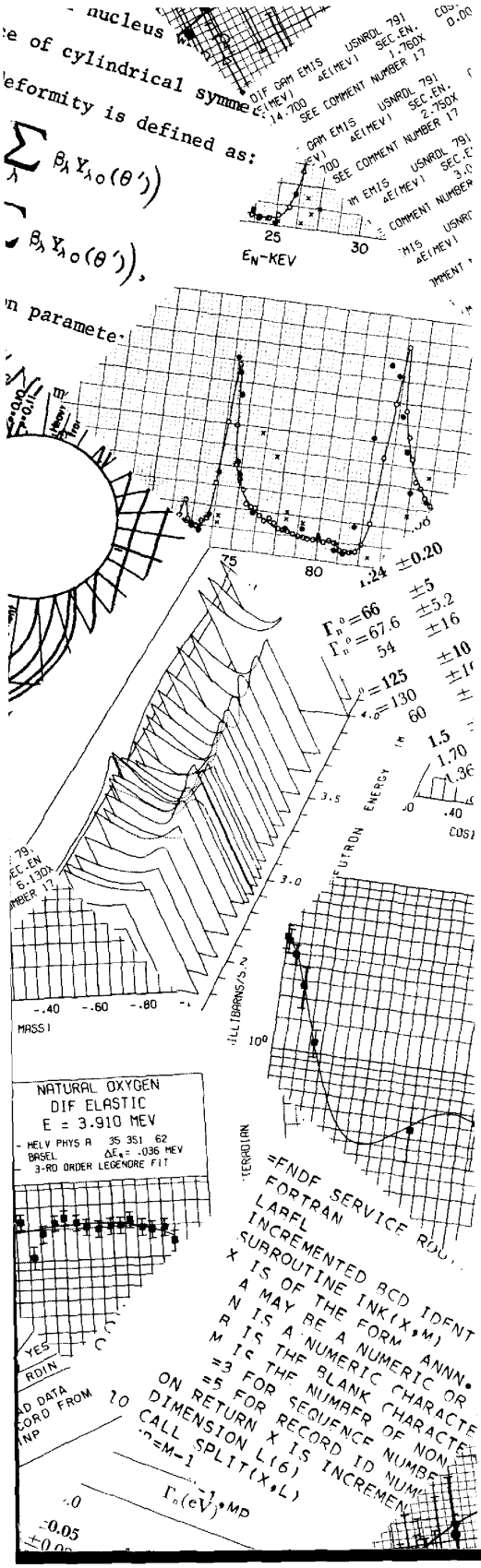

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PROCEEDINGS OF THE CSEWG
RESONANCE REGION SUBCOMMITTEE MEETING
HELD AT
BROOKHAVEN NATIONAL LABORATORY
MAY 8, 1972

M.R. BHAT (Editor)

April 1973

NATIONAL NEUTRON CROSS SECTION CENTER
BROOKHAVEN NATIONAL LABORATORY
UPTON, NEW YORK 11973

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AGENDA

Resonance Region Meeting

Monday, May 8, 1972

Location: National Neutron Cross Section Center
Conference Room, Building 197C
29 Cornell Avenue

Chairman of the Meeting: M. R. Bhat

	Time	Program
Monday	9:00 am	1. Resonance Reaction Formalisms G. de Saussure (ORNL)
	10:00 am	2. Calculations in the Unresolved Resonance Region R. N. Hwang (ANL)
	11:00 am	3. Reactor Applications C. L. Cowan (GE-BRDO)
		LUNCH
	2:00 pm	4. The Probability Table Method L. B. Levitt (AI)
	3:00 pm	5. Use of Pre-processed Data in the Resonance Region O. Ozer (BNL)
	4:00 pm	6. Summary of the Meeting M. K. Drake (BNL)

TABLE OF CONTENTS

INTRODUCTION

This report is a collection of the talks given at the Meeting of the Resonance Region Subcommittee of CSEWG, held at the Brookhaven National Laboratory on May 8, 1972. This was a special one-day meeting organized in connection with the CSEWG Meeting, held on the next two days. The purpose of this meeting, and its objectives were the following.

A number of formalisms are being used to analyse and represent the resolved resonance data of nuclei. Amongst these are the different multi-level formalisms in addition to the usual single-level Breit-Wigner representation. The need of the multi-level formalisms to give a good representation of the experimental data is well known. However, it is not at all clear whether the additional effort involved in obtaining such multi-level parameters and using them in reactor codes is necessary from the viewpoint of practical reactor calculations. Hence, one of the objectives of the meeting was to review and emphasise the salient features of each of these formalisms and arrive at some conclusions regarding their usefulness in reactor calculations.

In addition, there is the question of extending these formalisms to the unresolved resonance region and whether the parameters obtained in the resolved resonance region could readily be used in the unresolved region. This is related to the more general problem of data representation and calculations in the unresolved resonance region. It was hoped that discussions at the Meeting would resolve or clarify some of these difficulties

When an outline of the Meeting was drawn up in March 1972, the Probabilit Table Method was one of the newly proposed methods of data representation for the unresolved resonance region. It had been suggested by L. B. Levitt

as being particularly suited for Monte Carlo calculations. Its advantages are that it is fast, needing only a modest amount of computer storage as compared to the conventional methods using either a ladder of resonances or average parameters in the unresolved resonance region. Though the method was considered as being basically correct, there were a few reservations about it which could hopefully be settled by further calculations of suitable test cases. Hence, it was felt that extensive discussions on this new method would stress the basic principles on which it is based and emphasise those areas which needed further clarification before its final acceptance as a suitable alternate format of data representation in the unresolved resonance region.

Lastly, it was recognised that the time had come to assess the usefulness and determine the role of preprocessed data in the resonance region, its effect on the evaluated data files, reactor codes and future applications.

The Meeting was attended by thirty-nine persons and there were extensive discussions of the subject matter of the invited talks. A tape recording of the talks and the discussions was made but could not be reproduced verbatim due to the cost of labour involved. It was also felt that the discussions and exchange of ideas would be less inhibited if persons were not held responsible for the exact wording of their questions or comments. However, the tape recording was used to elaborate on some of the topics discussed during the course of the talk by M. K. Drake summarising the Meeting. There were also two extensive and significant contributions by M. S. Moore and D. E. Cullen, whose texts are reproduced along with those of the invited talks.

It has been nearly a year since the Meeting was held and perhaps one should summarise here what were its results and to what extent its objectives

were met. The different single-level and multi-level reaction formalisms were reviewed and their interrelationships clarified. As regards the estimates of multi-level effects in reactor calculations, during the course of discussions it became clear that there were no such calculations in published literature in spite of the claims of the authors. This led to a better understanding of what form such calculations should take and M. K. Drake, in summarising the Meeting, suggested procedures for such calculations. Some of these details and specifications were later distributed amongst the CSEWG Members and their criticism and suggestions solicited. These calculations are now being carried out in a few laboratories and it is hoped that the results would be available soon. At the Meeting, there was a general acceptance of the Probability Table Method as some of the questions of detail had been answered in the meantime. Though this method was originally proposed in connection with the Monte Carlo calculations, it was pointed out by D. E. Cullen that it could be extended to deterministic methods, e.g., multi-group calculations of neutron and photon transport problems using existing codes. Recently, he has also shown how the Probability Tables could be easily calculated using the parameters presently given in the evaluated data files. Such a procedure would obviate the need for separate programs for calculating the Probability Tables and make their extensive use more acceptable. The discussions at the Meeting also reviewed the role of pre-processed resonance region data and some useful comments and suggestions were made which would be helpful in planning future reactor codes.

It is my privilege to thank the speakers and all the participants at the Meeting who contributed to the fruitful discussions and exchange of

ideas. My thanks are due to M. K. Drake for agreeing to the difficult task of summarising the Meeting at short notice when the scheduled speaker could not come. Again, I would like to thank him and S. Pearlstein for their help in drawing up an agenda of the Meeting and its organization, and Georgia Irving for a commendable job of retyping parts of the manuscript.

April 23, 1973 M. R. Bhat

Text of an invited talk presented at Resonance Region Meeting
Brookhaven National Laboratory, Upton, New York, May 8, 1972

RESONANCE REACTION FORMALISMS FOR FISSILE NUCLEI*

by

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*Research sponsored by the U. S. Atomic Energy Commission, under contract with the Union Carbide Corporation.

ABSTRACT

In this paper we describe very briefly some of the multilevel formalisms most frequently used to represent the low-energy cross sections of the fissile nuclei. We also discuss some of the properties and applications of the resonance parameters.

I. Introduction

It is now well known that the neutron cross sections of fissile nuclei cannot be adequately represented by the single-level Breit-Wigner formula. Indeed there are asymmetries in the resonances of the reaction cross sections caused by interference in the fission channels.

Various multilevel formalisms have been developed which account for the observed asymmetries. These formalisms have proven very successful for representing the cross sections of the main fissile isotopes in the resolved resonance region.

The multilevel formalisms have been extensively described in the literature. In this paper we will very briefly discuss the formalisms which have been most frequently used to represent the cross sections of the fissile isotopes. In particular, we will review how these formalisms can all be derived from the Wigner-Eisenbud R-matrix theory.

We will also describe some of the properties of the resonance parameters entering the various multilevel formalisms, and discuss some applications of these formalisms, particularly to the interpretation of measured neutron cross sections.

II. Multilevel Formalisms

The different formalisms used to interpret the low-energy cross sections of the fissile nuclei have been reviewed by Moore.[1] The relations of these formalisms to different nuclear reaction theories have been discussed by Adler and Adler.[2] Complete reviews of the formal nuclear reaction theories have been given by Lane and Thomas[3] and by Lynn.[4]

Three different multilevel formalisms have been extensively used to describe the low-energy neutron cross sections of the fissile nuclei.

These formalisms, developed by Vogt,[5] Reich and Moore,[6] and Adler and Adler,[7] can be derived directly from the R-matrix theory.

The expression for the neutron cross section which proceeds through the outgoing channel c is given by:

$$\sigma_{nc} = \pi\lambda\!\!\!^{-2} \sum_J g^J |\delta_{nc} - U^J_{nc}|^2 \ , \tag{1}$$

where $\lambda\!\!\!^{-}$ is the neutron wave length divided by 2π and g^J is the statistical factor for resonances of spin J. The collision matrix element U^J_{nc} may be written as:[8]

$$U^J_{nc} = e^{i(\phi_n + \phi_c)} \left[\delta_{nc} + i \sum_{\lambda\lambda'} A_{\lambda\lambda'} (\Gamma_{\lambda n}\Gamma_{\lambda' c})^{\frac{1}{2}} \right], \tag{2}$$

where ϕ_n and ϕ_c are potential scattering phase shifts, $\Gamma_{\lambda c}$ is the partial width for the decay of the level λ into the channel c and the $A_{\lambda\lambda'}$ are elements of the Wigner level matrix. The inverse level matrix is given by

$$(A^{-1})_{\lambda\lambda'} = (E_\lambda - E)\,\delta_{\lambda\lambda'} - \frac{i}{2} \sum_c (\Gamma_{\lambda c}\Gamma_{\gamma' c})^{\frac{1}{2}} \ . \tag{3}$$

In order to obtain the cross sections from the R-matrix parameters E_γ and $\Gamma_{\gamma c}$, Vogt[5] inverts the inverse level matrix A^{-1} directly considering only a finite number N of levels. A smooth "background term" then accounts for the contribution of the neglected distant levels.

The technique developed by Adler and Adler[7] consists of diagonalizing the inverse level matrix by an orthogonal transformation:

$$D = S^{-1} A S$$

$$A_{\lambda\lambda'} = \sum_\nu \frac{S_{\lambda\nu} S_{\lambda'\nu}}{d_\nu - E} \tag{4}$$

The collision matrix is obtained by combining Eqs. (2) and (4):

$$U^J_{nc} = e^{i(\phi_n + \phi_c)} \left[\delta_{nc} + \sum_\nu \frac{r_{\nu c}}{d_\nu - E} \right] , \tag{5}$$

and

$$r_{\nu c} = i \sum_{\lambda\lambda'} (\Gamma_{\lambda n} \Gamma_{\lambda' c})^{\frac{1}{2}} S_{\lambda\nu} S_{\lambda'\nu} . \tag{6}$$

In terms of the new complex parameters d_ν and $r_{\nu c}$, the Adler and Adler cross-section formulae given in Table I can easily be derived. These expressions are particularly well suited for reactor calculations and "least-squares fitting" of experimental data.

When the number of levels, N, is large, and the number of fission channels, n_f, is known and small, the formalism of Reich and Moore[6] is very convenient. Reich and Moore exploit the fact that the sum $\sum_c (\Gamma_{\lambda c} \Gamma_{\lambda' c})^{\frac{1}{2}}$ over the many radiation channels can be assumed to be diagonal to obtain an expression for the collision matrix not in terms of the NxN level matrix A but in terms of a much smaller $(n_f + 1)$ x $(n_f + 1)$ channel matrix (I-K):

$$U^J_{nc} = e^{i(\phi_n + \phi_c)} \{2[(I - K)^{-1}]_{nc} - \delta_{nc}\} , \tag{7}$$

and

$$(I - K)_{cc'} = \delta_{cc'} - \frac{i}{2} \sum_\lambda \frac{(\Gamma_{\lambda c} \Gamma_{\lambda c'})^{\frac{1}{2}}}{E_\lambda - E - \frac{i}{2} \Gamma_{\lambda\gamma}} . \tag{8}$$

The Reich-Moore formulas for the neutron cross sections are obtained by combining Eqs. (1), (7), and (8) and are listed in Table 2.

It is interesting to note[9,10] here that the Adler-Adler formalism can also be derived by directly expanding the Reich-Moore cross sections into partial fractions, as is shown in Table 3.

Another representation of the cross sections of fissile nuclei has been much used in reactor calculations. This representation could be called "pseudo Breit-Wigner" and consists essentially of describing the symmetric part of the resonances with the Breit-Wigner single level formula. The "interference part," however, is not parametrized but described on a point-by-point basis and denoted as a "smooth background".[11,12,51] This pseudo Breit-Wigner representation can, of course, be derived from R-matrix theory, in fact it can be obtained directly from the Adler-Adler formalism by a trivial change of notation.

In Table 3 we illustrate the relation between various expressions for the fission cross section. The first equation in the table is the Reich-Moore expression for one fission channel. This expression can be rationalized as the ratio of two polynomials in E, by multiplying the numerator and denominator by the "rationalizing polynomial" indicated. The ratio of two polynomials can then be expanded in partial fractions with complex roots d_k. This expansion immediately yields the Adler-Adler expression which can be separated into symmetric and antisymmetric parts. A change of notation then yields the pseudo Breit-Wigner representation.

The parameters entering this representation [Eq. (III_4) of Table 3] have been denoted by primes to distinguish them from the resonance energies and partial widths entering into the R-matrix formulation [Eq. (III_1), for instance]. It is very important to realize that the parameters entering

the pseudo Breit-Wigner representation are not the usual R-matrix parameters. In particular the partial widths and spacings of the pseudo Breit-Wigner representation do not follow the Porter-Thomas[13] and Wigner[14] distribution laws.

III. Energy Dependence of the Multilevel Parameters

The R-matrix formalism of Wigner and Eisenbud is derived by assuming real, energy independent boundary conditions at the surface of the nucleus. Hence, the R-matrix resonance energies and reduced widths are energy independent. On the other hand, the Adler-Adler parameters and the parameters entering the Pseudo Breit-Wigner representation are somewhat energy dependent, for the transformation S [of Eq. (4)] which diagonalizes the level matrix, is a function of the neutron widths which are proportional to the neutron momentum. This energy dependence, however is negligible so long as the neutron width $\Gamma_n = \Gamma_n^\circ \sqrt{E}$ is very small compared to the total width, $\Gamma = \Gamma_f + \Gamma_\gamma + \Gamma_n$. This is the case for the main fissile nuclei up to 10 keV, at least. For instance for ^{235}U, $\langle \Gamma_n^\circ \rangle = 0.13$ mV, $\langle \Gamma_f + \Gamma_\gamma \rangle = 180$ mV, so that at 10 keV $\langle \Gamma_n \rangle = 13$ mV $\ll \langle \Gamma \rangle = 190$ mV.

IV. Nonuniqueness of Multilevel Parameters

It is well known that multilevel fits to measured cross sections are not unique. Different sets of parameters may describe the existing data equally well. This lack of uniqueness is due in part to the uncertainties in the measured cross sections: Precise scattering and capture measurements in the fissile nuclei are exceedingly difficult. Often there is very little information on the spin of the resonances so that assumptions must be made as to which resonances interfere with each other. Finally,

due to the natural width of the resonance and due to Doppler and instrumental broadening some levels are usually missed in the analysis because they are concealed in the wings of other levels.[15,16]

More fundamentally, Auchampaugh[21] has recently shown by a computer study, and Adler and Adler[23] have demonstrated mathematically that, in some cases, at least, different sets of partial fission widths will yield the same set of fission, capture, and scattering cross sections. Hence, even if the cross sections were known exactly, and for each spin state, some R-matrix parameters may not be determined uniquely. Of course, as pointed out by Moore,[22] the R-matrix parameters could still be determined uniquely if additional data were available, such as the partial fission cross section for each fission channel. One consequence of the nonuniqueness of multilevel parameters is that no meaningful uncertainty can be assigned to a given parameter. Hence, it would not in general be correct to average parameters from different sources for the same resonance. Because the multilevel parameters are not unique, their interpretation in terms of nuclear physics is subject to question; in some cases, for instance, it would be erroneous to conclude from the apparent interference of two levels that those levels belong to the same spin state. On the other hand, the multilevel parameters yield precise cross sections, hence they are very useful as a mathematical tool for data reduction or for reactor computations. As long as the parameters are used only as a tool to compute selfshielding, their nonuniqueness is not too important.

V. Applications of the Multilevel Formalisms

It is perhaps appropriate to discuss here some of the applications of resonance analysis, particularly in interpreting neutron cross-section measurements.

Not only does the resonance analysis of nuclear data provide information on the statistical distribution of resonance parameters which is of interest to nuclear physics, but it is also an indispensable tool to correct measured cross sections for a number of instrumental effects such as resolution broadening, selfshielding and multiple scattering effects, contamination of the data by resonances due to isotopes or chemical impurities, etc.

In the resolved resonance region, the multilevel formalisms permit a concise and precise analytical representation of the cross sections, which results in an appreciable economy of information storage[24] and allows easy comparison of data taken with different resolution or at different temperatures.[25] As an illustration, in Fig. 1 we show the low-energy capture and fission cross sections of ^{235}U and a multilevel fit to these data.[10,27] There are more than 8,000 data points in the figure, whereas the solid line is described by only 300 parameters. The multilevel representation is fully consistent with the data, in the sense that the difference between the data and the computed curve is always small compared to the uncertainties in the data.

In the unresolved resonance region, measured cross sections cannot usually be corrected reliably for the instrumental resolution broadening. For the selfshielding and multiple scattering corrections to the data, as well as for using the cross sections in reactor calculations, it is

necessary to rely on a resonance reaction theory. This is illustrated in Fig. 2. The upper curve in the figure represents the assumed behavior of the unbroadened ^{235}U fission cross section between 2,000 and 2,060 eV. The true shape of that cross section is, of course, not known, but it might look similar to the upper curve of Fig. 2. (This curve was obtained by assuming, in that energy region, the same spacing and reduced widths that are found between 0 and 60 eV. This is not unreasonable since p-wave contributions to the fission cross section are still very small at 2 keV and since the S-wave average spacings and reduced widths are not expected to change much over the small change in excitation energy.) The second curve in Fig. 2 was obtained by Doppler broadening the upper curve, for a temperature of 300°K. This Doppler broadened cross section is the cross section which should be used in computing selfshielding or multiple scattering corrections to a measurement done at room temperature, or to compute a reactor operating at that temperature. The lowest curve on Fig. 2 was obtained by Doppler and resolution broadening the upper curve. The resolution corresponds to that of a typical time-of-flight spectrometer. (It is the resolution corresponding to the ORNL-RPI measurement[27] on which the cross sections for ^{235}U in the ENDF/B III file[11] are partly based.) This lowest curve in Fig. 2 is the cross section that would be measured experimentally if the upper curve were the true unbroadened cross section. It is clear from the figure that at some energy the Doppler broadened cross section, which is the cross section required, cannot be obtained reliably from the measured cross section. As the resolution of time-of-flight spectrometers is improved, the measured cross section approaches the Doppler-broadened

cross section, but since the instrumental broadening is proportional to $E^{3/2}$ whereas the Doppler broadening is proportional to $E^{1/2}$, there will usually be some energy where the instrumental broadening dominates the Doppler broadening.

The statistical features of the Doppler broadened cross section may be obtained by generating a mock-up cross section by selecting parameters from the appropriate distributions. This mock-up cross section can then be resolution broadened to verify that it displays the same qualitative features and has the same average values as the measured cross section.[26] It is for such statistical study in the unresolved region that the multilevel formalisms and the statistical distributions of the parameters are most needed.

VI. Comparison of Multilevel Formalisms

There are now computer codes available to "least squares fit" measured cross sections to both the Adler-Adler and the Reich-Moore multilevel formalisms,[28-31] as well as sophisticated automated cross section analysis programs which use live visual display.[32,33] The question arises as to which of the formalisms is most desirable to represent the cross sections in the resolved and unresolved region. The Vogt and Reich-Moore formalisms are essentially equivalent, since they are based on the same parametric representation. These two formalisms differ mostly in the technique used to invert the channel matrix. The Vogt formalism is to be preferred when many channels and few levels must be considered simultaneously, whereas the Reich-Moore formalism is more convenient when many levels and few channels must

be considered, as is generally the case for the low-energy cross sections of the fissile isotopes.

The R-matrix formalisms and the Adler-Adler formalism are complementary in that the statistical properties of the R-matrix parameters are much better known,[13] but the Adler-Adler formulation is best suited for a variety of applications.[34] For this reason various techniques have been developed to transform a set of R-matrix parameters into an equivalent set of Adler-Adler parameters, using the mathematical connection between the R-matrix and Adler-Adler cross section formalisms.[9,35-37]

Hence, it is possible to rank the multilevel formalisms in the sense that it is relatively easy to obtain equivalent Adler-Adler parameters from a given set of R-matrix parameters. The inverse process, of converting Adler-Adler parameters into equivalent R-matrix parameters, is very difficult and impractical except in some very special cases.[38] Similarly the conversion of the Adler-Adler representation into an equivalent "pseudo Breit-Wigner" representation is a trivial operation, whereas the Adler-Adler parameters cannot be obtained from a "pseudo Breit-Wigner" representation except by fitting the smooth background with the appropriate parametric representation.

For ^{239}Pu a meaningful R-matrix analysis can be done, because the low-energy cross sections of this nucleus are relatively simple and because the spin of many resonances has been determined. For such a nucleus, an R-matrix simultaneous analysis of several partial cross sections[31] will yield valuable nuclear physics information and the

R-matrix parameters can always be transformed into equivalent Adler-Adler parameters. For ^{233}U, on the other hand, no meaningful R-matrix analysis can be performed at the present time: The resonance structure at low energy is very complicated, due to the larger value of Γ/D, and none of the resonance spins have been determined reliably.[19] For such a nucleus, an Adler-Adler type analysis is probably to be preferred[20] since it will yield a precise description of the cross section and it does not require an *a priori* decision as to which resonances belong to the same spin state and hence interfere. The nucleus ^{235}U falls between these two extreme cases.[26]

VII. Some Limitations in Extrapolating Cross Sections into the Unresolved Resonance Region

One of the most important application of the multilevel formalisms is the generation of mock-up cross sections in the unresolved region, in order to compute selfshielding effects, such as the Doppler coefficient, in that region where the measured cross section does not fully reflect the structure of the Doppler broadened cross section. Such applications require a knowledge of the statistical distribution of the resonance parameters and of the resonance spacings, and a knowledge of the variation with energy of the average values of the parameters.

The statistical properties of the R-matrix parameters and level spacings have been investigated extensively by Porter and Thomas[13] and by Wigner.[14] The statistical properties of the S-matrix parameters have been investigated analytically and numerically by using the connection between the R-matrix and the S-matrix parameters.[39-43]

In the neutron S-wave region, up to a few keV, it is usually assumed that the average capture width and reduced neutron width remain constant, and that the average fission width follows a Hill-Wheeler penetration law,[44]

$$\langle \Gamma_f \rangle = \frac{\langle D \rangle}{2\pi} \left[1 + \exp \left(-2\pi \frac{E - E_f}{\hbar w} \right) \right]^{-1}$$

where E_f is some threshold energy and $\hbar w$ some characteristic width.

Recently Lynn[45] has called attention to the possible influence of the (n, γf) process in which an excited nucleus emits a gamma ray before undergoing fission. If this process is important it will distort the apparent distribution of fission width, and more small widths will be observed than are expected from the Porter-Thomas distribution. Such a distortion of the fission width distribution has usually not been observed experimentally. However, there are large uncertainties in the observed fission width distributions, particularly toward the small width end, due to "missed levels," to ambiguities in the resonance analysis of the fissile nuclei and to the small statistical sampling of the distributions. The effect of the (n, γf) process on the calculation of average cross sections has been investigated by Stavinsky and Shaker,[46] Garrison,[47] and Lynn.[45]

The intermediate structure recently observed[48] in the fission cross section of various isotopes implies that the simple Hill-Wheeler formula is not applicable in the vicinity of a fission threshold. In

many cases the average fission cross section shows a considerable amount of intermediate structure that can be understood on the basis of the double-humped fission barrier recently introduced by Strutinsky.[49] The incorporation of this intermediate structure in the calculation of average cross sections has been investigated, particularly by Kikuchi.[50]

VIII. Conclusions

Adequate multilevel formalisms have been developed to describe the low-energy cross sections of the fissile nuclei. In the resolved resonance region, the cross sections can be parametrized with great precision by any of those formalisms. The generation of mock-up cross sections in the unresolved resonance region requires a knowledge of the statistical distributions and of the average values of the parameters. The statistical distribution of the R-matrix parameters can be derived from general considerations concerning the nuclear Hamiltonian. The statistical properties of the generalized Kapur-Peierls parameters can be investigated numerically and sometimes analytically, using the mathematical connection between the R-matrix and Kapur-Peierls formalisms.

Many problems remain to be solved, such as, for instance, the incorporation of processes like the $(n, \gamma f)$ reaction or the subthreshold fission through a double-humped potential, into the mechanism to compute cross sections in the unresolved region. Some information on these processes will probably come from more extensive investigations of the properties of the parameters obtained by fitting data in the resolved region.

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Table I

Adler and Adler Formulae for the Neutron Cross Sections

$$(I_1) \quad \sigma_{nT} = 2\pi\lambda^2 g[1 - \cos(2ka)] + \frac{C}{\sqrt{E}} \sum_{\lambda} \frac{\nu_\lambda G_\lambda^T + (\mu_\lambda - E) H_\lambda^T}{(\mu_\lambda - E)^2 + \nu_\lambda^2}$$

$$(I_2) \quad \sigma_{nA} = \frac{C}{\sqrt{E}} \sum_{\lambda} \frac{\nu_\lambda G_\lambda^A + (\mu_\lambda - E) H_\lambda^A}{(\mu_\lambda - E)^2 + \nu_\lambda^2}$$

$$(I_3) \quad \sigma_{nF} = \frac{C}{\sqrt{E}} \sum_{\lambda} \frac{\nu_\lambda G_\lambda^F + (\mu_\lambda - E) H_\lambda^F}{(\mu_\lambda - E)^2 + \nu_\lambda^2}$$

$$(I_4) \quad \sigma_{nS} = \sigma_{nT} - \sigma_{nA} \qquad \sigma_{n\gamma} = \sigma_{nA} - \sigma_{nF}$$

$$(I_5) \quad G_\lambda^T = \alpha_\lambda \cos(2ka) + \beta_\lambda \sin(2ka)$$

$$H_\lambda^T = \beta_\lambda \cos(2ka) - \alpha_\lambda \sin(2ka)$$

$$C = 6.52 \cdot 10^5 \text{ b·eV.}$$

σ_{nT}, σ_{nA}, σ_{nF}, σ_{nS} and $\sigma_{n\gamma}$ are respectively the total, absorption, fission, scattering and capture cross sections, k is the neutron momentum and a the nuclear radius. The other symbols are defined in the texts.

The smooth "background" which accounts for the neglected "far-away" levels has been omitted from I_1, I_2 and I_3 for simplicity.

Table II

Reich and Moore Formulae for the Neutron Cross Sections

$$(II_1) \quad \sigma_{nT}^{J} = 2\pi\lambda\!\!\!^{-2}\, g[1 - \cos(2ka)] + 4\pi\lambda\!\!\!^{-2}\, g\, \mathrm{Re}(e^{2ika}\, \rho_{nn})$$

$$(II_2) \quad \sigma_{nA}^{J} = 4\pi\lambda\!\!\!^{-2}\, g[\mathrm{Re}(\rho_{nn}) - |\rho_{nn}|^2]$$

$$(II_3) \quad \sigma_{nF}^{J} = 4\pi\lambda\!\!\!^{-2}\, g \sum_{c} |\rho_{nc}|^2$$

$$(II_4) \quad \rho_{nc} = \delta_{nc} - [(I - K)^{-1}]_{nc}$$

$$(II_5) \quad (I - K)_{cc'} = \delta_{cc'} - \frac{i}{2} \sum_{\lambda} \frac{(\Gamma_{\lambda c}\, \Gamma_{\lambda c'})^{\frac{1}{2}}}{E_\lambda - E - \frac{i}{2}\, \Gamma_{\lambda\gamma}}$$

The symbols are defined in Table I and in the text.

The scattering and capture cross sections can be obtained by (I_4).

The cross sections and parameters refer to one spin value.

The sum in (II_3) extends over the fission channels only.

A constant term representing the contribution of the neglected "far-away" levels has been omitted for simplicity.

Table III

Relation Between Multilevel Formalisms

1. Reich-Moore expression for the fission cross section (one fission channel)

$$\sigma_{nf} = \frac{cg}{E}\left|\frac{\sum_{\lambda}[(\Gamma_{\lambda n}\Gamma_{\lambda f})^{1/2}]/[E_\lambda - E - (i/2)\Gamma_{\lambda\gamma}]}{1-(i/2)\sum_{\lambda}\frac{\Gamma_{\lambda n}+\Gamma_{\lambda f}}{E_\lambda - E - (i/2)\Gamma_{\lambda\gamma}} - \frac{1}{8}\sum_{\lambda\lambda'}\frac{[(\Gamma_{\lambda n}\Gamma_{\lambda' f})^{1/2} - (\Gamma_{\lambda' n}\Gamma_{\lambda f})^{1/2}]^2}{[E_\lambda - E - (i/2)\Gamma_{\lambda\gamma}][E_{\lambda'} - E - (i/2)\Gamma_{\lambda'\gamma}]}}\right|^2 \qquad III_1$$

"Rationalizing" Polynomial $\prod_{\lambda}[E_\lambda - E - (i/2)\Gamma_{\lambda\gamma}]$

2. Adler-Adler expression for the fission cross section

$$\sigma_{nf} = \frac{cg}{\sqrt{E}}\sum_k\left(\frac{R_k}{d_k - E} + c.c.\right) = \frac{cg}{\sqrt{E}}\sum_k\frac{G_k\nu_k - H_k(\mu_k - E)}{(\mu_k - E)^2 + \nu_k^2} \qquad III_2$$

3. Pseudo Breit-Wigner representation

$$\sigma_{nf} = \frac{cg}{\sqrt{E}}\sum_k\frac{G_\nu\,\nu_k}{(\mu_k - E)^2 + \nu^2} + \frac{cg}{\sqrt{E}}\sum_k\frac{H_k(\mu_k - E)}{(\mu_k - E)^2 + \nu_k^2} \qquad III_3$$

$$\sigma_{nf} = \frac{cg}{\sqrt{E}}\sum_k\frac{(\Gamma'_{no}\Gamma'_f)_k}{(E'_0 - E)^2 + (\Gamma'/2)^2} + \text{"smooth background"} \qquad III_4$$

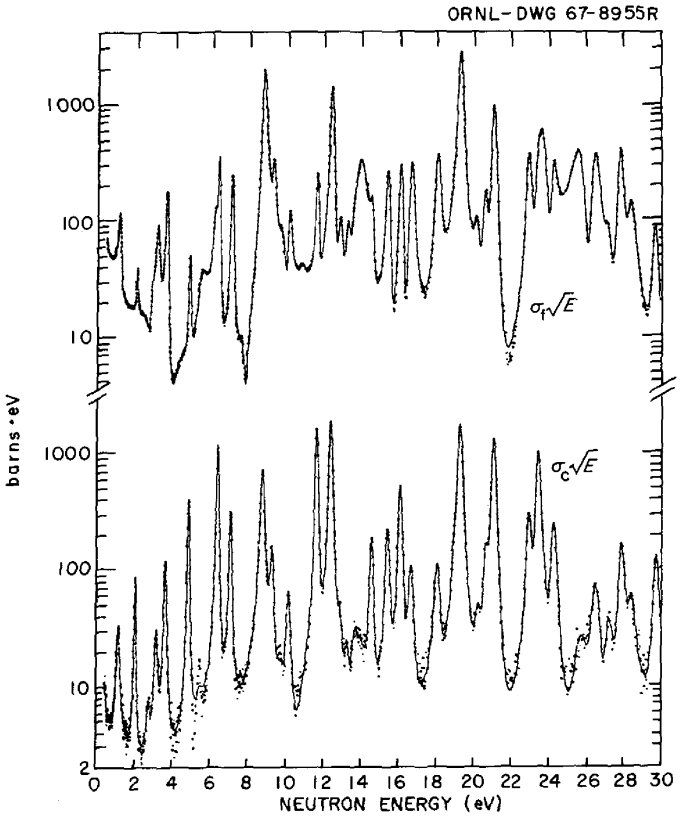

Figure 1. Least Squares Fit to the ^{235}U Capture and Fission Cross Sections.

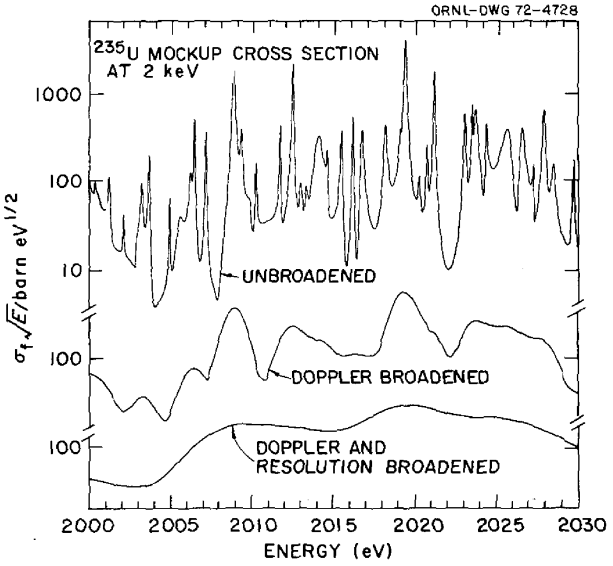

Figure 2. Mock-up Fission Cross Section for ^{235}U Between 2000 and 2060 eV.

Text of a talk presented at Resonance Region Meeting
Brookhaven National Laboratory, Upton, New York, May 8, 1972.

NEW HOPE AND WHY BOTHER*

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NEW HOPE AND WHY BOTHER

The purpose of this very brief discussion is to point out the importance of new data on spins and fission-channel quantum numbers for resolved resonances of fissile targets. Such data will help to resolve problems of nonunique multilevel descriptions. There is also some evidence that the data may be of importance for reactor design.

The variation of K, the projection of the total angular momentum on the nuclear symmetry axis, can be determined by measuring the anisotropy of fragments emitted in the fission of aligned target nuclei by slow neutrons. Measurements of this type, in which the target nuclei are aligned by quadrupole coupling at low temperatures, have been carried out for a number of years by J. W. T. Dabbs[1,2] and associates at ORNL. Most recently, significant new results have been obtained by Pattenden and Postma[3] at Harwell. A somewhat different experiment is planned by Keyworth et al.[4] (LASL), in collaboration with Dabbs[5] on the ORELA. In this measurement, the target nuclei will be polarized, to permit the determination of J; since the polarization also produces alignment, measurement of the anisotropy will allow them to determine K at the same time.

The results of this experiment will not remove the nonuniqueness of multilevel descriptions completely (because there are more than two fission channels in each spin state), but they will certainly help. In principle, if one could measure the A_4 and A_6 terms in the Legendre expansion describing the fragment angular distribution, the unique set of multilevel parameters

could be obtained. However, this will not be done in the Keyworth experiment.

Let us assume that J and K will be known in the near future. The next question to be asked is, "Why does one want to bother with a multilevel description?" The most important reason hinges on the variation of $\bar{\nu}$ from resonance to resonance, depending on J and K, and the concomitant variation of the fission width. This leads to an apparent effective $\bar{\nu}$ dependence of self-shielding and temperature. These are effects which have not yet been included in sensitivity calculations as far as I know, but they could be important--especially for ^{239}Pu.

The situation is perhaps best summarized by considering the lowest energy resonance, at 0.28 eV, in ^{235}U. Figure 1 shows some old data which Lowell Miller and I[6] reported at the Salzburg conference. Plotted (in arbitrary units) is the variation of the relative yield of the highest energy heavy binary fragments. The solid line is the multilevel fit to these data using the parameters reported by Vogt[7], and simply rotating the fission vectors in channel space until one gets the best fit.

Figure 2 shows the A_2 values determined by Pattenden and Postma.[8] The solid line is the same fit (to the data of Fig. 1). The simplest interpretation is that there are two channels effective, having K=0 and K=2, with no contributions from K=1 or 3.

Next, we want to ask about $\bar{\nu}$. Figure 3 shows the results of a rather crude experiment which Lowell Miller and I did in 1965. The four data points we obtained seem to show a K dependence over this resonance; the solid line is a best fit to these data, and represents a guess as to what the variation of $\bar{\nu}$ might be. Finally, after going through this exercise, I went back to Simon Weinstein's thesis[8,9] and plotted his data (slightly renormalized); again

there seems to be consistency with the same curve, as shown in Fig. 4. Unfortunately, there was no reported value for $\bar{\nu}$ between 0.28 and 1.1 eV; this would have perhaps been the definitive test.

Finally, to complete the picture, Fig. 5 shows the correlation between the Pattenden-Postma A_2 and the total width of the resonance. The correlation does exist, and indicates (somewhat surprisingly) that the widest resonances are associated with higher K values.

My own conclusions from this study are summarized as follows:

(1) J and K are associated with physical observables, in particular the fragment mass and kinetic-energy distributions, the fission widths, and $\bar{\nu}$.

(2) I believe that these results tend to corroborate the Weinstein measurements of $\bar{\nu}$. The reason there is no clear correlation of Weinstein's $\bar{\nu}$ with K is that there is also a strong J dependence as well, and the spins are not yet known. This implies that the Weinstein ^{239}Pu results are also correct.

(3) It is important to be able to account for such effects, both in the resolved and in the unresolved region. A multilevel description appears to be required.

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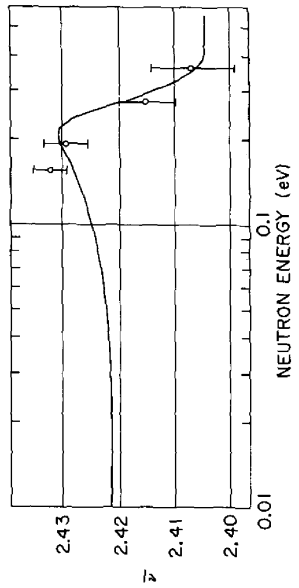

Figure 3

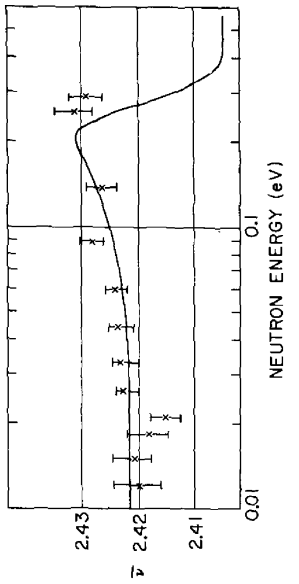

Figure 4.

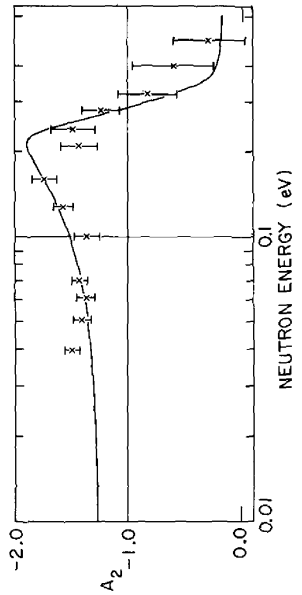

Figure 1

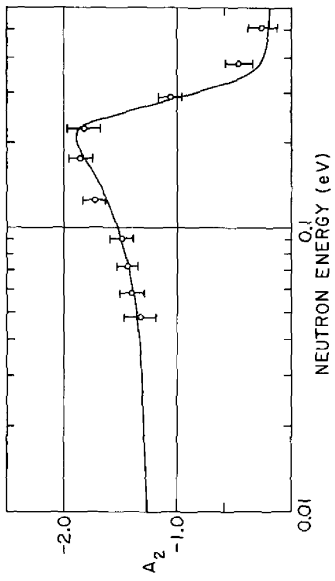

Figure 2

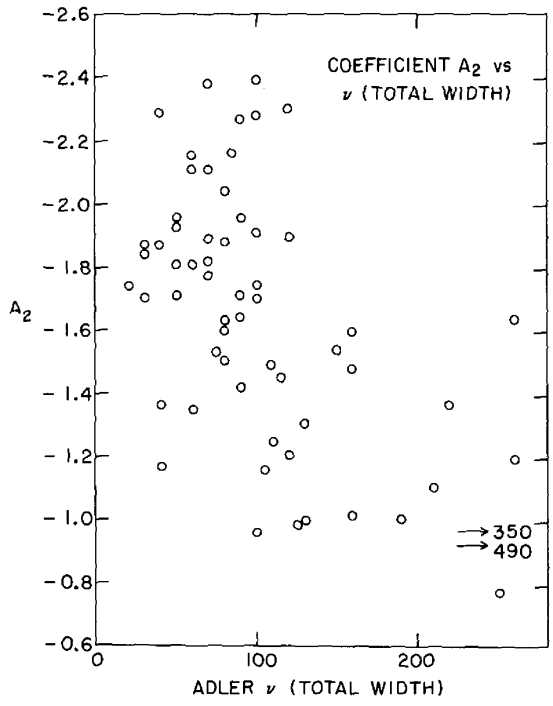
COEFFICIENT A_2 vs
ν (TOTAL WIDTH)
A_2
-2.6
-2.4
-2.2
-2.0
-1.8
-1.6
-1.4
-1.2
-1.0
-0.8
-0.6
0
100
200
ADLER ν (TOTAL WIDTH)
→350
→490

Figure 5.

Text of an invited talk presented at Resonance Region Meeting,
Brookhaven National Laboratory, Upton, New York, May 8, 1972;

THEORETICAL CONSIDERATIONS PERTINENT TO THE TREATMENT OF UNRESOLVED RESONANCES*

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May 8, 1972

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I. INTRODUCTION

The treatment of the resonance absorption in the unresolved energy region is generally based on concepts directly related to the statistical theory of nuclear reactions. In reactor applications, one of the most difficult problems is to estimate the resonance self-shielding effect and the related Doppler effect on a statistical basis. The resonance self-shielding effect is characterized by the correlation between the reaction cross section and the neutron flux in energy and space. The neutron flux is generally related to the cross sections in an extremely complicated way through the integral transport equation. The problem is further complicated by the fact that the temperature-dependence of the cross sections must be considered. Because of the important role that the Doppler effect plays in large fast reactors, there have been a great number of studies concerning this subject. Numerical methods and codes that treat the problem to various degrees of sophistication have recently become available. However, unlike the problem of treating the resolved resonances, the calculated results in the unresolved region are usually subject to significant statistical uncertainties which are difficult to estimate. The interpretation of the calculated results, the efficient use of various methods, and application of newly developed statistical methods and nuclear theory are still active fields of research.

The primary purpose of this paper is to improve understanding of the fundamental aspects of problems concerning the statistical treatment of the resonance absorption in the reactor applications. Section II describes some general problems that one encounters in estimating the resonance self-shielding effect. In Section III, various calculational methods and their theoretical justifications are discussed. Particular attention is devoted to the discussion of the cross-section sampling techniques. Finally, the role of the multilevel effect on reactor Doppler-effect analysis is examined in Section IV. Simple examples that illustrate the statistical behavior of the S-matrix parameters are given. Numerical results obtained using the single-level and the multilevel representations are compared.

II. Problems Associated with Estimation of Resonance Self-Shielding Effect

The treatment of the resonance self-shielding effect in the unresolved energy region is a natural extension of the statistical theory of average cross sections such as described by Moldauer[1] and Ericson.[2] Since the theoretical foundations may often be obscurred in routine applications, it is useful to summarize briefly some conceptual aspects of the problems prior to the detailed discussions of the basis for the calculational methods.

The quantities of interest in the reactor calculations are generally of the form

$$E(q) = \langle \sigma_x \phi \rangle \text{ ; and } \langle \phi \rangle \quad , \tag{1}$$

which represent the expectation values of the reaction rate of a given reaction process and the neutron flux over a large number of events within a given energy interval. Here, the neutron flux ϕ depends on the macroscopic total and scattering cross sections as described by the integral transport equation. Without loss of generality, the cross section of any given process x can be represented in the R-matrix formalism in terms of parameters E_{oi} and γ_{ci}

$$\sigma_x = \sigma_x\left(\gamma_{c1}, E - E_{01}; \gamma_{c2}, E - E_{02} \cdots \gamma_{c2}, E_{0i}\right) \quad , \tag{2}$$

where E_{oi} and γ_{ci} are the R-matrix state and the reduced width for various channels c, respectively. From the statistical theory of spectra,[4] the distributions of these parameters are well known. The distribution of E_{oi} for a given spin state is characterized by the Wigner distribution and by the long-range correlations described by Dyson.[4,5] γ_{ci} are statistically independent and normally distributed with zero means and variance of unity according to Porter and Thomas.[6] Given $\langle |E_{oi} - E_{oi+1}| \rangle$ and γ_{ci}^2 , Eq. 2, in principle, includes all the statistical information and the explicit energy dependence of the cross sections from which, and through the integral transport equation, the random variable q_i and its expectation values are completely specified.

For practical applications the R-matrix representation, which requires the inversion of a level matrix, is clearly too complicated, especially when the temperature dependence of the cross sections is considered. This, of course, excludes the cases where the natural widths of the resonances are much smaller than the level spacing and the Breit-Wigner equation becomes valid. For special cases where the Breit-Wigner equation is questionable, one convenient alternative is to use the S-matrix representation from which a simple energy and temperature dependence can be derived.[1,7,8,9] One disadvantage of the S-matrix representation is our lack of a statistical theory that will adequately describe the statistical behavior of the S-matrix parameters. The problem, therefore, becomes that of finding the statistical properties of the S-matrix parameters from those of the known R-matrix parameters. Numerical approaches are usually required in practical calculations with the exception of some oversimplified special cases. A further discussion of this subject will be given in Section IV.

Two special problems must be considered in the application of the statistical theory to self-shielded average cross sections. First, the presence of the neutron flux in Eq. (1), which attenuates as energy decreases, complicates the problem significantly. The statistical description of q within any given energy interval becomes meaningless if the neutron flux attenuates too rapidly. Consequently, significant uncertainties in the estimated self-shielding effect are expected in the low energy region where the resonance absorption becomes strong. Secondly, there does not appear to exist any simple way to relate the statistical behavior of the self-shielding effect in the unresolved energy region directly to the observed statistical behavior of cross sections from various experiments. The latter problem is particularly important in the application of Monte Carlo techniques.

The problem can be best illustrated by using the narrow resonance approximation which is widely used in the reactor applications. For simplicity, consider the case of a infinite homogeneous reactor system. Under the assumption that the extent of the resonance is small compared

to the maximum energy loss per collision, the neutron flux becomes inversel proportional to the total macroscopic cross section of all isotopes in the system. The self-shielded reaction rate for a given isotope i becomes simply

$$E\{q_i\} \simeq \left[\langle\sigma_{xi}\rangle - \left\langle\sigma_{xi}\frac{\Sigma_R}{\Sigma_p + \Sigma_R}\right\rangle\right] \Big/ \Sigma_p \ , \tag{3}$$

where Σ_p and Σ_R are the macroscopic total potential scattering and total resonance cross sections respectively. The quantity $\langle\sigma_{xi}\rangle$ is the unshielded average cross section which is temperature independent. The second term represents the degree of the self-shielding effect and is temperature dependent. In terms of the cross-section statistics, the self-shielding term clearly relates to the higher-order moments not only of σ_{xi} and σ_{ti} but also of the total cross section of different isotope i' in the mixture. Hence, an adequate statistical description of the means $\langle\sigma_{xi}\rangle$ alone may not be sufficient in estimating the self-shielding effect especially when the energy interval under consideration is relatively small in practical applications. Of particular interest from a theoretical point of view is a special case in which Eq. (3) approaches asymptotically to

$$E\left\{\frac{\sigma_{xi}}{\Sigma_t}\right\} \cong \frac{\langle\sigma_{xi}\rangle}{k} - \frac{\langle\sigma_{xi}\sigma_{ti}\rangle - \langle\sigma_{xi}\rangle\langle\sigma_{ti}\rangle}{k^2} + \cdots \tag{4}$$

in the limit of high energy where the Doppler width becomes relatively large. The constant k is the average macroscopic total cross section $\langle\Sigma_t\rangle$ per atom concentration of isotope i under consideration.

It is interesting to note that, under this limiting condition, the self-shielding effect can be identified directly with the correlation between the microscopic reaction cross section σ_{xi} and the corresponding total cross section σ_{ti}. This is, of course, true only under the idealized condition where the number of resonances for all the isotopes

present is large. Under such condition, the correlations between the uncorrelated resonances vanish. It is, therefore, reasonable to assume that the minimum requirement for any meaningful statistical method is to reproduce at least the first- and the second-order moments defined in Eq. (4) when compared to the observed values from the cross-section experiments. More realistic conditions appear to require the preservation of the correlation between σ_{xi} and Σ_t if the energy interval under consideration is relatively small. It appears that a reduction in statistical uncertainties may be possible if experimental information on such correlations is available. The importance of such conditions in practical calculations will be further discussed in the next section.

III. BASIS AND PROBLEMS CONCERNING THE EXISTING METHODS

The validity of the Breit-Wigner equation is usually assumed in practical reactor applications. The temperature and energy-dependent cross sections are expressed in terms of the well-known Doppler-broadened line shape functions. The joint distribution function is specified once the independently distributed probability functions for each partial width and the distribution of level spacing are known.

There are generally two methods in estimating E(q); namely (1) the Integral Mthod, in which a multiple integration is performed over the distribution functions and energy; and (2) the Discrete (or Monte Carlo) Method in which the expectation value is considered as the sum of the appropriate discrete values generated from known distribution functions. The detailed descriptions of these methods are available in the literature and will not be discussed in this paper. Instead, some important aspects of the statistical theory pertinent to these methods will be discussed.

A. Integral Method

The expectation value E(q) of interest is generally much too complicated to be treated by the integral method unless some simplified assumptions are made on the space and energy dependence of the flux. It is customary to assume that the narrow resonance approximation and the

Wigner rational approximation of collision probabilities and the equivalence relations are valid.[10,11] Under these assumptions, the expectation values of interest are of the form defined in Eq. (3) and can be written in the relatively simple forms:

$$\langle \sigma_x \phi \rangle_{E_0} \simeq \langle \Gamma_x J^* \rangle_{E_0} \Big/ \langle D \rangle \tag{5}$$

and

$$\langle \phi \rangle_{E_0} \simeq \frac{1}{\sigma_p^{(eq)}} \left(1 - \langle \Gamma J^* \rangle_{E_0} \Big/ \langle D \rangle \right) , \tag{6}$$

where $\sigma_p^{(eq)}$ and $\langle D \rangle$ are the "equivalent" potential scattering cross section and the average spacing respectively. The characteristic integral J^* is defined and discussed in Ref. 12. All the expectation values are evaluated at E_0 which may be conveniently taken to be the midpoint of the energy interval of interest. It should be noted that the J^*-treatment described in the previous work[12] has been improved in conjunction with the recent development of the MC^2-2 code. Efficient algorithms have been developed to treat $\langle \Gamma_x J^* \rangle$. In particular, the in-sequence overlap effect is treated more accurately taking into account the long-range correlation of levels described by Dyson.[5] The detailed discussions are given in Ref. 13.

Of particular interest in the present paper is the implicit assumption involved in the Integral Method. One of the most important assumptions is that the ergodic theorem must be valid. The validity of the ergodic theorem required that the following limit condition must exist for any given energy interval

$$\Delta E = E_1 - E_2$$

$$E(q) = \frac{1}{\Delta E} \int_{E_2}^{E_1} q(E)\, dE \simeq \frac{1}{\langle D \rangle} \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \Gamma_{xi}^{(L)} J_i^{*(L)}$$

$$\simeq \langle \Gamma_x J^* \rangle_{E_0} \Big/ \langle D \rangle \tag{7}$$

where $\{\Gamma_{xi}^{(L)} J_i^{*(L)}\}$ is a subset or a "ladder" of the stationary sequence of resonance integral $\{\Gamma_{xi} J_i^*\}$. The discrete sum is required to approach $\langle \Gamma_x J^* \rangle_{E_0}$ ergodically when N becomes large. This assumption provides a natural transition between the resolved resonances and the unresolved resonances. The results obtained using the integral method represents the theoretical mean values under the idealized conditions.

B. Discrete (or Monte Carlo) Method

In contrast to the integral method, the cross sections may be considered as an energy-dependent discrete sequence sampled from the appropriate distribution functions in estimating the expectation values. The discrete method is clearly less restrictive, and assumptions on energy and space dependence of neutron flux are not required. Hence, it is extremely useful in more rigorous calculations. If the same assumptions are used, the results obtained by the discrete method must approach those obtained by the integral method ergodically according to Eq. (7) under idealized conditions. In practical calculations, however, the energy interval in which the expectation values are defined is finite and sometimes small. Consequently, large dispersions in E(q) obtained using various cross-section sequences are expected if the sample size is small.

There are two methods of generating discrete cross sections. One method is to construct the resonance sequences directly from the distribution functions of the partial widths and level spacing and is often referred to as the "ladder" technique. Another method is to sample the cross sections from conditional distributions of various reaction cross sections deduced from the ladder technique. The latter method will be referred to as the cross-section sampling technique.

1. Ladder Method. This method is most straightforward. All the energy dependence of the cross sections within the energy region under consideration is included explicitly in the calculations. Considerable uncertainties in the self-shielding effect are expected when the total number of resonances within the given energy interval is small. From a practical point of view, some bias is obviously needed in order to reproduce the observed behavior of the microscopic cross sections as a func-

tion of energy. For this reason, Dyos[14] has suggested two criteria in selecting resonance ladders. First of all, the means and variances of the nuclear parameters for the selected ladder must match the theoretical values as closely as possible to be representative of the characteristics described by the theoretical distribution functions. Secondly, the unshielded average cross sections within the given energy interval must be equal to the observed value. It was hoped that the biased selection of resonance samples would reduce the uncertainties in the Doppler-effect calculations. As discussed in Section II, the self-shielding effect and the Doppler effect depend on the higher-order moments in a rather complicated way. Adequate statistical samples for the unshielded average $\langle \sigma_x \rangle$ may not be sufficient in estimating the Doppler effect.

Investigation of this problem has been carried out using the narrow resonance approximation.[15] The resonance integrals in Eq. (5) can be represented by the unshielded term $\langle \sigma_x \rangle$ and the self-shielding term (say $\langle S_x \rangle$) similar to that given in Eq. (3). The point in question is then to estimate the relationship between the variances of the discrete sum of temperature derivatives

$$\sum_{i=1}^{N} \frac{\partial}{\partial T} S_{xi}$$

for the unbiased and the biased samples. Two interesting results were found: (1) the variance of

$$\sum_{i=1}^{N} \frac{\partial}{\partial T} S_{xi}$$

was found to be approximately inversely proportional to N, the total number of levels present within a given energy interval; and (2) the conditional variance of $(\partial/\partial T)\, S_{xi}$ for any given σ_{xi} is related to the variance of $(\partial/\partial T)\, S_{xi}$ for the unbiased sample by the simple relationship

$$\mathrm{Var}\left[\frac{\partial}{\partial T}\langle S_{xi}\rangle \middle| \langle \sigma_{xi}\rangle\right] \simeq \mathrm{Var}\left[\frac{\partial}{\partial T}\langle S_{xi}\rangle\right] \cdot \left[1 - \rho^2\right] , \qquad (8)$$

where ρ is the correlation coefficient for σ_{xi} and S_{xi}. Hence, the biased sampling technique of Dyos[14] will generally reduce the dispersion of the calculated Doppler effect and its effectiveness is characterized by the correlation coefficient ρ. ρ, in turn, depends strongly on the composition of the system under consideration.

To illustrate the magnitude of ρ in practical applications, calculations have been carried out for two realistic cases in the energy interval around 1 keV with the temperature increment of ΔT = 750-300°K. Case 1 is equivalent to an isolated PuO_2 sample with $\sigma_p^{(eq)}$ = 71.7 barns per atom. Only the S-wave resonances are considered. Case 2 is equivalent to a system with ^{238}U:^{239}Pu = 7:1 with σ_p = 300 barns per ^{239}Pu atom. The resulting ρ for ^{239}Pu in two cases are given below:

	Fission	Capture
Case 1	-0.644	-0.953
Case 2	-0.408	-0.849

It is seen that the scheme of Dyos[14] will significantly improve the capture contribution to the Doppler effect, but the improvement for the fission contribution is much less. In the presence of a strongly overlapping sequence of ^{238}U resonances, however, ρ for the fission contribution is so small that the corresponding conditional variance, and the variance for the unbiased samples are substantially the same. Under such conditions, very little improvement is achieved by suing the scheme of Dyos.[14]

It is believed that the method can be further improved if the selected sample is chosen not only to reproduce the observed value in $\langle\sigma_x\rangle$ but also the "observed" correlation between σ_x and σ_t (and/or Σ_t). This requires additional experimental information which may not be obtained easily. Further studies are obviously needed.

2. Cross Section Sampling Technique. The most serious limitation of the ladder method is that it requires not only large storage but also considerable computing time in calculating the Doppler-broadened line-shape functions at various energy points for a given temperature. One

alternative to the ladder method is the cross section sampling method, whereby the cross sections are sampled directly from the probability distributions of various cross sections deduced from the known distributions of resonance parameters using Eq. (2). One simple but useful technique of this kind has been proposed by Levitt for the fast reactor applications.[16,17] Of particular interest in the following discussions are the theoretical foundations and limitations in the application of the cross-section sampling technique.

Let $h(\sigma_x, \sigma_s, \sigma_t)$ be the joint density function for random variables σ_x, σ_s, and σ_t corresponding to the reaction, scattering, and total cross sections respectively. In principle, $h(\sigma_x, \sigma_s, \sigma_t)$ can be deduced from the joint distribution of the resonance parameters through the transformation of variables as long as the Jacobian of the transformation does not vanish. It should be noted that, while the correlation of various resonances is described by the appropriate correlation functions, the energy correlation among cross-section values within a given resonance depends on the explicit description specified by the cross-section formalism. If one is only interested in the proper statistical description of the means and various moments in the cross sections, it is possible to construct $h(\sigma_x, \sigma_s, \sigma_t)$ numerically from the pointwise cross-section values determined from the resonance ladders. These values at various energy points within a given interval are assumed to follow uniform statistics. The joint distribution $h(\sigma_x, \sigma_s, \sigma_t)$ determined this way does not have the explicit energy dependence of the cross section. All moments of the forms $E\left(\sigma_x^n\right)$ and $E\left(\sigma_x^n \sigma_s^m \sigma_t^\ell\right)$ remain unchanged using this joint tributions. The joint distribution is related to the conditional densities by

$$h\left(\sigma_x, \sigma_s, \sigma_t\right) = h_t\left(\sigma_t\right) h_x\left(\sigma_x \middle| \sigma_t\right) h\left(\sigma_s \middle| \sigma_x, \sigma_t\right) . \qquad (9)$$

For practical applications, two questions arise immediately: (1) while $h(\sigma_x, \sigma_s, \sigma_t)$ is sufficient in determining all moments in cross sections, the question is whether it is also sufficient in estimating $E(\sigma_x \phi)$; and (2) Eq. (9) implies the need of multidimensional tables which may make this method unattractive. Extensive studies concerning these

questions have been carried out by Prael[18] at Argonne National Laboratory. These questions, which were found to be closely related, do not appear to present any serious problem in cases of practical interest. To illustrate what is relevant in practical applications, a simple example is given.

Without loss of generality, consider a two-region problem which is of considerable interest in reactor calculations. Let ϕ_1 and ϕ_2 be the neutron fluxes in spatial regions 1 and 2, respectively. The fluxes are related to the collision densities by

$$\phi_1 = F_1/\Sigma_t^{(1)} \quad \text{and} \quad \phi_2 = F_2/\Sigma_t^{(2)} , \tag{10}$$

and the collision densities are described by Chernick's equation[19]

$$F_1(u) = \left[1 - P_1\left(\Sigma_t^{(1)}\right)\right] \sum_i \int_{u-\epsilon_i}^{u} \frac{\exp[u' - u]}{1 - \alpha_i} \frac{\Sigma_{si}^{(1)}(u')}{\Sigma_t^{(1)}} F_1(u')\, du'$$

$$+ P_2\left(\Sigma_t^{(2)}\right) F_2 , \tag{11}$$

where P_1 and P_2 are the resonance escape probabilities for Regions 1 and 2 respectively; ϵ_i and α_i are the maximum increment in lethargy and the maximum fractional energy loss per collision for a given isotope i. For simplicity, $\Sigma_t^{(2)}$ and F_2 are taken to be constant. P_1 and P_2 vanish for an infinite homogeneous system.

Strictly speaking, F_1 depends not only on the cross-section values at a given u but also on those within the interval ϵ_i from u. Hence, the question is whether the energy-independent joint distribution function $h(\sigma_x, \sigma_s, \sigma_t)$ is sufficient in describing $\phi_1(u)$. Qualitatively, this question clearly does not arise if the extent of the resonance is small compared to the maximum energy loss per collision. Under this condition, the events taking place within a given resonance become

uncorrelated since the neutrons, when suffering elastic collisions, are scattered outside of the resonance for practical purposes. The question of what types of conditional distributions are actually needed in the calculations is also closely related to the narrowness of the resonance. The first-order solution to the slowing-down equation, say $f_1\left[\Sigma_t^{(1)},\Sigma_t^{(2)}\right]$, does not depend on the resonance-scattering cross sections explicitly. Hence, the corresponding first-order estimate of the expectation value $E(\sigma_x\phi_1)$ for the case of one resonance absorber becomes

$$E\left[\sigma_x^{(1)}\phi_1\right] \simeq \left\langle \int E\left[\sigma_x^{(1)}\middle|\sigma_t^{(1)}\right] \frac{f_1\left[\Sigma_t^{(1)}\right]}{\Sigma_t^{(1)}} h_t\left[\sigma_t^{(1)}\right] d\sigma_t^{(1)} \right\rangle_u , \qquad (12)$$

where $E\left[\sigma_x^{(1)}\middle|\sigma_t^{(1)}\right]$ is the conditional mean of $\sigma_x^{(1)}$ for any given $\sigma_t^{(1)}$ defined as

$$E\left[\sigma_x^{(1)}\middle|\sigma_t^{(1)}\right] = \int_0^{\sigma_t^{(1)}} \sigma_x^{(1)} h_x\left[\sigma_x^{(1)}\middle|\sigma_t^{(1)}\right] d\sigma_x^{(1)} . \qquad (13)$$

The relevant statistical descriptions that appear in the first-order estimate are the conditional mean and the marginal p.d.f. of the total cross sections, and the conditional densities do not enter the calculation explicitly. Both $E\left[\sigma_x^{(1)}\middle|\sigma_t^{(1)}\right]$ and $h_t\left[\sigma_t^{(1)}\right]$ are functions of the variable $\sigma_t^{(1)}$ only. The contribution of the resonance scattering cross section will appear in the second-order solution of the slowing-down equation. In the unresolved energy region of interest, the resonances of the heavy nonfissionable isotopes are generally narrow compared to the maximum energy loss per collision. For fissionable isotopes, the resonance-scattering cross sections are generally small compared to other reaction processes if the resonances are not narrow. Under the latter condition, the first-order estimates are generally satisfactory in problems of practical interest. For narrow resonances it can be shown that the contribution of the resonance-scattering cross section in the second-order estimates of $E\left[\sigma_x^{(1)}\phi_1\right]$ exhibits the same form as Eq. (12)

characterized by $E\left[\sigma_s^{(1)} \middle| \sigma_t^{(1)}\right]$ and $h\left(\sigma_t^{(1)}\right)$ if one replaces the lower limit of Eq. (11) by zero. Thus, only conditional means of various reaction processes and the marginal p.d.f. of σ_t are needed explicitly in estimating $E\left(\sigma_x \phi\right)$ if the resonances are narrow or if the first-order approximation is valid. It is fortunate that these conditions are generally satisfactory for practical problems of interest in the unresolved energy region. Since the statistical behavior is characterized by the functions of one variable, it is, therefore, feasible to construct one-dimensional tables of the cumulative density function $H_t\left(\sigma_t\right)$ and various conditional means for the practical application.

It is believed that the same theoretical foundations are implicitly used in the method proposed by Levitt.[16] After extensive studies by Prael,[18] it was found that the probability tables described by Levitt are, in fact, identifiable with $H_t\left(\sigma_t\right)$ and various conditional means. For numerically accurate tables, it is reasonable to expect that Levitt's method will estimate $E\left(\sigma_x \phi\right)$ adequately within the limit of the conditions described.

IV. APPLICATION OF MULTILEVEL FORMALISM FOR REACTOR CALCULATIONS

In reactor applications the explicit energy and temperature dependence is generally required. One convenient way of examining the multilevel effect is to extend the procedure described by Moldauer[1] for treating the average cross section in the unresolved region, using the S-matrix formulation in which the energy dependence of the cross sections is represented by means of the resonance pole expansion. The Doppler-broadened cross sections can be readily obtained by integrating the the unbroadened cross sections over the Maxwell-Boltzmann kernel. For our purpose, the Doppler-broadened cross sections can be written as

$$\sigma_x = 4\pi\lambda^2 g \sum_{c'} \sum_{\mu} \frac{1}{\Gamma_\mu^{(S)}} \mathrm{Im}\left[\zeta_\mu \cdot \frac{i\Gamma_\mu^{(S)}}{2\sqrt{\pi}\,\Delta} \int_{-\infty}^{\infty} \frac{e^{-(t/\Delta)^2}}{E - P_\mu - t}\, dt\right] \tag{14}$$

and

$$\sigma_t = \sigma_p + 4\pi\lambda^2 g_J \sum_{\mu} \frac{1}{\Gamma_\mu^{(S)}} \mathrm{Re}\left[\alpha_\mu \cdot \frac{i\Gamma_\mu^{(S)}}{2\sqrt{\pi}\,\Delta} \int_{-\infty}^{\infty} \frac{e^{-(t/\Delta)^2}}{E - P_\mu - t}\, dt\right], \tag{15}$$

where the complex pole P_μ and the complex amplitude of residues ζ_μ and α_μ are related to the usual S-matrix parameters by

$$P_\mu = \varepsilon_\mu - \frac{i\Gamma_\mu^{(S)}}{2} , \tag{16}$$

$$\zeta_\mu = g_{\mu c} g_{\mu c'} \sum_{\mu'} \frac{g_{\mu' c} g_{\mu' c'}}{\left(\varepsilon_\mu - \varepsilon_{\mu'}\right) - (i/2)\left(\Gamma_\mu^{(S)} + \Gamma_{\mu'}^{(S)}\right)} , \tag{17}$$

$$\alpha_\mu = g_{\mu c}^2 \cdot \exp[-i2R/\lambda] , \tag{18}$$

and the real and the imaginary parts of the complex probability integral with the appropriate constant can be directly identified with the usual symmetric and asymmetric-broadened functions respectively. The real and complex parts of various parameters are directly identifiable with those of Adler-Adler.[7] From a purely numerical point of view, there is a striking similarity between the multilevel representation to these forms and the single-level representation with the exception of the presence of the asymmetric-broadened line-shape function in the reaction cross section. It is, therefore, particularly amenable for reactor applications. It requires very little modification of the existing codes for calculating the resonance absorption to accommodate the use of the multilevel formalism.

In the practical calculations, however, the effect of using the multilevel formalism is generally difficult to estimate in spite of the similarity in the description of the energy and temperature dependence defined in Eqs. 14 and 15 and the conventional single-level representation. Qualitatively, the effect may arise from three main sources: (1) the statistical behavior of the S-matrix parameters is generally different from that of the R-matrix parameters; (2) the dependence of the reaction amplitude ζ_μ for a given μ on the separation $\varepsilon_\mu - \varepsilon_{\mu'}$ gives rise to an additional term in both the unshielded and shielded reaction cross sections which does not appear in the single-level equation; and (3) there exists an asymmetric contribution in the reaction cross section which does not appear in the single-level equation. One of the most difficult problems is to determine the precise statistical behavior of the S-matrix

parameters. There does not appear to exist a general statistical theory to describe these parameters with the exception of perhaps some over-simplified cases. The problem becomes then that of deducing the statistical behavior of the S-matrix parameters numerically from those of the R-matrix parameters well described in the statistical theory of spectra.[4] The formal approach requires the following computational procedures:

(1) The first step is to generate from appropriate distributions a set of random R-matrix parameters whereby the level matrix can be constructed.

(2) The level matrix, which is a complex symmetric matrix, must be diagonalized. The eigenvalues of this level matrix yield the S-matrix pole parameters ε_μ and $\Gamma_\mu^{(S)}$ directly and the channel pole amplitude $g_{\mu c}$ can be obtained from the corresponding eigen-vectors.

A computer code MATDIAG[20] which allows a level matrix with maximum size of 120 × 120 has been developed for this purpose. The computing time, of which a significant portion is required for computing the eigen-vectors, becomes large when the size of the level matrix is greater than 50 × 50. An alternative procedure of computing the Adler-Adler parameters has been developed by deSaussure and Perez[21] using the Reich-Moore formalism.[22] In this method the collision matrix is not expressed in terms of the level matrix but in terms of a channel matrix. The size of the channel matrix is determined by the total number of fission channels and is usually very small. This approach requires the inversion of a small channel matrix accompanied by the calculation of the S-matrix pole parameters from the complex roots of a N-*th* order polynomial. Since the method does not require the diagonalization of a large level matrix of which the computation of the eigen-vectors is most time consuming, it is, therefore, more economical for practical applications.

In Ref. 8, some quantitative and qualitative studies on the statistical distributions of the S-matrix parameters were carried out. The distributions of the S-matrix parameters are usually different from those of R-matrix parameters and are sensitive to the ratio of the average level spacing $\langle D \rangle$ and the average total width $\langle \Gamma \rangle$ used in the calculations. For S-matrix spacing $\varepsilon_\mu - \varepsilon_{\mu'}$, the distribution appears to deviate from the Wigner distribution near the origin if the ratio $\langle D \rangle / \langle \Gamma \rangle$ is small.

Figures 1 and 2 show some of the representative results obtained using MATIAG.[20] It is generally difficult to deduce the exact shapes of these distribution functions from the numerical results. For the purpose of illustration, analytical distributions have been derived for the simplified case of two-level and one-channel problems similar to those considered by Garrison.[23] Figures 3 and 4 show the analytical distributions of the S-matrix level spacing $D^{(S)}$ and $\Gamma^{(S)}$ for various values of $\langle D\rangle/\langle\Gamma\rangle$. The distributions of $D^{(S)}$ and $\Gamma^{(S)}$ begin to deviate from the Wigner distribution and the Porter-Thomas distribution, respectively, as $\langle D\rangle/\langle\Gamma\rangle$ becomes small. The results are qualitatively consistent with the case with many levels and channels. One of the advantages of the simple example is that the statistical behavior of the distributions can be examined more precisely. One quantity of particular interest is the dispersion of these distributions. Table I shows the variance of $D^{(S)}$ for various values of $\langle D\rangle/\langle\Gamma\rangle$. Similar results using the direct numerical technique were also obtained by deSaussure and Perez.[26]

In Refs. 9 and 24, the importance of the multilevel effect in reactor applications has also been examined. Judging from the magnitude of $\langle D\rangle/\langle\Gamma\rangle$, one expects that the multilevel representation may play a role only when the fissile isotopes are considered. Of particular interest in the practical applications is its role in conjunction to the analysis of Doppler experiments. Calculations using either the single-level or the multilevel formulation can be carried out using the modified RABBLE code[25] with the appropriate parameters generated from the MATDIAG code.[20]

The most difficult problem in these studies is to establish a reasonable basis for comparing the results obtained by using the different cross-section representations. The interpretation of the multilevel effect depends to a great extent on the basic assumptions used. Two possible assumptions are:

(1) The same set of R-matrix parameters generated from the appropriate distributions with given mean values is used for both the single-level and multilevel approaches. The resulting unshielded and the self-shielded average cross sections obtained by the two approaches are certainly expected to be different unless the level matrix is diagonal. The comparison of the results made on this basis will provide a test on the validity of the single-level equation.

(2) The random parameters for the multilevel and the single-level parameters must be chosen in such a way that the resulting unshielded average cross sections are identical with the observed value. This is the condition usually required in practical calculations regardless of what cross-section formalisms are used. The comparison of the results on the basis of the latter assumption will provide further understanding of the role that the multilevel formalism plays in the practical calculations.

Numerical calculations of the self-shielded cross sections for the highly enriched 1/2-in. UO_2 and PuO_2 samples have been carried out under various conditions using the assumption (1). It was found that the multilevel representation generally yields greater values of average capture cross sections and the capture-to-fission ratios than those single-level results obtained by using the same set of random R-matrix parameters generated from the appropriate distributions and means. Noticeable differences in the Doppler change of the self-shielded cross sections were also observed if $\langle D \rangle / \langle \Gamma \rangle$ is small. Tables II and III give some typical results obtained for 1/2-in. enriched samples of PuO_2 and UO_2 respectively. The multilevel approach, which yields higher values of $\bar{\sigma}_\gamma / \bar{\sigma}_f$ and $\delta\bar{\sigma}_\gamma / \delta\bar{\sigma}_f$, is expected to decrease the positive contribution to the Doppler reactivity. It is important to realize that only one S-wave state is considered in these calculations. The role of the multilevel representation is much less important for other S-wave states due to the larger $\langle D \rangle / \langle \Gamma \rangle$ ratios. The overall effect is certainly much smaller than those indicated in Tables II and III. Furthermore, there is the question of whether the basis of comparison using the assumption (1) is fair in the practical application. Regardless of the cross-section formalisms, the calculated results must be related to the observed values of cross sections. In absence of precise knowledge of the magnitude of the measured cross sections and their relevant higher-order moments, conclusions based on the calculated results are rather artificial. Further studies using the assumption (2) may help improve understanding of the problem.

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TABLE I

Average Spacing and Variances for Various Cases
(Two Levels, One Channel)

Distribution	$\frac{\langle D^{(S)} \rangle}{\langle D \rangle}$	$\frac{\langle D^{(S)^2} \rangle - \langle D^{(S)} \rangle^2}{\langle D^{(2)} \rangle^2}$
Wigner	1.0	0.2732
Random	1.0	1.0
$f_2\left(D^{(S)}\right)$:*		
$\langle D \rangle / \langle \Gamma \rangle = \pi$	0.9587	0.3150
$\langle D \rangle / \langle \Gamma \rangle = 2.0$	0.9273	0.3444
$\langle D \rangle / \langle \Gamma \rangle = 1.0$	0.8603	0.4057
$\langle D \rangle / \langle \Gamma \rangle = 0.5$	0.9876	0.4700
$\langle D \rangle / \langle \Gamma \rangle = 0.1$	0.714	0.4910

*$f_2\left(D^{(S)}\right)$, p.d.f. of $D^{(S)}$, is defined in Ref. 8.

TABLE II

Comparison of Multilevel and Single-Level Results
for the Highly Enriched 1/2-in. PuO_2 Sample
Using the Modified RABBLE ($J = 0^+$ only)

Penetration Probability p_f = 1.0; 1.0
Number of Poles = 80
ΔE = 1.0 - 1.725 keV

	Unshielded		Shielded		750-300°K	
	$\langle \sigma_\gamma \rangle$	$\langle \sigma_f \rangle$	$\tilde{\sigma}_{\gamma 300°K}$	$\tilde{\sigma}_{f300°K}$	$\delta\tilde{\sigma}_\gamma$	$\delta\tilde{\sigma}_f$
SL	0.1772	2.6131	0.1235	2.2373	0.0101	0.0379
ML	0.4044	2.7664	0.2300	2.3188	0.0315	0.0476

TABLE III

Comparison of Multilevel and Single-Level Results
for the Highly Enriched 1/2-in. UO_2 Sample
Using the Modified RABBLE (G = 3 only)

Number of Poles = 120

ΔE = 1.0 - 1.165 keV

	Unshielded		Self-Shielded			
					750-300°K	
	σ_γ	σ_f	$\tilde{\sigma}_{\gamma 300°K}$	$\tilde{\sigma}_{f 300°K}$	$\delta\tilde{\sigma}_\gamma$	$\delta\tilde{\sigma}_f$
	CASE I: p_f = 1.0, 0.9, 0.18					
SL	0.8868	4.3024	0.8112	3.9978	0.0218	0.0722
ML	1.0884	4.2503	0.9950	3.9190	0.0279	0.0759
	CASE II: p_f = 1.0, 1.0, 1.0, 1.0					
SL	0.4280	5.2726	0.3822	4.8797	0.0121	0.0963
ML	0.5728	5.2477	0.5059	4.7570	0.0194	0.1325

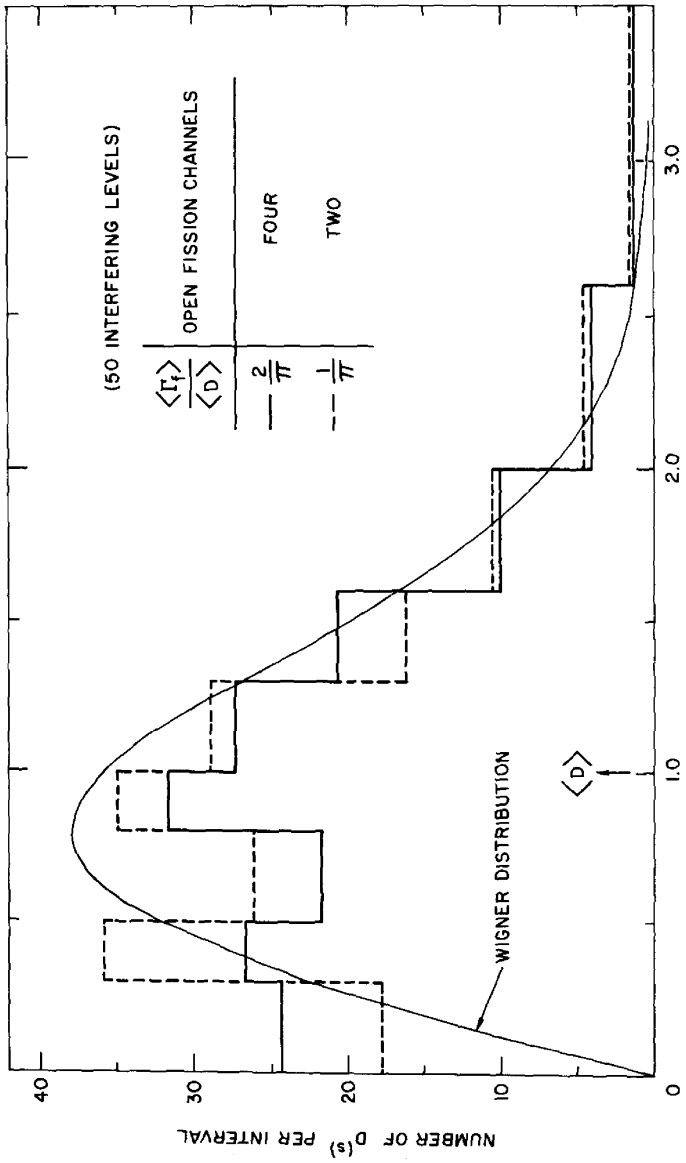

Figure 1. The distribution function for the S-matrix level spacing using 50 interfering levels. (Neg. No. 112-9813)

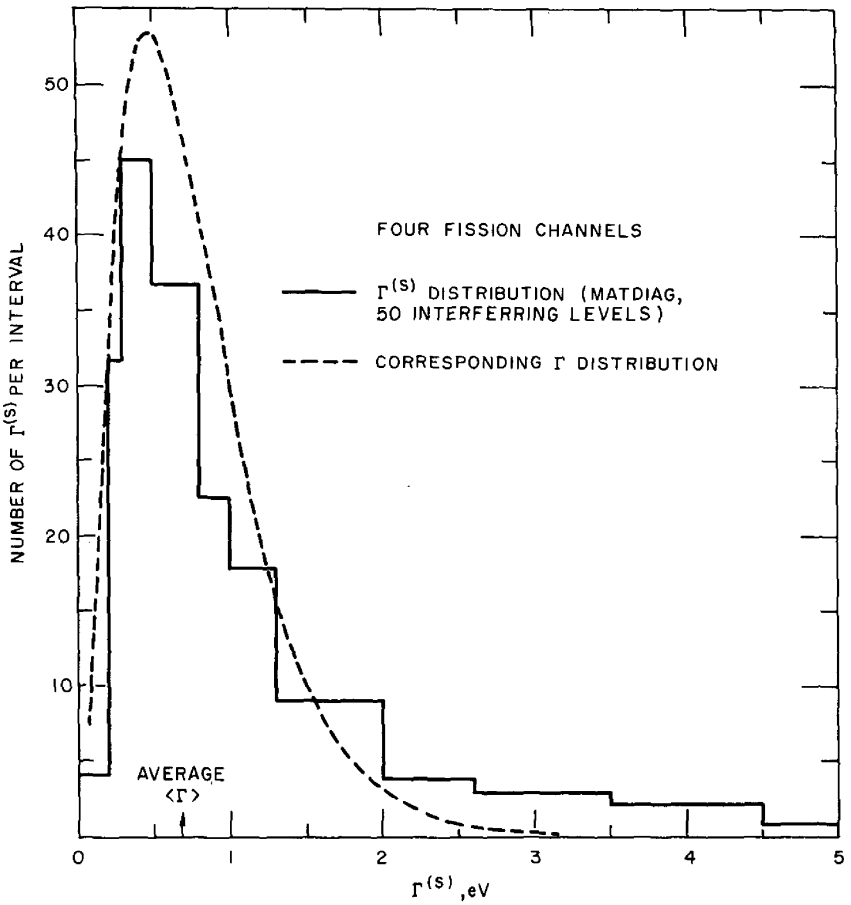

Figure 2. The distribution function for S-matrix level width using 50 interfering levels for $D / \Gamma = \pi/2$. (Neg. No. 112-9980)

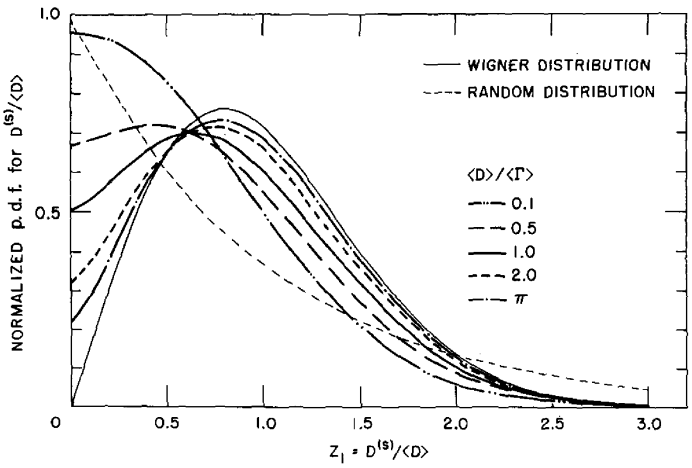

Figure 3. The analytical p.d.f. for the S-matrix level spacing using two levels. (Neg. No. 113-126)

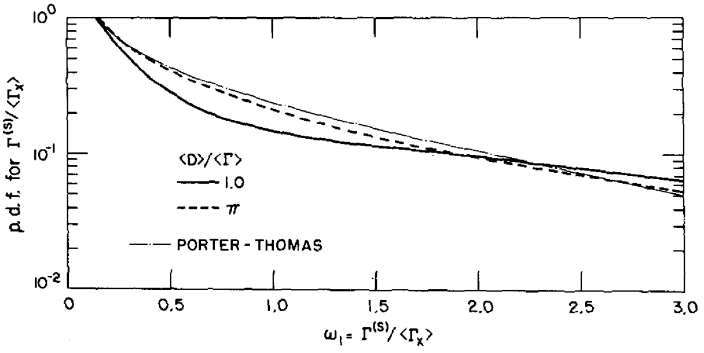

Figure 4. The analytical p.d.f. for $\Gamma^{(S)}$ using two levels. (Neg. No. 113-132)

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RESONANCE TREATMENT IN REACTOR APPLICATIONS

by

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I. INTRODUCTION

The treatment of resonances in ENDF/B-III is based, for the most part, upon the single level Breit-Wigner formalism with only a few materials described by multilevel parameters. This treatment is essentially satisfactory for the present reactor design applications. Later requirements for more accurate calculations may necessitate more elaborate treatments, particularly for fast reactors. However, it would be a mistake to anticipate such a need at this time because changes in the ENDF procedures lead to expensive and delaying modifications to the data processing codes.

There are a number of factors in the treatment of resonances in the ENDF libraries that are important in reactor design applications. These include the following:

a. The detail which is used to describe resolved resonances.
b. The averaging capability for unresolved resonances.
c. The adequacy of the resonance treatment for shielding studies.
d. The use of multilevel versus single level formulae.

Reactor designers are, for the most part, quite happy with the first two treatments as they are in the present ENDF files. Averaging of unresolved resonances seems to be sufficiently accurate and no surprises are expected in the near future which would change this conclusion. The Probability Table Method looks as though it may save some computing time and, of course, has a unique application in Monte Carlo, but it is not expected to improve the accuracy which is achieved with the present treatment in ENDF/B-III. If the Probability Table Method does save considerable computing time and is convincingly demonstrated to be accurate, it would be preferable to the present use of average parameters, keeping in mind the conversion which would be necessary for the processing codes.

With regard to resolved resonances, some thermal reactor designers may be somewhat unhappy with the resolved resonances in ENDF/B-III but necessary corrections should not involve modifications to the processing codes.

The increasing use of ENDF Libraries for shielding applications has pointed to the need for accuracy in the intermediate and high energy

resonance description. The resonance interference minima are of particular importance. However, the accuracy which is required is primarily a problem of interpretation and evaluation of basic data and should not require elaborate treatments.

Probably the most difficult question concerning resonance treatment is the utilization of multilevel versus single level formalisms. There is continuing pressure to go to the multilevel formalisms but this pressure is not from the reactor community. It is recognized that the multilevel equations give a more accurate discription of resonances for certain materials, in particular fissile materials, but it is not clear that the use of such formalisms will significantly improve the accuracy of reactor calculations. It is the consensus of most users that some direct evidence for the need of multilevel formulae is required. At the present time direct comparisons of the consequences of singel level and multilevel applications, based upon the same data, are essentially non-existent.

II. MULTILEVEL FORMALISM IN REACTOR APPLICATIONS

Reactor parameters which may be affected by the use of multilevel equations and which are of concern to the reactor designer include the Doppler coefficient, the capture to fission ratio (alpha value) for fissile materials, slowing down due to resonance scattering in materials of intermediate atomic weight and the cross section interference minima which are used for shielding applications.

As far as the Doppler coefficient is concerned, the most important material is ^{238}U and the use of multilevel parameters for this material is expected to have a negligible effect since the level spacing is large. The small level spacings in fissile isotopes and the small number of channels available for fission cause strong interference effects, which lead to asymmetry and other distortions in fission cross section resonances. Such distortions of the cross section shape can be expected to influence the Doppler effect. Thus, ^{233}U, ^{235}U, and to a lesser degree ^{239}Pu may have non-negligible Doppler contributions which are dependent upon the resonance treatment which is used. Significant differences in the

calculated and measured ^{239}Pu Doppler have been reported by Fischer, et al.[1] in the zoned ZPR-3 Assemblies 45 and 45A and by Davey[2] in ZPR-3 Assembly 48. There was considerable uncertainty in both sets of measurements but in all cases, except one where the sample was surrounded by B_4C, the measured Doppler effect was significantly less positive (and for Assembly 48 it was small and negative) than the calculated values. In contrast, the agreement between measured and calculated values for the ^{238}U Doppler was generally good. The ^{239}Pu results are an indication that the multilevel approach may be required to correctly evaluate the ^{239}Pu Doppler effect. However, the ^{239}Pu contribution to the total Doppler in fast power reactors is less than 5% and it would require a significant change in the ^{239}Pu cross sections to have an appreciable effect on the total Doppler. The agreement between the calculated and measured Doppler for SEFOR[3] is one indication that no large surprises are to be expected.

One of the disadvantages of most multilevel formulae is the difficulty in computing the Doppler broadened cross sections using the standard ψ and χ functions. Only the Adler-Adler equations which are specified for ENDF/B-III provide this capability.

There is some evidence that the alpha value for fissile materials increases in going from the single level to multilevel parameters. Pennington and Sargis[4] give the relationship between the single level and multilevel infinitely dilute resonance integral for two neighboring resonances in the unresolved resonance region as:

$$\bar{I}^{ML}_{\gamma\infty} = I^{SL}_{\gamma\infty}\left[1 + \frac{\Gamma_f^2}{D^2 + \Gamma_\gamma(\Gamma_\gamma + 2\Gamma_f)}\right]$$

$$\bar{I}^{ML}_{f\infty} = I^{SL}_{f\infty}\left[1 - \frac{\Gamma_\gamma\Gamma_f}{D^2 + \Gamma_\gamma(\Gamma_\gamma + 2\Gamma_f)}\right]$$

where D is the separation of the two interfering levels and the other terms have the usual meanings. It is apparent from these equations

that the multilevel alpha value will be larger than the single level value. However, it is not clear that the same resonance parameters should be used for both the multilevel and single level equations. Rather, it is to be expected that the resonance integrals would be the same regardless of the treatment which is to be used. Whether adequate fittings can be carried out to give the same multilevel and single level cross sections for capture, fission, and scattering remains to be shown.

The multilevel equation has been found to give a correct description of the very complicated scattering resonance structure of medium weight nuclei.[5] In particular, it describes correctly the interference between two closely spaced resonances, with the same quantum number, which destroys the single level shape of both resonances. The reactor designer is primarily concerned with the resonance scattering structural materials such as iron, nickel, and chromium. If the cross section shielding factors are not much different in multilevel or single level then the effect on fast reactors will be small. In the following section shielding factors based upon the single level data for iron from ENDF/B-II will be compared with the shielding factors for the multilevel data for iron in ENDF/B-III.

The adequacy or inadequacy of shielding data is also an important concern for reactor applications. Extreme accuracy in the interference minima is required both with respect to the cross section magnitude and for the energy distribution. An evaluation study is required to determine the effects that resonance treatment and Doppler broadening have on these minima and resulting shielding calculations.

III. STATUS OF DIRECT COMPARISONS OF MULTILEVEL AND SINGLE LEVEL EFFECTS

Direct comparisons of the effects of multilevel versus single level resonance treatment in reactor applications are few and are complicated by the uncertainty as to what constitutes a meaningful comparison. Taking account of multilevel effects poses difficulties from the standpoint of estimating the appropriate multilevel parameters (primarily in the unresolved resonance region) and of utilizing correct computational techniques.

A. Comparisons in the Resolved Resonance Region

Multilevel effects on the temperature change in the ^{235}U fission cross section in the 2.4 to 29.0 eV energy range have been reported by Cohen[6] and Adler-Adler[7] and were summarized by Hummel and Okrent.[8] Cohen's results indicated that $\Delta\sigma_f$ for a change in temperature from 1500° to 2500°K and based upon the multilevel treatment was about 15% less than that for the single level evaluation. The effective cross sections themselves were, on the average, 20 to 50% higher according to the multilevel numerical computations.

Adler and Adler compared cross sections from their parameters with those from single level parameters and their results appear to be reasonably consistent with those of Cohen.

Tmeperature-dependent group cross sections and their Doppler changes between 300° and 750°K using the single level and multilevel reparesntations were obtained by modified RABBLE calculations and reported by Hwang[9] for highly enriched UO_2 rods. This evaluation was carried out for six energy groups between 1.3 and 60 eV. The Doppler changes for both the capture and fission cross sections varied from 0 to over 40% lower for the multilevel results. Hwang substituted Γ_T^{ML} for Γ_T^{SL} in the Doppler integral of the single level formula while retaining the same single level amplitude and the "smooth" data.* The discrepancies in the $\Delta\sigma_f$'s and $\Delta\sigma_c$'s were much smaller than previously reported. From this it was concluded that the presence of the antisymmetric function is not a major contributor to the discrepancies for the case under consideration. This conclusion was based upon one group and was considered to be inconclusive because the existence of relatively large fluctuations of the "smooth" cross section in the ENDF files, in other groups, makes the comparison not meaningful.

B. Comparisons in the Unresolved Resonance Region

The treatment of unresolved resonances in the energy range around 1 keV and above is very important from the standpoint of fast reactor

*It was pointed out that the estimated average of the total width of the ENDF/B single level parameters was found to be considerably less than the corresponding average quantity for the multilevel parameters between 0 and 60 eV. However, the infinitely dilute resonance integrals were still different by as much as 5-15%.

applications. Doppler effect studies have been carried out for ^{239}Pu, in this energy range, at General Electric.[10] These studies involved the computations of the infinitely dilute fission cross section of ^{239}Pu ($\bar{\sigma}_f$) and the reduction of the cross section from its infinitely dilute value ($\Delta\sigma_f$), due to self shielding of Doppler broadened unresolved resonances and based upon both the multilevel and single level formalisms. The comparison was made for an energy of 1 keV, a fuel temperature of 300°K and a potential cross section per absorber atom of 400 barns. Only the $\ell = 0$, $J = 1$ state was considered. A $\nu = 10$ resonance spacing distribution was assumed with an average spacing <S> of 3.33 eV for this ^{239}Pu state.

A random sampling procedure was used with 40 resonances to represent the distribution of neutron width, fission width and resonance spacing. The results of the calculations are summarized as follows:

	$\bar{\sigma}_f$	$\Delta\sigma_f$	$\Delta\sigma_f/\bar{\sigma}_f$
Multilevel	5.98	0.87	0.145
Single level	5.69	0.84	0.148

The $\bar{\sigma}_f$ values computed with the use of multilevel and single level formalisms agree within about 5%, and the ratios $\Delta\sigma_f/\bar{\sigma}_f$ (representative of the change due to the Doppler effect) agree to within 2%. It was concluded that the multilevel methods in the unresolved resonance region would not markedly alter results obtained with single level methods.

The most comprehensive evaluations of the multilevel effects in the unresolved resonance region have been carried out for highly enriched UO_2 and PuO_2 rods and reported by Hwang (Reference 9). Six cases were considered for ^{239}Pu and all but one of them involved the $J = 0$ state, for which the multilevel interference effects were believed to be much more important than the $J = 1$ state due to the large ratio of the average total width to the level spacing. (That is, the fractional change in the $J = 0$ cross sections was expected to be much larger than

the fractional change for the J = 1 cross section. The J = 1 cross section is, of course, much larger than the J = 0 cross section.) The number of fission channels for the J = 0 state was taken to be two for all cases considered. It was assumed that the average parameters and distribution functions were the same for both the multilevel and single level representations.

Changes in the capture and fission cross sections between 300° and 750°K were computed (for J = 0 only) and were found to be significant. The multilevel $\Delta\sigma_c$'s were between 60 and 200% higher than the single level $\Delta\sigma_c$'s, whereas the multilevel $\Delta\sigma_f$'s were about 20 to 80% higher than the single level values. The larger magnitudes in $\Delta\sigma_c$ and $\Delta\sigma_f$ do not necessarily imply a larger Doppler coefficient. Table I gives the Doppler reactivity $\Delta K/K$ per unit flux per atom with an arbitrary assigned adjoint flux of unity with appropriate normalizations. The table includes the contribution of the J = 1 state.

TABLE I

An Illustrative Example of $\Delta K/K$ per Unit Flux per Atom for ^{239}Pu Including J = 1 (1.0 - 1.455 keV)

	$\Delta\sigma_c$ 300 - 750°K		$\Delta\sigma_f$ 300 - 750°K		$\Delta K/K$ Unit Flux/Atom	
	J = 0	J = 1	J = 0	J = 1	J = 0	J = 1
SL	0.0134	0.2874	0.0393	0.1945	0.0625	0.0879
ML	0.0432	0.2869	0.0517	0.1963	0.0565	0.0920

The results in Table I indicated that even though the magnitudes of $\Delta\sigma_x$ for the J = 1 state are much larger than $\Delta\sigma_x$ for the J = 0 state, the corresponding Doppler reactivities are of the same order of magnitude. The multilevel effect in this case is to reduce slightly the Doppler reactivity. Hwang concluded that the multilevel effects may become important in Doppler reactivity calculations in the energy range where the contribution from the J = 1 state is small.

^{235}U calculations were also reported by Hwang for several cases which used different values of the average fission width and various numbers of fission channels (an uncertainty). The multilevel values of $\Delta\sigma_\gamma$ for a temperature change from 300° to 750°K were found to be from 0 to 50% larger than the corresponding single level values depending upon the assumptions being used. Integral calculations of the Doppler effect were not carried out.

The results in Table I indicate that the capture cross sections based upon the multilevel evaluation is larger than the corresponding value for the single level evaluation. However, discrepancies in the fission cross section are not as significant. Hence, the multilevel approach tends to give a higher capture to fission ratio. The higher α values have also been reported by Pennington and Sargis (Reference 4) and are summarized in Table II for ^{239}Pu in the energy range from 100 to 300 eV.

TABLE II

Multilevel and Single Level Resonance Integrals for ^{239}Pu from 100 to 300 eV

Case		$\bar{I}_{\gamma\infty}$ (barns)	$\bar{I}_{f\infty}$ (barns)	$\bar{\alpha}$	$\overline{\alpha^{ML}/\alpha^{SL}}$
J = 0	SL	0.347	8.271	0.0459	1.249±0.179
	ML	0.422	8.107	0.0554	
J = 1	SL	13.789	9.208	1.540	1.006±0.005
	ML	13.809	9.171	1.549	
TOTAL	SL	14.136	17.479	0.8442	1.019±0.018
	ML	14.231	17.278	0.8578	

The results in Table II indicate a significant change in the J = 0 alpha. However, since almost all the capture involves the J = 1 resonances, the total multilevel $\bar{\alpha}$ was only $\sim$ 2% higher than the single level value.

Similar calculations were also performed by Pennington and Sargis for ^{235}U. These calculations gave $\alpha^{ML}/\alpha^{SL} \cong 1.07$. It was concluded that

multilevel effects on resonance integrals were not sufficiently large to justify the use of multilevel formulae in place of simpler single level formulae in reactor physics cross section codes.

C. A Comparison of Cross Section Shielding Factors for Iron

Iron is the only material in the ENDF files which has been specified by both multilevel and single level parameters. That is, the ENDF/B-II version of iron was described by single level parameters and "smooth" background cross sections whereas the ENDF/B-III iron was described with multilevel parameters. Scattering cross section shielding factors have been determined for the two versions of iron from ETOX calculations[11,12] and are compared in Table III for two different energy ranges. The shielding factors are tabulated as a function of the "other material" cross section, σ_o, and are defined as:

$$f_s = \frac{\int \frac{\sigma_s}{\sigma_T + \sigma_o} \frac{dE}{E}}{\int \frac{1}{\sigma_T + \sigma_o} \frac{dE}{E}} \Big/ \langle \sigma_s(\infty) \rangle$$

where $\langle \sigma_s(\infty) \rangle$ is the average infinitely dilute scattering cross section over the energy range of interest, and the other terms have the usual meanings.

TABLE III

Multilevel and Single Level Scattering Cross Section Shielding Factors for Iron

		σ_o				
Group*	$\sigma_s(\infty)$	10^3	10^2	10^1	10^0	10^{-1}
1 ML	20.903	0.977	0.846	0.603	0.487	0.462
1 SL	20.187	0.978	0.854	0.624	0.525	0.508
2 ML	12.330	0.998	0.981	0.914	0.862	0.853
2 SL	10.743	0.997	0.977	0.900	0.841	0.830

*GROUP 1: 25.5 to 40.9 keV.
GROUP 2: 5.5 to 9.1 keV.

The agreement between the multilevel and single level shielding factors is very good. This is probably not too surprising since the single level equation includes the "smooth" background. The important questions should probably be (a) how many data points are required to adequately represent the "smooth" effect, and (b) how do we treat "smooth" data that is very sharply peaked. At any rate, for the iron example given in Table III, the differences in resonance treatment appear to be not too important.

IV. SUMMARY AND CONCLUSIONS

Comparisons of the multilevel and single level resonance treatment for reactor applications have not indicated significant differences. There is some evidence that the multilevel effect on the ^{235}U Doppler may be large. However, changes in the ^{239}Pu Doppler effect were found to be small. The multilevel equations do complicate the techniques for computing the Doppler broadened cross sections. Only the Adler-Adler approach utilizes the standard ψ and χ functions and for this reason there is a tendency to favor this technique should the multilevel formalism be deemed necessary.

There are some comparisons that indicate that the use of multilevel equations may result in slightly larger ^{239}Pu alpha values. However, the comparisons have not taken into account the energy dependence of the unresolved resonance parameters which are now being used in the ENDF files and it is not clear how the resonance treatment affects the cross section shielding factors. The only direct comparison of multilevel and single level shielding factor effects has been for the scattering cross section of iron and the differences were found to be unimportant.

Probably the biggest objections to the comparisons of multilevel and single level formalisms have been the consistent use of the same resonance parameters and distribution functions in the unresolved range. This has, expectedly, led to different group averaged cross sections. A meaningful comparison should begin with resonance parameters which can be used to generate the same infinitely dilute cross sections.

It is concluded that the comparisons to date have been inconsistent and are inconclusive in demonstrating or dispelling the need for multilevel formalisms.

One final point concerns the use of pre-processed data. The degree of opposition by the reactor designers to putting more elaborate resonance treatments in the ENDF files and the use of multilevel formalisms will depend upon the success of any pre-processing and distribution scheme. If the ENDF data is centrally processed for both core and shielding applications, if the processing codes are modular and kept current with ENDF/B and if a successful distribution scheme is established then the conservative stance of the designers will shift from the ENDF files to the pre-processor output. In the final analysis, it appears that reactor applications would fare best, for the near term, with essentially no changes in the resonance treatment used in ENDF/B-III.

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THE PROBABILITY TABLE METHOD FOR TREATING UNRESOLVED RESONANCES IN MONTE CARLO CALCULATIONS*†

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1. Introduction

To derive maximum benefit from Monte Carlo reactor criticality and shielding calculations, one should use cross section data sets which are properties of the individual isotopes, rather than group averaged sets. Throughout most of the pertinent energy ranges this can be accomplished by using point cross section data with energy grids tailor made for each isotope.

However, development of a suitable method for producing such data sets in the unresolved resonance energy range which could be contained entirely within the confines of even the largest computers, is a difficult problem. Up to now, two methods have been available:

1) Generation of a point cross section data set based on a ladder of pseudo-resolved resonances selected randomly from known average parameters and statistical laws.
2) Generation of point cross sections during the Monte Carlo calculations, as needed, from stored average parameters.

The first method is hardly feasible in view of the enormous storage requirements, and furthermore would produce results based on only one ladder. As an example let us look at the point data storage requirements for ^{239}Pu. The unresolved energy range is from 300-25000 eV. Approximately 33000 resonances exist in this range. To describe each resonance adequately would require about 8 points per resonance, for each of total, scattering, and fission cross sections and the corresponding energy. This amounts to about one million words of computer storage to contain one continuous point data set based on only one ladder.

The second method would require too much computation time in fast reactor calculations since the neutrons would spend a significant fraction of their life in this energy range and each such calculation is quite lengthy if one considers interference effects and uses resonances of all ℓ, J values.

We are proposing a new approach which we shall call the probability table method.

2. The Probability Table Method

The basic idea is to represent the neutron cross section at a given energy, not by a unique value, $\sigma(E)$, obtained from table interpolation or resonance formulae, but by a distribution function whose mean value is the infinite dilution smooth average value $\bar{\sigma}(E)$. These distribution functions, in the tabular form in which they appear in a data set, are known as cross section probability tables.

They are generated from point data sets obtained from ladders produced about a small energy range, sufficient to contain 50 to 100 resonances, insuring an adequate sampling of resonance interference and overlap effects while preventing significant variation in the energy dependent average parameters.[1] The table size is dependent mainly on the application.

In VIM[2] a table size of 10 appears quite adequate. These tables are distributed through the unresolved energy range of a given isotope and used in the intervals containing the energies at which the tables were produced. The number of tables required for a given isotope is governed by the observed change in the tables as a function of energy. Thirty tables are sufficient except where there is siginficant variation in the average parameters. Such a set requires only 1230 storages in VIM.

The entries to the table $(\bar{\sigma}_J, P_J)$ are defined as follows. Let there be a set of σ_J's, J=1, N, such that $\sigma_J > \sigma_{J-1}$, $\sigma_1 \geq \sigma_{MIN}$, the lowest value

of $\sigma(E)$ between E_0 and E_M, and $\sigma_N \geq \sigma_{MAX}$, the highest value of $\sigma(E)$ in this energy range. Let

$$\int_{E_{MIN}}^{E_{MAX}} \sigma\ (E)\ dE = \sum_{i=1}^{M} \int_{E_{(i-1)}}^{E_i} \sigma\ (E)\ dE = \sum_{i=1}^{M} I_i$$

and let each $\sigma(E_i)$, $1 \leq i \leq M-1$, be equal to one of the σ_J's. Figure 1 shows typical point cross section data generated from a ladder of pseudo-resolved resonances. One can see that I_i would simply be the area under the curve from $E_{(i-1)}$ to E_i. In the example depicted, $\sigma[E_{(i-1)}] = \sigma_4$, (J=4), while $\sigma(E_i)$ and $\sigma[E_{(i+1)}] = \sigma_3$. Then $\sigma_{J-1} \leq \sigma(E) \leq \sigma_J$ with probability

$$p_J = \sum_{i=1}^{M} \Delta E_i\ \delta_{iJ}/(E_{MAX} - E_{MIN}) \text{ where } \Delta E_i = E_i - E_{i-1}, \text{ and}$$

$$\delta_{iJ} = \begin{cases} 1 & \text{if } \sigma_{J-1} \leq \sigma(E) \leq \sigma_J \text{ for } E_{i-1} \leq E \leq E_i \\ 0 & \text{otherwise.} \end{cases}$$

The probability that the cross section lies below σ_J is then

$$P_J = \sum_{k=1}^{J} p_k, \qquad \text{while } \bar{\sigma}_J = \frac{\sum_{i=1}^{M} I_i\ \delta_{iJ}}{\sum_{i=1}^{M} \Delta E_i\ \delta_{iJ}}$$

represents the mean value of the cross section between σ_{J-1} and σ_J.

The probability table method assumes that the resonance energies are so close together that the neutron enters a resonance randomly, and that the resonances are sufficiently narrow to ignore successive collisions in the same resonance.

3. Preparation of the Tables

In the preparation of cross section probability tables the following sequence of operations is observed:

1. An individual ladder of resonances is prepared in the prescribed energy region from known statistical laws and average parameters.

2. This individual ladder is used to generate a point data set. At this time the contributions to a probability table are computed and entered into a table at each of the desired temperatures. This entire process is then repeated over as many ladders as are deemed appropriate.

The details perhaps require further explanation. Starting with a given point data set prepared from a ladder of resonances, we have at any given energy in the set a total, scattering, capture, and possibly, a fission cross section. One of these, usually the total, is chosen as the basis for constructing a table. A set of total cross section magnitudes is constructed to serve as band limits, monotonically increasing. These may be erected arbitrarily, but at present start at some value above the minimum observed cross section and follow a geometric progression, i.e., σ_1, $k\sigma_1$, $k^2\sigma_1$, etc. where k is a constant such as 1.5 or 1.15, depending on the degree of detail required of the table. Assume for the moment that our point data set consists of a large number of equally spaced points to which we assign equal probability The actual set may not be so spaced but such a set can be obtained by interpolation, or a numerical integration scheme can be employed. The assumption of equally probable points is best for illustrative purposes. For each point in the set, the total cross section is entered in the band with appropriate magnitude limits. Simultaneously, a counter assigned to that band is advanced by unity. At the same time, in appropriate registers with the same band number, the corresponding values of scattering, capture

and fission cross sections are entered. When all points of the data set have been entered we have the following information: The average value of the total cross section in each band of monotonically increasing magnitude, obtained by dividing the sum of the cross section entries in each band by the number of entries in that band. Average cross sections for the other reactions are similarly obtained. The probability assigned to the band is obtained by dividing the number of entries in a given band by the total number of entries in all bands. Notice that in this way, only the total cross section band averages need be monotonically increasing. The other reaction cross section band averages are, in fact, the conditional averages corresponding to their respective total cross section band averages. Should they be observed to be also monotonically increasing, note that this is a consequence of the specific data and not the result of a realignment of the probability bands to be monotonically increasing for all reaction cross sections.

When, in a Monte Carlo calculation, the cross section of an isotope in its unresolved range is needed, it is obtained by a random selection from the appropriate probability table as follows:

Select a random number, $0 < r < 1$, and set $\sigma(E) = \bar{\sigma}_J$, where

$$P_{J-1} < r \leq P_J .$$

In actuality we select not only the total cross section but the scattering, fission, and capture cross sections associated with $\bar{\sigma}_J$, simultaneously. In this way the total and all reaction cross sections are correlated at every neutron collision.

4. A Test Problem

To establish the validity of the method a test program was set up using the AIRABL code. AIRABL is a modified version of RABBLE[3] which can obtain

effective cross sections using probability tables as well as point data. Since a given probability table is based on several ladders generated in the prescribed energy range, the accuracy of the method can be tested by comparing the mean effective cross sections obtained for a given problem using point data sets from each of several ladders with those obtained from several trials using a probability table based on these same point data sets. Effective capture and scattering cross sections for three isotopes in problems emphasizing different portions of their unresolved energy ranges are shown in Table I. In each case, the means were obtained from thirty samples of each method.[4]

The means based on the probability table method were in statistical agreement with their corresponding means from the point data set calculations While most of the calculations were performed using a table size of 45, no appreciable loss in quality was observed using a table size of 10.

The success of the method in predicting effective cross sections in both Monte Carlo and analytical calculations now permits full energy range neutron data sets to be independent of geometry and composition without requiring inordinately large blocks of computer storage. Probability tables, therefore, could serve as a standard way of representing neutron cross sectio in the unresolved energy range.

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TABLE I

COMPARISON OF AIRABL EFFECTIVE CROSS SECTIONS COMPUTED WITH POINT DATA FROM LADDERS AND THE PROBABILITY TABLES

Isotope	Effective Cross Section (b) Obtained Using		Difference	Table Size	Temp. (^{o}K)	Energy (eV)
	Point Data From Ladders	Probability Table				
Ta, σ_c	4.276 ± .157	4.204 ± .115	-.072 ± .195	45	300	300
Ta, σ_c	5.247 ± .201	5.240 ± .103	-.007 ± .226	45	700	300
Ta, σ_c	5.247 ± .201	5.383 ± .098	+.136 ± .224	10	700	300
Ta, σ_s	9.826 ± .166	9.639 ± .079	-.187 ± .184	45	300	300
Ta, σ_s	10.391 ± .199	10.220 ± .067	-.171 ± .210	45	700	300
Ta, σ_s	10.391 ± .199	10.326 ± .062	-.065 ± .208	10	700	300
U238, σ_c	.817 ± .014	.812 ± .009	-.005 ± .017	45	300	5500
U238, σ_c	.871 ± .015	.863 ± .008	-.008 ± .017	45	700	5500
U238, σ_s	13.39 ± .18	13.37 ± .10	-.02 ± .21	45	300	5500
U238, σ_s	13.80 ± .20	13.83 ± .09	+.03 ± .22	45	700	5500
Pu239, σ_c	5.007 ± .251	5.022 ± .064	+ .015 ± .259	45	300	825
Pu239, σ_c	5.196 ± .270	5.217 ± .053	+.021 ± .275	45	700	825
Pu239, σ_s	12.749 ± .273	12.723 ± .052	-.026 ± .278	45	300	825
Pu239, σ_s	12.886 ± .295	12.886 ± .044	.000 ± .298	45	700	825

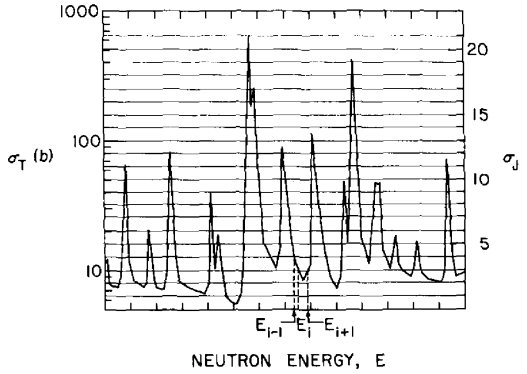

Figure 1. Typical Point Data
From Statistically Generated Ladder.

Text of a talk presented at the Resonance Region Meeting, Brookhaven National Laboratory, Upton, New York, May 8, 1972

APPLICATIONS OF THE PROBABILITY TABLE METHOD TO MULTI-GROUP CALCULATIONS*

by

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APPLICATION OF THE PROBABILITY TABLE METHOD

TO MULTI-GROUP CALCULATIONS

by

Dermott E. Cullen

May 1972

Consider the linear neutron Boltzmann equation:

$$\bar{\Omega} \cdot \bar{\nabla} N(\bar{r},\bar{\Omega},E) + \Sigma_T(\bar{r},E)N(\bar{r},\bar{\Omega},E) = \int_{\bar{\Omega}'}\int_{E'} f(\bar{r},\bar{\Omega}',E' \rightarrow \bar{\Omega},E)N(\bar{r},\bar{\Omega}',E)d\bar{\Omega}'dE' + S(\bar{r},\bar{\Omega},E) \qquad (1)$$

Multi-Group

In the multi-group approach the continuous energy range is divided into a number of adjacent intervals: $E_1 < E_2 < E_3 -- < E_{Kmax}$. Equation (1) is integrated over each energy range and divided by the width of the group to define group averaged quantities:

$$\bar{\Omega} \cdot \bar{\nabla} N_K(\bar{r},\bar{\Omega}) + \Sigma_{T_K}(\bar{r})N_K(\bar{r},\bar{\Omega}) = \sum_M \int_{\bar{\Omega}'} f(\bar{r},\bar{\Omega}',M \rightarrow \bar{\Omega},K)N_M(\bar{r},\bar{\Omega}')d\bar{\Omega}' + S_K(\bar{r},\bar{\Omega}) \qquad (2)*$$

where by definition:

$$N_K(\bar{r},\bar{\Omega}) = \int_{E_K}^{E_{K+1}} N(\bar{r},\bar{\Omega},E)dE/(E_{K+1} - E_K) \qquad \text{(group averaged flux)} \qquad (3)$$

$$\Sigma_{T_K}(\bar{r})N_K(\bar{r},\bar{\Omega}) = \int_{E_K}^{E_{K+1}} \Sigma_T(\bar{r},E)N(\bar{r},\bar{\Omega},E)dE/(E_{K+1} - E_K) \qquad \text{(group averaged cross sections)} \qquad (4)$$

$$f(\bar{r},\bar{\Omega}',M \rightarrow \bar{\Omega},K)N(\bar{r},\bar{\Omega}',M) = \int_{E_K}^{E_{K+1}}\int_{E_M}^{E_{M+1}} f(\bar{r},\bar{\Omega}',E' \rightarrow \bar{\Omega},E)N(\bar{r},\bar{\Omega}',E')dE'dE/(E_{K+1} - E_K) \qquad (5)$$

(group averaged transfer matrix)

*In practice the angular variable is eliminated by one of a number of available methods. It has been carried along to simplify the equations and to indicate the results of this paper are independent of the treatment of the angular variable.

Multi-Group, Multi-Band

The multi-group approach as defined above is of course not the only approach to defining group averages. In many applications Equation (1) is first multiplied by a function f(E) before performing the integration over the group. In this way it is possible to change the variable from the flux $N(\bar{r},\bar{\Omega},E)$ to $f(E)N(\bar{r},\bar{\Omega},E)$: e.g., in dose calculations, heating calculations, etc. However, in most applications f(E) is continuous and non-zero over any portion of the group. Therefore, the group is still treated as a single entity and the number of multi-group equations obtained by this approach would be the same as in the case of the multi-group approach as defined by Equations (2) through (5).

However, it is also possible to further sub-divide one or more groups according to ranges of the total cross section (other criteria are of course also possible). The resulting algorithm has the desirable property that the resulting equations can be cast in a form that is identical to the multi-group equations and the average flux and the input data (averaged cross sections and transfer matrix) can be simply related to the corresponding group averaged quantities. Therefore existing transport codes can be used simply by preprocessing the input data and correctly interpreting the flux output.

Defining a number of partition functions in each group (K) which are one (1) within a given cross section range and zero (0) outside of this range:

$$p_{KL}(E) = 1 \qquad \text{if } \Sigma_{T_{KL}} \leq \Sigma_T(E) \leq \Sigma_{T_{KL+1}} : \quad L = 1, 2, \ldots, L_{max}$$

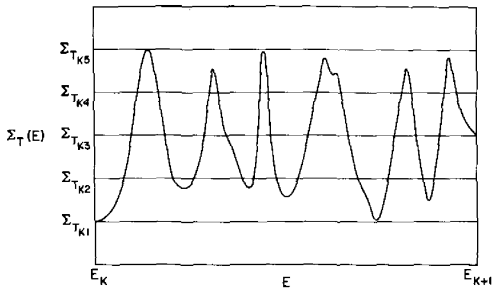
$$= 0 \qquad \text{if } \Sigma_{T_{KL}} > \Sigma_T(E) \text{ or } \Sigma_T(E) > \Sigma_{T_{KL+1}}$$

*Note that the partition functions $p_{KL}(E)$ are also functions of space and vary from region to region.

where:

$$\Sigma_{T_{K1}} = \min(\Sigma_T(E)) \quad E_K \leq E \leq E_{K+1}$$

$$\Sigma_{T_{KL_{max}}} = \max(\Sigma_T(E)) \quad E_K \leq E \leq E_{K+1} \tag{7}$$



some of the properties of these partition functions are:

1. The sum over all bands is one (1) within the group

$$\sum_L p_{KL}(E) = 1 \qquad E_K \leq E \leq E_{K+1} \tag{8}$$

2. The integral of one partition function over the group is merely the the cumulative probability of the cross section lying in the band (P_{KL}) times the width of the group ($E_{K+1} - E_K$)

$$\int_{E_K}^{E_{K+1}} p_{KL}(E)dE = P_{KL}(E_{K+1} - E_K) \tag{9}$$

3. Any integral over the group can be further partitioned using these partition functions:

$$\int_{E_K}^{E_{K+1}} f(E)dE = \sum_L \int_{E_K}^{E_{K+1}} p_{KL}(E)f(E)dE \tag{10}$$

In order to derive the multi-group, multi-band equations the linear neutron Boltzmann equation is first multiplied by one of the partition functions $p_{KL}(E)$, the continuous energy range is divided into a number of adjacent intervals: $E_1 < E_2 < E_3 \text{ -- } < E_{Kmax}$, Equation (1) is integrated over each energy range and divided by the width of the group to define group-band averaged quantities:

$$\bar{\Omega} \cdot \bar{\nabla} N_{KL}(\bar{r},\bar{\Omega}) + \Sigma_{T_{KL}}(\bar{r}) N_{KL}(\bar{r},\bar{\Omega}) = \sum_{M} \sum_{J(M)} \int_{\bar{\Omega}'} f(\bar{r},\bar{\Omega}',MJ \rightarrow \bar{\Omega},KL) N_{MJ}(\bar{r},\bar{\Omega}') d\bar{\Omega}' + S_{KL}(\bar{r},\bar{\Omega})$$

where by definition:

$$N_{KL}(\bar{r},\bar{\Omega}) = \int_{E_K}^{E_{K+1}} p_{KL}(E) N(\bar{r},\bar{\Omega},E) dE / (E_{K+1} - E_K) \quad \text{(group-band averaged flux)} \tag{11}$$

$$\Sigma_{T_{KL}}(\bar{r}) N_{KL}(\bar{r},\bar{\Omega}) = \int_{E_K}^{E_{K+1}} p_{KL}(E) \Sigma_T(\bar{r},E) N(\bar{r},\bar{\Omega},E) dE / (E_{K+1} - E_K) \tag{12}$$

(group-band averaged cross sections)

$$f(\bar{r},\bar{\Omega}',MJ \rightarrow \bar{\Omega},KL) N_{KL}(\bar{r},\bar{\Omega}) = \tag{13}$$

$$\int_{E_K}^{E_{K+1}} \int_{E_M}^{E_{M+1}} p_{KL}(E) p_{MJ}(E') f(\bar{r},\bar{\Omega}',E' \rightarrow \bar{\Omega},E) N(\bar{r},\bar{\Omega}',E') dE' dE / (E_{K+1} - E_K)$$

(group-band average transfer matrix)

In the definition of the group-band average transfer matrix, the partitioning property defined by Equation (10) above has been used to further sub-divide the integral over the source group (M) into a sum of integrals over the source group-bands (MJ).

Essentially sub-dividing one or more groups into cross section bands allows the flux within these groups to interact not with merely one cross section as in the multi-group approach but with any number of cross sections, properly weighted

according to the probability of these cross sections occurring within the group. The effect of this approach is that fairly broad groups can be used but since the population of each band (i.e., flux interacting in each cross section band) is allowed to vary as a function of position, the resulting "group" averaged cross sections (based upon reaction rates) can vary as a function of position. Furthermore, since the weighting function which is used to define the band averaged cross section and transfer matrix is not the group flux but rather the flux only within the cross section band, self-shielding effects due to cross section variation are minimized.

However, the applicability of this method depends upon the ability to actually calculate the group-band cross sections and transfer matrix and to relate the resulting group-band averaged flux to the group averaged flux.

It will be shown that the group averaged flux is merely the sum of the group-band averaged fluxes over all bands within the group. It will further be shown that the group-band cross sections can be simply related to the probability table and that at least in the unresolved energy range the group-band transfer matrix can be simply related to the group transfer matrix and the probabiltiy table.

To illustrate how to define the group averaged flux in terms of the group-band averaged fluxes consider the definition of the group averaged flux defined by Equation (3) and the partitioning property defined by Equation (10):

$$N_K(\bar{r},\bar{\Omega}) = \int_{E_K}^{E_{K+1}} N(\bar{r},\bar{\Omega},E)dE/(E_{K+1} - E_K) = \sum_L \int_{E_K}^{E_{K+1}} p_{KL}(E)N(\bar{r},\bar{\Omega},E)dE/(E_{K+1} - E_K) \quad (14)$$

or upon employing the definition of the group-band averaged flux (Equation (11)):

$$N_K(\bar{r},\bar{\Omega}) = \sum_L N_{KL}(\bar{r},\bar{\Omega}) \quad (15)$$

Therefore, the group averaged flux is merely the sum of the group-band averaged fluxes over all bands in the group.

Similarly from the definition of the total reaction rates within the group as a whole (Equation (4)) and the reaction rates within the individual bands (Equation (12)):

$$\Sigma_{T_K} N_K(\vec{r},\vec{\Omega}) = \sum_L \Sigma_{T_{KL}} N_{KL}(\vec{r},\vec{\Omega}) \tag{1}$$

Once a solution to a problem is obtained, Equations (15) and (16) may be used to define an equivalent group averaged cross section. Since the population of the individual bands are spatially dependent the resulting group averaged cross section can also be spatially dependent.

In order to define the group-band averaged cross sections, one could simply choose a median value of the cross section within the band $(1/2(\Sigma_{T_{KL}} + \Sigma_{T_{KL+1}}))$. This choice infers that all cross section values are equally probable within the band. However, since the probability table method supplies the true distribution of total cross sections within the group it can be used to define a more accurate average cross section for the band.

$$\Sigma_{T_{KL}} = \int_{\Sigma_{T_L}}^{\Sigma_{T_{L+1}}} \Sigma_T p_K(\Sigma_T) d\Sigma_T \Bigg/ \int_{\Sigma_{T_L}}^{\Sigma_{T_{L+1}}} p_K(\Sigma_T) d\Sigma_T \tag{1}$$

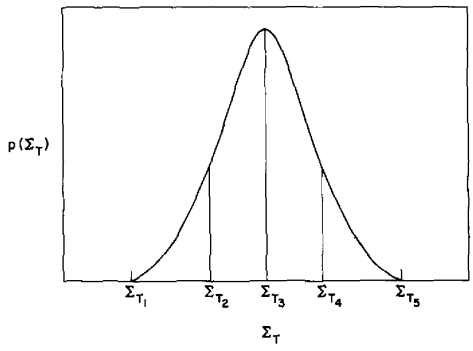
$$= \int_{\Sigma_{T_L}}^{\Sigma_{T_{L+1}}} \Sigma_T p_K(\Sigma_T) d\Sigma_T \Bigg/ P_{KL}$$

where $p_K(\Sigma_T)$ and P_{KL} are merely the partial and cumulative probabilities of the cross section lying between $\Sigma_{T_{KL}}$ and $\Sigma_{T_{KL+1}}$.

However, this approach ignores effects of the flux as a weighting factor in the definition of the cross section: both local effects (i.e., $1/\Sigma_T(E)$) and continuous trends (i.e., 1/E). In principle, for wide groups the 1/E weighting

can be significant, however, in practice in the unresolved region one has sufficient mixing of the cross section values over the entire group to virtually eliminate the influence of the 1/E factor (i.e., the 1/E factor will change averages over the group only in the case where the statistical distribution of cross sections is significantly varying as a function of E). However, if one wishes to eliminate the effect of the 1/E, consider using lethargy units instead of energy.

In considering the flux as a weighting function in the definition of the group-band cross sections and transfer matrices once consideration of the 1/E factor is eliminated the resulting approximate weighting function $N(\bar{r},\bar{\Omega},E)$ may be considered in the form $N(\bar{r},\bar{\Omega},\Sigma_T)$ and instead of considering the integrals in the $\Sigma_T(E)$ vs. E plane one can use the $p_K(\Sigma_T)$ vs. Σ_T plane (where $p_K(\Sigma_T)$ is the partial probability of obtaining a cross section Σ_T in the K-th group).



The inclusion of a $1/\Sigma_T$ weighting for the flux in the definition of the band cross sections is simple in this plane:

$$\Sigma_{T_{KL}} = \int_{\Sigma_{T_L}}^{\Sigma_{T_{L+1}}} \Sigma_T N(\bar{r},\bar{\Omega},\Sigma_T) p(\Sigma_T) d\Sigma_T \Big/ \int_{\Sigma_{T_L}}^{\Sigma_{T_{L+1}}} N(\bar{r},\bar{\Omega},\Sigma_T) p(\Sigma_T) d\Sigma_T \tag{18}$$

However in practice since the integral of the flux (weighting function) is only over bands of cross section the $1/\Sigma_T$ factor does not play as important a role as in the case of multi-group calculations where the integration is over all cross section values within the group.

In summary in order to define the group-band cross sections one can include the influence of the flux as a weighting function to compensate for 1/E and $1/\Sigma_T(E)$ effects, however, in practice it is not necessary and a straight weighting according to the probability of the cross section appearing within the band is sufficient (i.e., use Equation (17)).

Turning to the problem of defining the transfer matrix for the group-band, consider the differential definition of the transfer matrix:

$$p_{KL}(E) p_{MJ}(E') f(\bar{r},\bar{\Omega}',E' \rightarrow \bar{\Omega},E) N(\bar{r},\bar{\Omega}',E') \tag{19}$$

or simply re-grouping terms to a transfer probability and the definition of the band flux:

$$p_{KL}(E) f(\bar{r},\bar{\Omega}',E' \rightarrow \bar{\Omega},E) [p_{MJ}(E') N(\bar{r},\bar{\Omega}',E')] \tag{20}$$

From this grouping one can see that the transfer of the group-band flux is modified by a term $p_{KL}(E)$ which is simply the probability of the cross section lying within the band $\Sigma_{T_{KL}} \leq \Sigma_T(E) \leq \Sigma_{T_{KL+1}}$. In the unresolved region one has sufficient mixing of the cross section values over the entire group so that the probability of the final energy having a cross section in the range $\Sigma_{T_{KL}}$ to $\Sigma_{T_{KL+1}}$ is merely the cumulative probability of the cross section lying in this band averaged over the group: i.e.,

$$\int_{E_K}^{E_{K+1}} p_{KL}(E) f(\bar{r},\bar{\Omega}',E' \rightarrow \bar{\Omega},E)dE/(E_{K+1} - E_K) = P_{KL} f(\bar{r},\bar{\Omega}',E' \rightarrow \bar{\Omega},K) \tag{21}$$

which simply states that the probability of transfer to the L-th band of the K-th group is simply the probability of transfer to the K-th group times the cumulative probability of cross section lying in the L-th band (Σ_{T_L} to $\Sigma_{T_{L+1}}$) averaged over the group.

The remaining integration over the source group-band is of the form:

$$P_{KL} \int_{E_M}^{E_{M+1}} f(\bar{r},\bar{\Omega}',E' \rightarrow \bar{\Omega},K)[p_{MJ}(E')N(\bar{r},\bar{\Omega}',E')]dE' \tag{22}$$

In order to define this group-band averaged transfer matrix, one can proceed as in the case of the group-band averaged cross section to argue that effects such as 1/E play no significant role if the cross sections are significantly mixed and that the $1/\Sigma_T(E)$ is not that important since the integration is only being performed over a band of cross section values.

The transfer function $f(\bar{r},\bar{\Omega}',E' \rightarrow \bar{\Omega},E)$ can be represented as a cross section $\Sigma_T(E')$ times a normalized transfer function $g(\bar{r},\bar{\Omega}',E' \rightarrow \bar{\Omega},E)$, normalized to the average number of secondaries per event when integrated over all $(\bar{\Omega},E)$. When the term $p_{MJ}(E')N(\bar{r},\bar{\Omega}',E')$ is considered to be a statistically continuously distributed quantity over the group the integral becomes identical to that encountered in multi-group calculations with $\Sigma_{T_K} g(\bar{r},\bar{\Omega}',E' \rightarrow \bar{\Omega},E)$ replaced by $\Sigma_{T_{KL}} g(\bar{r},\bar{\Omega}',E' \rightarrow \bar{\Omega},E)$.

The result of these considerations is that the group-band transfer matrix can be simply related to the group transfer matrix properly normalized to the band reaction rate:

$$f(\bar{r},\bar{\Omega}',MJ \rightarrow \bar{\Omega},KL) = p_{KL} \frac{\Sigma_{T_{KL}}}{\Sigma_{T_K}} f(\bar{r},\bar{\Omega}',M \rightarrow \bar{\Omega},K) \tag{23}$$

However, before proceeding to a summary of these simple relationships between the group averaged values and the group-band averaged values it

should be pointed out that Equation (23) does not account for an effect that may be of importance in calculations. The transfer matrix as defined includes not only effects involving the probability of transfer for one energy group and cross section band to another, but also the probability of surviving (or multiplying) due to a collision in the source group-band. The group transfer matrix naturally also includes this effect, however, integrated over all cross section bands. Therefore, if the probability of survival is a strongly varying function of cross section (e.g., the ratio of $\Sigma_C(E)/\Sigma_T(E)$ in strongly absorbing resonances), the definition of the group-band transfer matrix must be modified to account for this effect by considering a probability table not only for the total cross section but also the "secondary" cross section.

In summary the following relationships can be established between available group averaged and probability table data and the required group-band averaged data:

$$\Sigma_{T_{KL}} = \int_{\Sigma_{T_L}}^{\Sigma_{T_{L+1}}} \Sigma_T p(\Sigma_T) d\Sigma_T \Bigg/ \int_{\Sigma_{T_L}}^{\Sigma_{T_{L+1}}} p(\Sigma_T) d\Sigma_T \qquad (2$$

(group-band averaged cross section)

$$f(\bar{r},\bar{\Omega}',MJ \rightarrow \bar{\Omega},KL) = P_{KL} \frac{\Sigma_{T_{KL}}}{\Sigma_{T_K}} f(\bar{r},\bar{\Omega}',M \rightarrow \bar{\Omega},K) \qquad (2$$

(group-band averaged transfer matrix)

The following relationships between group-band and group averaged fluxes and reaction rates can also be established:

$$N_K(\bar{r},\bar{\Omega}) = \sum_L N_{KL}(\bar{r},\bar{\Omega}) \qquad (2$$

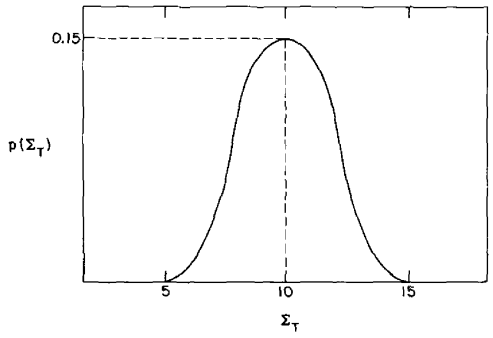
$$\Sigma_{T_K}(\bar{r}) N_K(\bar{r},\bar{\Omega}) = \sum_L \Sigma_{T_{KL}}(\bar{r}) N_{KL}(\bar{r},\bar{\Omega}) \qquad (2$$

These two equations can be used to define an equivalent group averaged cross section based upon a reaction rate balance:

$$\Sigma_{T_K}(\bar{r}) = \sum_L \Sigma_{T_{KL}}(\bar{r})\, N_{KL}(\bar{r},\bar{\Omega}) \Big/ \sum_L N_{KL}(\bar{r},\bar{\Omega}) \tag{28}$$

Since the population of the individual bands can vary as a function of position the resulting group averaged cross sections can also vary as a function of position.

Consider a simple application of the proposed group-band method. To illustrate the method, the unresolved region will be considered to be a single group with a number of bands. A flat flux distribution will be considered to be incident upon a slab which has the following total cross section probability table:



$$p(\Sigma_T) = 0.15 - 0.006(\Sigma_T - 10)^2$$

The effects of self shield as a function of probability of survival (i.e., Σ_S/Σ_T) will be studied.

In the case of a totally absorbing medium one obtains simple exponential attenuation within the various cross section bands. The effect is a clustering of the flux in the low cross section regions. The result is a continuous decrease in the group averaged cross section from 10 barns at the boundary toward a limit of 5 barns at infinity.

Using mean free path (MFP) units as defined by the cross section at the boundary (i.e., 1 MFP $\sim$ 10 barns) the following changes in the group averaged cross section occur:

Distance	$\bar{\Sigma}_T$
0.0	10.0
0.5	9.75
1.0	9.5
5.0	7.85
10.0	6.75

The difference in the scalar flux 10.0 units into the slab between using $\bar{\Sigma}_T = 10$ and the true self-shielding cross section is almost a factor of 10 (see: Figure 1).

For the case of a pure scattering medium one naturally obtains a somewhat different result. In this case a reaction balance is reached between the bands where the low cross section bands feed the high cross section band via spatial transport effects. The effect is to have a group averaged cross section that varies from $\bar{\Sigma}_T = 10.0$ at the boundary with a flat flux over the group to $\bar{\Sigma}_T = 9.47$ at infinity with a $1/\Sigma_T(E)$ flux over the group (i.e., $\Sigma_T(E)N(E)$ balance between the cross section bands).

In conclusion, calculations indicate that the method is a practical means of obtaining numerical solutions to transport problems involving the unresolved

resonance region. Furthermore, it has been demonstrated that starting from existing transport codes and an unshielded cross section library, one still obtains correct self-shielding effects such as spatially dependent group averaged cross sections.

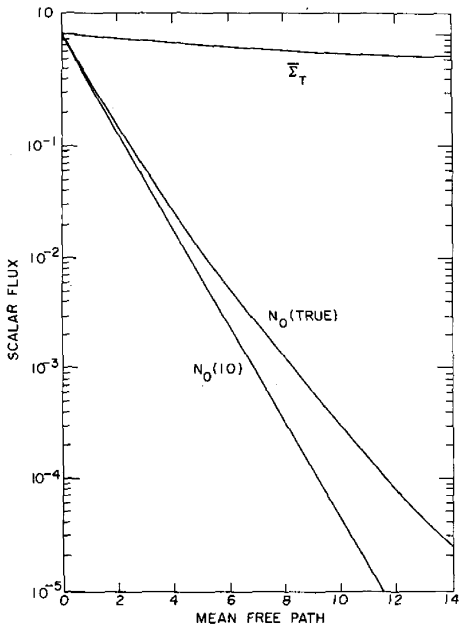


Figure 1. Flux in Totally Absorbing Medium.

Text of an invited talk presented at the Resonance Region Meeting, Brookhaven National Laboratory, Upton, New York, May 8, 1972

USE OF PRE-PROCESSED DATA IN THE RESONANCE RANGE*

by

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USE OF PRE-PROCESSED DATA IN THE RESONANCE RANGE

O. Ozer

May 1972

I Introduction

The increasing quality of the ENDF files has often resulted in the data being given in greater detail and use being made of more complex representations. This in turn has caused the files to become more expensive and difficult to process and use.

Even a simple problem such as the determination of a cross section at some specified energy may necessitate a rather lengthy calculation since for a large fraction of ENDF materials the cross sections are given in two separate parts: resonance and background. The resonance part must be reconstructed from resonance parameters according to a specified formalism. The corresponding background section must be interpolated and added to the former to give the final value of the cross section.

The ENDF processing codes are correspondingly becoming quite elaborate since they must have the capability of processing all combinations of permissible formalisms. In general changes in the ENDF formats or procedures or the addition of new formalisms have resulted in need for extensive reprogramming, updating or patching up of existing codes.

A great amount of computing time and effort can be saved by pre-processing and storing the ENDF data at an "intermediate" or simplified level.

Obviously a compromise must be made between the amount of "pre-processing" necessary to bring the data to this "intermediate" level,

and the general usefulness of the pre-processed data. Application and composition dependent group constant libraries will save a very large amount of time for a small number of users but will be useless to others. Whereas ENDF/B like files for which the only pre-processing consisted of replacing the resonance and background data by a set of reconstructed point cross sections will be useful in a wider range of applications but may still require a fair amount of processing.

This paper will discuss two levels of "pre-processed" files: The first level consists of an ENDF/B like file of point cross sections. The second level will be a multipurpose, multigroup library of group constants and transfer matrices to be used in reactor calculations. Since a Level I library has already been generated at NNCSC, the library, codes used in its preparation and its applications will be discussed in some detail.

Plans for formats and contents of a Level 2 library will be presented only briefly.

II Generation of Level I Pre-Processed Data

The Level I pre-processed files are generated using the code RESEND. The purpose of this code is to process all of the permissible ENDF/B resonance range formalisms and to generate infinitely dilute, unbroadened point cross sections in an ENDF/B like format.

The program is written in a modular fashion with two major sections operating as overlays on the PDP-10 system. The first section does the resonance calculation and stores its results on a scratch file. The second section combines the resonance points with the background and prints out the results. The program is written entirely in Fortran-4 with liberal use of

descriptive comment cards. It makes use of no machine dependent techniques.

A. Resonance Section

The resonance section operates by first reading all the resonance information of an ENDF material and storing it in a compact form in a dense array. However the data for the various sections (isotope/energy range) are kept separate. The calculation of the cross section at an energy point is done by calling a single subroutine SIGMA. This subroutine determines which sections contribute to the energy of interest and the formalisms to be used, then calculates the contribution of each section by calling a secondary subroutine depending on the formalism to be used. A separate subroutine is used for each of the formalisms to facilitate the addition of new formalisms or the replacement of the treatment of existing ones.

An advantage of calculating the contributions of each section separately is that correct results will be obtained even if some present ENDF/B procedures are violated on the input files. (eg. overlapping resolved-unresolved ranges, different ranges and/or formalisms for the different isotopes of the same material.

1. Formalism

The formulae specified in appendix D of the ENDF formats and procedures manual[1] are strictly followed for single or multilevel Breit-Wigner, Reich-Moore or Adler-Adler formalisms in the resolved resonance range. (Although Adler-Adler and Reich-Moore subroutines have not been implemented in the present version of the code).

Since only infinitely dilute and unbroadened point cross sections are calculated there are no ambiguities in the calculations and the formulae of Ref-I will not be repeated here.

The only ambiguity may appear in the treatment of the cross sections in the unresolved ranges. Here the RESEND code calculates only averaged cross sections in a manner similar to the one used by M.R. Bhat in the codes AVERAGE 3 AND AVERAGE 4[2]. This procedure is outlined on Table I. It basically consists of replacing the average of the ratio of resonance widths by a ratio of the average values times a fluctuation integral S. Since the resonance parameters are subject to statistical fluctuations according to a Chi-squared distribution the fluctuation integral S will in general consist of double integrals of products of Chi-squared distributions. In the present version of the code this integral is evaluated by using the standard 10 point numerical quadrature method of Greebler-Hutchins. However in the future a method developed by M. Beer[3] in which the double integral is reduced to a single integral ideally suited for gaussian quadratures will be implemented.

2. The Energy Grid

Great care must be applied in the selection of an adequate energy grid. The grid must be fine enough not to miss any important features of the cross section; yet it must be flexible enough in order not to generate an unnecessarily large number of points in areas where the variation of the cross section is slow.

The RESEND code uses a grid generated by a convergence algorithm develop ed by D.E. Cullen[4] and shown shematically on figure 1. The algorithm

consists of first assigning node points to each resonance energy (in order not to miss any resonance peaks). Next the cross sections of the node points are computed (exactly). The grid between two adjacent node points (points A and B in figure 1) is determined by calculating the cross section σ_1 at the mid-point X_1 and comparing it with a cross section $\bar{\sigma}_1$ that would be obtained at this energy by linear interpolution between the last two converged points (in this case A and B). If

$$\frac{|\sigma_1-\bar{\sigma}_1|}{\sigma_1} > \varepsilon$$

where ε is an input convergence criterion then the interval A-B is assumed not to have converged. X_1 becomes the new pivot point and the convergence of the interval $A-X_1$ is tested in a similar manner. The procedure is repeated until convergence. Note that the cross sections calculated at the intermediate points are not lost but are stored and used to test the convergence of later intervals. Thus for example if the interval $A-X_3$ was converged the next interval tested will be X_3-X_2 etc.

An additional convergence criterion is introduced in order not to generate an unnecessarily large number of points in areas where $\sigma_1 \simeq 0.0$. Thus the grid will be assumed to have converged within an interval if the cross section at both ends of the interval is less than an input number ε^1.

This method has been fairly successful in representing even highly structured cross sections. Figure 2 shows a small section of the cross section curve obtained for U-235. Figure 3 shows the distribution of the grid points between two resonances.

The total number of points generated depends very strongly on the

complexity of the material (number of resonances) and on the accuracy desired Table 2 shows the number of points generated for a selected number of ENDF materials with two different convergence criteria.

3. Acceleration

The running time of the code can be reduced by treating far away and weak resonances in an approximate manner. If this option is selected the cross section at the two nodes will be assumed to consist of two parts $\sigma_A=\sigma_A^R+\sigma_A^S$. The contribution of all resonances within n Γ of node A, where N is again an input no., is included in the "rapidly varying" section σ_A^R. The contribution of all other far away or weak resonances is included in the "slowly varying" section σ_A^S. Note that both of these parts are calculat exactly at the nodes. However in the calculation of the intermediate grid points only the resonances which contributed to σ_A^R will be treated exactly. The contribution of all other resonances will be obtained approximately by interpolating between σ_A^S and σ_B^S. (This technique has not been incorporated into the present version of the program).

B. Background Correction

The second section of the program RESEND combines the resonance data written out onto a scratch file by the first section with background cross sections read from the ENDF file. The unusual feature of this section is that the resonance data file as well as the background data file are read, combined and printed out in small fixed size blocks or pages. Thus the dimensions of the program are completely uncoupled from the size of the data arrays that are being generated. In fact only $24K_{10}$ of core is

required when running on the PDP-10 system.

III Description of the Level I Pre-processed data files.

The Level I pre-processed data files consist of infinitely dilute, un-Doppler broadened point cross sections in ENDF/B format with one possible exception: The present ENDF (version 2 and 3) formats restrict the maximum number of points that can be given for a reaction type to 5000. The dimensions of the data arrays in the pre-processed files are unlimited.

In order to conform to ENDF formats the pre-processed materials are supplied with a dummy file 1 Hollerith information section (MT=451) which only contains the accuracy criterion used in the reconstruction of the data file. A dummy file 2 is also supplied. The reconstructed cross sections appear in file 3 as reaction types 1, 2, 18 and 102. These cross sections are supplied over a master energy grid consisting of the union of the resonance and background grid. A linear-linear interpolation law is used in the resonance range. Outside this range the original interpolation law is left unchanged. In addition any other reaction types present in file 3 of the original ENDF material are also transfered to the pre-processed files without any changes. However in order to preserve space files higher than 3 are not included in the present version of the files.

Level I files for all ENDF/B Version 3 materials with resonance parameters have been generated using convergence criteria of 0.05% or 0.1%.

IV Uses of the level I preprocessed data

The steps followed in the generation and some of the applications of the pre-processed files are shown on the flow diagram on Figure 4.

A. Doppler Broadening: Program DOPEND

The pre-processed files generated by RESEND are not Doppler broadened. A numerical Doppler broadening program Dopend is being designed in order to broaden the data to any desired temperature.

The formalism followed by DOPEND is shown on Table 3. The Doppler broadened cross section σ^* at energy ϵ consists of two parts I_1 and I_2. However the I_2 part is only non negligible at very low energies or high temperatures and will only be calculated when

$$\epsilon < \frac{80\ kT}{A}$$

The integrals are evaluated numerically by Rhomberg integration. End proble near the very top and bottom of the data tables where the integration range exceeds the range over which the data is defined are avoided by adding two extrapolated points at $E_1-9\Delta$ and $E_n+9\Delta$ where E_1 and E_n are first and last energies of an array.

Since very large data arrays are expected to be processed the code will be designed in a manner that will allow the processing of these arrays a small section at a time.

Some important advantages are obtained by Doppler broadening the data after it has been processed through RESEND:

a. The broadening process becomes very simple since it is complete uncoupled from the formalism used in the generation of the point data set.

b. The broadening is not restricted to the resonance range but can be applied to the entire range over which the data is defined.

c. Problems caused by not broadening the "smooth background" are avoided. In principle this problem should be negligible however in

practice because of pressures to use single level formalisms it is possible to have a considerable amount of structure in the background cross section.

d. Because of the inclusion of the low energy correction term I_2 the code will be well suited for high temperature (or low energy) applications.

B. Plotting and Display Capability

The pre-processed point cross section files are well suited for displaying, plotting and publication. The only requirement on a plotting code is that it be capable of plotting the data a small section at a time. The interactive graphics code SCOPE[5] has been used to obtain plots of all the ENDF/B Version III materials and will be used for the publication of selected ENDF/B data.

The standard ENDF plotting and listing program PLOTFB however must be upgraded to process the larger data arrays.

C. Calculation of Integral Properties

Because of the pre-processing done in generating the Level I files the calculation of various integral properties of the cross sections becomes a particularly simple task. Thus a simple special purpose program INTER has been written to calculate the resonance integrals. Maxwellian averaged thermal cross sections and Westcott-"g" factors by numerically integrating the point data files with 1/E and Maxwellian weight functions. All of the ENDF/B Version III materials have been processed through INTER. Tables of the calculated values have been generated and are available for reference purposes.

A general purpose integration program INTEND is being planned as a logical extension of INTER. This program will be able to produce up to 1000 group constants with combinations of fission, 1/E, Maxwellian, $1/\Sigma_t$ or input weight functions.

V Level 2 Pre-Processed Libraries

Recently R. Neuhold of the AEC conducted a study to determine the need and feasibility of an ENDF/B based data file that would be pre-processed to a considerably higher degree. This Level 2 file would consist of a single set of group constant libraries that would satisfy the initial survey-design needs of the fast reactor, thermal reactor, shielding and possibly other design communities.

The purpose of the study was to examine the needs of the three major communities as well as the features of present day codes in order to determine specifications and desirable features for a new processing code to be used in the generation of the library.

It was determined that a single pseudo composition independent "Bodnaren" type library of cross sections and shielding factors (such as the ones generated by the codes ETOX or ENDRUN) would be quite desirable providing it had a number of additional features such as anisotropic transfer matrices, larger number of groups, a thermal sink group, etc.

Consequently specifications for two new codes were drafted. The first code will be used to generate group constants and shielding factors, the second to interpolate the shielding factor for a particular composition and energy and space collapse the group constants for use in reactor or shielding calculations.

The specifications for the first code include the following selected points:

A. Group Structure

The code is expected to process of the order of 100 groups which will include commonly used boundaries such as 10 and 15 Mev. and a thermal group with a flexible upper energy cut to accommodate cuts used at various installations. The basis for the mesh structure will consider in addition to important features of the neutron cross sections of important materials, also peculiarities in neutron-gamma production.

B. Weighting Spectra

A large variety of within-group weighting spectra including possibly analytical slowing down spectra will be considered.

C. Matrices

Matrices up to order P_8 should be calculated with algorithms based on analytic integration in the Laboratory system. f-factors should also be supplied.

Anisotropic angular dependence should be considered in the generation of the inelastic transfer matrices.

D. In the Resonance Range:

a. Interference scattering should be included.

b. Same sequence overlap effects [Hwang, NSE 21, 523 (1965)] should be implemented although not necessarily in the first version of the code.

c. All ENDF formalisms should be processable (Breit-Wigner, Reich-Moore and Adler-Adler)

d. The Intermediate Resonance Method should be considered in both resolved and unresolved ranges.

e. Use of probability table and integral slowing down theory method should be studied for future versions.

f. Provisions should be made for storing multilevel point data in Doppler broadened form so that it will be available for interpolatives re-use.

E. The output will conform to the CCCC (Computer Code Coordinating Committee) interface specification.

To accomodate thermal reactor needs the output will include a thermal edit with breakdown of contributions in the resonance range.

Moreover as a programming requirement it is strongly recommended that the program be written in such a manner that large ENDF/B arrays are not read in all at one time but in small blocks.

When this code is implemented, even though it will be possible to generate the Level 2 pre-processed files directly from ENDF/B, a great amount of time can be saved if except for a few materials with unresolved resonance regions-- the Level 1 files are used as the starting base. In the unresolved ranges however the present treatment in the code RESEND will have to be brought to a consistent level with the processing code.

REFERENCES

1. M. K. Drake, Ed., Data Formats and Procedures for the ENDF Neutron Cross Section Library. BNL-50274(T-601)ENDF-102, Vol. 1, October 1970.

2. M.R. Bhat, ENDF/B Processing Codes for the Resonance Region. BNL-50296, ENDF-148, June 1971.

3. M. Beer, MAGI internal memo to H. Steinberg etal September 13, 1971.

4. D.E. Cullen, Private Communication.

5. D.E. Cullen, Program SCOPE, BNL-16700, April 1972.

TABLE 1: Outline of Unresolved Range Formalism Followed in RESEND

$$\sigma_{n,\gamma}(E) = \frac{2\pi^2}{k^2} \sum_{\ell=0}^{NLS} \sum_{J}^{NJS_\ell} \frac{g_J}{\langle D \rangle_{\ell,J}} \left\langle \frac{\Gamma_n \Gamma_\gamma}{\Gamma} \right\rangle_{\ell,J}$$

$$\sigma_{n,n}(E) = \frac{4\pi}{k^2} \sum_{\ell=0}^{NLS} \sum_{J}^{NJS_\ell} (2\ell+1)\sin^2\varphi_\ell + \frac{2\pi}{k^2} \sum_{\ell=0}^{NLS} \sum_{J}^{NJS_\ell} \frac{g_J}{\langle D \rangle_{\ell,J}} \left[\left\langle \frac{\Gamma_n \Gamma_\gamma}{\Gamma} \right\rangle_{\ell,J} - 2\bar{\Gamma}_{n_{\ell,J}} \sin^2\varphi_\ell \right]$$

χ^2 distribution with "n" degrees of freedom $\rightarrow P_n(x)dx = \frac{n}{2} \frac{1}{\Gamma\left(\frac{n}{2}\right)} \left(\frac{nx}{2}\right)^{\frac{n}{2}-1} \exp\left(\frac{-nx}{2}\right) dx$

Replace $\left\langle \frac{\Gamma_n \Gamma_n}{\Gamma} \right\rangle_{\ell,J}$ by $\frac{\bar{\Gamma}_{n_{\ell,J}} \bar{\Gamma}_{n_{\ell,J}}}{\bar{\Gamma}_{\ell,J}} \cdot S_{n_{\ell,J}}$

and $\left\langle \frac{\Gamma_\gamma \Gamma_n}{\Gamma} \right\rangle$ by $\frac{\bar{\Gamma}_{n_{\ell,J}} \bar{\Gamma}_{n_{\ell,J}}}{\bar{\Gamma}_{\ell,J}} \cdot S_{\gamma_{\ell,J}}$

where the fluctuation integrals $S_{n_{\ell,J}}(f(x))$ are of the form

$$S_{n_{\ell,J}}(f(x)) = \int_0^\infty P_n(r) \int_0^\infty P_k(s)\, f(x)\, ds\, dr$$

Integrations computed by a 10 point numerical quadrature

$$S_{n_{\ell,J}} \simeq \frac{1}{10.10} \sum_{i=1}^{10} \sum_{i'=1}^{10} f(P_i P_{i'})$$

TABLE 2: Number of Points Generated in the Resonance Range for Selected ENDF/B Materials With Two Convergence Criteria.

Symbol	ENDF MAT Number	No. of Resolved Resonances	Unresolved Section	Number of Points ε = 1.0%	Number of Points ε = 0.05%
U-234	1043	21	Yes	2083	8124
U-235	1157	130	"	3146	14304
U-238	1158	457	"	16575	39632
Pu-238	1050	14	"	1268	5543
Pu-239	1159	123	"	5367	21683
Pu-240	1105	201	"	12491	33467
Pu-241	1106	44	"	997	4602
Fe	1180	29*	No	988	2045
Ni	1123	294	No	2874	11012

*Contains MLBW Parameters.

TABLE 3: Doppler Broadening Formalism Used by DOPEND

Doppler broadened cross section $\sigma^*(\epsilon) = I_1 + I_2$

where $I_1 \simeq \frac{1}{\sqrt{\pi}\,\Delta} \int_{\epsilon - 9\Delta}^{\epsilon + 9\Delta} \left[1 + \frac{E'-\epsilon}{\Delta}\right]^2 \sigma(E') \exp -\left(\frac{E-\epsilon}{\Delta}\right)^2 dE'$

and $I_2 = \frac{1}{\sqrt{\pi}\,\Delta} \int_0^{\infty} \frac{\sqrt{E'}}{\sqrt{\epsilon}} \sigma(E') \exp\left[-\beta(\sqrt{E'} + \sqrt{\epsilon})^2\right] dE'$

in above expressions $\Delta = \frac{2\sqrt{\epsilon}}{\sqrt{\beta}}$ and $\beta = \frac{A}{kT}$

Note that $I_2 \simeq 0.0$ for all $\epsilon > \frac{80}{\beta}$

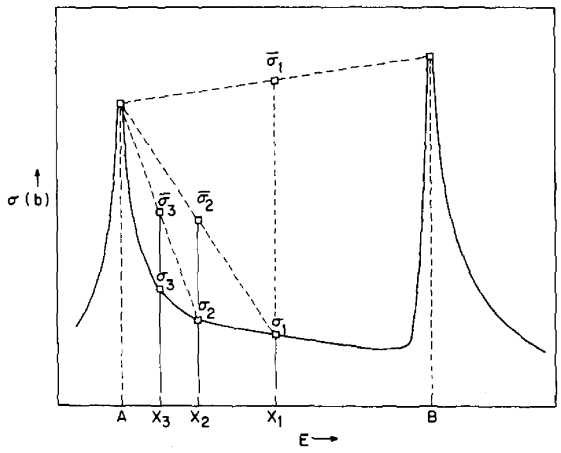

Figure 1. Generation of Energy Grid in Program RESEND.

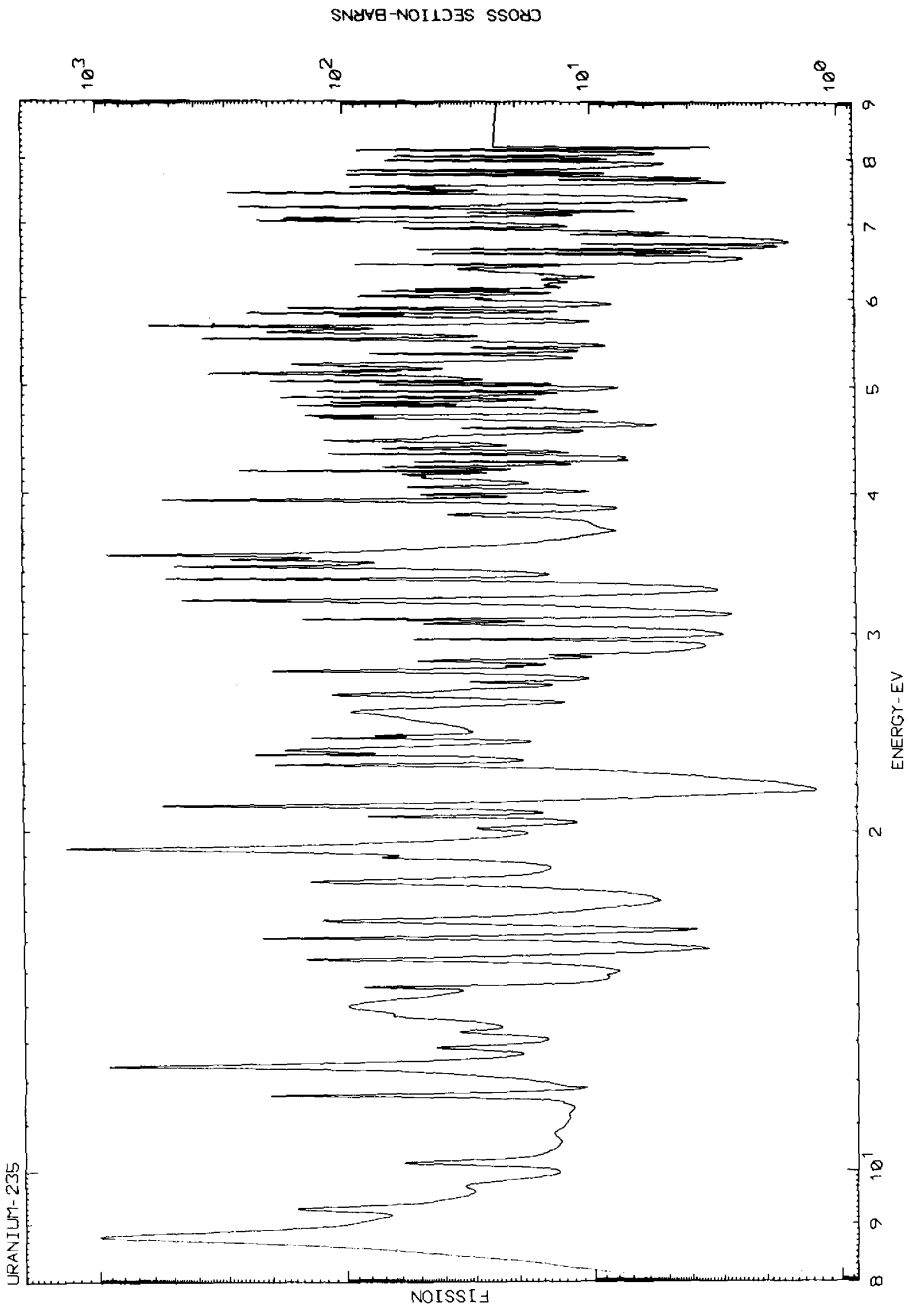

Figure 2. Fission Cross-Section of U-235.

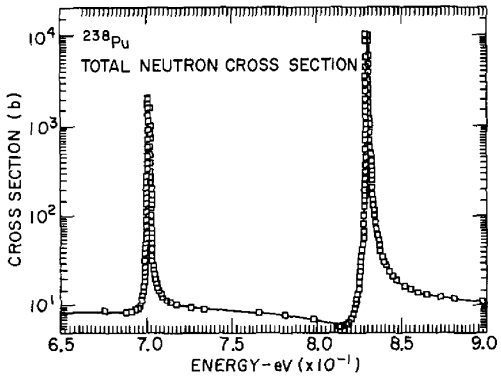

Figure 3. Sample Grid for Pu-238 with 1 % Accuracy.

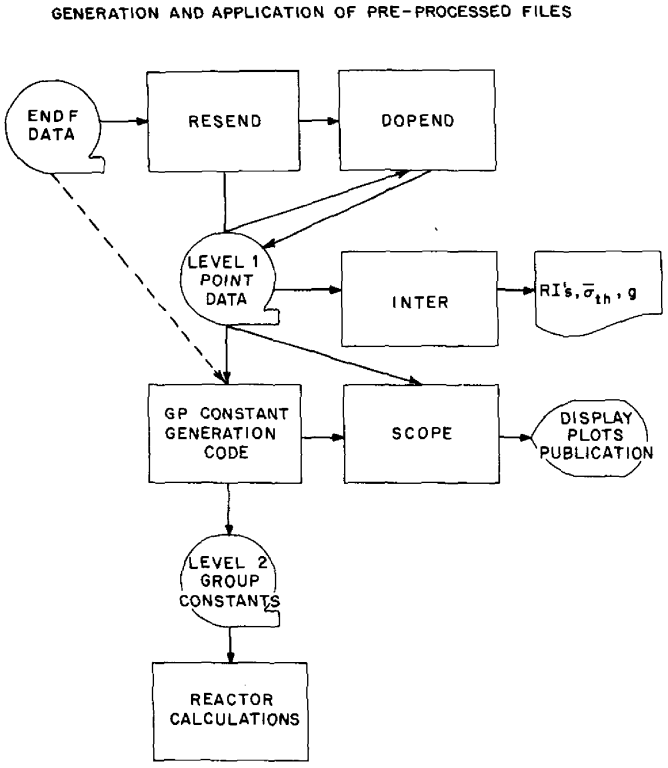

Figure 4. Generation and Application of Pre-Processed Data Files.

Text of an invited talk presented at the Resonance Region Meeting, Brookhaven National Laboratory, Upton, New York, May 8, 1972.

SUMMARY OF THE MEETING

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S U M M A R Y

M. K. Drake

The speakers did a tremendous job today. I don't feel under a severe obligation to give a detailed summary since most of the speakers have been kind enough to prepare written summaries of their presentations.

At the beginning of the meeting, Mulki Bhat asked two questions: "Are multi-level resonance parameters required for accurate application oriented calculations, such as reactor physics?" and "Is the probability table method completely understood and valid for use in reactor physics calculations?"

First, let me say that at the time we put this meeting together the probability table method was under much more controversy than it is today. Most of the controversy was due to the fact that it was not understood by many people. I didn't see the controversy at this meeting that we expected several months ago. The participants at this meeting agreed that the method was valid and appears to be very useful for preparing multi-group constants for Monte Carlo calculations. In fact, Dr. Cullen presented a scheme for using the method for preparing multi-group constants for use in transport calculations.

The question about the need to use multi-level parameters generated much more controversy. The question was really never resolved. The theoreticians and the experimentalists stressed the need for multi-level formalisms to accurately represent the physics and experimentally observed cross sections, particularly the fission cross sections. The reactor physicists tended to agree that the statements made by the experimentalists were true but they didn't agree that anyone had demonstrated that multi-level

representations had any significant effect on reactor physics calculations. I think it is important that we have gathered here and exchanged ideas on this subject. It is unfortunate that no one has bothered to attack the problem in such a manner that would demonstrate whether or not one must use multi-level parameters in reactor physics calculations.

I will digress from my summary to make a few points. I think that the sought after demonstrated need lies in qualified numerical or experiment studies. Oh yes, several groups have done numerical experiments and there have even been a few experimental measurements. As one can observe from the comments made here, neither approach has thus far been very successful.

Some very good people have done numerical experiments but I don't think that the answers proved anything. Most of these experiments have used the following line. First a set of unresolved resonance parameters were selected. These parameters were selected by studying the statistical properties of the resolved resonances. The average resonance parameters were then used in application oriented calculations. First the parameters were called single level parameters and a calculation was done. Then the exact same parameters were called multi-level parameters and the calculation was repeated. The two calculated results were compared and the difference was called the multi-level effect. I don't think that such calculations prove anything.

I think that it would be more meaningful to perform another type of numerical experiment. Such an experiment could be done by the following steps:

1. Select a nucleus such as ^{239}Pu.
2. Evaluate the total, fission, and radiative capture (or alpha) cross sections using the best experimentally consistent data

available. The energy range should cover the unresolved range, from about 300 eV to 40 keV.

3. Divide the energy range into bands. Each band should be wide enough to represent a statistically significant average ($\geq$ 100 resonances). The bands should not be so wide that they would represent an average over the gross structure (intermediate structure effects).
4. Select resolved single level resonance parameters for each energy band. The resonance energies and widths should be selected in such a manner that they collectively obey the usual distribution laws. Calculate pointwise cross sections from the parameters and then average cross sections for each band. If the average cross sections do not agree with the averages calculated from the experimental data from step number 2, then a new ladder must be generated. If the bands contain enough resonances, each band can be represented by the average parameters obtained from the ladder for the band.
5. Step number 4 is repeated. In this case multilevel parameters will be selected. The same constraint must be used. The final parameters must predict the same average cross sections for the band. The average multi-level parameters will likely be different than the average single level parameters but they will both predict the same average infinitely dilute Doppler broadened cross sections (to room temperature or the experimental sample temperature).
6. At this point two application oriented calculations can be made. The calculations should include several different temperatures

and varying degrees of resonance self-shielding. It is true that the above mentioned experiment still has problems. For example, there is no unique set of parameters that will predict the average cross sections for a band. Also, one does not know which fission width to vary in order to predict the gross structure in the cross section.

Question: What experimental measurements can be done?

Answer: I would think that there are some experiments that can be done. They might be very difficult and expensive. One could measure the fission and/or the capture cross sections over the energy region from 500 eV to about 10 keV. In this same measurement, various sample thicknesse and temperatures should be used. It may be difficult to measure accurate cross sections with thick samples and at elevated temperatures.

Comment: I think an experiment of the type you are talking about was done by Bramblett.[1,2]

Comment: There were problems with that experiment and the results were not very conclusive.

Comment: Marvin, in view of the divided communities on multi-level vs. single level data, could I suggest that in the future when an evaluation is done giving multi-level parameters, could the evaluator also provide an equivalent set of single-level parameters?

Answer: This topic has come up in the past. The CSEWG philosophy states that the evaluator is free to use the formalism that he feels best describes the particular data set. If CSEWG recommends the data set, it becomes the officially distributed material. It is possible to create an equivalent data set containing single-level parameters and appropriate background cross section.

References

1. J. B. Czirr and R. L. Bramblett. Nucl. Sci. and Eng. 28, 62 (1967).

2. R. L. Bramblett and J. B. Czirr. Nucl. Sci. and Eng. 35, 350 (1969).

List of Attendees

Adler, F. T. - University of Illinois, Urbana, Illinois

Alter, H. - Atomics International, Canoga Park, California

Bhat, M. R. - Brookhaven National Laboratory, Upton, New York

Cowan, C. L. - General Electric Co. - BRDO, Sunnyvale, California

Cullen, D. E. - Brookhaven National Laboratory, now at Lawrence Livermore Laboratory, Livermore, California

Dannels, R. A. - Westinghouse Electric Corporation, Pittsburgh, Pennsylvania

de Saussure, G. - Oak Ridge National Laboratory, Oak Ridge, Tennessee

Drake, M. K. - Brookhaven National Laboratory, now at Science Applications Incorporated, La Jolla, California

Finch, D. R. - E. I. Dupont de Nemours and Co., Savannah River Laboratory, Aiken, South Carolina

Garber, D. I. - Brookhaven National Laboratory, Upton, New York

Goldberg, M. D. - Brookhaven National Laboratory, Upton, New York

Goldstein, R. - Cumbustion Engineering Inc., Winsor, Connecticut

Hardy, J. - Bettis Atomic Power Laboratory, West Mifflin, Pennsylvania

Harris, D. R. - Los Alamos Scientific Laboratory, Los Alamos, New Mexico

Hemmig, P. B. - U. S. Atomic Energy Commission, Washington, DC

Hockenbury, R. W. - Rensselaer Polytechnic Institute, Troy, New York

Hwang, R. N. - Argonne National Laboratory, Argonne, Illinois

Jenkins, J. D. - Oak Ridge National Laboratory, Oak Ridge, Tennessee

Krieger, T. J. - Brookhaven National Laboratory, Upton, New York

LaBauve, R. J. - Los Alamos Scientific Laboratory, Los Alamos, New Mexico

Levitt, L. B. - Atomics International, Canoga Park, California

Lubitz, C. R. - Knolls Atomic Power Laboratory, Schenectady, New York

Magurno, B. A. - Brookhaven National Laboratory, Upton, New York

Moore, M. S. - Los Alamos Scientific Laboratory, Los Alamos, New Mexico

Attendees

Mughabghab, S. F. - Brookhaven National Laboratory, Upton, New York

Ozer, O. - Brookhaven National Laboratory, Upton, New York

Neuhold, R. J. - U. S. Atomic Energy Commission, Washington, DC

Pearlstein, S. - Brookhaven National Laboratory, Upton, New York

Petrie, L. - Oak Ridge National Laboratory, Oak Ridge, Tennessee

Pitterle, T. A. - Westinghouse Electric Corp., Madison, Pennsylvania

Prince, A. - Brookhaven National Laboratory, Upton, New York

Rahn, F. J. - Columbia University, New York, New York

Semler, T. T. - NASA - Lewis Research Center, Cleveland, Ohio

Smith, J. R. - Aerojet Nuclear Co., Idaho Falls, Idaho

Stehn, J. R. - Brookhaven National Laboratory, Upton, New York

Takahashi, H. - Brookhaven National Laboratory, Upton, New York

Walker, W. - Atomic Energy of Canada Ltd., Chalk River, Ontario

Weisbin, C. R. - Los Alamos Scientific Laboratory, Los Alamos, New Mexico

Wietzberg, A. - General Electric Co. - APED, San Jose, California