_k^o / v_k \quad \text{for total cross sections} \quad (16)$$

The phase shift ω for the total cross section is expressed by

$$\omega = 2 \text{WN} \sqrt{E} \quad (17)$$

where WN is a constant representing the "radius a " of the compound nucleus in units of $(\text{eV})^{-1/2}$. In using (12) to represent reaction cross sections, WN is set equal to zero.

In Eq. (12) the broadening of the background terms is neglected, being $\sqrt{E}$ a slowly varying function of E across each resonance term. The functions ϕ_k , χ_k are the well-known line shape functions^{3/}

$$\phi_k + i\chi_k = \frac{1}{\sqrt{\pi} \sqrt{T_D} v_k} \int e^{-\frac{(E-E')^2}{T_D}} \frac{dE'}{1 - i(\mu_k - E')/v_k} \quad (18)$$

$$T_D = 4T_c E / (A+1) \quad (19)$$

where T_c is the sample effective temperature (in eV), A the atomic mass number, and E the neutron energy.

In the actual construction of the trial function three different types of resonance lines are included in the number N , for a given energy interval:

- (1) Resonances internal to the energy interval to be fitted (NR)
- (2) Resonances neighboring the same interval, which also are to be fitted (NEIGH)
- (3) Resonances having known parameters, which may be internal or external to the same interval (NOUT) .

The resonances of the second group contribute only with the asymptotic "tail" of their resonance lines, so that broadening is unnecessary, and one can write

$$\Phi_k^{(s)} \approx 1/(1 + x^2) \quad (20)$$

$$\Phi_k^{(a)} = 1/(1 + x^2)$$

where $x = (\mu_k - E)/v_k$, for $k = 1, \text{NEIGH}$. The use of this option in the fitting procedure is necessary only for negative energy resonances for which direct shape analysis is impossible.

The NOUT resonances, of the third group, contribute as a known background, which in the least square procedure is subtracted from the data values. The larger this number, the less meaningful (or important) become the background terms A, B, to be fitted.

In the following, the total number of resonance to be fitted is indicated with NRT

$$\text{NRT} = \text{NR} + \text{NEIGH} \quad (21)$$

and the total number of unknowns, for a given data set, by

$$\text{NG} = 2 \text{NRT} + \text{KNEG} + \text{KPOS} \quad (22)$$

Separating in (12) the known terms from those containing the unknown parameters one can write

$$\begin{aligned} \sigma_{\text{DB}}^{(x)}(E) \sqrt{E}/C = & \sum_{k=1}^{\text{NRT}} (G R_k^{(x)} \Phi_k^{(s)} + G I_k^{(x)} \Phi_k^{(a)}) + \sum_{j=1}^{\text{KNEG}} A_j^{(x)} \sqrt{E}^{1-j} + \sum_{j=1}^{\text{KPOS}} B_j^{(x)} \sqrt{E}^j \\ & + \sigma_0^{(x)}(E) \sqrt{E}/C \quad (23) \end{aligned}$$

$$\sigma_0^{(x)}(E) \sqrt{E}/C = \sum_{k=1}^{\text{NOUT}} (GR_k^{(x)} \bar{\Phi}_k^{(s)} + GI_k^{(x)} \bar{\Phi}_k^{(a)}) + 2(1 - \cos u)/\sqrt{E} . \quad (24)$$

In subsequent fits, when known parameters for the NRT resonances, or for some of them, are given, $\sigma_0^{(x)}$ may also contain these contributions. The parameters $GR^{(x)}$, $GI^{(x)}$ appearing in the "unknown" term of Eq. (23) represent in this case the change of the initial set of values, obtainable through the data fitting.

B. Resolution Effects on Reaction Cross Sections

The measured data are in this case the values of the reaction rate, $\sigma^{(x)}(E) \sqrt{E}$, related to $\sigma_{DB}^{(x)}$ through the resolution function: ^{24, 3 /}

$$\sigma^{(x)}(E) \sqrt{E} = \int R(E, E') \sigma_{DB}^{(x)}(E') dE' . \quad (25)$$

Because the convolution of Eq. (25) can be applied term-by-term to the expansion (23), the trial function can be written, similarly to (23), as a linear superposition of convoluted line shape functions

$$\bar{\Phi}_k(E) = \int R(E, E') dE' \bar{\Phi}_k(E') \quad (26)$$

having the same coefficients:

$$Y_t^{(x)}(E) = \sum_{k=1}^{\text{NRT}} (GR_k^{(x)} \bar{\Phi}_k^{(s)} + GI_k^{(x)} \bar{\Phi}_k^{(a)}) + \sum_{j=1}^{\text{KNEG}} A_j^{(x)} \sqrt{E}^{1-j} + \sum_{j=1}^{\text{KPOS}} B_j^{(x)} \sqrt{E} + Y_0^{(x)}(E) \quad (27)$$

where

$$Y_0^{(x)}(E) = \int R(E, E') dE' \sigma_0^{(x)}(E') \sqrt{E}/C . \quad (28)$$

The expression of $\bar{\Phi}$ of Eq. (26) simplifies when the resolution kernel $R(E, E')$ is of Gaussian form. The resolution kernel and the Gaussian Doppler kernel combine into one, ^{24/} with a resulting square width T given by

$$T = T_D + T_{\text{res}} \quad (29)$$

Where T_D is defined in (19). The square resolution width, T_{res} , is related to the nature of the experiment. For time-of-flight measurements, T_{res} has the form: ^{19/}

$$T_{\text{res}} = BE^2 + CE^3 \quad (30)$$

where B and C are parameters depending on the experiment, and are in general variable over the energy range of the experiment itself. In this case the functions $\bar{\Phi}_k$ can be calculated as Doppler broadened line shape functions as defined in Eqs. (13) and (14) with an "apparent" Doppler width as given in (29).

C. Total Cross Section

The rigorous treatment of the total cross section data, ^{24, 25/} obtained from transmission measurements, requires the use of the expansion (12) in a non-linear form.

The experimental data are given in this case as transmission yield

$$Y_x(E) = e^{-n\sigma^{\text{tot}}(E)} \quad (31)$$

where n is the sample thickness (in atm/barn) and σ^{tot} is the measured total cross section. Correspondingly the trial function becomes

$$Y_t(E) = \int R(E, E') dE' e^{-n\sigma_{\text{DB}}(E')} \quad (32)$$

where R represents again the resolution kernel and σ_{DB} the Doppler broadened total cross section, as defined in Eq. (12).

In order to apply the least squares procedure it is necessary to linearize the trial function given in (32).

When $n \ll 1$ (thin sample measurements), and

$$Y_x(E) \approx 1 - n\sigma^{\text{tot}}(E) \quad (33)$$

$$Y_c(E) \approx 1 - n \int R(E, E') \sigma_{DB}(E') dE' \quad (34)$$

the equations are linear, to a good approximation.

The least squares analysis proceeds in this case as for a reaction cross section, through a trial function of the form (27), and line shape functions of the form (26).

In the general case the equation (32) can be linearized, if in σ_{DB} the contribution of the unknown terms can be considered to be smaller than σ_0 , as defined in Eq. (23). This is possible when known sets of parameters for the resonances to be fitted are available (either obtained from previous analysis, or from known fission and capture parameters). The NOUT group includes in this case also the known contributions of the NRT resonances:

$$\sigma_0(E) \sqrt{E} = C \left\{ \sum_{k=1}^{\text{NRT}} \left(GR_k^{(T)(0)} \Phi_k^{(s)} + GI_k^{(T)(0)} \Phi_k^{(a)} \right) + 2 (1 - \cos w) / \sqrt{E} \right. \\ \left. + \sum_{k=1}^{\text{NOUT}} \left(GR_k^{(T)} \Phi_k^{(s)} + GI_k^{(T)} \Phi_k^{(a)} \right) \right\} \quad (35)$$

and the unknown part of σ_{DB} can be interpreted as containing the increments δGR , δGI :

$$\sigma_1(E)\sqrt{E} = C \sum_{k=1}^{NRT} (\delta GR_k^{(T)} \phi_k^{(s)} + \delta GL_k^{(T)} \phi_k^{(a)}) + \text{background terms} \quad (36)$$

so that

$$\sigma_1(E) \ll \sigma_0(E) \quad (37)$$

With this provision, the trial function given in eq. (32) can be safely linearized,^{5/} to give:

$$Y_t(E) \approx \int R(E, E') e^{-n\sigma_0(E')} (1 - n\sigma_1(E')) dE' \quad (38)$$

hence, separating the known transmission term from the unknown one has the expansion

$$Y_t(E) = Y_0(E) + \sum_{k=1}^{NRT} (X_k^{(s)} \bar{\phi}_k^{(s)} + X_k^{(a)} \bar{\phi}_k^{(a)}) + \sum_{j=1}^{KNEG} a_j f_j^{(-)} + \sum_{j=1}^{KPOS} b_j f_j^{(+)} \quad (39)$$

in form equivalent to (27).

In Eq. (39) one defines

$$Y_0(E) = \int R(E, E') e^{-n\sigma_0(E')} dE' \quad (40)$$

$$X_k^{(s)} = -nC \delta GR_k^T \quad (41)$$

$$X_k^{(a)} = -nC \delta GL_k^T$$

$$\bar{\phi}_k^{(s)} = \int R(E, E') e^{-n\sigma_0(E')} \phi_k^{(s)}(E') dE' \quad (42)$$

and similar relation for $\bar{\phi}^{(a)}$, where σ_0 , $\phi_n^{(s)}$ and $\phi_n^{(a)}$ are the Doppler broadened functions defined in equations (24), (13), and (14). One has furthermore

$$a_j = -nC A_j \quad j = 1, KNEG \quad (43)$$

$$b_j = -nC B_j \quad j = 1, KPOS$$

and

$$f_j^{(-)} = \int R(E, E') e^{-n\sigma_0(E')} dE' / (\sqrt{E})^j \quad (44)$$

$$f_j^{(+)} = \int R(E, E') e^{-n\sigma_0(E')} dE' (\sqrt{E})^{j-1} \quad (45)$$

In practice it is sufficient in these cases to introduce only the constant

$$\alpha_1$$

and to a good approximation pose

$$f_1^{(-)} \approx e^{-n\sigma_0(E)} / \sqrt{E} \approx 1/\sqrt{E} \quad (46)$$

In most cases where the initial set of parameters GR^0 , GI^0 , gives already a close fit, and where other NOUT terms are present to form a background, one can proceed without the background terms ($KNEG = KPOS = 0$) .

V. CONSTRAINTS FOR THE TRIPLE FIT

The constraints utilized in the triple fit depend on the types of cross sections chosen to be fitted simultaneously.

Program TRIPLE includes five options, two of which treat with different modes total fission and capture data. The other three options combine two different data sets for the same cross section type, with a third different type. These choices are controlled by the input index IFIT.

A. Simultaneous Analysis of Total Fission and Capture Data (IFIT = 1, and IFIT = 5)

This grouping of cross section types allows to apply as a constraint the conditions that for each resonance k , the sum of the reaction parameters equals the corresponding total cross section parameter, as given in Eq. (1). These conditions follow from the unitarity of the R-matrix formalism, and are essential in order to obtain compatibility among the parameters describing each cross section type. As a consequence the trial function for the total cross section is expressed in terms of the parameters fitting the fission and the capture cross sections.

Indicating with

$$\begin{aligned} \ell = 1 & \quad \text{the fission cross section} \\ \ell = 2 & \quad \text{the capture cross section} \\ \ell = 3 & \quad \text{the total cross section,} \end{aligned}$$

in the notations of Section III, Eq. (1) can also be written as:

$$\left. \begin{aligned} GR_k^{(3)} &= GR_k^{(1)} + GR_k^{(2)} + GR_k^{(n)} \\ GI_k^{(3)} &= GI_k^{(1)} + GI_k^{(2)} + GI_k^{(n)} \end{aligned} \right\} \quad (47)$$

where $GR^{(n)}$ and $GI^{(n)}$ are the line shape parameters of the scattering cross section. The resonance scattering contribution to the total cross section in principle cannot be neglected, although $GR^{(n)}$ and $GI^{(n)}$ are usually smaller than the other parameters. Interference effects can enhance the resonance scattering, as evident from measurements of ^{239}Pu ^{26/} and ^{235}U ^{27/} scattering cross sections.

On the other hand, it is well-known that the scattering parameters depend non-linearly on those of the total cross section, ^{2/} and therefore cannot be fitted rigorously, in a linear fit, while fitting the total cross section data.

Two approximate approaches have been introduced in TRIPLE, according to the options IFIT = 1 and IFIT = 5.

In the branch IFIT = 1, the parameters $GR^{(n)}$, $GI^{(n)}$ are fitted as independent parameters, compensating the difference between total and absorption cross sections.

This mode of fitting might, however, provide scattering parameters which are too large, or incompatible with those of the total, when tested against values calculated independently from the parameters of the total cross section. ^{13/} The reason for this discrepancy is that the effects of errors in the fission, total, and capture parameters, and of the systematic errors inherent in the measurements, combine and accumulate in the scattering parameters when fitted in this manner.

The alternate branch, IFIT = 5, has been introduced to be used especially in preliminary triple fits of total, fission, and capture data. In this case initial values of $GR^{(n)}$ and $GI^{(n)}$ are chosen before fitting, and introduced as known parameters, together with the appropriate value of the statistical factor g . Initial values for $GR^{(n)}$ and $GI^{(n)}$ can be obtained from previous runs with CODILLI II, ^{14/} either from total cross section data, or from direct fitting of scattering data. This option has the advantage also of reducing the number of unknowns with respect to the previous choice.

Because this branch of TRIPLE is most suited for preliminary analysis, it also contains the option of fitting, if necessary, the capture lines as symmetrical. This is of course an approximation, but the effects of the asymmetries in the capture cross section are in general small, and of the order of those of the scattering, so that one can select a priori symmetrical lines for the capture when the precalculated asymmetries of the scattering are very small, or negligible.

While in the mode $IFIT = 1$ the total number of unknown is $NX = 3 NG$, for $IFIT = 5$

$$NX = 2NG + KNEG + KPOS - NSYM , \quad (48)$$

$NSYM$ being the number of symmetrical capture lines. Thus, of all the modes included in TRIPLE, $IFIT = 1$ has the largest NX , $IFIT = 5$ the lowest, if $NSYM > KNEG + KPOS$, for the same values of NRT , $KNEG$, and $KPOS$.

The vector X , defined in Eq. (7) is described in Table I for $IFIT = 1$, and in Table II for $IFIT = 5$.

B. Simultaneous Analysis of Three Data Sets for Two Cross Section Types

The three other branches of TRIPLE combine the following cross section grouping:

Fission, and two sets of total cross sections: $IFIT = 2$

Two fission sets and one total cross section set: $IFIT = 3$

Two fission sets, and one capture: $IFIT = 4$.

The constraints used in each of these options are obvious: the same set of line shape parameters is expected to be shared by the two data sets representing the same cross section type. In each of these cases the total number of unknowns is

$$NX = 2 NG .$$

These options can be used advantageously in comparing data for the same reaction type measured under different experimental conditions. Discrepancies and apparent ambiguities of representations can be analyzed in this manner.

Table III gives the detailed definition of the vector X for each of the cases $IFIT = 2, 3$, and 4 .

VI. PRELIMINARY CALCULATIONS: ENERGY SCALE, STATISTICAL ERRORS, and
RESOLUTION FUNCTIONS. SUBROUTINES ALIGN, WEIGHT, SIGRES, WIDTH

The problem of making compatible with each other the energy scales of the three data sets, as described in Section II, is treated in the Subroutine ALIGN.

For time-of-flight measurements, the problem is discussed by G. de Saussure,^{19/} and is summarized here, using the same notations.

The measured neutron energy is defined by

$$E = \mu^2 L^2 / \tau^2 \quad (49)$$

where L is the effective flight path (in m), τ the time of flight (in μ sec), and $\mu = 72.3 \text{ eV}^{\frac{1}{2}} \mu\text{sec/m}$.

Errors in L and τ induce in E the error:

$$\delta E = 2E (\delta L - \delta \tau \sqrt{E/\mu}) / L. \quad (50)$$

In adjusting the energy scale E' of one data set to the scale E of another, one selects according to convenience one of the two as "correct." The second appears then affected by a relative error of the type (50), and one can write

$$E = E' (A + B\sqrt{E'}). \quad (51)$$

The values of A and B can be determined by comparing two pairs of corresponding points in the two data sets.

In the subroutine ALIGN the comparison is made between two narrow resonances of each data set, which are selected by input. The "wrong" energy scale is then "re-aligned" to the "correct" scale using Eq. (51). This operation is necessary as, in the least squares analysis, the values of the resonance energies, μ_k , are assumed to be the same for all data sets.

Because on the other hand the correction of the energy scale is only relative, each data set independently should be described by apparent values of the resonance energies, μ'_k , related to the μ_k values by Eq. (51). In view of the possible use of the results of TRIPLE for the independent analysis of each data set, the original energy scale is restored, after the fitting, and the apparent values, μ'_k , are punched on cards. The printed output provides the adjusted values of μ_k , as used in the triple fit, and the original value, μ'_k .

The statistical weights are calculated in the Subroutine WEIGHT.

The least squares equations involve statistical weights, which are here calculated following the same pattern used in CODILLI II.^{3,5} These are three options, controlled by the index JWE, one for each data set. At each energy point the weights w_i are calculated as:

JWE = 1 equal weights: $w_i = \text{constant}$.

JWE = 2 weights calculated from the statistical errors $\delta\sigma$:
 $w_i = \text{constant}/(\delta\sigma)^2$

JWE = 3 weights calculated as inverse of the experimental datum:
 $w_i = \text{constant}/Y_{\text{exp}}(i)$.

In each case the weights are scaled so that the sum of the weights over the totality of the data points equals the number of the data points.

In most cases the statistical errors are given at each point, along with the data.

For the ORNL-RPI simultaneous measurements of fission and capture data, the errors are instead given by analytic relations correlating the two data sets. In these cases, it has been preferable to pre-treat the errors and generate data decks containing data and calculated statistical errors, along with the energy values. Other cases can be included by adding extra options (JWE = 4, 5, etc.).

The resolution effects are introduced in the triple fit through two related subroutines: Subroutine SIGRES and Subroutine WIDTH.

For each data set, the independently given information on the condition of the measurement is assessed in SIGRES and WIDTH, for the purpose to calculate the resolution function.

Subroutine SIGRES (EN, ES, L, G, HR) contains for each data set L the calculation of the pertinent resolution kernel, denoted with G. Using the notations of Eq. (14), SIGRES provides

$$G = R(EN, ES, HR) \quad (52)$$

for every value of $E = EN$, $E' = ES$. The energy dependent parameter HR, for a large class of functions, represents the resolution width. The value of HR, at each value of E is obtained from the Subroutine WIDTH (L, EN, KP, HR), where, again, for different L values different functions HR are calculated.

It is not possible to include in a "universal" calculation the variety of functions R which relate to varieties of experiments reported in the literature. Because at present most high resolution measurements are obtained from LINAC experiments, the Subroutines SIGRES and WIDTH reported here are adjusted to this case:

SIGRES returns a Gaussian kernel for each L,

WIDTH returns the related Gaussian width (as total width at 1/e of the maximum) which is given by the relation (30):

$$HR = (BE^2 + CE^3)^{\frac{1}{2}}.$$

The parameters B and C, in general different from one measurement to another, also can vary (differently, for different data sets) over the energy range of the experiment. The Subroutine WIDTH used in TRIPLE is limited to the ORNL-RPI ^{19,20}/ measurements of ²³⁵U and ²³⁹Pu fission and capture data, and to the low-temperature SACLAY measurements of ²³⁵U and ²³⁹Pu total cross sections. ^{24,21}/
-133-

For the ORNL ^{239}Pu data, Dr. R. Gwin kindly supplied the values of the parameters B, C. For all other cases B and C are calculated from the parameters describing the conditions of the experiment (channel width, burst width, flight path, etc.) using the equations of ref. (19).

The implementation of these subroutines is left to the user, according to the data intended to be fitted.

The argument KP in WIDTH is not used. It reflects the possible need of an extra index when other functions HR, for different measurements, were to be added to the same calculation (e.g., Saclay fission cross section measurements of ^{235}U or ^{239}Pu).

VII. CALCULATION OF THE TRIAL FUNCTION FOR SINGLE DATA SETS: SUBROUTINES

YPHI, PHIDO, SIGAP, SIGIN, SIGOUT.

As discussed in Section III, the normal equations are calculated through the definition of trial functions, $Y_t^{(L)}$ one for each data set, defined in Eq. (7).

The solutions of the normal equations are the NX components X_j of the vector $\vec{X}$, which is defined over the entire group of the three data sets. The matrix elements M_{lj} form a $3 \times NX$ rectangular matrix, calculated at the points of the l -th data set, and provide the values of the matrix Q and of the vector $\vec{R}$ appearing in Eq. (9).

The calculation of M_{lj} has been split into two separate steps:

(1) For each data set, l , calculation of a vector $\phi_j^{(L)}$, having NG components and defining the individual trial function of the set l .

(2) Rearrangement of the vector $\phi^{(L)}$ in the matrix M , according to the constraints, and subsequent construction of the normal equations.

This section describes Step 1; Section VIII describes Step 2, which forms the first part of the Subroutine SIGTRE.

(1) Vector $\phi^{(L)}$

For any one of the three data sets the trial function can be written in the form:

$$Y_t^{(L)}(E) = \sum_{j=1}^{NG} \phi_j^{(L)}(E) P_j^{(L)} + Y_0^{(L)}(E) \quad (53)$$

where, referring to the notations of Eq. (27) and (39)

$$\begin{aligned} \text{for } j = 1, \text{ NRT} \quad \phi_j^{(L)} &= \bar{\Phi}_k^{(s)} \\ \text{for } j = \text{NRT} + 1, 2 \text{ NRT} \quad \phi_j^{(L)} &= \bar{\Phi}_k^{(a)} \end{aligned} \quad (54)$$

and $k = 1, \text{ NRT}$;

for $j = 2NRT + 1$, $2NRT + KNEG$, and $j = 2NRT + KNEG + 1$, $2NG$ $\varphi_j^{(\ell)}$ represents the corresponding functions for the background terms, as defined in Eqs. (27) or (39).

The unknowns $P_j^{(\ell)}$ for reaction cross section are:

$$\begin{aligned} \text{for } j = 1, NRT & P_j^{(\ell)} = GR_k^{(x)} \\ j = NRT + 1, 2NRT & = GI_k^{(x)} \quad k = 1, NRT \end{aligned} \quad (55)$$

$$\begin{aligned} j = 2NRT + 1, 2NRT + KNEG & = A_k \quad k = 1, KNEG \\ j = 2NRT + KNEG + 1, NG & = B_k \quad k = 1, KPOS \end{aligned} \quad (56)$$

Similar relations apply to transmission calculations, where $X_k^{(s)}$ replaces $GR^{(x)}$, $X^{(a)}$ replaces $GI^{(x)}$, and a_k , b_k replace respectively A_k , B_k (See Eq. (39)).

In the actual calculation of the vector $\varphi^{(\ell)}$, and of $\gamma_0^{(\ell)}$, four resolution modes have been distinguished, in the same manner as originally done in Programs CODILLI^{4/} and TANDEM^{8/}

JS = 1. This mode includes only Doppler broadening of "reaction cross sections." This is the fastest branch of the program. It can be used for example for (a) code checking with precalculated data, (b) in the analysis of low energy data (1 eV region) for rapid survey of the parameters μ , ν , chosen to represent negative energy resonances.

JS = 2. This mode is suitable for reaction cross section convolutions with resolution functions not of Gaussian type (See. Eqs. (26) and (28)).

JS = 3. This mode includes the case of transmission convolutions, in which the resolution kernel may or may not be of Gaussian type (See. Eqs. (40), (42), and (43)).

JS = 4. This mode, the second fastest of the program, includes the treatment of reaction cross sections with Gaussian resolution function, in which the broadening effects of temperature and instrumental resolution are combined.

The array $\varphi^{(\ell)}$ is evaluated at each energy point of the set (ℓ) in the Subroutine YPHI, through the Subroutines PHIDO, SIGIN, SIGOUT, SIGRES, WIDTH, and SHAPE.

The Subroutine PHIDO provides Doppler broadened vectors Φ , as defined in Eq. (13) and (14), which, for JS = 1 and JS = 4, are directly stored into the array $\varphi^{(\ell)}$ and returned to the calling Subroutine YPHI. The cases JS = 2 and JS = 3 are treated in the Subroutine YPHI through a Simpson integration scheme with a prescribed number of integration steps, NINT. For JS = 2, YPHI provides integrals of the form (26) with the convolution kernel $R(E, E')$ supplied by the Subroutine SIGRES. The Doppler broadened vector Φ , as defined in Eqs. (13) and (14), and entering the convolution integral, is supplied at each E' , by the subroutine PHIDO. The resulting integral, $\bar{\Phi}$, is stored in the array $\varphi^{(\ell)}$.

For JS = 3, YPHI provides convolutions of the form (42), where the resolution kernel $R(E, E')$ is again supplied by SIGRES, and the vector Φ entering the convolution is again calculated in PHIDO. The transmission factor

$$e^{-\alpha\sigma_0(E')} \quad (57)$$

is calculated through the Subroutines SIGIN and SIGOUT. The calculated array $\bar{\Phi}$ is again stored in the array $\varphi^{(\ell)}$.

The Subroutine SIGIN at each energy point evaluates the expansion of the form (23), purely for temperature broadened resonance lines. An index, transmitted as argument, controls the inclusion (JIN = 1) or exclusion (JIN = 2) of the background terms. The specific calculation of the distant resonance contributions

($\sum^{NOUT}$) and of the potential scattering term is made separately in the Subroutine SIGOUT, in which the arguments MJS controls inclusion (MJS = 1) or exclusion (MJS = 2) of the Gaussian resolution effect. Thus MJS = 1 is equivalent to JS = 1, MJS = 2, equivalent to JS = 4. This (internal) distinction makes the use of the Subroutine SIGOUT adaptable to the different modes of calculation. SIGIN is mostly used for convolution calculations (JS = 2,3).

The function $Y_0^{(L)}$ of Eq. (53) is calculated in the Subroutine SIGAP, according to the modes JS. For JS = 1, 4 the calculation is straightforward, as given in Eq. (24).

For JS = 2 and JS = 3, convolution calculations, with the same kernels used in YPHI for each case, provide Y_0 as in Eq. (28) and (40), respectively, through Subroutine SIGIN.

The Simpson integration scheme of the subroutines YPHI and SIGAP is set between the limits

$$\begin{aligned} E_{\max} &= E + 4 \text{ HR} \\ E_{\min} &= E - 4 \text{ HR} \end{aligned} \quad (58)$$

HR being the resolution width at E, supplied by the Subroutine WIDTH. The number of integration steps, which may be input as different from a set (L) to another, by default is set equal to 32.

VIII. SOLUTION OF THE NORMAL EQUATIONS: SUBROUTINES SIGTRE, INVERT, TEST, SIGPLT, GRAPH

The normal equations given in (9) are solved in the Subroutine SIGTRE.

The calculation of the matrix Q and of the vector R, given in Eqs. (10) and (11) is based on the following notations.

For NX unknowns X, the matrix M of Eq. (7) is defined as a rectangular matrix ξ with NX columns and NP rows, where

$$NP = \sum_{\ell=1}^3 NP_{\ell} \quad (59)$$

is the total number of points entering the least squares sum. Similarly, $Y_x^{(\ell)}(i)$ and $Y_0^{(\ell)}(i)$ are written as vectors with NP components:

$$Y^{(\ell)}(i) = Y(p) \quad (60)$$

and

$$Y_t^{(\ell)}(i) = Y_t(p) = \sum_{j=1}^{NX} \xi_{pj} X_j \quad (61)$$

where

$$\xi_{pj} = M_{\ell j}(i) \quad (62)$$

and where for $\ell = 1$, $p = i$, $i = 1, NP_1$, for $\ell = 2$, $p = NP_1 + i$, $i = 1, NP_2$, etc.

Writing also

$$w_p = \lambda_{\ell} w_i^{(\ell)} \quad (63)$$

R and Q of Eqs. (9) and (10) can be written as

$$R_j = \sum_{p=1}^{NP} W_p \left(Y_x(p) - Y_0(p) \right) \xi_{pj} \quad (64)$$

$$Q_{kj} = \sum_{p=1}^{NP} W_p \xi_{kp} \xi_{pj} \quad (65)$$

At each point p , the vector $\varphi^{(\ell)}(E_i)$ is returned to SIGTRE from the Subroutine YPHI in its original length NG and stored (on disc) in the column locations j according to the particular type of constraints.

At the same time the function $Y_0^{(\ell)}(E_i)$, returned from the Subroutine SIGAP, is stored as vector $Y_0(p)$.

The use of the disc, controlled by the Subroutines WRITE, READ, REWIND (See Section X) makes it possible to rapidly reconstruct the trial function after the inversion of the normal equations, avoiding repetitions of lengthy calculations (particularly for $JS = 2, 3$).

The matrix Q is stored in turn in a vector of length $NX(NX + 1)/2$, and its inversion is made through the Subroutine INV2Z,^{5/} employing the decomposition method of Cholesky for real symmetrical positive definite matrices.

An intermediary, Subroutine INVERT, permits to evaluate, after inversion, the values of the unknowns X_j and their variances.

The different fitting modes controlled by IFIT (See Section V) require different arrangements of the vectors $\varphi^{(\ell)}$ in the matrix ξ .

For IFIT = 1, the vector $\varphi^{(3)}$ of the total cross section is constraint to enter the partial trial functions of fission and capture as discussed in Section V, and to fit separately the "scattering" contribution, as difference between total and absorption. The total number of unknowns in this case is

$$NX = 3 NG \quad (66)$$

and the same values of $\varphi^{(3)}$ will enter the column indices $j = 1, 2NRT$,
 $j = NG + 1, NG + 2NRT$ (of fission and capture) and $j = 2NG+1, 2NG+2NRT$ (of total).
 Thus for $p = NP_1 + NP_2 + 1, NP$, and for $j = 1, 2NRT$:

$$\xi_{pj} = \xi_{p, NG+j} = \xi_{p, 2NG+j} \quad (67)$$

as shown in Table I.

For $IFIT = 5$, where the scattering contribution is postulated by input, the rearrangement of the vector $\varphi^{(3)}$ results in a contraction: for $p = NP_1 + NP_2 + 1, NP$, and for $j = 1, 2NRT$

$$\xi_{pj} = \xi_{p, NG+j} \quad (68)$$

so that the number of columns in this case reduces at most to

$$2NG + KNEG + KPOS \quad (69)$$

as shown in Table II.

The inclusion of the option, that capture lines can be individually taken as symmetrical further reduces the number of unknowns:

$$NX = 2NG + KNEG + KPOS - NSYM \quad (70)$$

where $NSYM$ is the number of capture lines assumed to be symmetrical ($GI = 0$).

These two modes ($IFIT = 1$, and $IFIT = 5$) are those having respectively the highest and, depending on the value of $KNEG + KPOS - NSYM$, the lowest number of unknowns NX , for the same number of resonances NRT and same choice of $KNEG$ and $KPOS$.

The branches $IFIT = 2, 3, 4$ similarly require contractions of the vectors $\varphi^{(l)}$ into

$$NX = 2NG \quad (71)$$

columns, as two of the three data sets are represented by the same form of the trial function $Y_t^{(\ell)}$.

After completion of the matrix inversion, in the second part of SIGRE, the over-all "goodness of fit" is evaluated as

$$\chi = \left(\sum_{p=1}^{NP} \left(Y_x(p) - Y_o(p) - \sum_{j=1}^{NX} \xi_{pj} X_j \right)^2 W_p / N \right)^{\frac{1}{2}} \quad (72)$$

where

$$N = NP - NX - 1 \quad (73)$$

is the number of degrees of freedom.

From the array X the values of the fitted parameters are calculated, and given with their errors (as obtained from Q^{-1}).^{5/} This calculation requires stretching the array X into the arrays

$$GR(\ell, k) \equiv GR_k^{(x)}, \quad GI(\ell, k) \equiv GI_k^{(x)} \quad (74)$$

etc., thus inverting the initial operation of contraction.

The quantity χ , given in Eq. (72), is however not sufficient to indicate in detail the "goodness" of the results.

To obtain an appreciation of it, three additional types of calculations are included, in a manner similar to the one used for programs CODILLI^{5/} and TANDEM^{8/} these calculations involve the Subroutines TEST, SIGPLT, GRAPH:

The Subroutine TEST^{5/} has two branches.

In the first branch the value of the partial goodness of fit around each resonance peak is calculated, as weighted sum of square deviations, for each data set:

$$\chi_k^{(\ell)2} = \sum_{i=n_1}^{n_2} \left(Y_x^{(\ell)}(i) - Y_t^{(\ell)}(i) \right)^2 / m Y_x^{(\ell)}(i) \quad (75)$$

The weighting factor in this case is $1/Y_x$, and m represents the number of points of the (ℓ) set ranging from n_1 to n_2 in an interval of width $6v_k$, centered at μ_k . In (75) $Y_t^{(\ell)}(1)$ is the value of the trial function at E_1 , as defined in Eq. (7).

In the second branch of TEST the unbroadened cross section values; as defined in Eq. (2) or (3) are calculated, and their sign is tested. If values occur which are not positive, an error flag is displayed, giving the related energy point. This provision allows the user to revise the values of μ and v , or the general definition of the trial function, as a complement to the information otherwise obtainable from SIGPLT and GRAPH.

The Subroutine SIGPLT provides (as printed output) the experimental data, the values of the trial function, the values of the Doppler broadened cross section (as in Eq. (12)) the deviations of the trial function from the data, the percent errors and the standard deviations.^{4/} For each data set, a partial goodness of fit is also calculated using the definition given in Eq. (72): indicating with $\chi^{(\ell)}$ the partial goodness of fit, and with N_ℓ the corresponding number of degrees of freedom, one has

$$\chi^2 = \sum_{\ell=1}^3 \chi^{(\ell)2} N_\ell / N \quad . \quad (76)$$

In SIGPLT the contribution of each trial function to the thermal cross section is also evaluated. This output can become useful in the fitting of low-energy data with negative energy resonances, or to test the effects of background contributions.

The Subroutine GRAPH provides a graphic display of data, trial function and deviations for each data set. This is a CALCOMP $8\frac{1}{2} \times 11$ " semilog plot, in which the trial function is plotted either point by point, or as a continuous curve (input index ISEL).

IX. EDITORIAL SUBROUTINES: SUBROUTINES LEGE and SCRIBE

The original test version of TRIPLE was written for the IBM 7094 of the University of Illinois, in FASTRAN, and adapted later to the IBM 360-75, in FORTRAN IV.

Envisaging the possibility of adapting TRIPLE to computers at other installations, and in particular to the SCORE package, the reading of the input and the writing of the outputs with a few exceptions (TEST, SIGPLT, and error flags) were relegated to two independent subroutines, LEGE and SCRIBE. These can be therefore changed, or removed (for example, with SCORE the reading is done interactively) according to the need.

The input to TRIPLE is provided by the Subroutine LEGE, where the data set are read in according to three different modes, controlled by the input index ICOD:

For ICOD = 1, each data set is input from independent decks;

For ICOD = 2, the data sets 1 and 2 are read from the same deck, and the set 3 is read independently. This option in particular accommodates the simultaneous measurements of fission and capture of ORNL-RPI.^{19,20} /

For precalculated data, e.g., obtained from Program LEMA-CHAMA²⁸ / the option ICOD = 3 reads in data stored in one single deck. This branch has been added for code-checking purposes, as discussed in Part 2 of this report.

The energy scale is aligned to the scale of the first set through a call to the Subroutine ALIGN, and subsequently the data are scaled, according to the option JS, in the first branch of the Subroutine WEIGHT. The second branch of WEIGHT evaluates the statistical weights, according to the index JWE, individually chosen for each data set.

The detailed description of the input is given in Part 2 of this report.

The printed and punched output of TRIPLE is almost entirely controlled by the Subroutine SCRIBE.

While the detailed description of the output is given in Part 2 of this report, the physically important branches of the output are outlined below.

Before the fit, the initial input values for

$$\mu, \nu, GR, GI$$

and distant resonance parameters (NOUT) for each data set are printed, where the μ values appear in the original energy scale. After the fit, similar arrays are output with the common values of μ and ν , and the fitted parameters.

From GR, GI are evaluated the parameters G, H, α^0 , β^0 , as given in Eqs. (13) and (14) and the value of the sums

$$\begin{aligned} \sum_k H_k^{(x)} \\ \sum_k \beta_k^0 \end{aligned} \quad (77)$$

For IFIT = 1, and IFIT = 5, additional output is given:

- (1) The values of the parameters GRN, GIN.
- (2) The zero-order partial reaction width $\frac{18}{18}$

$$\Gamma_{k(x)} = 2\nu_k G_k^{(x)} / \alpha_k^{(0)} \quad (78)$$

- (3) The first order scattering parameters, given by

$$G_k^{(n)} \approx \Gamma_{kn}^0 \Gamma_{kn} / 2\nu_k \quad (79)$$

where

$$\Gamma_{kn}^0 \approx \alpha_k^0 \quad (80)$$

and

$$\Gamma_{kn} \approx \sqrt{\mu_k} \alpha_k^0 / 2g_k \quad (81)$$

This calculation requires input values for the statistical factor g for each resonance k ; if not given, g_k by default is taken equal to one.

The parameters G , H , with the related values of μ and ν are also punched on cards as to be directly used for further calculations:

- (1) As NOUT of subsequent runs, either with TRIPLE, or CODILLI II
- (2) To evaluate cross section curves at different temperatures and in mixtures
- (3) To calculate values of α , or η and their temperature dependence
- (4) As input for Program GAMPLEX,^{19/} in order to extract compatible R-matrix parameters.

X. AUXILIARY SUBROUTINES: SUBROUTINES WRITE AND SKIP

The evaluation of the vector Φ from which the normal equations are constructed, and from which later the trial function is calculated (See Section VIII) can be time consuming, not only if the number of points is large, but especially if the options JS = 2,3 are wanted. It is convenient to store on a scratch unit these values as they are calculated: Unit 9 in this case. The group of Subroutines WRITE (READ, REWIND) is used to reduce the number of calls to the FORTRAN I/O support package by blocking data. In many systems this is desirable if the overhead for each READ or WRITE is large compared to the overhead of a subroutine call.

Finally, the Subroutine SKIP is used to write page headings with the day's date and the run identification number (specified by input).

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Table I

BRANCH IFIT = 1 : $\ell = 1, 2, 3$

Storage of the Vector X: $NG = 2NRT + KNEG + KPOS$

For $k = 1, NRT$

$$X_j = GR_k^{(\ell)} (1 - \delta_{\ell 3}) + \delta_{\ell 3} GR_k^{(n)} \quad j = (\ell-1)*NG + k$$

$$X_j = GI_k^{(\ell)} (1 - \delta_{\ell 3}) + \delta_{\ell 3} GI_k^{(n)} \quad j = NRT + (\ell-1)*NG + k$$

For $k = 1, KNEG$

$$X_j = A_k^{(\ell)} \quad j = 2 NRT + (\ell-1)*NG + k$$

For $k = 1, KPOS$

$$X_j = B_k^{(\ell)} \quad j = 2 NRT + KNEG + (\ell-1)*NG + k$$

Storage of the arrays $\varphi^{(\ell)}$ into the array ξ : $KB = KNEG + KPOS$

For $p = 1, NP_1$

For $p = NP_1 + 1, NP_1 + NP_2$

For $p = NP_1 + NP_2 + 1, NP$

BRANCH IFIT = 5 : $\ell = 1, 2, 3$

Storage of the Vector X: $NG = 2NRT + KNEG + KPOS$

For $k = 1, NRT$ and $\ell = 1, 2$

$$\begin{aligned} X_j &= GR_k^{(\ell)} (1 - \delta_{\ell 3}) & j &= (\ell-1)*NG + k \\ &= GL_k^{(\ell)} (1 - \delta_{\ell 3}) & j &= NRT + (\ell-1)*NG + k \end{aligned}$$

For $k = 1, KNEG$

$$\begin{aligned} X_j &= A_k^{(\ell)} & j &= 2NRT + (\ell-1)*NG + k, \text{ for } \ell = 1, 2 \\ & & j &= 2NG + k \text{ for } \ell = 3 \end{aligned}$$

For $k = 1, KPOS$

$$\begin{aligned} X_j &= B_k^{(\ell)} & j &= 2NRT + KNEG + (\ell-1)*NG + k \text{ for } \ell = 1, 2 \\ & & j &= 2NG + KNEG + k \text{ for } \ell = 3 \end{aligned}$$

Storage of the arrays $\varphi^{(\ell)}$ into the array ξ : $KB = KNEG + KPOS$

For $p = 1, NP_1$

For $p = NP_1 + 1, NP_1 + NP_2$

For $p = NP_1 + NP_2 + 1, NP$

Table III

BRANCH IFIT = 2: $\ell = 1, 2$ ($\ell = 3$ same cross section type as $\ell = 2$)

Storage of the vector X: $NG = 2NRT + KNEG + KPOS$

For $k = 1, NRT$

$$X_j = GR_k^{(\ell)} \quad (GR^{(3)} \equiv GR^{(2)}) \quad j = (\ell-1)*NG + k$$

$$X_j = GI_k^{(\ell)} \quad (GI^{(3)} \equiv GI^{(2)}) \quad j = (\ell-1)*NG + NRT + k$$

For $k = 1, KNEG$

$$X_j = A_k^{(\ell)} \quad j = (\ell-1)*NG + 2NRT + k$$

For $k = 1, KPOS$

$$X_j = B_k^{(\ell)} \quad j = (\ell-1)*NG + 2NRT + KNEG + k$$

Storage of the arrays $\varphi^{(p)}$ into the array ξ

For $p = 1, NP_1$

For $p = NP_1 + 1, NP_1 + NP_2$

For $p = NP_1 + NP_2 + 1, NP$

Table IV

BRANCH IFIT = 3: $\ell = 2, 3$ ($\ell = 1$ same cross section type as $\ell = 2$)

Storage of the vector X: $NG = 2NRT + KNEG + KPOS$

For $k = 1, NRT$ and $\ell = 2, 3$

$$\begin{aligned} X_j &= GR_k^{(\ell)} & (GR^{(1)} &= GR^{(2)}) & j &= (\ell-2)*NG + k \\ X_j &= GI_k^{(\ell)} & (GI^{(1)} &= GI^{(2)}) & j &= (\ell-2)*NG + NRT + k \end{aligned}$$

For $k = 1, KNEG$

$$X_j = A_k^{(\ell)} \quad j = (\ell-2)*NG + 2NRT + k$$

For $k = 1, KPOS$

$$X_j = B_k^{(\ell)} \quad j = (\ell-2)*NG + 2NRT + KNEG + k$$

Storage of the arrays $\varphi^{(\ell)}$ into the array ξ

For $\gamma = 1, NP_1$

For $p = NP_1 + 1, NP_1 + NP_2$

For $p = NP_1 + NP_2 + 1, NP$

Table V

BRANCH IFIT = 4 : $\ell = 1, 2$ ($\ell = 3$ same cross section type as $\ell = 1$)

Storage of the vector X: $NG = 2NRT + KNEG + KPOS$

For $k = 1, NRT$

$$\begin{aligned} X_j &= GR_k^{(\ell)} & (GR^{(3)} &\equiv GR^{(1)}) & j &= (\ell-1)*NG + k \\ &= GI_k^{(\ell)} & (GI^{(3)} &\equiv GI^{(1)}) & j &= (\ell-1)*NG + NRT + k \end{aligned}$$

For $k = 1, KNEG$

$$X_j = A_k^{(\ell)} \quad j = (\ell-1)*NG + 2NRT + k$$

For $k = 1, KPOS$

$$X_j = B_k^{(\ell)} \quad j = (\ell-1)*NG + 2NRT + KNEG + k$$

Storage of the arrays $\varphi^{(\ell)}$ into the array ξ

For $p = 1, NP_1$

For $p = NP_1 + 1, NP_1 + NP_2$

For $p = NP_1 + NP_2 + 1, NP$

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APPENDIX F

INTERACTIVE USE OF PROGRAM CODILLI 2 WITH SCORE III-A:
LEAST SQUARES DATA FITTING OF ^{239}Pu USING PROGRAM CODILLI WITH SCORE

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TABLE OF CONTENTS

	Page
A. Introduction	156
B. Performance of CODILLI with SCORE III-A	157
C. Present Limitations of SCORE III-A	158
D. Desirable Improvements in SCORE III-A	160
E. Comments and Conclusions	161
Figures	162-174
References	175

A. Introduction

During the weekend of September 18-19, 1971, Program SCORE III-A was used for the first time, not for demonstration purposes, but for actual data fitting of the Pu-239 fission, capture, and total cross sections in the 0.1 to 50 eV range, using the single level and multilevel option of Program CODILLI - 2 (CODILLI with SCORE).⁽¹⁾ SCORE III-A, in its present state, provides a versatile tool having many advantages over normal batch mode data processing schemes. While the program is not yet perfect, it can be used in the mode incorporating CODILLI-2 to excellent advantage for preliminary least squares fitting of individual cross sections.

Least squares fitting with Program SCORE has many advantages:

(1) Work with SCORE provides for a continuity of effort and thinking by the practically instant turn-around time; results can easily be compared and immediately improved by the interactive mode of operation.

(2) The possibility of selecting different groups of neighboring resonances and of rapid changes in resonance energies μ and total line widths γ provides an intuitive insight into the sensitivity of the parameters obtained to the choices made.

(3) The interactive fitting, using changes of resonance energies and line widths makes non-linear iterative fitting routines unnecessary in preliminary fits, resulting in substantial savings in use of central processor time.

(1) Collaboration of D. B. Adler (UI), P. F. Rose (AI), N. H. Marshall (CSC - Idaho), and F. T. Adler (UI).

(4) For adequate data and with sufficient preliminary preparation, it appears possible to analyze narrow energy bands within a few minutes of real time scope use.

The performance of the program can best be illustrated by considering sequences of scope pictures generated during the data analysis; present limitations of SCORE III-A and suggested improvements will then be discussed and summarized in a section on conclusions.

B. Performance of CODILLI with SCORE III-A

Operation of SCORE III-A requires first of all the preparation of suitable data tapes (experimental cross sections, experimental errors) and of a preliminary library of assumed resonance energies and line widths for the nuclide being investigated, as well as for the nuclides which appear as impurities in the experimental targets; a subroutine dealing with the resolution function needed in Program CODILLI-2 must also be provided. At present a subroutine suitable for the analysis of Linac measurements is built into CODILLI-2.

In the actual operation of SCORE, the first five interactive panels are standard panels, as described by Dunford.^{1/} The subsequent panels are specific for the use of CODILLI-2 with SCORE and are described elsewhere.^{2/} Fig. 1 to 7 obtained as hardcopy from the content of the IBM 2250 scope display illustrate the choices open during the initialization of the fitting process and the first display of experimental data. Fig. 7 shows one of the three main option lists. These "menus" are at present too large and appear to be not fully implemented. After an expanded data display the resonance

fitting is entered, as discussed elsewhere,^{1/} and another set of options (again not fully implemented, and mostly not pertinent to this application) appear.

The crucial step in the resonance analysis is the choice of resonance energies and half widths (at present not displayed in the initial panel shown in Fig. 8) for the least squares fitting process; the relevant panel is shown in Fig. 8. After the fitting is completed the data and the theoretical curve are displayed as illustrated in Fig. 9; the "menu" on the right is used to proceed to further fitting steps or to display an enlarged picture allowing better interactive judgment. The key decisions are made by considering the "residuals" i.e., the χ values over the region of an individual resonance displayed on a separate panel (Fig. 10). By light pen, one can then choose one resonance for an expanded display from the panel shown in Fig. 10. Fig. 11 shows the expanded view of a single resonance where changes in resonance energy and half widths can be introduced either in the numerical values by means of the keyboard or by changing through the light pen the vertical lines defining the position of the resonance energy and the half width of the resonance line. This picture can also be expanded in energy scale to show several resonances around the resonance being investigated. Fig. 12 shows such an expanded view, containing also the lines defining the resonance considered. The possibility of using the visual appearances together with computed χ values practically simultaneous is a distinct advantage for iterative fitting with SCORE III-A.

C. Present Limitations of SCORE III-A

(1) The most serious limitation of SCORE III-A is the requirement that only 500 data points are to be used in display and/or data analysis. This does not

allow to fit more than one or two resonances at a time if good data (many closely space data points) are used.

(2) The data-point limitation is not consistent: many data points and other information get lost because of present hardware limitations due to the limited size of the buffer memory on the IBM 2250 currently in use at the CSC at Idaho. For example:

(a) data are eliminated in uncontrollable manner; to avoid this many runs were made using only 300-400 data points;

(b) the possibility of exiting from an option is lost because of loss of information; this makes it necessary to stop the run, exit from computer and restart a problem with loss of computer time and need to restart problem from start.

(c) information essential for interactive use of SCORE III-A is suppressed and lost; for example, the cross section pictures may have no longer an energy scale, and/or the numerical magnitude of the cross sections may no longer be indicated.

(d) the routine ADLISP, which should allow final judgment on an interactive operation for a given energy range cuts out too much detail (150 calculated points) and frequently allows no estimate on the quality of fit near a strong resonance peak.

(e) too many options are provided which take up buffer space, and which are not germane to least-squares data analysis.

(f) the flicker of the scope in the "time slice" mode of central computer operation can occasionally be disturbing in considering a picture frame.

D. Desirable Improvements in SCORE III-A

(1) The most important improvement would be to increase the number of acceptable data points to at least 1000, preferably 1500, with assurance that the useful options can be reached without need of terminating a run.

(2) Cross section and energy scales should be provided for all pictures, and without cut-off of scales.

(3) Provisions should be made to display by option $\sqrt{E}\sigma(e)$ or $\sigma(E)$ [and not only $\sigma(E)$]; this would facilitate the visual analysis of broad resonances, and such a feature may be essential for work on fertile or low Z elements.

(4) Frequently, one needs to reconsider previous "display pages" on the scope. Provisions should be made to go backwards in panels, without losing information.

(5) The routine "ADLISP" needs access to more calculated points.

(6) Space for a temporary library (including updating due to the fit in progress) would be most helpful so that no time is lost in re-entering resonance energies and halfwidths by starting a new problem. This aspect is of special importance if several data sets corresponding to different reactions (σ_T , σ_F , σ_C) have to be fitted, or if data sets due to different authors have to be compared.

(7) At present only LINAC times resolution functions are provided within CODILLI-2 because of space limitations imposed by SCORE III-A; other resolution functions (especially for bomb shot data) are needed, and space and a suitable interactive choice panel should be provided in SCORE III-A.

E. Comments and Conclusions

(1) SCORE III-A, in its present state, is an excellent tool for interactive data fitting if adequate care is taken in the preparation for the least-squares data fitting.

(2) SCORE III-A appears most useful for preliminary fitting, and probably for final detailed adjustments of parameter. It cannot be the only tool for data analysis; the interdependence and interaction of the use of SCORE III-A and of simultaneous fitting routines such as TANDEM and TRIPLE need further investigation following more extensive practical use of all programs.

(3) The provision of hard copy from SCORE III-A fitting is an essential improvement; comparison of results of analyzing fission, capture, and total data cannot be performed on one scope; one needs hard copy to make the necessary judgments before completing the fitting, and, above all, before altering the permanent data file library.

(4) CODILLI-2 (Subrouting TEST) provides warning flags if the multilevel parameters obtained would lead to some negative values of the unbroadened cross sections; these and other warning flags should be displayed to guide the interactive fitting procedure.

September 27, 1971

LABORATORY: CSC

EVALUATOR: DAPRFANM

DATE: 9/18/71

PROBLEM I.D.: 15

Figure 1

SELECT DESIRED ISOTOPES

74	0	1.00000E 00	92	233	1.00000E 00
92	235	5.00000E-01	92	335	5.00000E-01
92	238	1.00000E 00	94	239	2.50000E-01
94	239	7.50000E-01	94	240	1.00000E 00

-163-

ATOM FRACTION: 1.00

POTENTIAL SCATTERING (BARN): 10.0

ATOMIC WEIGHT (AMU): 239.0

REACTION TYPES AVAILABLE FOR Z = 94 A = 339 ARE

NF

NG

TOT

-164-

MINIMUM ENERGY (MEV):

6.48E-06

MAXIMUM ENERGY (MEV):

23.48E-06

Figure 3

SELECT EXPERIMENTAL DATA WEIGHTING FUNCTION

-165-

UNIT WEIGHTING

EXPERIMENTAL ERROR WEIGHTING

CALCULATED INVERSE WEIGHTING

Figure 4

SELECT RESOLUTION TREATMENT

JS=1 CONSTANT GAUSSIAN RESOLUTION WIDTH

JS=2 CONVOLUTION ON REACTION CROSS SECTION

JS=3 CONVOLUTION ON TRANSMISSION

JS=4 ENERGY DEPENDENT GAUSSIAN RES. WIDTH

-991-

BACKGROUND CONSTANT EVALUATION
(ENTER NEW VALUES FROM KEYBOARD)

ISOTOPE IDENTIFICATION

Z = 94 A = 239 G = 7.50000E-01

FORMULA

$$A1 + A2/E + A3/E**2 + A4/E**3 + (B1 * E + B2 * E**2) / \text{SQRT}(E)$$

CURRENT VALUE OF CONSTANTS

	TOTAL	FISSION	CAPTURE
A1	0.0	0.0	0.0
A2	0.0	0.0	0.0
A3	0.0	0.0	0.0
A4	0.0	0.0	0.0
B1	0.0	0.0	0.0
B2	0.0	0.0	0.0

Figure 6a

NUMBER OF FITTED BACKGROUND TERMS

NEGATIVE POWERS	1
-----------------	---

POSITIVE POWERS	0
-----------------	---

-168-

SELECT RESONANCE ISOTOPES

Figure 6 b

-169-

C
R
O
S
S
S
E
C
T
I
O
N
D
A
R
N
S

ADLER-ADLER MULTILEVEL

RES 1/3
MODEL
CHANGES
ADD RES
MOD RES
LOAD RES
COMPARE
FIT
CALC
MAIN OPT

Figure 7

INCIDENT NEUTRON ENERGY (eV)

Z = 94

A = 239

G = 7.50000E-01

-170-

ENERGY	CALCULATE	FIT	MULTILEVEL
7.00103E 00	YES	YES	YES
1.00120E 01	YES	YES	YES
1.10777E 01	YES	YES	YES
1.43086E 01	YES	YES	YES
1.046583E 01	YES	YES	YES
1.76329E 01	YES	YES	YES
2.22342E 01	YES	YES	YES
2.38758E 01	YES	NO	YES
2.62228E 01	YES	NO	YES
2.72329E 01	YES	NO	YES
3.54220E 01	YES	NO	YES
4.13731E 01	NO	NO	NO
4.16230E 01	NO	NO	NO
4.44350E 01	NO	NO	NO
5.00330E 01	NO	NO	NO
5.25331E 01	NO	NO	NO
5.55022E 01	NO	NO	NO
5.91536E 01	NO	NO	NO

Figure 9

Z = 94	A = 239	G = 7.50000E-01
ROLE		RESIDUAL
ENERGY	CURRENT	PREVIOUS
7.84816E 00	• 6.52643E 01	8.18215E 03
1.09957E 01	• 2.49766E 03	8.70871E 03
1.19261E 01	• 5.33701E 02	1.23587E 04
1.43540E 01	• 1.27974E 02	2.37176E 03
1.47404E 01	• 2.52790E 02	1.48877E 04
1.77034E 01	• 2.53098E 02	9.78237E 03
2.23246E 01	• 4.54042E 02	6.59495E 03

-172-

Figure 10

Figure 11

Z = 34

A = 239

G = 2.50000E+01

FISSION

FISSION

POLE ENERGY

1.55200E 01

HALF WIDTH

3.30000E-01

FISSION G

6.72720E-04

Figure 12

References

1. C. L. DUNFORD: SCORE, an Interactive Cross Section Evaluation System. AI-AEC-12994 Vol. I. May 15, 1971.
2. F. T. ADLER: Memorandum #3 on the Adaptation of Program CODILLI to Program SCORE. Dec. 9, 1970.

A MULTILEVEL ANALYSIS OF THE ^{239}Pu CROSS SECTIONS IN THE 6 to 70 eV REGION [†]

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TABLE OF CONTENTS

	Page
Summary	177
1. Introduction	178
2. Preliminary remarks on the fitting procedure with the multilevel expansion	183
3. Multilevel analysis of fission capture and total cross section of ^{239}Pu between 6 and 70 eV	190
a) General Procedure	190
1. Impurities	190
2. Spin assignments	191
3. Capture data	192
4. Analysis of the total cross section data	192
5. Gwin resonance parameters.....	192
6. R-matrix parameters of Derrien	193
7. Comparison of fits of Gwin and Derrien	193
b) Results of Triple Fit for ^{239}Pu from 6 to 70 eV	195
4. Determination of R-Matrix parameters	200
a) Spin state $J = 1^+$	200
b) Spin state $J = 0^+$	206
c) Comparison with single level analysis	206
5. Conclusions.....	208
Tables	210-226
Figure Captions	227
References	243-245

Summary

Results of a correlated analysis of fission, capture, and total cross sections of ^{239}Pu with the multilevel formalism are presented. R-matrix parameters are derived, and it is shown that because of the inaccuracies of the data several sets of R-matrix parameters can be obtained, for the $J = 1^+$ state, where the results should be unique.

Effects of missed levels and quasi-resonances have been studied numerically. Comparisons have been made with the results of recent single level analysis of the same data, pointing to appreciable differences in the average $\langle\Gamma_f\rangle$ and $\langle\Gamma_\gamma\rangle$ values for the energy range between 7 and 70 eV.

1. INTRODUCTION

One of the aims of the analysis of fissile nuclide cross sections is to obtain sets of resonance parameters, ideally independent from the experimental conditions of the measurement (sample temperature and impurities, resolution, calibration, etc.) so as to be consistent with other measurements (e.g., predict cross section values at different temperatures), and to satisfy general physical requirements such as the unitarity of the resulting collision matrix and the possibility of constructing and predicting the energy dependence of all the partial cross sections of the nuclide studied. For fissile elements the analysis must account for the effects of the fission channel interferences, as originally made evident by Shore and Sailor.^{1/} For fissile elements the simultaneous analysis of fission, capture, and total cross sections appears therefore essential in order to derive parameter sets satisfying these requirements.

Data analysis of fission and capture,^{2,3/} or of fission and total cross sections^{4,5/} provide less complete information, leaving open ambiguities, which in the first case affect the role of the resonance scattering, and in the second case the prediction of the capture widths.

Any analysis based on least squares fits of experimental data necessarily leads to results which depend on the choice of the trial function, and are therefore not uniquely defined.^{6/} The procedure based on the correlated analysis of the cross sections representing a "complete experiment," such as coordinated measurements of fission, total, capture, and scattering cross sections, in providing parameters which describe simultaneously each individual reaction, will reduce ambiguities.^{7/}

These considerations appear necessary in any type of least squares analysis, independently from the specific type of formalism utilized in the analysis and in defining the trial function. Until now, two types of approaches have been widely used in the data analysis of fissile element cross sections:

(1) the multilevel-multichannel model based on the R-matrix theory of nuclear reactions;^{1,6,7,8,9,10,11} /

(2) the single level model.

The single level model represents a limiting case of the general R-matrix theory, valid if the channel interferences are either negligible or, as for radiative capture, cancel as effect of the large number of open channels. The well-known fact that at low energies only a few fission channels are open, so that interference effects produce observable asymmetries in the fission and total cross sections, should in principle rule out the single level model as a nonpertinent description of the fissile element cross sections. Thus, only reasons of convenience can justify the use of single level analysis. Although formally simple, this type of analysis has also proven to be not unique in its results,^{12/} aside from the considerations involving missed levels,^{14/} and the arbitrariness in choosing additional levels to represent asymmetries in the cross sections. Perhaps the strongest objection to this model is related to the physical meaning of the parameter values derived, whether they can constitute a basis for statistics, as to provide for the evaluation of the cross sections in the unresolved region. The fact that in the high energy region the interference effects may become negligible may justify the use of single level formulas at high energies, but does not seem to justify the use of single level analysis in the resolved resonance region.

Recently, a single level analysis with a compensating "smooth background" has been produced.^{12/} The "smooth background" appears as a continuous curve,

oscillating from positive to negative values around resonance peaks. While it is not evident which type of broadening technique would be applied in calculating temperature effects, it is instead clear, from a straightforward comparison with the data, that this background describes the "missing" effect of interferences such as it would be given by superpositions of asymmetrical line shape functions. Figure 1 shows a plot for the low energy resonances of ^{239}Pu , using the symmetrical line shape parameters derived from Derrien's evaluation discussed in Section 2. In Figure 2 the continuous line represents the contribution of the asymmetrical parameters deduced from the same compilation: the plot shows only the positive part of this curve.

The R-matrix formalism has been used repeatedly in different forms as a basis for least squares data analysis: as early as 1958, Vogt^{8/} utilized the level matrix algorithm, while more recently Derrien^{5/} based his analysis of fission and total cross sections in ^{239}Pu on it. Auchampaugh^{9/} has presented the results of a simultaneous analysis, based on the computer program MULTI and utilizing the Reich-Moore partitioning of the channel matrix. This type of analysis, requiring the selection of the spin states and assumptions on the number of fission channels implies solutions of systems of nonlinear equations which are computer-wise time consuming. The inherent non-uniqueness of the results obtained from the least squares fits with MULTI for cases of well-spaced resonances with two fission channels have been discussed by Auchampaugh.^{9/} ^{235}U fission and capture data, assuming two fission channels, have been analyzed recently by de Saussure^{15/} using program MULTI. Although this author does not discuss the problem of the uniqueness of his results it is to be expected that the same procedure using program MULTI should lead to the same conclusions, that is, to more than one set of R-matrix parameters describing the same data.

The analysis based on the multilevel expansion in terms of symmetrical and asymmetrical line shape functions^{16/} provides parameters which, in describing the cross section shape, are related non-linearly to the R-matrix parameters. The non-linearities of the trial function in this case occur only in the complex resonance energies: the values of the symmetrical and asymmetrical line shape parameters differ, as can be anticipated, if different values of the poles of the level matrix are assumed at start. This type of non-uniqueness is obviously analogous to the one inherent to single level or to R-matrix analysis when changing the initial values of the resonance energies and partial widths.

Examples of this non-uniqueness (which is strongly affected by the uncertainties inherent in the data, as discussed in Section 2) have been given previously.^{17/} In these cases the goodness of fit was systematically calculated so as to gauge the quality of the parameters, although the calculated curves differ inappreciably from one case to another, and although the cross section at higher temperatures than at that prevailing at measurement would not be distinguishable.

The ²³⁵U parameters ^{17,18/} as well as the ²³⁹Pu parameters ^{7/} presented previously were obtained constraining the chosen resonance energies μ and half widths ν to fit both fission and total cross section data. This type of constraint is essential in the correlated analysis of total, fission, and capture data,^{18,19/} as contrasted to the interpretation of the same approach recently published by Bhat,^{20/} who parameterizes the fissile nuclide cross sections assuming different values of μ and ν for fission, capture and total cross sections.

The multilevel expansion is economical in computer use so that the fitting procedure can readily be iterated, to include effects of distant resonances, and to converge to better fitting sets of μ , ν values. The use of the parameters obtained in calculating Doppler broadened cross sections is straightforward.^{21/}

An apparent criticism to the use of the multilevel parameters for statistical studies is based on the fact that, although attempted,^{22,23/} statistical distributions of general utility have not been obtained. Because, however, R-matrix parameters are derivable from the multilevel expansion,^{24,25/} their use in data fitting appears at least as advantageous as the use of procedures based directly on the channel matrix or level matrix inversion. The calculations used to derive R-matrix parameters from the multilevel expansion require solutions of non-linear equations which can be solved on the computer efficiently after the data fitting is completed.

In the context of ^{239}Pu , for the one-channel case ($J = 1$) the multilevel analysis of fission, capture and total cross section data provides multilevel parameters which in principle should be uniquely related to the R-matrix parameters, but may differ from those of other compilations. It is shown that in particular the Derrien evaluation proposes Γ_{γ} widths, and occasionally Γ_f widths, which, although fitting the total, do not fit the capture cross section. The reason for this discrepancy is that in the Derrien compilation the Γ_{γ} values were taken from an independent single level analysis,^{2/} and not obtained from a correlated analysis of the three cross sections. It has become apparent that in the single level analysis for narrow resonances Γ_{γ} is generally overestimated, while Γ_f is generally underestimated^{15/} in comparison with a multilevel analysis.

2. PRELIMINARY REMARKS ON THE FITTING PROCEDURE WITH THE MULTILEVEL EXPANSION

The multilevel fitting procedure used in this report has been based on two interrelated computer programs, CODILLI 2,^{26/} and TRIPLE.^{19/}

While the numerical experiments made in testing these programs will be reported separately,^{27/} some of the conclusions reached in the phase of testing these programs are recalled here, as essential to illustrate their use.

(a) Synthetic data, obtained from given sets of R-matrix parameters with the program LEMA-CHAMA,^{28/} have been Doppler and resolution broadened (and, for the total, transmission-broadened) using one of the branches of CODILLI 2. These fictitious data, of which the line-shape parameters were calculated initially from LEMA-CHAMA, and therefore exactly known, have been subsequently used as "experimental data" to be fitted with either program.

The test runs have been shown that, by initiating the fit from mathematically correct values of μ and ν , the correct values of the line-shape parameters are obtained^(*) independently from the choice of:

- (1) statistical weight
- (2) type of constraint used in the fit
- (3) type of background constants added to the trial function.

Modifications of the values of μ and ν in the input for a "linear fit" lead to values of the line-shape parameters, different from the exact values, with errors which are larger, the coarser is the initial "guess."

Replacing the resolution function used in originating the "data set" with a slightly different function (e.g., changing the value of the flight path, or of the

(*) Aside from deviations in the 7th to 5th digit, as inherent to the computer accuracy.

moderator thickness), or introducing a temperature value different from the original value, alters accordingly the final answer, even when the exact μ , ν values were used.

For use with TRIPLE additional data sets were formed, by assigning to the same data shifted energy values, altered with a law of the form^{29/}

$$E = E' (A + \sqrt{E'} B) . \quad (1)$$

The inaccurate definition of the "bench-mark" values of the energy needed in TRIPLE^{19/} to re-align the data, leads again to errors in the fitted parameters. It can be concluded that this fitting procedure provides the exact values of the line-shape parameters if the exact values of μ and ν are used, and if all the variables affecting the shape of the cross section lines (resolution, alignment, etc.) are precisely known.

In data fitting, not only the "true" values of μ and ν are not known a priori, but the number of resonances is at times uncertain (effect of hidden resonances, discussed below). For a given choice of the values of μ and ν , and of the number of resonances to be fitted, a different set of line-shape parameters is derived. Of this, examples were reported previously as obtained from the original version of CODILLI.^{17,30,31/}

The use of program TRIPLE allows to introduce constraints among the line-shape parameters, so as to give a description of the data compatible with a given choice of the μ , ν values, which are bound to be shared by the three data sets. Although not pointing to a unique choice of the μ , ν values, this procedure has the function of narrowing the ambiguities in the parameter values thus derived. In particular, in fitting fission, total and capture the unitarity of the

formalism requires that, for each fitted resonance, k,

$$\sum_{(x)} G_k^{(x)} = \alpha_k^0 \quad (2)$$

$$\sum_{(x)} H_k^{(x)} = \beta_k^0 \quad (3)$$

where $G^{(x)}$, $H^{(x)}$ represent the line-shape parameters of fission, capture and scattering, and α^0 , β^0 , those of the total cross section.

The consistency of these results is further tested by comparing the zero order perturbation value of Γ_n , as derived from the total cross section, with the difference

$$2v - \Gamma_f - \Gamma_y$$

where Γ_f , Γ_y are in turn the zero order perturbation widths for fission and capture derived from the line-shape parameters.^{25/} For well fitted resonances (and for a consistent choice of the g_J value)

$$\Gamma_n \approx 2v - \Gamma_f - \Gamma_y \quad (4)$$

Failure to reproduce this relation indicates usually an inadequate fit which may be caused by a poor choice of μ , v , g_J , thus the need of correcting the fit.

The non-linear searching routine of the original version of CODILLI^{30/} and TRIPLE^{19/} have been eliminated from the current versions of these programs, because the experience made with interactive displays^{32,33/} has shown that a more efficient convergence to values of μ and v providing good fits is attainable with interactive procedures.

In the batch-mode operations of these programs, the availability of CALCOMP routines for graphic display, and of the "graphics package" GRASS,^{34/} developed at Illinois, has allowed to avoid lengthy and often disappointing non-linear iterations.

(b) Numerical experiments have been made with "missing levels" and "quasi-resonances."

The fact, that resonances with small neutron width and situated close to larger resonances (small spacing) are not detectable by anyone of the fitting techniques currently in use, has been pointed out and discussed by Michaudon,^{14/} while the existence of "quasi resonances" has been indicated by Lynn.^{35/}

For a numerical study of these problems with CODILLI and TRIPLE, synthetic data were constructed using the program LEMA-CHAMA for a sample energy interval from 6 to 30 eV, with R-matrix parameters simulating those of the ^{239}Pu resonances. Two small single levels were added to the $J = 1$ levels, on the wings of the resonances at 7.8 and 10.9 eV. Two small levels were added to the $J = 0$ resonances, very close to the 7.8 and 14.3 eV peaks, to be used as "hidden resonances." At 15.5 eV a quasi-resonance was also postulated (in shape unrelated to the existing $J = 0$ resonance of ^{239}Pu). Thus, five levels were added to the eleven resonances currently assigned to ^{239}Pu in the same energy interval.

As shown elsewhere^{36/} the multilevel formalism allows to fit readily a quasi-resonance. The "missing levels" however remain hard, if not impossible, to resolve, due to the smallness of the natural widths.

The synthetic data of this example were used to investigate which changes occur in the line-shape parameters and in the "goodness of fit" value if the small levels and(or) the "hidden resonances" are ignored in the fit.

The original resonance parameters of this example, as obtained from LEMA-CHAMA, are listed in Table 1. The fit with CODILLI of the total cross section, using the entire group of resonances calculated in CHAMA gave the parameters listed in Table 2, and the curve shown in Fig. 3. As already mentioned, the differences between the exact parameters (Table 1) and the fitted parameters (Table 2) are in the 6th to 7th decimal figure (that is the accuracy is to the 4th significant figure in parameters of the order 10^{-3} or 10^{-4}).

Test runs were made by fitting the total cross section in the region from 6 to 20 eV as follows:

- Case 1: ignoring the quasi-resonance, the two single levels and the hidden levels.
- Case 2: fitting the quasi-resonance as a doublet and ignoring single levels and hidden resonances.
- Case 3: fitting the quasi resonance and the two single levels, but ignoring the hidden levels.

These numerical experiments lead to the following conclusions:

(1) When fitted as originating only from one pole (μ, ν), the quasi resonance at 15 eV shows deviations which are very large. Moreover, in the triple fit it becomes impossible to match the three peaks: in this example the fission peak is small as compared with those of capture and total, and the differences cannot be reduced by fitting with one set of μ, ν values. Fig. 4 illustrates these deviations for the total cross section. Thus it is seen that, in presence of data measured with high resolution, a quasi resonance can be detected, if not too close to other resonances.

(2) the two small levels at 8.5 and 9.9 eV have been purposely omitted, although in a regular fitting procedure they could be readily taken into account. These resonances can be expected to disappear from the curve as effect of broadening. The temperature and resolution effects of the Derrien measurements, however, are not sufficient to flatten the contributions of these resonances, reducing the peaks of the total by only 30%. The temperature and resolution effects of the Gwin measurement reduce the fission of more than 50%, so that these levels would not be obvious in an independent analysis of the fission and capture cross sections thus broadened. In the case of the ^{239}Pu data of Derrien only resonances with a width

$$\gamma \ll \Delta \sim 0.2 \times 10^{-2} \text{ eV}$$

(where Δ is the combined temperature and resolution width at 8 eV) and very low Γ_n^0 in value would become undetectable.

The omission of these resonances had the purpose of testing the changes induced in the line-shape parameters of the fitted resonances, with respect to the exact values. In Fig. 4 the deviations arising from this procedure are obvious.

(3) The presence of the two hidden levels at 7.9 and 14.2 eV is however harder to establish, in accordance with the prediction of Michaudon.^{14/} Figs. 4 and 5 show deviations under the peaks at 7.8 and 14.3 eV which do not outline the omission of a resonance line as plainly as for the case (2). Rather, the deviations could hint to the need of shifting the μ values in the attempt of adjusting the shape of the peaks.

As discussed below, the effects of temperature and resolution broadening could, to some extent, indicate the presence of a hidden level, if data with different broadening were to be compared.

Tables 3 and 4 show the parameters of the fitted resonances in these cases. It is apparent that the symmetrical parameters, α^0 , vary by a small amount around the exact values, while the asymmetrical parameters, β^0 , change in magnitude, to a maximum of 30% for the resonances close to the missed levels. The fact, that "hidden resonances" alter the wings of the cross section curve, was studied by Michaudon in the context of a single level analysis,^{14/} and lead to the introduction of small levels to match the asymmetries of the large ^{239}Pu peaks.^{37/} Because, however, the contribution of a symmetrical line broadens differently than the contribution of the interferences (asymmetrical component of the line), a comparison of data taken at different temperatures could possibly hint to a decision between the two cases.

It is however striking that, although the magnitude of the asymmetries is highly sensitive to the "hidden levels," their signs are stable. This fact is explained, if one considers that the sign of the asymmetry shows the skewness of the line with respect to the peak. Because the hidden levels are characterized by low Γ_n^0 values, they may contribute by enhancing, or reducing the apparent asymmetry, but only in extreme cases reverse the direction of the asymmetry around the peak. In conclusion, the presence of hidden levels near a large peak can be considered as a relatively large perturbation on the asymmetrical parameters, which however does not preclude detecting the existence of interferences. As shown in Section 4, this fact permits to determine the signs of the fission width amplitudes in a one-channel case and to reach compatible sets of R-matrix parameters, even when the magnitude of the asymmetries could change by introducing hidden levels.

3. MULTILEVEL ANALYSIS OF FISSION CAPTURE AND TOTAL CROSS SECTIONS OF

^{239}Pu BETWEEN 6 and 70 eV

a) General Procedure

The data selected for this analysis were the total cross section of Derrien,^{5,37/} and the fission and capture data of Gwin.^{3,38/} These data were chosen because Gwin's measurement is the only existing simultaneous measurement of capture and fission of ^{239}Pu , and Derrien's total data still appear to have the highest resolution in the low energy region. Each of these measurements is characterized by different resolution functions and slightly different energy scales. Moreover, the types and concentrations of the impurities differ from Gwin's capture to Derrien's total.

For these reasons it has been necessary to obtain preliminary independent fits of each data set with Program CODILLI,²⁶ before using TRIPLE. In particular, the following aspects of the fit were investigated:

(1) Impurities. Although parameters for the impurities (^{240}Pu for total, Tungsten and ^{240}Pu for capture) are available in the BNL tables, it was necessary first of all to assess exactly the values of the resonance energies for the two different measurements, which differ slightly from those of the BNL tables. It was also necessary to fit the ^{240}Pu levels with exactly the same ν values. This led to considerations on the resolution widths, which are discussed below.

After good fits were obtained, new data sets were calculated, by subtracting from the original data the contributions of the impurities, and scaling the data of 100% concentration, for use on TRIPLE.

2. Spin assignments. Although most of the spins of the ^{239}Pu low energy levels are known, tests on the spin assignments have been made with CODILLI 2, comparing in each case the "goodness of fit" values

$$\chi = \sqrt{\sum_{i=1}^{NP} \left(Y_x(i) - Y_a(i) \right)^2 \omega_i / (NP - ND)} \quad (5)$$

where:

NP = number of data points

ND = number of fitted parameters

Y_x = experimental value

Y_a = trial function

ω_i = statistical weight.

} at the energy point E_i

The choice of the statistical factor g_j is necessary in order to use TRIPLE profitably.^{19/} In cases in which the spin assignment was satisfactory, and a certain number of known resonances could be included in the trial function, the constraint^{26/}

$$\sum_{k=1}^N H_k = 0 \quad (6)$$

for resonances of the same spin state was used. Results with and without this constraint were compared. Large differences between line shape parameters in the two cases usually indicate that some μ values are ill-posed. If all μ , ν values are satisfactory, the use of the constraint (6) induces only minor differences in the values of the line shape parameters (that is, if the true μ and ν values were reached, the condition (6) would automatically be verified among the interfering resonances of the same spin state, as verified in the tests with synthetic data).

(3) When fitting the capture data, it has become evident that the asymmetries of the capture lines are negligible, as opposed to the similar multilevel analysis of Gwin.^{3/}

It should be noted that this result does not imply necessarily that an independent single level analysis of the same data would provide parameters consistent with those of the total and of the fission, but rather points to the fact that, for the specific case of ^{239}Pu (relatively large spacing among resonances) a first order perturbation approximation 7,31/ suffices in relating R-matrix parameters to the line shape parameters. This approach was used earlier in relating existing R-matrix compilations to the multilevel parameters obtained from the analysis of Bollinger's data,^{31/} and has been used here in deriving R-matrix parameters from the fitted line shape parameters, as discussed in Section 4.

(4) The analysis of the total cross section data with CODILLI 2 provides also a set of line shape parameters for the resonance scattering, which become useful in the triple fit of the data, when using one of the options of Program TRIPLE,^{19/} and which can be used in testing the spin assignment, by comparison with the results of scattering cross section measurements.^{39/}

(5) The first group of calculations was made using as input for the fission and capture data the GWIN values for μ and ν .^{3/} The results obtained represent good fits to the data. However, the parameter values obtained from CODILLI 2 are not identical to those given by GWIN. Because the resolution function used was exactly the same^{40/} the reason for this discrepancy seems to reside in differences between CODILLI and the Oak Ridge multilevel program, or possibly in the mode the ORNL program is used.

In Table 5 are compared the values of the line-shape parameters of Gwin's report with the values obtained from CODILLI fitting the same data with the μ , ν values of Gwin, for the region between 6.5 and 39 eV.

(6) The R-matrix parameters of Derrien^{5/} were used to obtain from program LEMA-CHAMA values of μ , ν of line-shape parameters, which are listed in Table 6. Table 6 shows the comparison with the values obtained by fitting the Derrien data with the same μ , ν values, using CODILLI in the region 6.5 to 39 eV. The discrepancies shown in Table 6 between calculated Derrien parameters and fitted parameters are less surprising than those of the Gwin's data. One reason might be a possible difference in the calculation of the potential scattering (chosen here to reproduce the thermal value of the BNL tables^{13/}) for which the Derrien publication does not contain information. Another reason is that, although reproducing accurately the total cross section data, the R-matrix fit of Derrien is not unique, so that the related values of μ , ν differ slightly from the (unknown) "true" values. Only if the mathematical curve calculated with Derrien parameters fitted exactly the experimental curve, the CODILLI fit with the same μ , ν values would reproduce the same parameters as obtained from LEMA-CHAMA (as it is the case for synthetic data).

(7) In comparing separate fits of Gwin and Derrien data it has become obvious that the ν values of Gwin are in general larger than those of Derrien. In particular, the ν value for the ²⁴⁰Pu level at 38 eV differs drastically from one case to another. Because this resonance is isolated, it was used as a "bench-mark" to attempt a unification of the values of ν to be treated in the triple fit.

This discrepancy points at insufficient information on the resolution width, or perhaps on the type of function describing the resolution effects, as discussed

by Simpson and Simpson.^{12/} Assuming that at low energy a gaussian function is an adequate description for the resolution function of the time-of-flight measurements,^{3/} it became necessary to analyze the definition of the resolution width, and to compare Michaudon's ^{41/} definition to de Saussure's ^{29/} definition. In the first case, the square gaussian half-width at 1/e of the maximum is given by:

$$\Delta^2 = \frac{(.0276)^2}{4 \ln 2} \left(\sum_i \Delta t_i^2 \right) \frac{1}{L^2} E^3. \quad (7)$$

In the second, the square gaussian width at 1/e of the maximum is given by:

$$(2\Delta)^2 = \frac{2}{3} \frac{(.0276)^2}{L^2} \left(\sum_i \Delta t_i^2 \right) E^3 \quad (8)$$

where E is the neutron energy, L the flight-path in meters, and Δt_i are the burst width, channel width, slowing down time, delay due to detector thickness, (the latter two following a 1/E dependence), etc. Eq.(7) gives a resolution width larger than the one prescribed by Eq.(8). Using the first definition [Eq. (7)] in fitting Gwin's data, it has been possible to obtain again good fits with ν values compatible with those of the Derrien data. For the latter the resolution width was calculated from (7) with the numerical values of Δt_i reported in Ref. 37.

(b) Results of Triple Fit for ^{239}Pu from 6 to 70 eV

The Program TRIPLE^{19/} allows to treat the different data sets with the original energy scales, and to re-align the data to a common scale, which in this case was chosen for convenience to be the one of the Gwin data. In this way it becomes possible to interpret the data with a unified set of resonance energies, so as to obtain parameters which permit readily to evaluate compatible cross section curves.

Two modes of fitting are possible with TRIPLE^{19/}:

- (1) Mode IFIT = 1. The difference between total and absorption cross sections is fitted so as to provide scattering parameters, through Eqs.(2) - (3).
- (2) Mode IFIT = 5. The scattering parameters are introduced as initial values, and the total cross section parameters are constrained to the fission and capture by eqs (2) - (3). In the present case, the incertitudes inherent in the data (e.g. resolution function, energy scale, statistical errors) do not always permit to use the mode (1) meaningfully. The mode (2) has proven more useful. The values of the scattering parameters were obtained from preliminary analysis with CODILLI. Values obtained from single level compilation could also be used, as a first approximation. Scattering parameters are also calculated as a result of the triple fit, so that in second approximation their values may be used to initiate a subsequent fit. Mode (2) includes also the option of treating the capture lines as symmetrical. This option has given satisfactory fits to the Gwin data for the region from 6 to 70 eV.

Background terms have been included, as the effects of the distant resonances in ^{239}Pu are large (owing to the large Γ_n^* values). For the cases presented here, a $1/\sqrt{E}$ background term was sufficient to fit the data.

The separation between spin states was investigated with CODILLI, selecting at first the resonances with the largest v values as $J = 0^+$ levels, and for which $G^F \gg G^Y$. The resonance at 65.5 eV could be fitted as a $J = 0^+$ level, or as a component of a doublet resonance of $J = 1^+$, pairing with the 65.8 eV level. Both interpretations gave equivalent fits, so that the assignment of the 65.5 eV level to the $J = 0^+$ state was chosen, in agreement with Derrien (and as most likely to occur).

Thus of the 27 resonances observed in the range from 6.5 to 70 eV 20 were assigned to the $J = 1^+$ state, 7 to the other.

The multilevel parameters obtained from the triple fit are presented in Tables 7 and 8, while Fig. 6 - 11 show the comparison between fitted curves and experimental data.

The μ and ν values of Table 7 gave better fits to the data than those of Table 5. There is a good agreement between the symmetrical parameters of G^F and G^Y of Table 7 with those of Table 5, especially for the large resonances, while the asymmetrical parameters H^F differ from one case to another. Similar comments apply to the total cross section parameters of Tables 7 and 6. These discrepancies can be explained, numerically, because the constraints used in the triple fit are not utilizable in the fit of individual data sets (CODILLI). These discrepancies would disappear if the values of the resonance energies μ and half-width ν represented exactly the "true" values, that is, the values of those uniquely defined theoretical curves ideally representing the nuclear properties of ^{239}Pu . The measured data naturally hide the "true" curve allowing only for related, but not identical interpretations, as remarked by de Saussure^{15/} in the context of a ^{235}U evaluation. In addition, it should be noted that the resolution width used with the Gwin data in the triple fit was slightly larger than the one used in testing Gwin's parameters with CODILLI (Table 5). In the particular case of the capture data, the discrepancies are necessarily larger, owing to the two different interpretations: that is, asymmetrical lines in Gwin's analysis, symmetrical lines in this evaluation. Similarly, the capture cross section predicted by Derrien does not agree with this evaluation. The reason is partly due to the fact that Derrien did not analyze directly capture data and predicted the Γ_γ values on the basis of a single level analysis^{37/}.

The comparison with a single level analysis of the same data^{12/} is presented in Section 4.

The neutron width obtained from the triple fit, as in eq (4), was used to obtain also the scattering parameters:

$$G^N \approx \Gamma_n \Gamma_n^* / 2\nu \quad (4a)$$

which can be compared to results of scattering measurements. In Table 9 the values of Γ_n of Derrien^{5/} are compared with those derived in the same fit providing the parameters of Tables 7 and 8. In the same table, the scattering area calculated from (4a) is compared with the values of Sauter and Bowman^{39/}, for the first 11 levels below 40 eV. Both comparisons show very good agreement.

Although small with respect to the other parameters, the scattering parameters cannot be neglected in a triple fit, as they can be used not only within the least squares fit, but also in testing the consistency of the spin assignments, and of the total cross section parameters with the other parameters.

(c) Physical Meaning of Parameters

The impossibility of resolving the "hidden levels" from the measured data has been shown by Michaudon, with the conclusion that the apparent parameters derived from data analysis differ from the true parameters, thus affecting the value of the number of the effective fission channels. Although the numerical experiments reported by Michaudon are based on the single level analysis of synthetic data, it can be expected that the same conclusions apply, at least qualitatively, to the results of a multilevel analysis.

In the actual fitting of the ^{239}Pu data, it appeared that resonances could be added, especially in the energy region above 50 eV, without altering the quality of the fit. On the other hand, as discussed in Section 3, the presence of hidden levels overlapping the apparent levels, change the symmetrical line shape parameters only in the second order, and do not alter the signs of the asymmetrical parameters. Therefore the parameters derived from the data analysis represent to a good approximation the cross section curves. As remarked by de Saussure,^{15/} they can be used for cross section evaluations with a good degree of confidence.

The derivation of average properties of the R-matrix parameters obtained through the data fitting, and in particular of the average level spacing, is instead doubtful, unless appropriate corrections are introduced to account for the missed levels. These considerations apply in general to any one of the data fitting procedures currently in use, while the distortions on the average values appear to differ from a single level analysis to a multilevel fit. It is perhaps relevant to note that, in fitting with a single level procedure the synthetic data calculated with the multilevel approach of Vogt, Michaudon shows that the average Γ_γ of the fit is larger than the true values used in creating the "data," while the opposite occurs for the fission width Γ_f .^{14/}

The effect quoted for the capture width is, however, not exclusively due to the missed resonances, but also to the interferences, as proposed by Lynn.^{35/} If, as for Michaudon's cases, Γ_γ is constant, the symmetrical parameters G^γ can be

written, to a good approximation, as:

$$G_{\lambda}^{\gamma} \approx \frac{\Gamma_{\lambda n}^{\circ}}{2\nu_{\lambda}} \Gamma_{\gamma} V_{\lambda\lambda} \quad (17)$$

where $V_{\lambda\lambda} > 1 - \frac{24}{\lambda}$. Because the single level analysis corresponds to the approximation

$$G_{\lambda}^{\gamma} \approx \frac{\Gamma_{\lambda n}^{\circ}}{2\nu_{\lambda}} \Gamma_{\lambda\gamma} \quad (18)$$

it is evident that, from an identical value of the area under the cross section line (given by G^{γ}), the value of $\Gamma_{\lambda\gamma}$ results larger than Γ_{γ} , the more, the stronger are the interferences. This comparison also gives the qualitative reason why, fitting the same data with the same number of resonances, the single level analysis predicts Γ_f values smaller than those derived from the multilevel analysis (ignoring the effects of the missing levels).

Simple relations can be used to express the changes of the observed average widths, $\langle \Gamma \rangle_{\text{obs}}$ and spacing, d_{obs} , to the corresponding "true" values $\langle \Gamma \rangle$ and d :

$$\frac{\langle \Gamma \rangle}{\langle \Gamma \rangle_{\text{obs}}} = \frac{d}{d_{\text{obs}}} + \frac{M}{N+M} \frac{\langle \Gamma \rangle_{\text{missed}}}{\langle \Gamma \rangle_{\text{obs}}} \quad (19)$$

$$\frac{d}{d_{\text{obs}}} = \frac{N}{N+M} \quad (20)$$

where N = number of observed levels

M = number of missed levels

$\langle \Gamma \rangle_{\text{missed}}$ = average width of missed levels.

A quantitative investigation of the effects of the missed levels on the $\langle \Gamma \rangle$ or d was however not contained in the task of this evaluation. It is evident, however, that, if most of the missed fission widths are large, most of the missed levels in ^{239}Pu are either $J = 0^+$ levels, or the broad component of a quasi-resonance, as it is expected that 14/

$$\langle \Gamma_f \rangle > \langle \Gamma_f \rangle_{\text{obs}} \quad .$$

The capture width of the $J = 0^+$ resonances is however regularly very small, so that it is unlikely that $\langle \Gamma_{\gamma} \rangle > \langle \Gamma_{\gamma} \rangle_{\text{obs}}$, because the quasi resonances are expected, in ^{239}Pu , to occur with less high probability than the overlapping resonances of different spin state. 35/

Therefore the average values presented above would point at even lower

$$\langle \Gamma_{\gamma} \rangle / \langle \Gamma_f \rangle$$

ratios than those obtained from the present multilevel analysis.

It should be pointed out that the parameters listed in Tables 7 and 8 could not be presented in the ENDF format. Two reasons prevented this task:

(1) The ENDF format 20,44/ anticipates μ and ν values different from one reaction type to another (arrays DET, DWT, DEF, DWF, DEC, DWC) for the same resonance, as shown in page D-7 of Ref. 44. This requirement contrasts the multilevel fitting procedure used in this and related work, 15,17,31 / so that it was not possible to satisfy it.

(2) The background constants requested in the ENDF format are defined once and for all for the whole set of parameters, while they should relate to the specific energy range on which the data were fitted, and vary therefore from region to region. 17/

4. DETERMINATION OF R-MATRIX PARAMETERS

(a) Spin State $J = 1^+$

It is known that the ^{239}Pu resonances of the spin state $J = 1^+$ have one partially open fission channel^{35/} in the low-energy region. In using R-matrix formalisms the analysis of these resonances is facilitated by constraining the fission width amplitudes to be either parallel or anti-parallel to a selected direction.^{11,5/}

This assumption, when used in deriving R-matrix parameters from the line shape parameters of the multilevel expansion, simplifies the procedure which is in general based on solutions of systems of nonlinear equations.^{24/} The relatively large spacing among the ^{239}Pu resonances allows moreover the use of a first order perturbation approximation, which further simplifies the treatment. The validity of this approximation has been tested previously^{31/} in deriving line-shape parameters from existing R-matrix compilations for ^{239}Pu . Evidence for its validity is also apparent from the lack of asymmetries in the capture cross section, as discussed in Section 3.

Among the resonances analyzed in the region to 70 eV, a few are mostly capture resonances, that is, present (negligibly) small asymmetries (e.g. at 27.3 eV and 35.4 eV). They are characterized by small neutron width and small fission width, so that the interference effect is smaller than for other resonances, and may be neglected.

Within the first order perturbation, the asymmetrical parameters H^F are given by the relations

$$H_{\lambda}^{(F)} \approx 2 \sum_{\lambda'=1}^N \rho_{\lambda\lambda'} \cos(\theta_{\lambda} - \theta_{\lambda'}) \quad (9)$$

$$H_{\lambda}^Y \approx 0 \quad (10)$$

where

$$\rho_{\lambda\lambda'} = \frac{\sqrt{\Gamma_{\lambda n}^0 \Gamma_{\lambda' n}^0} \sqrt{\Gamma_{\lambda f} \Gamma_{\lambda' f}}}{E_{\lambda'} - E_{\lambda}}, \quad \rho_{\lambda\lambda} = 0 \quad (11)$$

To this order of approximation also

$$E_{\lambda} \approx \mu_{\lambda} \quad (12)$$

$$2\nu_{\lambda} \approx \Gamma_{\lambda n} + \Gamma_{\lambda \gamma} + \Gamma_{\lambda f} \quad (13)$$

$$G_{\lambda}^{(x)} \approx \frac{\Gamma_{\lambda n}^0 \Gamma_{\lambda x}}{2\nu_{\lambda}} \quad (14)$$

$$\alpha_{\lambda}^0 \approx \Gamma_{\lambda n}^0 = 2g \Gamma_{\lambda n} / \sqrt{E_{\lambda}} \quad (15)$$

These equations are valid for instance, to about 1% for the case of Derrien's R-matrix parameters, so that the exact calculation is very closely approximated with the previous relations. The restrictive condition that only one fission channel ($\theta_{\lambda} = 0, \pi$) is available reduces Eq.(9) to the form

$$H_{\lambda}^F = \sum_{\lambda'} \rho_{\lambda\lambda'} \epsilon_{\lambda} \epsilon_{\lambda'} \quad (16)$$

where $\epsilon_{\lambda} = \pm 1$, inducing constraints for the asymmetrical parameters. In deriving in the general case R-matrix parameters from line-shape parameters, in the first-order perturbation, the partial reaction widths are obtained from the relations (14), and the only remaining unknowns are the angles θ_{λ} , representing the orientations of the reduced width amplitudes, $\gamma_{\lambda c}$, in the space of the fission channels.

It has been shown^{42,43} / that, for more than one fission channel, and more than two interfering levels, the same set of parameters G, H , can be interpreted with different sets of $\gamma_{\lambda c}$, so that the ensuing R-matrix representation is not unique.

For one fission channel, however, there exists only one set of values of ϵ_{λ} corresponding to the same set of H_{λ} , which can readily be obtained by solving $N-1$ of the equations (16), for a chosen sign of one of the ϵ_{λ} .

This procedure is not applicable, however, to values of H^F derived from data fitting, because of the uncertainties inherent to the fit. A straightforward numerical search can instead be applied, by combining in all possible ways the ϵ_{λ} , calculating for each combination the expressions (16), and comparing them with the fitted values. This calculation, which scans 2^{N-1} possible sign combinations, is easily routinized, and has the advantage of providing first-order perturbation H^F values compatible with the one channel assumption. Of all the 2^{N-1} cases those giving H^F values closest in magnitude and sign to the original ones are considered as meaningful.

During the course of this analysis two extreme cases have been met:

- (1) Cases in which no acceptable values of H^F were obtained from the one-channel calculation, for a given group of interfering resonances. These cases correspond to either ill-posed initial μ values, or to a wrong spin assignment.
- (2) On the other hand, cases were found in which more than one combination of the ϵ_{λ} gave equivalently good values for the H^F . These different combinations do not correspond to reflections of the channel amplitudes, and provide different values of H^F , all of which are compatible with the data.

Table 10 gives the multilevel parameters obtained from the Triple fit of the ²³⁹Pu data from 6.5 to 30 eV which were used for this preliminary investigation.

Table 11 presents the partial widths and three acceptable combinations of signs calculated in perturbation from the first ten resonances of Table 10. In Table 11 under column (1) are listed the Derrien R-matrix parameters $\frac{5}{\lambda}$, and under column (2) the R-matrix parameters derived from the Triple fit with the perturbation approximation. For the fission width column (2) gives the absolute values of the partial widths, while the columns (2a), (2b), (2c) give the three compatible combinations of the signs ϵ_λ for the same $|\Gamma_{\lambda f}|$. It should be noted that the set (a) reproduces the channel orientations of Derrien, aside from a reflection. Column (b) describes a situation in which the first six vectors are reflected with respect to the corresponding vectors of column (a), while the last four remain fixed. Column (c) similarly shows a reflection of the three intermediate resonances (14.3, 14.6, 17.6 eV) with respect to (a) while the other remain fixed. These results may indicate for the $J = 1^+$ state a natural grouping of three strongly interfering resonances, weakly coupled to the others.

The corresponding three sets of R-matrix parameters were then used as input in the Program LEMA-CHAMA, to obtain values of the line-shape parameters. These parameters are shown in Tables 12 and 13, and compared with those derived from Derrien compilation.

It is apparent that, while the symmetrical parameters G^F , G^Y , α^O do not change appreciably from cases (2a) to (2c), the asymmetrical parameters H^F , β^O , change sizeably in magnitude from one case to another, while their signs are invariant.

These values were used subsequently to calculate the cross section curves and to compare them with the experimental data, in the region between 6.5 and 20 eV. Figs. 12, 13, 14 show the comparisons of each of the three sets with the Derrien data.

Each set provides a good fit to the data. For comparison, Fig. 15 shows the similar calculation using the parameters of the Derrien compilation, listed under (1) in Tables 12 and 13. The "goodness of fit" χ for each set is shown in Table 14. Thus three equivalently good sets of R-matrix parameters were determined, providing equivalently good representations of the data for the same energy region. Because the capture lines are to a good approximation symmetrical, very little change occurs in the capture parameters from one set to the other. A test for the fission cross section shows that the same R-matrix parameter set also provide a satisfactory fit to the fission data.

This multiplicity of choices is possibly induced by the impossibility of resolving completely the data, and of deciding, on the grounds of a least-squares analysis, which is the "true" representation of the data, because for the case of one fission channel, no degeneracy of R-matrix parameters^{43/} is expected to occur on theoretical grounds. Only if backed by assumptions related to a given physical model could a least-squares analysis predict unambiguously resonance parameters.

Among the three sets derived from the same triple fit, set (2b) is the one giving the least value of χ , and could be thus chosen as the R-matrix set more closely fitting the data, as alternative to the one of Derrien. The fact that neither of the three R-matrix parameter sets reproduces the values of H^F derived from the fit (and that the fit with the multilevel expansion is slightly better than any one with the R-matrix parameters) is explainable if one considers that no assumption (i.e., no constraint) on the number of fission channels is introduced in the multilevel analysis, so that the line-shape parameters, in adjusting to the shape of the measured data point to a band of best fitting values, among which the one-channel interpretation will select the most adequate values.

In Table 15 are reported the R-matrix parameters obtained from the lineshape parameters of Table 7 for the 20 levels of the spin state $J = 1^+$ in the region from 6 to 70 eV. The resonance energies seem to follow closely the pattern of Derrien's analysis.^{5/} The values of the partial widths point to two groups of resonances:

- (1) resonances having fission and capture widths of comparable magnitude,
- (2) resonances with predominant Γ_Y and small Γ_f , at the energies 27.29, 35.53, 41.46, 44.52, 50.12, 52.62 eV.

The levels of this second group are obviously less asymmetrical than those of the first group. As seen from Table 7, the asymmetrical parameters are in general small, and regularly very small compared with α^0 , and G^F is much smaller than G^Y .

The levels of the first group cannot, however, be described without asymmetries, that is, without taking into account the interferences. The one-channel perturbation analysis of the 20 resonances of the spin state $J = 1^+$ was made neglecting the resonances of group (2), as their contributions to the asymmetrical parameters is of the second order or higher.

For the 9 resonances below 27 eV which belong to the first group, three different sets of ϵ_λ were found, in a manner similar to the one discussed for the resonances of Table 10. Of these three sets, the set $\epsilon^{(3)}$ reproduces values of H^F and β^0 closest to the corresponding values of Table 7. Set $\epsilon^{(2)}$ reproduces the Derrien assignments, set $\epsilon^{(1)}$ is its mirror image.

For the resonances above 40 eV only one set of ϵ_λ was found, not related to Derrien's assignments.

(b) Spin state $J = 0^+$

These resonances are recognized as having large ν values, small or negligible G^Y values as compared with G^F ; while they are widely spaced, interference effects may still be appreciable because of the large values of Γ_f . In the range from 6 to 70 eV Derrien has introduced seven $J = 0^+$ resonances, of which six certainly fall into this class. The resonance at 65.5 eV could, on the other hand, be fitted also as a $J = 1^+$ level; the quality of the data, however, did not permit to resolve this case, and the selection of Derrien was followed.

The multilevel parameters for these resonances are given in Table 8; R-matrix parameters are presented in Table 16. It should be noted that the quality of the fission and capture data above 35 eV limits the possibility of a two-channel analysis of the multilevel parameters. The results given in Table 16 can therefore be considered only as preliminary, especially with regard to the channel space angles θ_λ . In the preliminary analysis the first four resonances were fitted in pairs, while the last three levels were treated together. The uncertainty in the spin assignment for the 65.5 eV level also affects this result.

(c) Comparison with single level analysis

A comparison with the evaluation of Simpson and Simpson^{12/} shows systematic differences in the partial widths: for the majority of the levels analyzed between 6.5 and 70 eV the single level capture widths are larger than those of this evaluation. Although there is no spin assignment to the resonances fitted by Simpson and Simpson, it seems straightforward to relate them to those of this analysis. For the large $J = 0$ resonances above 50 eV this single level

evaluation shows additional resonances, possibly because, in presence of large interferences, the compensating "smooth file" is not adequate to account for the line shape. The average values of the capture and fission widths of each spin state, obtained by the single level and by the multilevel analysis are compared in Table 17. The difference in the ratios $\langle \Gamma_Y \rangle / \langle \Gamma_f \rangle$ are of the order of 12% for $J = 1^+$ and 50% for $J = 0^+$. The implications of these results for the study of statistical distributions are straightforward: whether the asymmetries need being taken into account, or not, in the unresolved resonance region, the statistical parameters will be chosen on the basis of average values established in the resolved region. It is surprising to detect so large a discrepancy, as shown in Table 17, among evaluations which appear to provide equally good representations of the data.

5. CONCLUSIONS

The correlated analysis of the Derrien total cross section data, measured at 77°K, and of the Gwin capture and fission measurements, made near room temperature, allows for a consistent description of the ^{239}Pu cross sections by the multilevel parameters reported in Tables 7 and 8 for the region from 6 to 70 eV. Perturbation methods have been used successfully to derive the R - matrix parameters shown in Tables 15 and 16 from the multilevel parameters. Some of these parameters are close to but not identical to those obtained by Derrien.

A least squares data analysis cannot provide a unique set of parameters because of the arbitrariness involved in the choice of the trial function and the criteria used in evaluating a fit; the parameters obtained appear however significant, not only for direct nuclear reactor applications, but also as guides for determining average values of resonance widths and spacings relevant for investigating the unresolved resonance region. Values for $\langle\Gamma_\gamma\rangle$ and $\langle\Gamma_f\rangle$ have been obtained for the spin states $J = 1^+$ and $J = 0^+$ which differ significantly from the results of a recent single level analysis, as shown in Table 17.

To ascertain the self-consistency of the results, the scattering area has been calculated for some of the levels of the spin state $J = 1^+$. Although the resonance scattering parameters are small, the agreement of the values deduced from the analysis of total, fission, and capture cross sections with the experimental results of Sauter and Bowman is surprisingly good, indicating that the parameters have a physical relevance. Comparisons with other data compilations have also shown that the values $G_k^{(x)}$ deduced from various sources are in good agreement while the magnitudes of $H_k^{(x)}$, but not the signs of $H_k^{(x)}$, show variations, depending on the measurement and evaluation made. The near constancy of G_k^F and G_k^γ , and of the sign of H_k^F for the resonances considered in different approaches makes it possible to obtain reliable estimates for $\Gamma_k^{(\gamma)}$, $\Gamma_k^{(f)}$, and Γ_{kn}^* .

The role of the small levels, missed in the data analysis, has been pointed out by Michaudon. This point has been investigated by adding small levels to a set of levels simulating the low-energy ^{239}Pu cross sections. It is apparent that some levels are missed even at low temperature measurements, but that a significant reduction of missed levels is observed at 77°K as compared to the Gwin measurements. Numerical experiments indicate that these missed levels may modify the value, but not the sign, of the $H_k^{(x)}$ parameters of a neighboring level, while their effect on

the $G_k^{(\alpha)}$ is practically insignificant. In the framework of a first order perturbation treatment applicable to ^{239}Pu , the values of $\Gamma_k^{(f)}$, $\Gamma_k^{(\gamma)}$, and $\Gamma_{kn}^{(b)}$ are therefore influenced but little by the missed levels.

Numerical experiments with synthetic data indicate that the quasi-resonances postulated by Lynn should be observable in cross sections simulating the low-energy ^{239}Pu data. No indications for the occurrence of quasi-resonances have been found in this data analysis; it is of course possible to add broad resonances which could be combined with existing levels to form a "quasi-resonance." The quality of the data however does not allow a clear indication for the existence of a quasi-resonance in the energy region investigated.

The uniqueness of the R - matrix representation was also considered: three sets of fission widths amplitudes for the $J = 1^+$ state have been obtained from the same set of multilevel parameters which give practically equivalently good representations of the three cross section data sets, indicating the limitations imposed by the accuracy of the data on the fitting procedure, since for theoretical reasons the $J = 1^+$ state should have a unique R - matrix parametrization.

The results of this evaluation indicate the value a high precision measurement of σ_c and σ_f made at a low temperature would have for determining accurately resonance parameters of ^{239}Pu over a wide energy range.

Table 1

Multilevel Parameters Generating Synthetic Data for Testing
Effects of Hidden and Quasi-resonances.

$(g = 3/4)$ $\mu(\text{eV})$	$\nu(\text{eV})$	$\alpha^o(1)$	$\beta^o(1)$	$G^F(1)$	$H^F(1)$	$G^Y(1)$	$H^Y(1)$
7.8079	.0432	4.2344	.0809	2.2657	.0748	1.9301	0.0
10.9118	.0920	8.4398	-.7219	6.5516	-.7344	1.7487	-.0032
11.8825	.0294	4.3111	.4657	1.5299	.4650	2.7056	.0030
14.3096	.0510	2.6019	.6758	1.7175	.6561	.8673	.0056
14.6562	.0351	7.6489	-.5322	3.4091	-.5120	4.0270	-.0055
17.6347	.0353	6.6445	.0128	3.0198	.0179	3.4493	0.0
22.2390	.0494	8.3422	-.0569	4.9395	-.0504	3.1809	0.0
23.8794	.0436	.2661	.0562	.1361	.0565	.1296	0.0
26.2776	.0329	4.4174	.0023	2.3037	.0085	2.0125	0.0
27.2370	.0095	.3187	.0171	.1600	.0180	.1567	0.0
8.500	.0215	.0300	0.0	.0056	0.0	.0244	0.0
9.900	.0250	.0300	0.0	.0120	0.0	.0180	0.0
$(g = 1/4)$							
7.9002	.0215	.0400	-.0024	.0074	-.0024	.0327	0.0
14.2023	.0245	.0425	-.0233	.0121	-.0232	.0303	-.0003
15.4987	.3362	1.7678	-.0453	1.6714	-.0396	.0799	-.0058
15.5188	.0164	3.2300	.0710	0.0	.0652	2.9656	.0061
(1) In units of $(\text{eV})^{\frac{1}{2}} \times 10^{-4}$							

Table 2

Lineshape Parameters from CODILLI Fitting the Total Cross Section Generated from the Parameters of Table 1 in the Region Between 6 and 20 eV.

$(g = 3/4)$ $\mu(\text{eV})$	$\nu(\text{eV})$	$\alpha^{(1)}$	$\beta^{(1)}$
7.8079	.0432	4.2342	.08005
10.9118	.0920	8.4394	-.7239
11.8825	.0294	4.3111	.4648
14.3096	.0510	2.6019	.6752
14.6562	.0351	7.6485	-.5338
17.6347	.0353	6.6443	.0117
9.900	.0250	.0300	0.0
8.500	.0215	.0300	0.0
$(g = 1/4)$			
7.9002	.0215	.0400	-.0023
14.2023	.0245	.0426	-.0234
15.4987	.3362	1.7670	-.0452
15.5188	.0164	3.2300	.0709
(1) In units of $(\text{eV})^{\frac{1}{2}} \times 10^{-4}$			

Table 3

Values of $\alpha^{(1)}$ for the cases discussed in Sec. 2.b

$\mu^{(2)}$	Exact values from CHAMA	Case 1	Case 2	Case 3
7.808	4.2344	4.2658	4.2826	4.2784
10.912	8.4398	8.3743	8.4325	8.4347
11.883	4.3110	4.3170	4.3168	4.3106
14.310	2.6019	2.5575	2.6480	2.6503
14.656	7.6489	7.5413	7.6580	7.6576
17.635	6.6445	6.6181	6.6459	6.6424
χ	---	$.7580 \times 10^{-4}$	$.1048 \times 10^{-4}$	$.405 \times 10^{-5}$

(1) in $\text{eV}^{\frac{1}{2}} \times 10^{-4}$

(2) in eV .

Table 4
Values of $\beta^{(1)}$ for the cases discussed in Section 2.b

$\mu^{(2)}$	Exact values from GHAMA	Case 1	Case 2	Case 3
7.808	.08099	.07128	.05716	.07058
10.912	-.7219	-.6869	-.6987	-.7249
11.882	.4657	.4979	.4694	.4669
14.310	.6758	.6805	.6788	.6751
14.656	-.5322	-.4478	-.5406	-.5458
17.635	.01283	-.0384 ^(*)	.01136	.01053

(1) in $\text{eV}^{\frac{1}{2}} \times 10^{-4}$

(2) in eV

(*) discrepancy due to coarse fit of the 15.5 resonance.

Table 5

Fission and capture line-shape parameters for ^{239}Pu in $(\text{eV})^{\frac{1}{2}} \times 10^{-4}$: Comparison between Gwin's evaluation and this evaluation using Gwin's values of μ and ν .

(g = 3/4) $\mu(\text{eV})$	$\nu(\text{eV})$	G^F		H^F		G^Y		H^Y
		(1)	(2)	(1)	(2)	(1)	(2)	(1)
7.85088	.04638	2.3224	2.3526	.1392	.1104	1.9747	1.9865	.0188
10.97580	.10560	6.4594	6.4372	-.4392	-.4648	1.6936	1.6708	.0831
11.93653	.05900	1.6201	1.6380	.3535	.3705	2.8062	2.7933	-.0499
14.37746	.058020	1.7329	1.7340	.5524	.6072	.8560	.8835	.0602
14.72565	.037590	3.3833	3.4550	-.3921	-.4513	4.0029	3.9982	.0404
17.70590	.039560	2.9473	2.9234	.1243	.1185	3.4049	3.3379	.0835
22.31846	.05748	4.8849	4.7985	-.0136	-.0559	3.5310	3.1404	.1185
23.96776	.12357	.2209	.1689	.0859	.0680	.2403	.1524	.0745
26.31851	.05203	2.3861	2.2597	.0943	.1199	2.2687	2.0554	.1306
27.28879	.07169	.0684	.0695	-.0480	-.0443	.7699	.3424	0.0
35.56785	.03278	.0647	.0626	.0263	.0041	.7406	.6960	.1055
(g = 1/4)								
15.48510	.36115	2.5333	2.4149	-.1455	-.1857	.2211	.1135	.0192
32.41014	.10048	.5726	.5299	.0624	-.0178	.2259	.1500	.0225
(1) Gwin (Reference 3) (2) CODILLI (symmetrical capture)								

Table 6

Total Cross Section Lineshape Parameters for ^{239}Pu in Units of $(\text{eV})^{\frac{1}{2}} \times 10^{-4}$: Comparison Between the Values Calculated from Derrien and Those Obtained from CODILLI Fitting the Data with the Same Values of μ and ν , in the Region Between 7 and 40 eV.

$(g = 3/4)$ $\mu(\text{eV})$	$\nu(\text{eV})$	$\alpha^{\circ(1)}$	$\beta^{\circ(1)}$	$\alpha^{\circ(2)}$	$\beta^{\circ(2)}$
7.8009	.0437	4.1339	.07322	4.2214	.07316
10.9117	.0885	8.3965	-.6253	8.3778	-.5131
11.8778	.03198	4.2708	.4255	4.3414	.3675
14.3085	.04791	2.6095	.6530	2.6081	.5797
14.6582	.0382	7.5301	-.5879	7.8004	-.5191
17.6328	.0405	6.5382	.1056	6.5087	.1176
22.2340	.0555	8.2391	-.2101	8.2989	-.1475
23.8757	.0150	.2737	.0672	.2225	.0342
26.2226	.04126	4.4537	.0892	4.4654	.0022
27.2329	.0211	.4315	.0115	.3956	0.0
35.4220	.0238	.6300	0.0	.6296	.0104
$(g = 1/4)$					
15.4291	.2690	2.2190	-.1656	2.2518	-.0924
32.2619	.0779	.7404	.0077	.7000	.0924
<p>(1) Calculated with program LEMA-CHAMA from Ref. 5.</p> <p>(2) From CODILLI fit using the same μ, ν values.</p>					

Table 7

Multilevel parameters for ^{239}Pu from triple fit of fission, capture
and total cross section data in the region from 6 to 70 eV

$(g = 3/4)$ $\mu(\text{eV})$	$\nu(\text{eV})$	$\alpha^o(*)$	$\beta^o(*)$	$G^F(*)$	$K^F(*)$	$G^Y(*)$
7.849	.0432	4.2704	.1279	2.2933	.1226	1.9388
10.9718	.0920	8.5255	-.4258	6.7098	-.4399	1.7274
11.935	.0294	4.3351	.3335	1.5713	.3355	2.6913
14.375	.0509	2.6814	.5592	1.7765	.5457	0.8865
14.725	.0352	7.6476	-.5136	3.4317	-.4978	4.0115
17.702	.0352	6.4351	.0645	2.9555	.0704	3.3218
22.324	.050	8.2776	-.0465	4.8623	-.0393	3.2017
23.935	.038	0.2590	.0127	0.1343	.0133	0.1243
26.317	.033	4.3980	.0544	2.2446	.0610	2.0530
27.290	.022	0.4007	.0097~0	0.0597	.0094~0	.3419
35.530	.015	0.6159	.0312	0.0343	.0319	.5767
41.460	.0209	9.0051	.2900	0.3294	.2052	7.8345
41.720	.0473	3.1029	-.1084	1.8183	-.0702	1.2349
44.520	.0275	13.4205	.0194	1.0974	0.0	10.8678
50.120	.0279	6.4293	.0861	1.1405	.0629	4.9390
52.590	.0283	19.9905	.0307	2.5145	.0406	14.0539
55.680	.0275	2.8699	.0271	.9985	.0335	1.7965
59.270	.0850	9.6245	-.1520	7.5798	-.1405	1.7647
63.140	.0300	1.2200	.0233	.8042	.0224	.4024
65.810	.0470	20.2674	-.2166	7.5465	-.1620	10.3560

Background constants for the spin-state $J = 1$, in units of $(\text{eV})^{-\frac{1}{2}} \times 10^{-5}$			
Region	A_1^T	A_1^F	A_1^Y
6-40 eV	1.5	3.5	1.02
40-70 eV	.75	2.6	0.

(*) in units of $(\text{eV})^{\frac{1}{2}} \times 10^{-4}$.

Table 8

Multilevel parameters for ^{239}Pu from triple fit of fission, capture and total cross section data in the region from 6 to 70 eV.

$(g = 1/4)$ $\mu(\text{eV})$	$\nu(\text{eV})$	$\alpha^o(*)$	$\beta^o(*)$	$G^F(*)$	$H^F(*)$	$G^Y(*)$
15.490	.330	2.414	.2300	2.2639	.2276	.1181
32.379	.052	.6448	.0548	.4848	.0536	.1550
47.650	.140	3.7260	-.4200	2.9828	-.4360	.7179
49.83	.350	2.5575	.4362	2.4063	.4256	.1349
57.540	.480	15.6600	-2.4740	13.9600	-2.4680	1.020
61.40	3.600	11.6880	2.6730	11.5500	2.6735	0.0
65.52	.090	3.42	-.268	3.420	-.240	0.0

Background constants for the spin state $J = 0$, in units of $(\text{eV})^{-\frac{1}{2}} \times 10^{-5}$

Region	A_1^T	A_1^F	A_1^Y
6-40 eV	.45	1.45	.35
40-70 eV	0.	0.	0.

(*) in units of $(\text{eV})^{\frac{1}{2}} \times 10^{-4}$.

Table 9
Comparison of values of neutron width and scattering area

μ	Γ_n (mV) (1)	Γ_n (mV) (2)	$(g \Gamma_n^2 / \Gamma) \times 10^3$ (mV) (3)	$(g \Gamma_n^2 / \Gamma) \times 10^3$ (mV) (2)
7.849	.770	.798	6.7 ± 1.9	5.9
10.972	1.850	1.883	$12. \pm 2.4$	14.5
11.935	.980	.998	$16. \pm 3.1$	12.9
14.375	.660	.678	< 4.5	3.4
14.725	1.920	1.956	$40. \pm 8.4$	41.0
17.702	1.830	1.805	$30. \pm 6.6$	35.
22.324	2.590	2.607	51.0 ± 13.5	51.5
23.935	.090	.084	----	-
26.317	1.520	1.504	----	25.7
27.290	.150	.126	----	-
35.53	.250	.245	----	1.5
(1) Derrien (reference 5) (2) Triple fit (3) Sauter and Bowman (reference 39)				

Table 10

Total fission and capture parameters from TRIPLE fit originating the parameters of Table 11

$\mu^{(a)} (1)$	$\nu (1)$	$\alpha^0 (2)$	$G^F (2)$	$G^Y (2)$	$\beta (2)$	$H^F (2)$
7.848	.0432	4.2369	2.2695	1.9293	.1295	.1242
10.972	.0920	8.4523	6.5887	1.7753	-.4831	-.4973
11.935	.0294	4.3027	1.5697	2.6606	.3707	.3737
14.375	.0509	2.5993	1.6908	.8902	.5386	.5250
14.725	.0352	7.6506	3.4191	4.0272	-.4022	-.3864
17.702	.0352	6.4406	2.9354	3.3474	.1026	.1085
22.324	.0500	8.3408	4.8787	3.1410	-.0702	-.0710
23.935	.0380	.2683	.1501	.1180	.0272	.0272
26.317	.0330	4.4171	2.3007	2.0060	.0278	.0278
27.290	.0220	.4007	.0597	.341	.007	.007

(a) energy scale of GWIN measurement: correspond to the μ values of Table 2.

(1) in eV

(2) $10^4 \text{ eV}^{\frac{1}{2}}$

Table 11

 ^{239}Pu R-matrix parameters for 10 resonances of $J = 1^+$

E_λ (eV)		$\Gamma_{\lambda n}^o$ (mV)		$\Gamma_{\lambda \gamma}$ (eV)		$\Gamma_{\lambda f}$ (eV)		ϵ_λ		
(1)	(2)	(1)	(2)	(1)	(2)	(1)	(2)	(a)	(b)	(c)
7.800	7.807	.4136	.4237	.0397	.0393	-.0470	.0463	+	-	+
10.910	10.911	.8401	.8452	.0551	.0386	-.1200	.1434	+	-	+
11.878	11.882	.4265	.4303	.0420	.0364	.0210	.0214	-	+	-
14.307	14.309	.2617	.2600	.0340	.0349	.0610	.0662	-	+	+
14.660	14.656	.7522	.7651	.0376	.0371	.0370	.0314	-	+	+
17.633	17.634	.6537	.6441	.0387	.0366	-.0405	.0321	+	-	-
22.234	22.239	.8239	.8341	.0443	.0377	-.0640	.0585	+	+	+
23.876	23.879	.0276	.0268	0.00	.0412	.0300	.0459	-	-	-
26.223	26.228	.4452	.4417	.0371	.0300	.0440	.0344	-	-	-
27.233	27.238	.0431	.0401	.0340	.0317	-.0080	.0096	+	+	+

(1) Derrien (Ref. 5)

(2) From perturbation analysis of triple fit line shape parameters: The energy scale is the one of Derrien's measurements.

Table 12

Capture and Fission line shape parameters obtained from the R-matrix parameters of Table 11

Level	$\mu^{(a)}$ (eV)		$G^Y \cdot 10^4$ (eV) ^{$\frac{1}{2}$}		$G^F \cdot 10^4$ (eV) ^{$\frac{1}{2}$}		$H^F \cdot 10^4$ (eV) ^{$\frac{1}{2}$}			
	(1)	(2)	(1)	(2)	(1)	(2)	(1)	(2a)	(2b)	(2c)
1	7.801	7.808	1.8771	1.9298	2.2204	2.2650	.0647	.0953	.0748	.1734
2	10.912	10.912	2.6411	1.7975	5.6633	6.5546	-.6434	-.6661	-.7344	-.2608
3	11.878	11.883	2.8366	2.7044	1.3663	1.5314	.4214	.4440	.4650	.2823
4	14.308	14.309	.9045	.8663	1.6873	1.7247	.6314	.6155	.6561	.4309
5	14.658	14.656	3.6926	4.0253	3.6472	3.4032	-.5743	-.5610	-.5120	-.7526
6	17.633	17.635	3.1248	3.4496	3.2654	3.0208	.1042	.1050	.0179	.1620
7	22.234	22.239	3.2938	3.1807	4.7523	4.9395	-.2138	-.1648	-.0504	-.1881
8	23.876	23.879	.0053	.1306	.2723	.1337	.0672	.0709	.0566	.0759
9	26.223	26.228	2.000	2.0131	2.3718	2.3038	.0881	.0485	.0085	.0668
10	27.233	27.239	.3491	.1565	.0808	.1601	.0120	.0128	.0180	.0102

-221-

(a) Energy scale of Derrien measurement, corresponding to the μ values of Table 4.

Table 13

Total cross section parameters derived from the R-matrix parameters of Table (11)

$\alpha^o * 10^4 \text{ (eV)}^{\frac{1}{2}}$		$\beta^o * 10^4 \text{ (eV)}^{\frac{1}{2}}$			
(1)	(2)	(1)	(2a)	(2b)	(2c)
4.1339	4.2293	.0732	.1015	.0810	.1796
8.3965	8.452	-.6253	-.6534	-.7219	-.2471
4.2708	4.3094	.4255	.4446	.4657	.2820
2.6095	2.6346	.6530	.6354	.6758	.4518
7.5301	7.6114	-.5880	-.5815	-.5322	-.7741
6.5382	6.6458	.1056	.1000	.0128	.1570
8.2391	8.3415	-.2101	-.1714	-.0569	-.1947
.2737	.2642	.0671	.0706	.0562	.0757
4.4537	4.4186	.0892	.0423	.0023	.0606
.4315	.3985	.0115	.0119	.0171	.0936

Table 14

Values of the χ values for the parameters of table 13 used for fits of the total cross section.

$$\chi^2 = \sum_{i=1}^{NP} (Y_{ex}(i) - Y_{trial}(i))^2 w_i / (NP - ND)$$

NP = number of points, ND = number of fitted parameters

Parameters of Table 13 Column (1) (Derrien)	$\chi = .360-04$
Column (2a)	$\chi = .383-04$
Column (2b)	$\chi = .274-04$
Column (2c)	$\chi = .332-04$
Parameters of Table 10; (Triple fit)	$\chi = .192-04$

Table 15

R-matrix parameters obtained from the multilevel parameters of Table 7

(g = 3/4)

E(eV)	Γ_n^o (mV)	Γ_Y (eV)	Γ_f (eV)	$\epsilon^{(1)}$	$\epsilon^{(2)}$	$\epsilon^{(3)}$
7.849	.427	.0392	.0464	+	-	+
10.972	.853	.0373	.1448	+	-	+
11.935	.434	.0365	.0213	-	+	-
14.375	.268	.0337	.0674	-	+	+
14.725	.765	.0369	.0316	-	+	+
17.702	.644	.0363	.0323	+	-	-
22.324	.828	.0387	.0587	-	-	-
23.935	.026	.0365	.0394	+	+	+
26.317	.440	.0308	.0337	+	+	+
27.290	.040	.0386	.0065	+	+	+
35.530	.616	.0281	.0017	+	+	+
41.460	.904	.0366	.0015	+	---	---
41.720	.308	.0385	.0547	+	---	---
44.520	1.342	.0446	.0045	+	---	---
50.120	.643	.0429	.0099	+	---	---
52.590	1.999	.0397	.0071	+	---	---
55.680	.287	.0344	.0191	+	---	---
59.270	.962	.0312	.1339	+	---	---
63.140	.122	.0197	.0396	-	---	---
65.809	2.027	.0480	.0350	+	---	---

Table 16

R-matrix parameters obtained from the multilevel parameters of Table 8

$(g = 1/4)$ E(eV)	Γ_{μ}^0 (mV)	Γ_Y (eV)	Γ_F (eV)	$\theta^{(1)}$	$\theta^{(2)}$
15.49	.241	.033	.640	0°	0°
32.38	.065	.024	.076	25°	25°
47.65	.363	.049	.229	313°	313°
49.83	.255	.033	.660	135°	135°
57.54	1.390	.0625	.7638	118°	118°
61.40	1.168	0.	7.200	0°	0°
65.52	.3430	0.	.180	298°	82°
<p><u>Note:</u> These values are preliminary owing to the uncertain spin assignment of the resonance at 65.5 eV.</p>					

Table 17

Comparison of observed average reaction widths resulting
from single- and multilevel evaluations

Spin-state	Singlelevel analysis (ref 12)	Multilevel analysis (this work)
$J = 1^+$	$\langle \Gamma_Y \rangle = .0433$ $\langle \Gamma_f \rangle = .0416$ $\langle \Gamma_Y \rangle / \langle \Gamma_f \rangle = 1.04$	$\langle \Gamma_Y \rangle = .0364$ $\langle \Gamma_f \rangle = .0394$ $\langle \Gamma_Y \rangle / \langle \Gamma_f \rangle = .92$
$J = 0^+$	$\langle \Gamma_Y \rangle = .046$ $\langle \Gamma_f \rangle = 1.068$ $\langle \Gamma_Y \rangle / \langle \Gamma_f \rangle = .043$	$\langle \Gamma_Y \rangle = .029^{(*)}$ $\langle \Gamma_f \rangle = 1.392^{(*)}$ $\langle \Gamma_Y \rangle / \langle \Gamma_f \rangle = .020$
$(*)$ These values are preliminary owing to the uncertain spin-state of the resonance at 65.5 eV.		

FIGURE CAPTIONS

	Page
Fig. 1. <u>Effects of asymmetries.</u> The continuous curve represents the contribution of the symmetrical line shape parameters; the experimental points are those of Derrien measurement	228
Fig. 2. <u>Effects of asymmetries.</u> The continuous curve represents the contribution of the asymmetrical line shape parameters, (smooth background). Only positive values of the continuous curve are plotted	229
Fig. 3. Synthetic total cross section fitted with the parameters of Table 2	230
Fig. 4. Synthetic total cross section fitted ignoring the quasi-resonance and the small single levels and two hidden levels	231
Fig. 5. Synthetic total cross section fitted ignoring the small single levels	232
Fig. 6. Gwin's fission total cross section data fitted with the parameters of Tables 7 and 8, from 6 to 40 eV	233
Fig. 7. Gwin's capture cross section data fitted with the parameters of Tables 7 and 8, from 6 to 40 eV.....	234
Fig. 8. Derrien's total cross section data fitted with the parameters of Tables 7 and 8, from 6 to 40 eV	235
Fig. 9. Gwin's fission cross section data fitted with the parameters of Tables 7 and 8, from 40 to 70 eV	236
Fig. 10. Gwin's capture cross section data fitted with the parameters of Tables 7 and 8, from 40 to 70 eV.....	237
Fig. 11. Derrien's total cross section data fitted with the parameters of Tables 7 and 8, from 40 to 70 eV	238
Fig. 12. Derrien's total cross section in the region from 7 to 20 eV; the continuous curve is obtained from set (2a) of Table 13	239
Fig. 13. Derrien's total cross section in the region from 7 to 20 eV; the continuous curve is obtained from set (2b) of Table 13	240
Fig. 14. Derrien's total cross section in the region from 7 to 20 eV; the continuous curve is obtained from set (2c) of Table 13	241
Fig. 15. Derrien's total cross section in the region from 7 to 20 eV; the continuous curve is obtained from the parameters of Table 6.	242

Fig. 1. Effects of asymmetries. The continuous curve represents the contribution of the symmetrical line shape parameters; the experimental points are those of Derrien measurement.

x EXPERIMENTAL DATA
 + POSITIVE DEVIATION
 o NEGATIVE DEVIATION
 - CALCULATED POINTS

Fig. 2. Effects of asymmetries. The continuous curve represents the contribution of the asymmetrical line shape parameters (smooth background). Only positive values of the continuous curve are plotted.

× EXPERIMENTAL DATA
+ POSITIVE DEVIATION
◊ NEGATIVE DEVIATION
- CALCULATED POINTS

Fig. 3. Synthetic total cross section fitted with the parameters of Table 2.

x EXPERIMENTAL DATA
 + POSITIVE DEVIATION
 o NEGATIVE DEVIATION
 - CALCULATED POINTS

Fig. 4. Synthetic total cross section fitted ignoring the quasi-resonance and the small single levels and two hidden levels.

x EXPERIMENTAL DATA
 + POSITIVE DEVIATION
 o NEGATIVE DEVIATION
 - CALCULATED POINTS

Fig. 5. Synthetic total cross section fitted ignoring the small single levels.

- x EXPERIMENTAL DATA
- + POSITIVE DEVIATION
- ◇ NEGATIVE DEVIATION
- CALCULATED POINTS

Fig. 6. Gwin's fission cross section data fitted with the parameters of Tables 7 and 8, from 6 to 40 eV.

x EXPERIMENTAL DATA
 + POSITIVE DEVIATION
 o NEGATIVE DEVIATION
 - CALCULATED POINTS

Fig. 7. Gwin's capture cross section data fitted with the parameters of Tables 7 and 8, from 6 to 40 eV.

x EXPERIMENTAL DATA
 + POSITIVE DEVIATION
 o NEGATIVE DEVIATION
 - CALCULATED POINTS

Fig. 8. Derrien's total cross section data fitted with the parameters of Tables 7 and 8, from 6 to 40 eV.

- × EXPERIMENTAL DATA
- + POSITIVE DEVIATION
- ◊ NEGATIVE DEVIATION
- CALCULATED POINTS

Fig. 9. Gwin's fission cross section data fitted with the parameters of Tables 7 and 8, from 40 to 70 eV.

x EXPERIMENTAL DATA
 + POSITIVE DEVIATION
 o NEGATIVE DEVIATION
 - CALCULATED POINTS

Fig. 10. Gwin's capture cross section data fitted with the parameters of Tables 7 and 8, from 40 to 70 eV.

× EXPERIMENTAL DATA
 + POSITIVE DEVIATION
 ◊ NEGATIVE DEVIATION
 - CALCULATED POINTS

Fig. 11. Derrien's total cross section data fitted with the parameters of Tables 7 and 8, from 40 to 70 eV.

Fig. 12. Derrien's total cross section in the region from 7 to 20 eV: the continuous curve is obtained from set (2a) of Table 13.

x EXPERIMENTAL DATA
 + POSITIVE DEVIATION
 o NEGATIVE DEVIATION
 - CALCULATED POINTS

Fig. 13. Derrien's total cross section in the region from 7 to 20 eV: the continuous curve is obtained from set (2b) of Table 13.

× EXPERIMENTAL DATA
 + POSITIVE DEVIATION
 ○ NEGATIVE DEVIATION
 - CALCULATED POINTS

Fig. 14. Derrien's total cross section in the region from 7 to 20 eV: the continuous curve is obtained from set (2c) of Table 13.

x EXPERIMENTAL DATA
 + POSITIVE DEVIATION
 o NEGATIVE DEVIATION
 - CALCULATED POINTS

Fig. 15. Derrien's total cross section in the region from 7 to 20 eV: the continuous curve is obtained from the parameters of Table 6.

× EXPERIMENTAL DATA
 + POSITIVE DEVIATION
 ◊ NEGATIVE DEVIATION
 - CALCULATED POINTS

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C00-2022-18

THE MULTILEVEL EXPANSION AND ITS APPLICATION TO NEUTRON RESONANCE ANALYSIS

Final Report

Contract AT(11-1)-2022-1

NOTICE

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July 1972

14

TABLE OF CONTENTS

	Page
Summary	1
(1) Correlated Analysis of the ^{239}Pu fission, capture, and total cross sections	1
(2) Computer Program Development	1
(3) Exploratory Work	1
Task (1)	2
Task (2a)	2
Task (2b)	3
Task (2c)	3
Task (3a)	3
List of Publications and Technical Reports supported in part by Contract AT(11-1)-2022 and 2022-1.....	4
I. Introduction	7
II. Multilevel description of low energy neutron reactions in fissile elements	11
III. Ambiguities in the R-matrix representation	14
IV. Development of computer programs	15
V. References	21

APPENDICES

A. Multilevel description of neutron resonance reactions in fissile elements. ^{a) c)}	
B. Ambiguities in R-matrix representations of fissile element cross sections with two fission channels. ^{b) c)}	
C. Program CODILLI-2	24
D. Program LEMA-CHAMA	54
E. Program TRIPLE	106
F. Interactive Use of Program CODILLI 2 with SCORE III-A: Least Squares Data Fitting of ^{239}Pu Using Program CODILLI with SCORE	155
G. Multilevel analysis of ^{239}Pu cross sections in the low energy region	176

(a) This manuscript has been submitted for publication to Nuclear Physics,
and is being revised.

(b) This report will be published in Physical Review C, 1972.

(c) In view of the fact that this report will be published in a journal, a copy
of it is not appended here. Copies may be obtained upon request from the
Department of Physics of the University of Illinois, Urbana, Ill. 61801.

Summary

The scope of the work under this contract consisted of a continuation of the work supported under contract AT(11-1)-2022, and it included the following specific tasks:

(1) Correlated Analysis of the ^{239}Pu fission, capture, and total cross sections, to be reported in the ENDF-B format, with the aim of obtaining consistent generalized Kapur-Peierls and R-matrix parameters in the context of operational testing of Program TRIPLE.

(2) Computer Program Development

(a) Operational checks of Program TRIPLE, and deposition of the Program, with suitable test cases at the ANL code center.

(b) Development of Program GAMPLEX, to include three modes of deriving R-matrix parameters from the generalized Kapur-Peierls parameters obtainable from Programs CODILLI and TRIPLE, using a least-squares procedure, (GAMPLEX I), a perturbative method for the few channel case (GAMPLEX II), and a method permitting at least in principle the direct calculation of level matrix parameters from the generalized Kapur-Peierls parameters. (GAMPLEX III).

(c) To make Program CODILLI a part of the SCORE package, and to analyze and prepare Program TRIPLE for eventual inclusion in the SCORE package.

(3) Exploratory Work

(a) To investigate the usefulness of programs CODILLI and TRIPLE for the analysis of fertile and other non-fissile elements, and the necessary computer implementation of these programs for such purposes.

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