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

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ABSTRACT

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

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

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

I. INTRODUCTION

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

- (I) To be utilized as a subprogram of Program SCORE.⁽²⁾
- (II) To be used independently, as a least-squares fitting program, similarly to the original version.⁽¹⁾

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

(a) SCORE provides the possibility of interactively changing input parameters and of rapidly displaying the calculated cross section curve for comparison with the fitted data. This feature of SCORE becomes particularly attractive in relation to a least squares analysis, as the parameters occurring non-linearly in the trial function can be modified interactively, rather than evaluated through cumbersome iterative calculations. This potential of SCORE is of special relevance for the use of Program CODILLI, where the multilevel trial function contains as nonlinear parameters only the values of the poles of the collision matrix (resonance energy μ and half width ν), in contrast with other approaches based on the R-matrix formalism.^{(3) (4)} The least squares branch of CODILLI therefore has been compacted to the linear fitting (providing the line shape parameters), with the assumption that the "conversational mode" between evaluator and SCORE will supply a rapidly convergent definition of

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

(*)

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

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

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

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

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

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

II. TRIAL FUNCTION:

Multilevel Expansion with Doppler Broadening

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

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

where:

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

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

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

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

$NISO$ represents the number of isotopes present,

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

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

This condition is controlled only by input.

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

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

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

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

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

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

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

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

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

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

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

$$\phi_k = [v_k^2 \cos w - v_k (\mu_k - E) \sin w] / [(\mu_k - E)^2 + v_k^2] \quad (7)$$

$$\phi_{NR+k} = [v_k (\mu_k - E) \cos w + v_k^2 \sin w] / [(\mu_k - E)^2 + v_k^2]$$

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

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

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

where

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

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

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

$X, A, B,$

and the broadening effects on the backgrounds are considered negligible.

III. THE TRIAL FUNCTION WITH RESOLUTION EFFECTS

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

(1) Reaction Cross Sections

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

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

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

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

where the known term is:

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

and the trial function accordingly is given by:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

2. Total Cross Section

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

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

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

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

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

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

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

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

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

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

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

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

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

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

where

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

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

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

Defining:

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

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

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

the trial function acquires the form

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

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

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

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

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

and:

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

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

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

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

IV. TRIAL FUNCTION WITH CONSTRAINTS

This version of CODILLI provides for options (through the index IFIT (1)) which introduce two different types of constraints for the asymmetrical parameters. Each case has the consequence of reducing the number of the free parameters in the fitting.

(1) Constraints obtainable from unitarity

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

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

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

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

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

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

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

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

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

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

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

2. Constraints introduced by assuming symmetrical lines

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

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

$$MS(K, I)$$

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

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

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

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

where (x) represents capture or scattering.

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

$$G1_k^{(\gamma)} = 0 \quad (35)$$

represents only an approximation. (4) (17)

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

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

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

The normal equations are:⁽¹⁾

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

where

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

VII. INTERFACE WITH SCORE: ROUTINES PREAMB AND EDIT

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

The input information can be classified in two types:

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

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

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

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

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

IDOP = 2 experimental sample temperature
DOPPAR(2) ≠ 0 in °K

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

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

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

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

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

(6) selection of the weighting option:

JWE = 1 equal weight

JWE = 2 weight calculated from experimental statistical errors

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

where JWE is the index controlling the subroutine WEIGHT.

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

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

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

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

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

A(250,1) resonance energies μ

A(250,2) resonance half widths ν

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

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

where

ITP = 1 represents total cross section

ITP = 2 represents fission cross section

ITP = 3 represents capture cross section

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

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

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

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

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

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

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

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

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

CODILLI is finally called as a subroutine from PREAMB.

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

VIII. COMMENTS

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

The specifications of the current version are outlined below:

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

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

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

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

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

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

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