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SCORE-III-A
AN INTERACTIVE DISPLAY SYSTEM
FOR EVALUATION OF MULTILEVEL
RESONANCE PARAMETERS
IN THE ADLER FORMAT

AEC Research and Development Report

Atomics International
North American Rockwell

P.O. Box 309
Canoga Park, California 91304

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P. F. ROSE

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ABSTRACT

A study of techniques for using interactive computer graphics as an aid to neutron cross-section evaluation has been underway for some time. The result of this study is a computing system called SCORE. This document describes an experimental version of SCORE, detailing its use and explaining its capabilities. This version of SCORE, called SCORE-III-A, has been developed to provide a semi-automated procedure to fit experimental data with multilevel resonance parameters in the Adler-Adler formalism.

I. INTRODUCTION

A study of methods for using interactive computer graphics as an aid to neutron cross-section evaluation has been underway for quite some time. The result of this study is a computing system, using IBM computer hardware, called SCORE.

The SCORE system consists of four computer programs — SCORE and three library-generation programs, SAP, SCOFF, and RAP. SAP is a program to convert SCISRS I data tapes to the packed format required by SCORE; SCOFF converts ENDF/B data tapes to the SCORE format; and RAP generates resonance parameter libraries. The SCORE program has been fully referenced⁽¹⁾ as to operation and use.

One of the more difficult and time-consuming problems of data evaluation is the analysis of resonance data. Experimental data consist of the desired cross-section enfolded with a Doppler and a resolution function. The task of the evaluator is to unfold these unwanted effects from experimental data containing experimental uncertainties.

Three models for the resonance region have been used for evaluation of data. These models are the Breit-Wigner single level, the Reich-Moore multi-level, and the Adler-Adler multilevel resonance theories. A data library in the direct access format is provided in SCORE for storage of resonance parameters for each of the three models. In addition, space is provided for several Doppler and resolution functions which may be selected by the evaluator.

A semi-automated fitting procedure for single level and Reich-Moore multi-level resonance parameters is included in SCORE-III. The methods were developed by O. D. Simpson and co-workers at the Idaho Nuclear Corporation.⁽²⁾ The semi-automated fitting of Adler-Adler resonance parameters has been implemented in an experimental version of SCORE (SCORE-III-A) which is presently described.

The adaption of program CODILLI⁽³⁾ to the SCORE program was initiated in the summer of 1970. In this first phase, a special reduced version of CODILLI⁽⁴⁾ (CODILLI-2) was incorporated into the SCORE package to permit linear least-squares fitting procedures, followed by interactive changes that

could accelerate the nonlinear fitting steps. The fruition of this effort represented a close collaboration between Doctors Felix and Donatella Adler of the University of Illinois at Urbana and personnel at Atomics International. The preparation and code checking of CODILLI-2, including the writing of subroutine PREAMB and EDIT, was done at Illinois under Contract AT(11-1)-2022-1. In January 1971 six synthetic data sets were prepared at Illinois and were used for code checkout at Atomics International. Final complete system checkout and computer graphics work was done in collaboration with Neldon H. Marshall at the Computer Science Center in Idaho Falls using their IBM 360/75 and an IBM-2250 (CRT) Display Device.

Production runs at the Computer Science Center to analyze resonance data of Pu²³⁹ have fully demonstrated the successful use of interactive graphics for the rapid and quantitative analysis of resonance data.

II. TREATMENT OF EXPERIMENTAL DATA

All problems in SCORE-III-A start with the retrieval of experimental data from a tape file. The retrieval scheme chosen uses both tape and disk storage. The experimental cross-section data for an isotope or a natural element are stored as a hexadecimal sequential data file on a magnetic tape. The tapes are prepared by program SAP, and are referred to as SAP tapes. A description of the SAP tape for SCORE is given in the SCORE reference document.

When the SAP program creates a new SAP hexadecimal tape the first file of that tape has a single 16-word record containing the tape identifier. The second record contains the isotope atomic number, the isotope mass number, the atomic weight, and the date of entry. The succeeding records are a transformation of corresponding information from a SCISRS-I data tape. Each entry is detailed in the SCISRS document.⁽⁵⁾

Several problems were encountered which resulted in modifications to the SAP input procedure.

1. Experimental data for analysis is generally no longer available in the SCISRS-I format. The new format called CSISRS-II⁽⁶⁾ is in such a form as to invalidate the use of SAP.
2. The SCISRS-I format does not allow for enough significant figures in the data values for accurate least-squares analysis.

For this reason, the SAP code was modified for this SCORE application. The modified SAP program reads a pseudo SCISRS-I format data tape (80 column card image) and produces a normal SAP tape as described in the SCORE document. Informal computer routines have been written to manipulate the basic data (such as CSISRS-II) and write a tape in the pseudo format. The particular format for these tapes is given in Table 1.

TABLE 1
PSEUDO SCISRS FORMAT

Symbol	Card Column	Data Format*	Explanation
ZN	1-2	F	Charge Z
AN	3-5	F	Mass A
STYPE	6-8	A	Cross Section Type, See SCISRS-I Document
EN	9-24	E	Energy, Mev, in Ascending Order
SIG	25-40	E	Cross Section, Barns
ERS	41-56	E	Cross Section Error, Percent
EERU	57	A	"L"
EERT	58	A	"E"
ERST	59	A	"P"
SOURCE	60	A	See SCISRS-I Document
REF(1)	61-63	A	See SCISRS-I Document
REF(2)	64-67	A	See SCISRS-I Document
XMARK	68	A	See SCISRS-I Document
REF(3)	69-72	A	See SCISRS-I Document
DATE	73-75	A	SCISRS-I (not used)
CØM	76	A	SCISRS-I (not used)

*F = fixed point data, E = floating point data, and A = text field.

III. THE RESONANCE PARAMETER LIBRARY

The resonance library is divided into three parts; one part for Breit-Wigner single level parameters, one for Reich-Moore multilevel parameters, and one for Adler-Adler multilevel parameters. The library also contains Doppler and resolution models for each of the three parameter types.

The experimental version of SCORE admits a background expression for each isotope and cross-section type of the form:

$$(A_1 + A_2/E + A_3/E^2 + A_4/E^3 + B_1E + B_2E^2)/\sqrt{E}.$$

The resonance library program RAP has been modified to read and process background constants. The standard input to RAP is described in Vol. 2 of the SCORE reference document. The modification for the new version introduces a change in the individual isotope data card Type 4.2. This card now contains an additional parameter IBK which is set either to 0 or 1 in Card Column 72. If set to 1, three additional cards must be supplied containing the background constants for total, fission, and capture cross-sections respectively. On each card the constants A_1 , A_2 , A_3 , A_4 , B_1 and B_2 are specified in order in a 6E 12.8 format. If IBK=0, all background constants are set to zero for all 3 reaction types, and no additional input cards are needed.

All associated SCORE service routines have been modified to operate with the presence of background terms. A subroutine BKGD has been written to display the isotopic background constants, and is always called prior to displaying resonance parameters through the operation of SCORE.

In order to prepare library parameters in the "Adler Format" two auxiliary computer routines were written to process data.

The first program produces parameters from single level parameters, and the second, MINIBWSIG, calculates multilevel parameters from R-matrix parameters by perturbation. The prescription for these routines were transmitted by D. B. Adler and F. T. Adler, and the theory is discussed in Appendix B of COO-1546-7.⁽⁷⁾

For the preliminary fits of the Pu^{239} resonances made at the Computer Science Center in Idaho Falls, a multilevel library was prepared for Pu^{240} and the tungsten isotopes from single level parameters, and for Pu^{239} from the multilevel parameters of H. Derrien, et al.,⁽⁸⁾ using MINIBWSIG.

IV. AUTOMATED DATA FITTING

It is standard in SCORE for all problems to start with the retrieval of the experimental data from a SAP tape. Case identification is entered in the first graphic display. When the identification information has been supplied a new display is generated which lists all the nuclides having experimental data that are available to the system. A selected nuclide is indicated by having large characters identifying its charge and mass number. Any other nuclide may be selected by a light pen detect. When the desired nuclide has been selected, the END key is depressed.

The next display lists all the reaction types recognized by SCORE for which experimental data exist for that nuclide. The desired reaction type is selected by light pen. Space to enter the energy range desired is provided. Figure 1 shows this display. Data retrieval stops when 500 data points have been found or when there are no more data points for energies less than the maximum specified. When all entries are made the END key is pressed.

Data retrieved based on a user request is displayed as shown in Figure 2. In Figure 2, the upper box contains the reference from the pseudo SCISRS format. The lower right box contains the option list available to the user as described in the SCORE manual. The expanded version of the basic display is shown in Figure 3. This display grid fills the entire 12 in. by 12 in. screen. The resonance region analysis module is initiated by selecting the RESFIT option from the menu list.

On initial entry to the resonance region module, the evaluator must supply model, resolution, Doppler, and target composition details. Subsequent entries do not permit changes in these data except when the evaluator decides to change data in one of the four categories and selects one of the individual options.

The evaluator must select one of three models for the resonance region cross section. The display for the choice of models appears automatically on the initial entry to the resonance region module.

Two different displays allow the evaluator to select the Doppler and resolution function he desires. He must interactively supply the necessary function parameters. Available Doppler and resolution function titles are obtained from

*
REACTION TYPES AVAILABLE FOR Z = 94 A = 339 ARE

NF

NG

TOT

MINIMUM ENERGY (MEV):

6.503 E-06

MAXIMUM ENERGY (MEV):

19.00 E-06

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Figure 1. Display of Selected Reaction Type and Energy Range Data

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Figure 2. Basic SCORE Data Display

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Figure 3. Expanded Data Display

a list in the contents of the RAP library for each of the resonance theory models. The currently selected function appears in large characters and the others in small characters. When a choice is made with the light pen, the selected function appears in large characters and a list of required parameters for that particular function appears in the lower half of the display. The parameters may be supplied in the usual manner from the alphanumeric keyboard. When the information has been completed, the END key is depressed to continue the evaluation.

For the Adler-Adler multilevel option, the Doppler functions available are:

1. NO DOPPLER
2. GAUSSIAN

Selection of NO DOPPLER causes the index IDOP to be set to unity and the target temperature to be set to 0° Kelvin. Selection of GAUSSIAN allows the evaluator to enter a temperature from the keyboard and the index IDOP is set to 2.

The resolution function choice built into SCORE at present transfers only limited information to CODILLI.

The following choices can be made for the Adler model:

1. NO RESOLUTION	IRES = 1
2. CONSTANT WIDTH	IRES = 2
3. GAUSSIAN	IRES = 3

The choice IRES = 1 sets the special resolution width variable RESPAR(1) to zero. For IRES = 2 or 3 further information is requested:

IRES = 2 requires

1. RESOLUTION WIDTH (EV)	RESPAR(1)
2. SAMPLE THICKNESS (ATOMS/BARN)	RESPAR(2)

The choice IRES = 3 is for Linac experiments. The required input is:

1. FLIGHT PATH (METERS)	RESPAR(1)
2. MODERATOR THICKNESS (CM)	RESPAR(2)

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SELECT DESIRED ISOTOPES

74	0	1.00000E 00	92	233	1.00000E 00
92	235	5.00000E-01	92	335	5.00000E-01
92	238	1.00000E 00	94	239	2.50000E-01
94	239	7.50000E-01	94	240	1.00000E 00

ATOM FRACTION: 1.00000E 00

POTENTIAL SCATTERING (BARNs): 10.0

ATOMIC WEIGHT (AMU): 239.0

DELETE

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Figure 4. Selected Resonance Isotopes and Required Parameters

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3. SAMPLE EFFECTIVE THICKNESS (CM)	RESPAR(3)
4. SAMPLE THICKNESS (ATOMS/BARN)	RESPAR(4)
5. BURST WIDTH (MICROSEC)	RESPAR(5)
6. CHANNEL WIDTH CONSTANT (MICROSEC)	RESPAR(6)

Pressing the END key enters the values of RESPAR into the calculation. A new display allows the keyboard entry of break point energies E_N for changes in the variable channel index N , as described in ORNL-TM-1804.⁽⁹⁾ At present there is no implementation for the choice IRES = 3. The necessary information is now specially programmed in the CODILLI subroutine WIDTH for the experimental data being analyzed.

When the option to specify the isotopic composition of the target is initiated, a list of nuclides appear for which resonance parameters for the selected reaction model are available. Nuclides already selected as part of the target composition appear in large characters.

The light pen is used to select a nuclide for the target composition used in the measurement of the data being analyzed. Data for the atom fractions, the potential scattering, and the atomic mass can be supplied or modified from the alphanumeric keyboard. When the required data have been supplied, the END key is depressed. The new nuclide is included in the composition and another nuclide can be selected. The display also contains the word DELETE. When DELETE is chosen by light pen, the selected nuclide is deleted from the target composition and control is returned to allow action on other available nuclides. Figure 4 shows this display.

Upon completion of the selection of available nuclides, the END key is depressed again. A display appears which can allow an additional nuclide, not in the resonance parameter library to be added through the choice of YES or NO.

The selection of YES causes a display to appear requesting an identification. Resonance parameters are then specified for the chosen MODEL. When the specification for a single resonance is complete the END key is depressed. The data are stored and the picture reappears so that parameters for additional resonances may be supplied.

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Figure 5. Flow Diagram of Subroutine ADLER

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When complete, the CANCEL key is depressed. The "Isotope addition" question reappears. Another new nuclide could now be added by answering YES. The selection of NO terminates the option.

The option RESMOD permits the modification of resonance parameters currently in the program. When selected, a list of resonance energies for a nuclide appears. The user then selects the resonance he wishes to modify with the light pen. A display appears with the parameters for that resonance listed. These parameters can be changed from the alphanumeric keyboard. When modifications are complete, the END key is depressed.

Options are provided to move resonance parameters for an entire nuclide from storage (disk) to the program and from the program to storage. The LOAD RES option will move selected nuclide resonance parameters from storage to the in-core parameter arrays. The STORERES option permanently updates the disk with the current in-core resonance parameters. This option would be exercised when the evaluator feels that he has made sufficient improvements in the parameters for one or more nuclides, and wishes to store these parameters for a future reference point.

A Doppler- and resolution-broadened line shape is calculated for selected resonances when CALC is selected by light pen, or from the function keyboard. This selection has not been implemented for the Adler-Adler model. The calculation uses the Doppler model, resolution model, and the target compositions previously described to calculate the line shape for the reaction type and grid limits for the data being displayed. The calculated curve is overlaid on the experimental data and the root mean square residual is displayed in the right center box.

The semi-automated fitting procedure for single level and Reich-Moore multilevel resonance parameters implemented in SCORE is described in Reference 1. The option for semi-automated fitting of Adler parameters using CODILLI-II in SCORE is made via a light pen selection of FIT in the resonance menu. If the Adler multilevel model was previously selected, the SCORE program enters the Adler subroutine which controls the entire multilevel fitting procedure. A simplified flow diagram of this routine is shown in Figure 5.

The subroutine SCODOP controls the input of the data weighting function and the resolution mode.

The type of statistical weight to be used in the least-squares fit is made by selecting one of the three possible values of an index JWE:

Unit Weighting of Data	JWE = 1
Experimental Error Weighting	JWE = 2
Inverse Cross-Section Weighting	JWE = 3

In CODILLI-II, a distinction is made between the treatment of the resolution function and the calculation of the pertinent resolution width as a function of energy. The mode by which the resolution function is folded into the theoretical cross-section curve is made by selecting one of the four values of the index JS:

Gaussian broadening combining Doppler and resolution effects with constant or zero resolution width	JS = 1
Convolution for a reaction cross section	JS = 2
Convolution for transmission data	JS = 3
Gaussian broadening combining Doppler and resolution effects with an energy dependent resolution width	JS = 4

The choices JS = 2 and JS = 3 require also the interactive selection of the (even) number of integration steps, NI, which by default is set equal to 32. Finally KNEG and KPOS defining the number of fitted background coefficients of negative or positive powers of E are chosen interactively.

Subroutine FITSEL is used for the classification of resonances. The resonance energies are displayed, and for each resonance the logical index ISEL must be defined interactively according to the following algorithm: For the Kth resonance, the following (light pen) choices are possible:

ARRAYCHOICE

	. TRUE. (YES)	. FALSE. (NO)
ISEL(1,K)	Include resonance in calculation	Do not include resonance in calculation
ISEL(2,K)	Resonance is to be fitted	Resonance treated as background
ISEL(3,K)	Multilevel parameter fit	Single level (symmetric) fit

An example of this display is shown in Figure 6.

The least squares constraint $\sum_K H_K = 0$ is also selected for each isotope via the parameter IFIT as follows:

Introduce fitting constraint	IFIT = 1 (YES)
Ignore this constraint	IFIT = 0 (NO)

A special case is also encountered in a refitting sequence. IFIT = -1 indicates that all resonances were treated as "background" in the previous iteration. IFIT is then set to zero so that the SCORE display indicates NO. IFIT could again be reset to -1 at a later point in the calculation.

The subroutine PREAMB sets up the SCORE/CODILLI interface. The information transmitted is partly experimental data points, indices, and parameters directly usable in CODILLI-II. However, there is a part (specifically the resonance parameter array A and the ISEL array) which is in a form which requires pre-processing before the information can be utilized.

The array A may contain 250 resonances of which only a fraction (resonances NOR and NEIGH in CODILLI) will be fitted; others (resonances NOUT in CODILLI) may serve as background while still others will be omitted altogether, as predetermined through the array ISEL.

In formulating the least-squares equation in CODILLI, the resonances are regrouped in arrays recognizable within the structure of CODILLI. To this end, PREAMB processes the information provided by SCORE.

Z = 94

A = 239

G = 7.50000E-01

ENERGY	CALCULATE	FIT	MULTILEVEL
7.80103E 00	YES	NO	YES
1.09120E 01	YES	NO	YES
1.18777E 01	YES	NO	YES
1.43086E 01	YES	NO	YES
1.46583E 01	YES	NO	YES
1.76329E 01	YES	YES	YES
2.22342E 01	YES	YES	YES
2.38758E 01	YES	NO	YES
2.62228E 01	YES	NO	YES
2.72329E 01	YES	NO	YES
3.54220E 01	NO	NO	NO
4.13731E 01	NO	NO	NO
4.16230E 01	NO	NO	NO
4.44350E 01	NO	NO	NO
5.00330E 01	NO	NO	NO
5.25331E 01	NO	NO	NO
5.55822E 01	NO	NO	NO
5.91536E 01	NO	NO	NO

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Figure 6. Display of Resonance Classification

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SCORE stores the resonance parameters in the array A dimensioned (250,8) in the following sequence:

A(250,1): resonance energies

A(250,2): resonance widths

A(250, 2*ITP + 1): symmetrical line shape parameters

A(250, 2*ITP + 2): asymmetrical line shape parameters.

where ITP, the cross-section type index, is as follows:

Total Cross Section	ITP = 1
Fission Cross Section	ITP = 2
Capture Cross Section	ITP = 3

The ISEL array is utilized in rearranging the selected parameters in an order required internally by CODILLI-II for setting up the normal equations. The coefficient matrix for the normal equations is in double precision, and the computer memory allocation is large. Temporary disk storage is provided through the SCORE program.

For ISEL (1,K) = .TRUE., the Kth resonance is included in the calculation. The parameters for resonances to be fitted, ISEL (2,K) = .TRUE., are stored in the array MU(J,I) and NU(J,I) for each isotope I. The index J runs from 1 to NNR, where NNR is the number of resonances to be fitted for isotope I. An array NOR(I) and NEIGH(I) contain the number of resonances for the fitting procedure within the selected energy interval, and neighboring the energy interval, respectively. NNR is determined from the sum of NOR(I) and NEIGH(I). The array NOUT(I) contains the number of resonances for which ISEL (2,K) = .FALSE. The parameters for these resonances are stored in the DMU(J,I) and DNU(J,I) arrays. These parameters are used to evaluate a cross-section contribution which is subtracted from the experimental data. It is possible to include only known contributions of a given nuclide, as for example for one spin state, by choosing interactively every value of ISEL (2,K) = .FALSE. for

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Z = 94	A = 239	G = 7.50000E-01
POLE ENERGY	CURRENT	RESIDUAL PREVIOUS
7.84816E 00	• 5.97783E 01	8.09856E 03
1.09745E 01	• 3.40491E 02	8.24918E 03
1.19350E 01	• 5.43554E 01	1.23276E 04
1.43700E 01	• 6.24807E 01	2.26548E 03
1.47245E 01	• 1.32749E 02	1.39795E 04
1.77140E 01	• 2.00620E 02	9.27237E 03

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Figure 7. Display of Current and Previous Goodness of Fit

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the Ith isotope in consideration. This case is transmitted to CODILLI through PREAMB by the index IFIT(I)=-1. IFIT(I) is automatically set to -1 if NOR(I) + NEIGH(I)=0. Finally, the selection of ISEL (3,K) (between multilevel or single level parameters to be fitted) is translated to CODILLI-II by giving to the index MS(K,I) the value 1 or 0 corresponding to ISEL = .TRUE. or .FALSE.

After completion of these tasks, CODILLI-II performs the least squares fit. When the calculations are completed, the results are rearranged by the routine EDIT, which returns the resonance parameters and pole energies back into the main body of SCORE. The values of the theoretical (calculated) cross section, evaluated at the energies corresponding to the experimental points, are also returned from CODILLI-II to SCORE.

It is at this stage that the interactive use of SCORE becomes crucial in the data evaluation. The subroutine EXMFIT performs this role, and was specially written for SCORE-III-A. EXMFIT displays the various fits about selected resonances as well as the goodness of fit, and allows interactive adjustments to the pole and half width energy for the succeeding fitting cycle.

The existing subroutine TEST in CODILLI was adapted by F. T. Adler and D. B. Adler to supply, at the completion of each linear fit, a value of the partial χ^2 around each resonance k , and transmit the value to the subroutine EXMFIT. The "residual" is calculated after each linear fit as $\chi_k^2 = \sum_i W_i (Y_{\text{exp}}^i - Y_{\text{app}}^i)^2 / N_k$ for the number N_k of data points i in the interval $\mu_k - 5\nu_k$, $\mu_k + 5\nu_k$. Here Y_{exp} is a scaled experimental data point and Y_{app} is the corresponding value of the trial function or apparent cross section.

Subroutine EXMFIT displays both the current value of χ_k^2 as well as its previous value from the preceding iteration. Figure 7 shows such a display from a SCORE run. Observing Figure 7, we note that this display provides a quantitative guide in evaluating the degree of improvement (or worsening!) for each individual fitted resonance.

In subroutine TEST, a check of the positiveness of the theoretical (unbroadened) cross section is also given, displaying an error flag in the printed SCORE output when values occur which are less or equal to zero. The failure to reproduce positive cross-section values can occur from input errors, poor selection of the values of μ and ν , or from wrong assignments to the constraint indices.

Z = 94 A = 239 G = 2.50000E-01

POLE ENERGY 1.55200E 01

HALF WIDTH 3.30000E-01

FISSION G 6.53936E-04

FISSION H 3.11812E-06

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Figure 8. Basic Display of Fit Showing Pole and Half Width Energies

For any resonance chosen by light pen from the table displayed in Figure 7, a new display is generated showing the calculated cross-section curve (straight lines connecting the calculated point at each experimental energy point) and the experimental data points, together with vertical lines indicating the pole energy μ and the half width ν of the resonance. This display is shown in Figure 8. The display is logarithmic in cross-section and linear in energy. The range of the data is $\mu_k - 10\nu_k, \mu_k + 10\nu_k$.

If, as shown in Figure 9, the fit is poor, the values of μ and ν can be rapidly adjusted for the next iteration using the light pen. This is easily accomplished by touching "R" or "L" on the pole energy line or the half width line. The half width line moves simultaneously with the pole energy line when the pole energy is selected. Motion of the line is stopped when a light pen detect is made of the moving line itself. The moving lines will reverse direction if they travel too far either in the positive or negative energy direction. The values of μ and ν scaled from the position on which the line stops (updated value) are entered into the calculation by pushing the END key.

New values of μ and ν may also be entered directly into the display from the alphanumeric keyboard. This is done by pushing the END key which displays the cursor. The new values are typed in and the END key is again depressed to enter in the values. Figure 8 shows a stage in the fit which would require only minor improvements, and which could be effected by typing in slight changes in μ and ν . Depressing the CANCEL key advances the display sequence to the next isotope. After the last isotope is selected a final display appears which offers three choices:

FIT PARAMETERS AGAIN	IRET = 1
RESET FITTING REQUIREMENTS	IRET = 2
FITTING COMPLETE	IRET = 3

As shown in the flow diagram of Figure 5, the choice IRET = 1 transfers control to subroutine PREAMB for another linear fit. For IRET = 2, new fitting constraints may be introduced through subroutine SCODOP. After satisfactorily fitting the data, a final display is initiated (IRET = 3) through the subroutine ADLISP which generates the apparent line shape using energy points

Z = 94 A = 239 G = 7.50000E-01

FISSION

FISSION

POLE ENERGY

7.84816E 00

HALF WIDTH

4.50000E-02

FISSION G

4.14790E-03

FISSION H

-1.94664E-04

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6524-4640

Figure 9. Basic Display of a Poor Fit

previously determined in subroutine RSETUP. Figure 10 shows the final display in the resonance module. This display corresponds to the choice CALC in other models. The menu to the right offers various choices for the evaluator to continue his study. The options are selected by light pen detect. Figure 11 shows the same display with a continuation of the menu (RES 2/3) to the right of the display. This figure is significant as it shows one of the display problems associated with an IBM 2250 SCOPE with a small (4K) buffer. Note the scissoring of the scope display involved in displaying the ordinate and abscissa. This is caused by a need for more than 4K bytes of buffer to create the full display. The subroutine FILL transfers the contents of the computer in-core buffer to the 2250 buffer. If the transmitted string of orders exceeds the available space in the 2250, the string is truncated and a flag is set to indicate a full 2250 buffer. Graphic orders can be lost and parts of the display, as observed, are scissored from the CRT screen.

Figure 12 shows the "expanded" version of the resonance fit display. A return to the resonance menu is made by pressing the END key, and a return to the main program is made by light pen detect of MAIN OPT in the menu. At this point, a new calculation may be started or the run terminated.

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Figure 10. Final Display of the Calculated Line Shape
and Experimental Data Over the Selected
Energy Range

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Figure 11. Final Display Showing a Continuation of the Menu for the Resonance Module

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2250 HARDCOPY

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Figure 12. Expanded Display of Calculated Line Shape

AI-AEC-13018

V. CONCLUSIONS

The incorporation of CODILLI-2 in SCORE has permitted the rapid evaluation of resonance parameters in the "Adler" format for the fitting of experimental data. The interactive mode allows for rapid changes of resonance energies and line widths which has proved to be surprisingly effective compared to the nonlinear fitting procedures in the batch mode version of CODILLI.

The possibility of selecting various combinations of resonances over different energy ranges, and performing fits of capture, fission, and total cross section by visual inspection and interaction on a CRT screen has provided a most valuable insight into the quality and sensitivity of the resultant parameters to the choices made.

The reduction in both calendar time and personnel effort to perform these analyses has proven to be dramatic. Several months of tedious effort can be contracted to a few fitting sessions. Much planning and preparation is, of course, required before and after a fitting session using SCORE-III-A. Initially the experimental data must be selected and the SCORE input tapes generated in the required format. The preliminary resonance library must be prepared for the isotopes of interest, and the necessary energy resolution functions programmed into CODILLI. Following the fitting session, the large amounts of printed output from CODILLI and the hardcopy record of the CRT displays must all be recorded and analyzed.

APPENDIX

SCORE-III-A, operational at the Computer Science Center in Idaho Falls, is also the first version of SCORE to provide hard copy of the 2250 Scope displays.

The introduction of this feature was made possible by the use of a subroutine SNAPG which interfaces the 2250 buffer and an FR-80 Microfilm unit. This subroutine was distributed in a software package for the microfilm unit. A modification was made to SNAPG which bypasses a termination effected by an End Order Sequence instruction.

In order to efficiently use SNAPG, the Fortran Interactive Graphics Package⁽¹⁰⁾ used for SCORE had to be modified.

The subroutine INPICT initializes the parameters for a new graphic display. Normally the status for function keys are preset, such that the first two are active and the remaining 30 inactive. INPICT was modified to activate the 32nd function key for use in handling a request for hard copy.

The subroutine EXINGR controls the dynamic interaction between the computer program and the user at the 2250 console. When input is required from the graphics terminal, this subroutine is executed. The return gives information to the calling program about the nature of the interaction. EXINGR has been modified to call the subroutine SNAPG when it senses that an interrupt was caused by activation of the 32nd function key.

All the figures in this document (except Figure 5) were produced from 8 by 10 photographs enlarged from a 35-mm SNAPG film record of the first working session using SCORE-III-A. The hard copy feature has proved invaluable in keeping a permanent record of the evaluation process when using interactive graphics.

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