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NUMERICAL ANALYSIS OF NEUTRON RESONANCES

Susie E. Atta  
John A. Harvey

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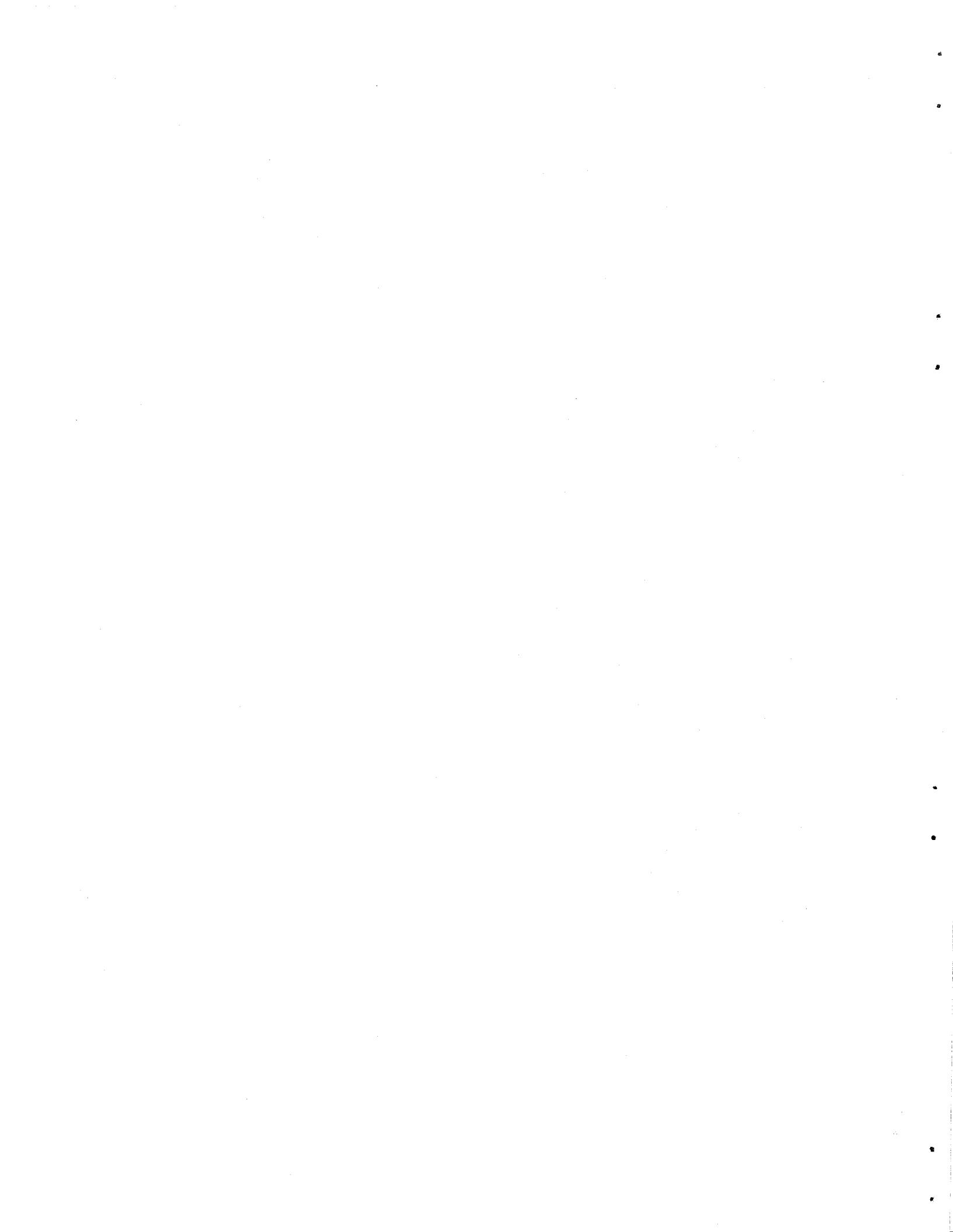


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# NUMERICAL ANALYSIS OF NEUTRON RESONANCES

Susie E. Atta      John A. Harvey

## ABSTRACT

Neutron resonances are analyzed numerically by determining the resonant energies, the total widths, and the neutron widths of the resonances. It is assumed that the total cross section can be represented by the sum of single-level Breit-Wigner formulas, with interference between resonance and potential scattering but no interference between resonances; that the Doppler broadening is represented by a Gaussian function; and that the instrument resolution is represented by a Gaussian function. Gauss' method is used to reduce the nonlinear problem to one in which linear methods can be applied. Some unusual techniques are used for evaluating the integrals in the function for calculating the transmission.

Two programs for analyzing transmission data to obtain the parameters of the resonances have been written for the IBM 7090 computer. The first program is a shape analysis for determining the resonant energies, the total widths, and the neutron widths of the resonances. This program analyzes the transmission data for as many as six resonances at once. The second program is an area analysis for determining the neutron widths of the resonances for assumed total widths. This program analyzes transmission data containing as many as 20 resonances at once.

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## INTRODUCTION

In recent years the resolutions of time-of-flight neutron spectrometers in the intermediate neutron energy region have improved by more than an order of magnitude. Transmission measurements are now being made where  $\sim 100$  resonances are observed in a single nuclide. An example of a transmission measurement is shown in Fig. 1. As a general rule the existing techniques for the analysis of neutron resonances are very time consuming, and sometimes not very accurate when the resonances are not well resolved from one another.

The total cross section,  $\sigma$ , as a function of neutron energy,  $E$ , can be computed from the transmission by the relationship

$$T(E) = e^{-N\sigma(E)}$$

where  $N$  is the thickness of the sample. However, there are two factors which greatly complicate the relationship between the observed transmission and the nuclear cross section when resonances are present. Distortions in the experimentally observed shape of a resonance arise because of imperfect instrument resolution and the Doppler broadening resulting from the thermal motion of the nuclei in the sample material. Figures 2 and 3 demonstrate these effects.

The distortions to the transmission curve become more serious for resonances at higher energies and for those having smaller total widths. In the high-energy region the shape of the dip in the transmission curve is determined almost completely by the resolution function and the sample thickness. Hence different methods of analysis are required for the high- and low-energy regions.

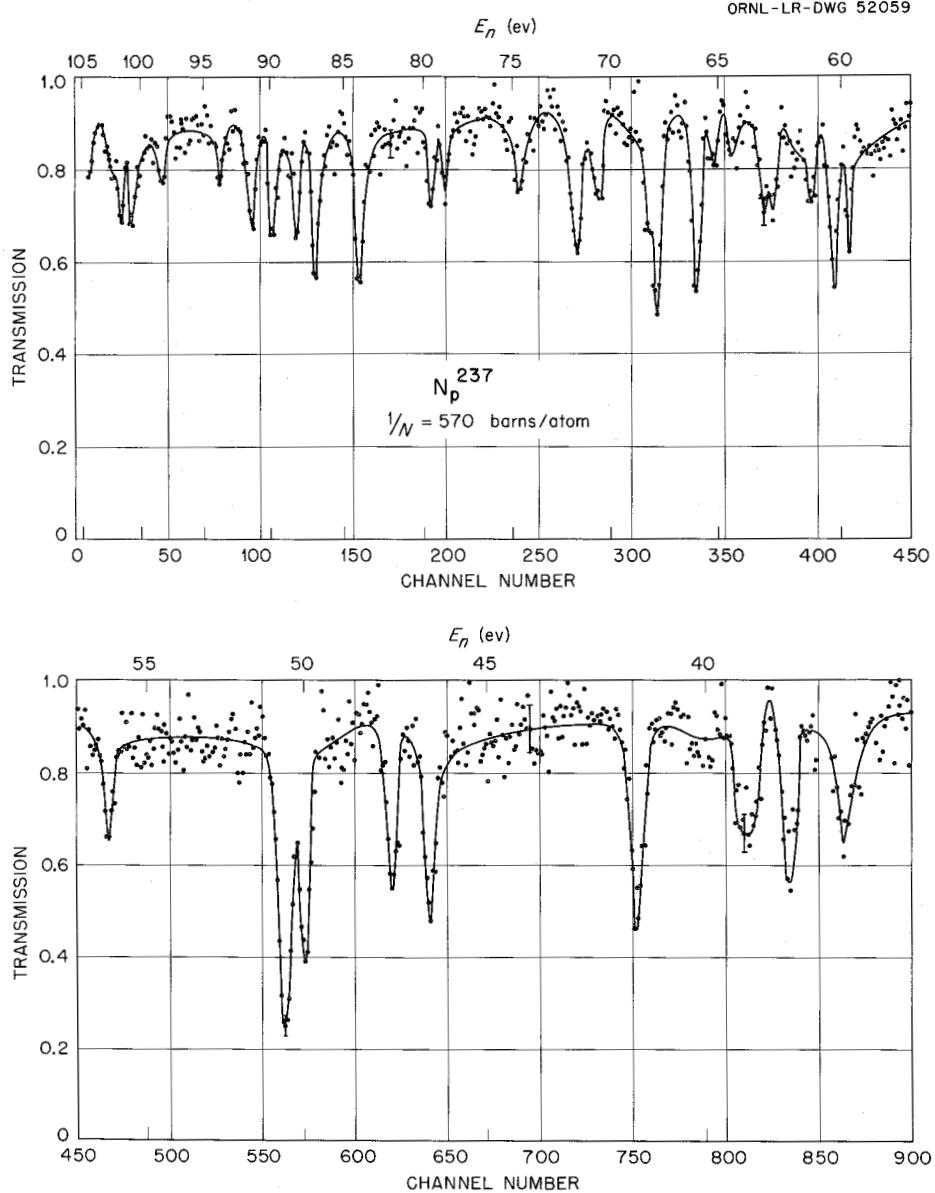


Fig. 1. Graph of a Transmission Measurement.

The problem was to find an adequate and practical method of analysis of the nonlinear function for the transmissions to determine the resonant energies, the total widths, and the neutron widths of the resonances.

Two programs for analyzing transmission data have been written for an IBM 7090<sup>1</sup> computer. These programs include the effects of Doppler broadening and instrument resolution on the transmission measurements.

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<sup>1</sup>Initially, the programs were written for the IBM 704 computer.

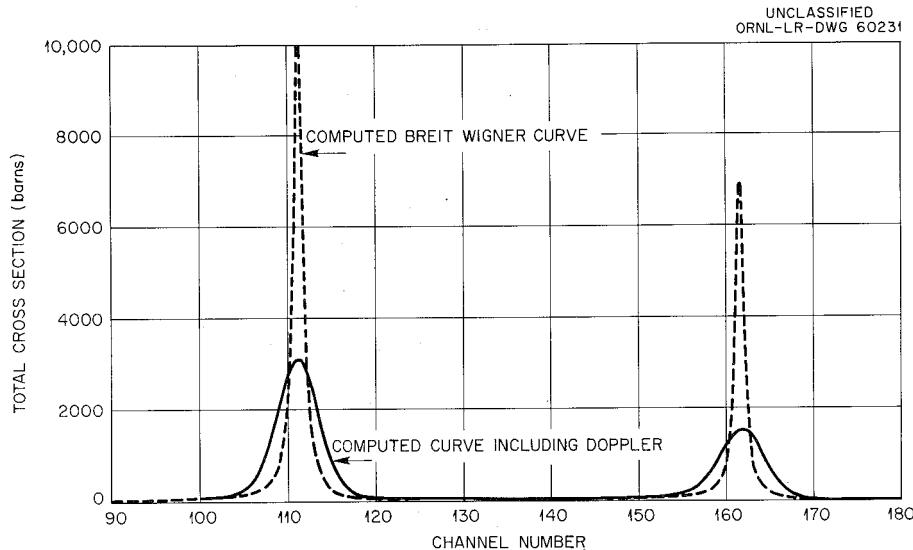


Fig. 2. Effect of Doppler Broadening on the Theoretical Cross Section of the Resonances at 23.5 and 21.9 ev in Th.

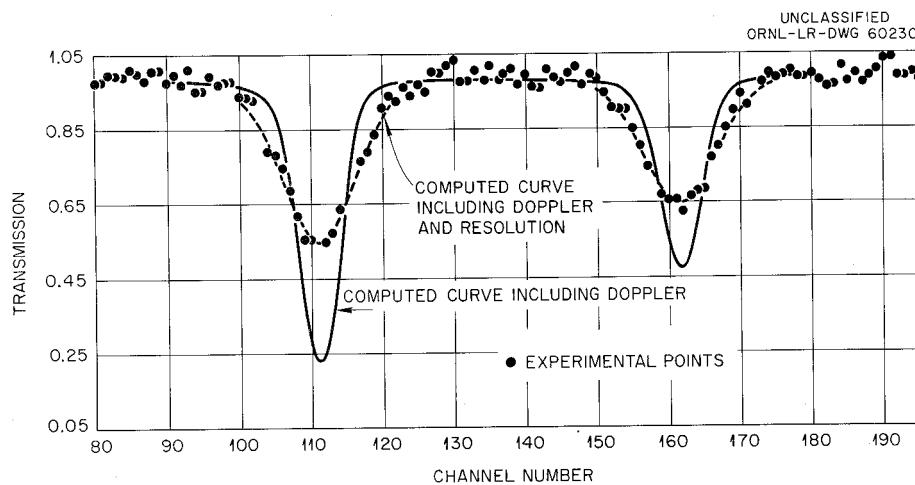


Fig. 3. Effect of Instrument Resolution on the Computed Transmissions for the 23.5- and 21.9-ev Resonances in Th.

## METHODS OF ANALYSIS

### FORMULAS

The single-level Breit-Wigner resonance formula [1] is used to describe the total cross section. The single-level formula for a single isotope,  $j$ , may be written

$$(1) \quad \sigma_j = \frac{\sigma_0(\cos 2\alpha + x \sin 2\alpha)}{1 + x^2} + 4\pi\chi^2 \sin^2 \alpha,$$

where

$$\sigma_0 = 4\pi\chi^2 g \frac{\Gamma_n}{\Gamma},$$

$$x = \frac{(E'' - E_0)}{\Gamma/2},$$

and

$$\alpha = a_j/\chi.$$

For low energies ( $E'' < 1$  kev)  $a_j/\chi \ll 1$ . Hence, one can write

$$(2) \quad \sigma_j = 4\pi a_j^2 + 4\pi\chi^2 g \frac{\Gamma_n}{\Gamma} \left[ \frac{1 - \left( \frac{E_0 - E''}{\Gamma/2} \right) \frac{2a_j}{\chi}}{1 + \left( \frac{E_0 - E''}{\Gamma/2} \right)^2} \right].$$

If  $E''$  is measured in electron volts, and  $4\pi\chi^2$  in barns,

$$4\pi\chi^2 = \frac{2.608 \times 10^6}{E''}$$

and

$$\Gamma_n = \Gamma_n^0 \sqrt{E''}.$$

Hence, it follows that

$$(3) \quad \sigma_j = 4\pi a_j^2 + \frac{6.52 \times 10^5}{\sqrt{E''}} \left[ \frac{\Gamma g \Gamma_n^0}{(\Gamma/2)^2 + (E_0 - E'')^2} \right] - 5.725 \times 10^3 \left[ \frac{(E_0 - E'') g \Gamma_n^0 a_j}{(\Gamma/2)^2 + (E_0 - E'')^2} \right].$$

Since a transmission measurement may be made upon elements which contain several isotopes, the cross section of the element is computed from the sum of the cross sections of the individual isotopes weighted by their fractional abundance  $f_j$ , where  $\sum_j f_j = 1$ . Since many resonances can be observed in a single isotope, let  $\lambda$  represent the resonances of the isotopes. Let

$E^\lambda$  represent the resonant energy of resonance  $\lambda$ ,

$\Gamma^\lambda$  represent the total width of resonance  $\lambda$ ,

$\Gamma_n^{0\lambda}$  represent the reduced neutron width of resonance  $\lambda$ ,

$f^\lambda$  represent the fractional abundance of the isotope which contains resonance  $\lambda$ ,

$g^\lambda$  represent the statistical weight factor of resonance  $\lambda$ ,

$r$  represent the effective nuclear radius (for all isotopes),

$a$  represent the potential scattering amplitude (for all isotopes where resonances are present).

Thus the total cross section is computed from the sum of single-level formulas,

$$(4) \quad \sigma(E'') = 4\pi r^2 + \frac{6.52 \times 10^5}{\sqrt{E''}} \sum_{\lambda} \frac{\Gamma^{\lambda} (fg\Gamma_n^0)^{\lambda}}{(E^{\lambda} - E'')^2 + (\Gamma^{\lambda}/2)^2} - 5.725 \times 10^3 \sum_{\lambda} \frac{(E^{\lambda} - E'') (fg\Gamma_n^0)^{\lambda} a}{(E^{\lambda} - E'')^2 + (\Gamma^{\lambda}/2)^2}.$$

The object of the analysis is to obtain the parameters  $E^{\lambda}$ ,  $\Gamma^{\lambda}$ , and  $(fg\Gamma_n^0)^{\lambda}$  which best satisfy the experimental points. Equation (4) includes interference between resonance and potential scattering, but does not include interference between resonances.

Assuming that the Doppler broadening follows a Gaussian function, one may compute the Doppler-broadened cross section,  $\sigma_{\Delta}(E')$ , by convoluting the nuclear cross section,  $\sigma(E'')$ , and a Gaussian function. Thus

$$(5) \quad \sigma_{\Delta}(E') = \frac{1}{\Delta\sqrt{\pi}} \int_0^{\infty} \sigma(E'') \exp \left[ -\left( \frac{E' - E''}{\Delta} \right)^2 \right] dE''.$$

Denote the effective temperature of the sample by  $T_{\text{eff}}$ , the neutron energy measured in electron volts by  $E'$ , and the atomic weight by  $AW$ . Then the Doppler width,  $\Delta$ , in electron volts is given by

$$\Delta = 2 \left( \frac{kT_{\text{eff}}^0 E'}{AW} \right)^{1/2} = D_0 \left( \frac{E'}{AW} \right)^{1/2},$$

where

$$D_0 = 0.318(T_{\text{eff}}^0/293)^{1/2}.$$

Assuming that the instrument resolution can also be represented by a Gaussian function, one may compute the theoretical transmission by another convolution. That is,

$$(6) \quad T(E_i) = \frac{1}{R(E_i)\sqrt{\pi}} \int_0^{\infty} \exp[-N\sigma_{\Delta}(E')] \exp \left\{ -\left[ \frac{E_i - E'}{R(E_i)} \right]^2 \right\} dE',$$

where  $R(E_i)$  is the resolution width at energy  $E_i$ . The resolution function is made up of many factors; some of these (such as the burst width, the collection time in the detectors, and the channel width) are independent of neutron energy, and others (such as the detector depth) vary as the time-of-flight of the neutron. It is assumed that the resolution in  $\mu\text{sec}/\text{meter}$  at channel  $i$  can be represented by the form

$$R_0 + R_1 i,$$

where  $R_0$  is the resolution (full width at half maximum in channels) at the zeroth channel of the run and  $R_1$  is the change in resolution (full width at half maximum in channels) per channel.

Expressing the resolution (half width in ev at  $1/e$  of peak) as a function of energy gives

$$(7) \quad R(E_i) = \frac{2}{1.665} \left[ \frac{R_0 t - R_1 (\text{delay})}{72.3 (\text{distance})} E_i^{3/2} + R_1 E_i \right] = B_0 E_i^{3/2} + B_1 E_i,$$

where

$$B_0 = \frac{1}{0.8325} \left[ \frac{R_0 t - R_1 (\text{delay})}{72.3 (\text{distance})} \right],$$

$$B_1 = R_1 / 0.8325.$$

The energy  $E_i$ , for channel  $i$ , is computed from the formula

$$(8) \quad E_i = \left[ \frac{72.3 (\text{distance})}{\text{delay} + it} \right]^2,$$

where

distance = flight path in meters,

delay = delay in  $\mu\text{sec}$ ,

$t$  = channel width in  $\mu\text{sec}$ .

In some cases the experimental data which we wish to analyze are not true transmission points, but the data have a shape which varies with energy exclusive of the resonances in the energy region which is measured. For example, there may be a large resonance outside the energy region under consideration whose effect is important in the energy range under consideration, or the data may represent the number of counts with the sample in the neutron beam whose spectrum is a function of neutron energy. It is assumed that this effect can be represented by the polynomial

$$(9) \quad P(E_i) = K_0 + \frac{K_1}{\sqrt{E_i}} + \frac{K_2}{E_i}.$$

Thus Eq. (6) becomes

$$(10) \quad T(E_i) = P(E_i) \frac{1}{R(E_i)\sqrt{\pi}} \int_0^\infty \exp[-N\sigma_\Delta(E')] \exp\left\{-\left[\frac{E_i - E'}{R(E_i)}\right]^2\right\} dE'.$$

## TECHNIQUES

The difficulty connected with any method of approach to the problem was the unreasonably large amount of computer time needed to evaluate so many double integrals. However, by using the following techniques and tricks for economy of time this difficulty is reduced to a reasonable amount of computer time.

The convolution of the Breit-Wigner total cross section with Doppler broadening,

$$(11) \quad \sigma_\Delta(E') = \frac{1}{\Delta\sqrt{\pi}} \int_0^\infty \left[ \frac{6.52 \times 10^5}{4\pi r^2 + \sqrt{E''}} \sum_\lambda \frac{\Gamma^\lambda (fg\Gamma_n^0)^\lambda}{(E^\lambda - E'')^2 + (\Gamma^\lambda/2)^2} \right. \\ \left. - 5.725 \times 10^3 \sum_\lambda \frac{(E^\lambda - E'')(fg\Gamma_n^0)^\lambda a}{(E^\lambda - E'')^2 + (\Gamma^\lambda/2)^2} \right] \exp\left[-\left(\frac{E' - E''}{\Delta}\right)^2\right] dE'',$$

is represented in terms of the real and imaginary parts of the complex probability integral [2],

$$(12) \quad \omega(z) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{ye^{-s^2}}{(x-s)^2 + y^2} ds + \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{(x-s)e^{-s^2}}{(x-s)^2 + y^2} ds.$$

A method [3]<sup>2</sup> is available for evaluating the complex probability integral very accurately with a small amount of computer time as compared with the Gaussian method for evaluating the integral in Eq. (11).

The derivative of the complex probability integral is also used in the evaluation of the partial derivatives of the nonlinear function, Eq. (10), with respect to the parameters  $E^{\lambda}$ ,  $\Gamma^{\lambda}$ , and  $(f_g \Gamma_n^0)^{\lambda}$ .

Since the integral in Eq. (11) does not contain values of  $E_i$ , the values of the Doppler-broadened integral are computed only once and stored in a table for later use in the computational procedure.

The trapezoidal rule is used for evaluating the convolution of the Doppler-broadened transmission with the resolution function, Eq. (6). This method was selected because the partitioning of equal intervals permitted the use of a recurrence formula for evaluating the exponential function

$$\exp \left\{ - \left[ \frac{E_i - E'}{R(E_i)} \right]^2 \right\}.$$

If  $b$  is the lower limit of the integral,  $b$  is the width of the intervals, and  $j$  is the partition number ( $j = 0, 1, \dots, n$ ), then

$$(13) \quad \exp \left\{ - \left[ \frac{E_i - (b + jb)}{R(E_i)} \right]^2 \right\} = \exp \left\{ - \left[ \frac{E_i - b}{R(E_i)} \right]^2 \right\} \exp \left\{ \frac{2(E_i - b)jb}{R^2(E_i)} - \left[ \frac{jb}{R(E_i)} \right]^2 \right\}.$$

Thus, the exponential function is evaluated each time from the previous value by making only two multiplications.

To use the recurrence formula for the exponential function, it is necessary that the value for the exponential at the lower limit not equal zero. Thus it is important that the computed finite limits of this integral not include portions of the resolution function which make insignificant contributions to the value of the integral. To avoid this, as well as to reduce the number of intervals needed to evaluate the integral, new finite limits for this integral are computed at each  $E_i$ . A spread of four times the resolution width  $R(E_i)$  on each side of  $E_i$  gives finite limits sufficient to obtain 99.99% of the value of the integral. However, changing the limits of the integral at each  $E_i$  requires intricate planning in order to pick values of  $E'$  which will be the same in the Doppler-broadened integral and the instrument-resolution function.

The number of partitions used to evaluate this integral is approximately equal to the number of channels included between the limits for the integral. However, this number may be multiplied by a designated integral factor in order to increase the accuracy of the evaluation of the integral.

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<sup>2</sup>The Gautschi and Beam subroutine for computing the complex probability integral is an IBM 704 SAP subprogram named WOFZ. For use in these programs it was compiled as a FORTRAN subprogram and named PFCN.

## SHAPE ANALYSIS

In the low-energy regions where the Doppler width,  $\Delta$ , and the resolution width,  $R$ , are small compared to the natural width,  $\Gamma$ , of the resonance, the parameters  $E$ ,  $\Gamma$ , and  $(fg\Gamma_n^0)^\lambda$  can be determined for each resonance. The method of least squares [4, 5] is used to determine the best estimates of these parameters. The nonlinear function, Eq. (10), is linearized by expanding it into a truncated Taylor's series at the initial estimates of the parameters and retaining only first-order terms. Thus

$$(14) \quad T[E_i; \Gamma^\lambda + \delta\Gamma^\lambda, E^\lambda + \delta E^\lambda, (fg\Gamma_n^0)^\lambda + \delta(fg\Gamma_n^0)^\lambda] \approx T[E_i; \Gamma^\lambda, E^\lambda, (fg\Gamma_n^0)^\lambda] \\ + \frac{\partial T[E_i; \Gamma^\lambda, E^\lambda, (fg\Gamma_n^0)^\lambda]}{\partial \Gamma^\lambda} \cdot \delta\Gamma^\lambda + \frac{\partial T[E_i; \Gamma^\lambda, E^\lambda, (fg\Gamma_n^0)^\lambda]}{\partial E^\lambda} \cdot \delta E^\lambda \\ + \frac{\partial T[E_i; \Gamma^\lambda, E^\lambda, (fg\Gamma_n^0)^\lambda]}{\partial (fg\Gamma_n^0)^\lambda} \cdot \delta(fg\Gamma_n^0)^\lambda$$

is a linear function in  $\delta\Gamma^\lambda$ ,  $\delta E^\lambda$ , and  $\delta(fg\Gamma_n^0)^\lambda$ . The least-squares estimates of  $\delta\Gamma^\lambda$ ,  $\delta E^\lambda$ , and  $\delta(fg\Gamma_n^0)^\lambda$  are used to modify the initial estimates of  $\Gamma^\lambda$ ,  $E^\lambda$ , and  $(fg\Gamma_n^0)^\lambda$ . With the improved estimates for the parameters, the process is repeated until the convergence criteria,

$$(15) \quad \left| \frac{\delta\Gamma^\lambda}{\Gamma^\lambda} \right| \leq 0.009, \quad \left| \frac{\delta E^\lambda}{E^\lambda} \right| \leq 0.0001, \quad \text{and} \quad \left| \frac{\delta(fg\Gamma_n^0)^\lambda}{(fg\Gamma_n^0)^\lambda} \right| \leq 0.002,$$

are satisfied.

The standard deviation of the last estimate of each parameter is computed from the relation

$$(16) \quad \text{standard deviation} = \sqrt{a_{jj} s^2},$$

where

$$s^2 = \frac{\sum_{i=1}^n [T_c(E_i) - T_e(E_i)]^2}{n - k}$$

and  $a_{jj}$  is the diagonal element of the inverse coefficient matrix of the normal equations which corresponds to the  $j$ th parameter. The theoretical transmission is represented by  $T_c(E_i)$ , the experimental transmission is represented by  $T_e(E_i)$ , the number of points is represented by  $n$ , and the number of parameters is represented by  $k$ . The covariance of  $\Gamma$  and  $(fg\Gamma_n^0)$  for each resonance is computed from the relation

$$\text{cov.} [\Gamma, (fg\Gamma_n^0)] = s^2 a_{ij},$$

where  $a_{ij}$  is the off-diagonal element of the inverse coefficient matrix of the normal equations which corresponds to  $\Gamma$  and  $(fg\Gamma_n^0)$ .

In order to determine how well the theoretical transmission curve fits the experimental transmission points, the two quantities chi-square ( $\chi^2$ ) and the number of degrees of freedom are computed. The number of degrees of freedom is defined by

$$d.f. = n - k - 1 ,$$

and chi-square is computed from the relation,

$$\chi^2 = \sum_{i=1}^n \frac{[(100/\text{PSA})^2 T_c(E_i) - (100/\text{PSA})^2 T_e(E_i)]^2}{(100/\text{PSA})^2 T_c(E_i)}$$

where PSA is the per cent statistical accuracy of a representative point of the resonances.

#### AREA ANALYSIS

For the higher-energy regions where the Doppler width,  $\Delta$ , or the resolution width,  $R$ , is greater than the natural width,  $\Gamma$ , of the resonance it is not possible to obtain meaningful values of  $\Gamma$  from the experimental data. Resonances at these higher energies are analyzed by an area-analysis technique to give  $(/g\Gamma_n^0)$  for an assumed  $\Gamma$ . The area under a transmission dip is independent of the resolution function. However, if the resonances are close together the accuracy of the area method can be increased if the resolution function is included in the analysis. By using the above methods and techniques, the resolution can be included with only a small amount of additional computing time.

In the area-analysis technique, estimates of  $E^\lambda$  and  $\Gamma^\lambda$  are provided. Initial estimates for  $(/g\Gamma_n^0)^\lambda$  are either estimated or computed by the program from the relation

$$(/g\Gamma_n^0)^\lambda = \frac{-\sqrt{E^\lambda} \Gamma^\lambda [\ln T(E^\lambda) - \ln T(E_w)]}{N(2.608 \times 10^6)} \cdot \text{CF} ,$$

where  $T(E^\lambda)$  is the experimental transmission at the resonant energy  $E^\lambda$ ,  $T(E_w)$  is the larger of the experimental transmissions at the first and last channels of the resonance, and

$$\text{CF} \approx 0.62 + \frac{1.66 \sqrt{\Delta^2(E^\lambda) + R^2(E^\lambda)}}{\Gamma^\lambda}$$

is an approximate correction for the effects of Doppler broadening and instrument resolution in order to increase the accuracy of the estimates. These estimates of the parameters are used in the function

$$T_e(E_i) = P(E_i) \exp [-N\sigma(E_i)]$$

to solve for  $P(E_i)$ , where  $T_e(E_i)$  are experimental transmission data from the flat regions between resonances, and  $\sigma(E_i)$  is defined in Eq. (4). These values,  $P(E_i)$ , are used by the method of least squares to determine the estimates of the coefficients of the polynomial equation (9). By using the estimates for the coefficients of  $P(E_i)$  and the estimates of the parameters, the sum of the calculated transmissions is compared with the sum of the experimental transmissions over each resonance. Corrections to the estimates

of  $(fg\Gamma_n^0)^\lambda$  are computed if the absolute value of the difference of these sums for each resonance is less than  $0.005 (\text{PSA}) (\text{number of channels in the resonance})^{1/2}$ , where PSA is the per cent statistical accuracy of a representative transmission point between resonances.

To obtain corrections for the estimates of  $(fg\Gamma_n^0)^\lambda$ , the sum over a resonance of the nonlinear function, Eq. (10), is linearized by expanding it into a truncated Taylor's series at the initial estimates of  $(fg\Gamma_n^0)^\lambda$  and retaining only first-order terms. If  $i_{\lambda=m}$  denotes the channels over a resonance  $m$ , then

$$(17) \quad \sum_{i_{\lambda=m}} T[E_i; \Gamma^\lambda, E^\lambda, (fg\Gamma_n^0)^\lambda + \delta(fg\Gamma_n^0)^\lambda] = \sum_{i_{\lambda=m}} T[E_i; \Gamma^\lambda, E^\lambda, (fg\Gamma_n^0)^\lambda] \\ + \sum_{\lambda} \frac{\partial \sum_{i_{\lambda=m}} T[E_i; \Gamma^\lambda, E^\lambda, (fg\Gamma_n^0)^\lambda]}{\partial (fg\Gamma_n^0)^\lambda} \cdot \delta(fg\Gamma_n^0)^\lambda$$

is a linear function with respect to the  $\delta(fg\Gamma_n^0)^\lambda$ , the corrections to the estimates of  $(fg\Gamma_n^0)^\lambda$ . It is assumed that only the adjoining resonances on each side of a resonance  $m$  have a significant effect on the area under the resonance  $m$ . If one denotes by  $M$  the number of resonances in the region of analysis, then the linear system of  $M$  equations,

$$(18) \quad \sum_{\lambda=m-1}^{m+1} \frac{\partial \sum_{i_{\lambda=m}} T[E_i; \Gamma^\lambda, E^\lambda, (fg\Gamma_n^0)^\lambda]}{\partial (fg\Gamma_n^0)^\lambda} \cdot \delta(fg\Gamma_n^0)^\lambda = \sum_{i_{\lambda=m}} T_e(E_i) - \sum_{i_{\lambda=m}} T_c(E_i)$$

is solved simultaneously to obtain  $\delta(fg\Gamma_n^0)^\lambda$  for each resonance  $m$  where  $m = 1, 2, \dots, M$ , and  $\delta(fg\Gamma_n^0)^0 = \delta(fg\Gamma_n^0)^{M+1} = 0$ . The  $\delta(fg\Gamma_n^0)^\lambda$  are added to the estimates of  $(fg\Gamma_n^0)^\lambda$  to give new estimates of  $(fg\Gamma_n^0)^\lambda$  which are used to repeat the process until the convergence criterion is satisfied.

A number which can be used to assess the accuracy of the estimate of  $(fg\Gamma_n^0)^\lambda$  is computed from the absolute value of the relation

$$\frac{(\text{PSA}/100) (\text{number of points over the resonance } \lambda)^{1/2}}{\partial \sum_{i_\lambda} T(E_i)/\partial (fg\Gamma_n^0)^\lambda}$$

### DERIVATION OF EQUATIONS

#### Doppler-Broadened Cross Section Integral in Terms of the Complex Probability Integral

In order to represent the Doppler-broadened cross section integral in terms of the real and imaginary parts of the complex probability integral, consider the Doppler-broadened integral,

$$(19) \quad \sigma_{\Delta}(E') = 4\pi r^2$$

$$+ \frac{1}{\Delta\sqrt{\pi}} \sum_{\lambda} (f_g \Gamma_n^0)^{\lambda} \left\{ 6.52 \times 10^5 \int_0^{\infty} \frac{1}{\sqrt{E''}} \cdot \frac{\Gamma^{\lambda}}{(E^{\lambda} - E'')^2 + (\Gamma^{\lambda}/2)^2} \exp \left[ - \left( \frac{E' - E''}{\Delta} \right)^2 \right] dE'' \right. \\ \left. - 5.725 \times 10^3 \int_0^{\infty} \frac{(E^{\lambda} - E'')a}{(E^{\lambda} - E'')^2 + (\Gamma^{\lambda}/2)^2} \exp \left[ - \left( \frac{E' - E''}{\Delta} \right)^2 \right] dE'' \right\} .$$

Let

$$s = \frac{(E'' - E')}{\Delta}, \quad \xi^{\lambda} = \frac{(E^{\lambda} - E')}{\Delta}, \quad \eta^{\lambda} = \frac{\Gamma^{\lambda}/2}{\Delta}.$$

Then

$$(20) \quad \int_0^{\infty} \frac{1}{\sqrt{E''}} \frac{\Gamma^{\lambda}}{(E^{\lambda} - E'')^2 + (\Gamma^{\lambda}/2)^2} \exp \left[ - \left( \frac{E' - E''}{\Delta} \right)^2 \right] dE'' \\ = 2 \int_{-E'/\Delta}^{\infty} \frac{1}{\sqrt{E' + s\Delta}} \frac{\eta^{\lambda}}{(\xi^{\lambda} - s)^2 + (\eta^{\lambda})^2} e^{-s^2} ds$$

and

$$(21) \quad \int_0^{\infty} \frac{(E^{\lambda} - E'')a}{(E^{\lambda} - E'')^2 + (\Gamma^{\lambda}/2)^2} \exp \left[ - \left( \frac{E' - E''}{\Delta} \right)^2 \right] dE'' = a \int_{-E'/\Delta}^{\infty} \frac{(\xi^{\lambda} - s)}{(\xi^{\lambda} - s)^2 + (\eta^{\lambda})^2} e^{-s^2} ds .$$

Since  $(s\Delta)^2 < (E')^2$  in the physical problems considered, one can approximate the factor  $1/\sqrt{E' + s\Delta}$  in the right side of Eq. (20) by expanding it into a truncated Taylor's series,

$$(22) \quad \frac{1}{\sqrt{E' + s\Delta}} \approx \frac{1}{\sqrt{E'}} \left( 1 - \frac{s\Delta}{2E'} \right).$$

Substitution of Eq. (22) in Eq. (20) gives

$$(23) \quad \int_0^\infty \frac{1}{\sqrt{E''}} \frac{\Gamma^\lambda}{(E^\lambda - E'')^2 + (\Gamma^\lambda/2)^2} \exp \left[ -\left( \frac{E' - E''}{\Delta} \right)^2 \right] dE'' \\ = 2 \int_{-E'/\Delta}^\infty \frac{1}{\sqrt{E'}} \left( 1 - \frac{s\Delta}{2E'} \right) \frac{\eta^\lambda}{(\xi^\lambda - s)^2 + (\eta^\lambda)^2} e^{-s^2} ds .$$

Adding and subtracting  $\Delta\xi^\lambda/2E'$  to the factor  $[1 - (s\Delta/2E')]$  in the right side of Eq. (23), one obtains

$$(24) \quad \int_0^\infty \frac{1}{\sqrt{E''}} \frac{\Gamma^\lambda}{(E^\lambda - E'')^2 + (\Gamma^\lambda/2)^2} \exp \left[ -\left( \frac{E' - E''}{\Delta} \right)^2 \right] dE'' \\ = \frac{2}{\sqrt{E'}} \left[ \int_{-E'/\Delta}^\infty \left( 1 - \frac{\Delta\xi^\lambda}{2E'} \right) \frac{\eta^\lambda}{(\xi^\lambda - s)^2 + (\eta^\lambda)^2} e^{-s^2} ds \right. \\ \left. + \int_{-E'/\Delta}^\infty \left( \frac{\Delta\eta^\lambda}{2E'} \right) \frac{\xi^\lambda - s}{(\xi^\lambda - s)^2 + (\eta^\lambda)^2} e^{-s^2} ds \right] .$$

Since, in the physical problems considered,  $\Gamma^\lambda/2E^\lambda \ll 1$ , the values of the integral for limits below  $-E'/\Delta$  are too small to add a significant contribution to the integral. Therefore the lower limit of the integral can be replaced by  $-\infty$ .

Let

$$\pi U(\xi^\lambda, \eta^\lambda) = \int_{-\infty}^\infty \frac{\eta^\lambda}{(\xi^\lambda - s)^2 + (\eta^\lambda)^2} e^{-s^2} ds ,$$

(25)

$$\pi V(\xi^\lambda, \eta^\lambda) = \int_{-\infty}^\infty \frac{\xi^\lambda - s}{(\xi^\lambda - s)^2 + (\eta^\lambda)^2} e^{-s^2} ds .$$

If one first substitutes Eq. (25) in Eqs. (21) and (24) and then substitutes the results in Eq. (19), the desired representation for the Doppler-broadened integral is derived,

$$(26) \quad \sigma_\Delta(E') = 4\pi r^2 + \frac{2\sqrt{\pi}}{\Delta} \cdot \sum_\lambda (fg\Gamma_n^0)^\lambda \left\{ (6.52 \times 10^5) \left[ \frac{1}{\sqrt{E'}} - \frac{\Delta\xi^\lambda}{2(E')^{3/2}} \right] U(\xi^\lambda, \eta^\lambda) \right. \\ \left. + \left[ 6.52 \times 10^5 \frac{\Delta\eta^\lambda}{2(E')^{3/2}} - 2.8625 \times 10^3 a \right] V(\xi^\lambda, \eta^\lambda) \right\} .$$

To simplify Eq. (26) let

$$\sigma_p = 4\pi r^2, \quad S = \frac{2\sqrt{\pi}}{\Delta}, \quad G = \frac{6.52 \times 10^5}{\sqrt{E'}}, \quad H = \frac{6.52 \times 10^5 \Delta}{2(E')^{3/2}}, \quad K = 2.8625 \times 10^3 a.$$

Substitution of Eq. (26) with its simplifications in Eq. (10) gives the desired formula for calculating the transmission data,

$$(27) \quad T(E_i) = \exp(-N\sigma_p) P(E_i) \frac{1}{R(E_i)\sqrt{\pi}} \int_0^\infty \exp \left\{ -NS \sum_{\lambda} (fg\Gamma_n^0)^{\lambda} [(G - H\xi^{\lambda}) U(\xi^{\lambda}, \eta^{\lambda}) + (H_{\eta}^{\lambda} - K) V(\xi^{\lambda}, \eta^{\lambda})] \right\} \exp \left\{ -\left[ \frac{E_i - E'}{R(E_i)} \right]^2 \right\} dE'.$$

#### Partial Derivatives from the Derivative of the Complex Probability Integral

In order to obtain partial derivatives by using the derivative of the complex probability integral, consider the complex probability integral,

$$(28) \quad \omega(z) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-s^2}}{z-s} ds,$$

or

$$\omega(z) = U(\xi, \eta) + iV(\xi, \eta),$$

where  $U(\xi, \eta)$  and  $V(\xi, \eta)$  are defined by Eq. (25), and

$$z = \xi + i\eta.$$

The derivative of Eq. (28) is

$$(29) \quad \omega'(z) = \frac{2i}{\sqrt{\pi}} - 2z\omega(z).$$

Substitution of the representations for  $z$  and  $\omega(z)$  in Eq. (29) gives

$$(30) \quad \begin{aligned} \omega'(z) &= \frac{2i}{\sqrt{\pi}} - 2(\xi + i\eta)[U(\xi, \eta) + iV(\xi, \eta)] \\ &= 2[\eta V(\xi, \eta) - \xi U(\xi, \eta)] + 2i \left[ \frac{1}{\sqrt{\pi}} - \xi V(\xi, \eta) - \eta U(\xi, \eta) \right]. \end{aligned}$$

Thus

$$(31) \quad \begin{aligned} \frac{\partial U}{\partial \xi^{\lambda}} &= 2[\eta^{\lambda} V(\xi^{\lambda}, \eta^{\lambda}) - \xi^{\lambda} U(\xi^{\lambda}, \eta^{\lambda})], \\ \frac{\partial V}{\partial \xi^{\lambda}} &= 2 \left[ \frac{1}{\sqrt{\pi}} - \xi^{\lambda} V(\xi^{\lambda}, \eta^{\lambda}) - \eta^{\lambda} U(\xi^{\lambda}, \eta^{\lambda}) \right]. \end{aligned}$$

Since the Cauchy-Riemann conditions,

$$\frac{\partial U}{\partial \xi} = \frac{\partial V}{\partial \eta} \quad \text{and} \quad \frac{\partial U}{\partial \eta} = -\frac{\partial V}{\partial \xi},$$

are necessary [6] for the existence of Eq. (29),

$$(32) \quad \begin{aligned} \frac{\partial U}{\partial \eta^\lambda} &= -2 \left[ \frac{1}{\sqrt{\pi}} - \xi^\lambda V(\xi^\lambda, \eta^\lambda) - \eta^\lambda U(\xi^\lambda, \eta^\lambda) \right], \\ \frac{\partial V}{\partial \eta^\lambda} &= 2[\eta^\lambda V(\xi^\lambda, \eta^\lambda) - \xi^\lambda U(\xi^\lambda, \eta^\lambda)]. \end{aligned}$$

By using the rule for the differentiation of composite functions,

$$(33) \quad \frac{\partial \omega(z)}{\partial E^\lambda} = \frac{\partial U}{\partial \xi^\lambda} \cdot \frac{\partial \xi^\lambda}{\partial E^\lambda} + \frac{\partial U}{\partial \eta^\lambda} \cdot \frac{\partial \eta^\lambda}{\partial E^\lambda} + i \left( \frac{\partial V}{\partial \xi^\lambda} \cdot \frac{\partial \xi^\lambda}{\partial E^\lambda} + \frac{\partial V}{\partial \eta^\lambda} \cdot \frac{\partial \eta^\lambda}{\partial E^\lambda} \right).$$

Since  $\partial \eta^\lambda / \partial E^\lambda = 0$ , Eq. (33) becomes

$$(34) \quad \frac{\partial \omega(z)}{\partial E^\lambda} = \left( \frac{\partial U}{\partial \xi^\lambda} + i \frac{\partial V}{\partial \xi^\lambda} \right) \frac{\partial \xi^\lambda}{\partial E^\lambda}.$$

Similarly,

$$(35) \quad \frac{\partial \omega(z)}{\partial \Gamma^\lambda} = \left( \frac{\partial U}{\partial \eta^\lambda} + i \frac{\partial V}{\partial \eta^\lambda} \right) \frac{\partial \eta^\lambda}{\partial \Gamma^\lambda}.$$

By using equalities (31), (32), (34), and (35) as well as the rule for differentiation under the integral sign, the partial derivatives with respect to each of the parameters  $E^\lambda$ ,  $\Gamma^\lambda$ , and  $(fg\Gamma_n^0)^\lambda$  are obtained. The partial derivatives, Eqs. (36), are given below:

(36)

$$\begin{aligned} \frac{\partial T(E_i)}{\partial E^\lambda} &= \exp(-N\sigma_p) P(E_i) \frac{1}{R(E_i) \sqrt{\pi}} \int_0^\infty \exp \left\{ -NS \sum_\lambda (fg\Gamma_n^0)^\lambda [(G - H\xi^\lambda) U(\xi^\lambda, \eta^\lambda) \right. \\ &\quad \left. + (H\eta^\lambda - K) V(\xi^\lambda, \eta^\lambda)] \right\} \left( -NS(fg\Gamma_n^0)^\lambda \left\{ 2(G - H\xi^\lambda) [\eta^\lambda V(\xi^\lambda, \eta^\lambda) - \xi^\lambda U(\xi^\lambda, \eta^\lambda)] - H U(\xi^\lambda, \eta^\lambda) \right. \right. \\ &\quad \left. \left. + 2(H\eta^\lambda - K) \left[ \frac{1}{\sqrt{\pi}} - \xi^\lambda V(\xi^\lambda, \eta^\lambda) - \eta^\lambda U(\xi^\lambda, \eta^\lambda) \right] \right\} \left( \frac{1}{\Delta} \right) \right) \exp \left\{ - \left[ \frac{E_i - E'}{R(E_i)} \right]^2 \right\} dE', \end{aligned}$$

$$\begin{aligned}
\frac{\partial T(E_i)}{\partial \Gamma^\lambda} &= \exp(-N\sigma_p) P(E_i) \frac{1}{R(E_i) \sqrt{\pi}} \int_0^\infty \exp \left\{ -NS \sum_\lambda (fg\Gamma_n^0)^\lambda [(G - H\xi^\lambda) U(\xi^\lambda, \eta^\lambda) \right. \\
&\quad \left. + (H\eta^\lambda - K) V(\xi^\lambda, \eta^\lambda)] \right\} \left( -NS(fg\Gamma_n^0)^\lambda \left\{ -2(G - H\xi^\lambda) \left[ \frac{1}{\sqrt{\pi}} - \xi^\lambda V(\xi^\lambda, \eta^\lambda) - \eta^\lambda U(\xi^\lambda, \eta^\lambda) \right] \right. \right. \\
&\quad \left. \left. + 2(H\eta^\lambda - K) [\eta^\lambda V(\xi^\lambda, \eta^\lambda) - \xi^\lambda U(\xi^\lambda, \eta^\lambda)] + H V(\xi^\lambda, \eta^\lambda) \right\} \left( \frac{1}{2\Delta} \right) \right) \exp \left\{ - \left[ \frac{E_i - E'}{R(E_i)} \right]^2 \right\} dE' , \\
\frac{\partial T(E_i)}{\partial (fg\Gamma_n^0)^\lambda} &= \exp(-N\sigma_p) P(E_i) \frac{1}{R(E_i) \sqrt{\pi}} \int_0^\infty \exp \left\{ -NS \sum_\lambda (fg\Gamma_n^0)^\lambda [(G - H\xi^\lambda) U(\xi^\lambda, \eta^\lambda) \right. \\
&\quad \left. + (H\eta^\lambda - K) V(\xi^\lambda, \eta^\lambda)] \right\} \left\{ -NS [(G - H\xi^\lambda) U(\xi^\lambda, \eta^\lambda) \right. \\
&\quad \left. + (H\eta^\lambda - K) V(\xi^\lambda, \eta^\lambda)] \right\} \exp \left\{ - \left[ \frac{E_i - E'}{R(E_i)} \right]^2 \right\} dE' .
\end{aligned}$$

### HIGH-SPEED-COMPUTER PROGRAMS

Since these methods of analysis are feasible only for high-speed computers, programs were written for the IBM 7090 computer. The FORTRAN language was used to write these programs.

Both the shape program and the area program analyze the transmission data by regions or portions of the data. A set of transmission data may contain data for as many as 2048 channels. Many regions for a set of transmission data as well as many sets of transmission data may be analyzed in a run of the program. The program will end an analysis of a region either when the convergence test is met or when a prescribed number of iterations has been made. A run is finished when all designated regions of all sets of data have been analyzed.

### SHAPE-ANALYSIS PROGRAM

The shape-analysis program makes a least-squares shape fit of the transmission data to the nonlinear function, Eq. (10), to determine the best estimates of the parameters  $E^\lambda$ ,  $\Gamma^\lambda$ , and  $(fg\Gamma_n^0)^\lambda$  for the resonances. The program requires good initial estimates for these parameters as well as the coefficients for the base-line polynomial,  $P(E_i)$ . The estimates for the parameters of each resonance and the coefficients for  $P(E_i)$  can be obtained by first running the transmission data in the area-analysis program. The parameters  $B_0$  and  $B_1$  for computing the resolution width  $R(E_i)$  may also be obtained from the output sheet from the area analysis program.

Regions of transmission data can be analyzed for as many as six resonances at once.

A description for using the program, illustrated with a sample problem, is given in Appendix A. A list of the FORTRAN statements for the program is given in Appendix B.

#### AREA-ANALYSIS PROGRAM

The area-analysis program determines the best estimates of  $(fg\Gamma_n^0)^\lambda$  for assumed values of  $\Gamma^\lambda$  and  $E^\lambda$  for the resonances. Initial estimates for  $(fg\Gamma_n^0)^\lambda$  are either furnished by the user or computed by the program. If  $(fg\Gamma_n^0)^\lambda$  is to be computed, it is given the value zero on the input-data card. Experience in using the area program has shown that convergence is more uniform when the initial estimates of the parameters are small compared to the true parameters. If the initial estimates of the parameters are too large by approximately a factor of 10, the program is unstable. If an estimate of  $(fg\Gamma_n^0)$  results in a negative number, the iterative procedure is terminated with the previous iteration.

The coefficients of the polynomial,  $P(E_i)$ , are either given to the program or determined by the method of least squares from the flat regions of the data between resonances. If the coefficient matrix of the normal equations is near singular, a unique set of estimates for the coefficients of  $P(E_i)$  cannot be determined. The program recognizes the near-singularity of the coefficient matrix by testing the sign<sup>3</sup> and relative magnitude of the determinant. If the determinant is negative or too small, its value is given on the output sheet and the analysis is discontinued.

The program will estimate a constant for the base line or will estimate coefficients for  $P(E_i)$  as a first- or second-degree polynomial, as desired by the user. The above requests must be designated by IC as follows:

IC = 0 means that the coefficients  $K_0$ ,  $K_1$ , and  $K_2$  will be furnished;

IC = 1 means to compute  $K_0$  and set  $K_1 = K_2 = 0$ ;

IC = 2 means to compute  $K_0$  and  $K_1$  and set  $K_2 = 0$ ;

IC = 3 means to compute  $K_0$ ,  $K_1$ , and  $K_2$ .

Regions of transmission data can be analyzed for as many as 20 resonances at once.

A description for using the program, illustrated with a sample problem, is given in Appendix A. A list of the FORTRAN statements for the program is given in Appendix B.

#### ACKNOWLEDGMENTS

We would like to thank Walter Gautschi and H. H. Bottenbruch for their valuable suggestions of some of the mathematical techniques used in this paper and G. J. Atta for assistance with some of the statistical aspects.

<sup>3</sup>The coefficient matrix is symmetric and positive definite, since it is formed from a nonsingular matrix times its transpose. Therefore its determinant is greater than zero.

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$$w(z) = e^{-z^2} \left( 1 + \frac{2i}{\sqrt{\pi}} \int_0^z e^{t^2} dt \right) \text{ot Kompleksnogo Argumenta ,}$$

Gosudarstv. Izdat. Tehn. – Teor. Lit., Moscow, 1954. [Tables of Values of the Function

$$w(z) = e^{-z^2} \left( 1 + \frac{2i}{\sqrt{\pi}} \int_0^z e^{t^2} dt \right) \text{for Complex Argument ,}$$

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**Appendix A**  
**DESCRIPTION OF PROGRAMS**  
**SHAPE-ANALYSIS PROGRAM**

**Input**

The shape-analysis program requires the following input data on IBM cards.

The first card, format (I6, 2A6),<sup>4</sup> is for the problem identification. It requires the problem identification number, the IBM 7090 run identification number, and the element and isotope identification.

The second card, format (6I5), is for the problem control data. It requires the number of channels of experimental transmission data, the numbers for the first and the last channels of the region to be analyzed, the number of resonances in this region, the multiplication factor for determining the number of partitions to be used in the evaluation of the integral of Eq. (6), and the maximum number of iterations to be run.

The third card, format (3E12.6), is for the coefficients of  $P(E_i)$ . It requires the coefficients  $K_0$ ,  $K_1$ , and  $K_2$ .

The next group of cards, format (3E12.6), is for the parameters of the resonances, with one card for each resonance. Each card requires  $\Gamma^\lambda$ ,  $E^\lambda$ , and  $(/g\Gamma_n^0)^\lambda$  for a resonance  $\lambda$ .

The next two cards, format (6E12.6), are for fixed parameters of the problem. They require the potential scattering radius in  $10^{-12}$  centimeters, the sample thickness in atoms of the element per barn, the atomic weight, the effective nuclear radius in  $10^{-12}$  centimeters, the flight path in meters, the channel width in microseconds, the delay in microseconds, the Doppler constant,  $B_0$  and  $B_1$  for computing the resolution width, and the factor which represents the per cent statistical accuracy.

The last group of cards, format (6I12), require the experimental transmission data.

If other regions of the transmission data are to be included in a run, then for each additional region the experimental-transmission data are followed by the input-parameter cards numbered one through three plus the cards for the parameters of the resonances. The last two cards for the fixed parameters and the experimental transmissions are omitted.

If other sets of transmission data are to be included in a run, then cards for the input parameters and the experimental transmissions follow in the order described above.

A blank card should be placed at the end of the deck to indicate the end of a run on the computer.

An example of an input data sheet is shown in Figs. 4 and 5.

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<sup>4</sup>Designators in parentheses are FORTRAN's Format specifications; in this case, I6 means an Integer decimal number having a field width of 6 columns, 2A6 means 2 Alphanumeric numbers having a field width of 6 columns.

Fig. 4. Input Data for Shape-Analysis Program.

INPUT PARAMETERS FOR SHAPE ANALYSIS JOB 1910

Card 1 for Problem Identification

Problem Number	7090 Run Number	Element and Isotope			...	80		
1	6	7	12	13	18	19	...	80
169		169S		LU176		not used		

Card 2 for Program Control Data

Channel Numbers								
For Input Data		For Analysis			Number of Resonances	Interval Factor for Integration	Maximum Number of Iterations	
1	5	6	10	11	15	16	20	21 25 26 30 31 ... 80
1023		400		600		4	1	8 not used

Card 3 for Coefficients of  $P(E_i)$

$K_0$	$K_1$	$K_2$	...	80				
1	12	13	24	25	36	37	...	80
.888600+00		.000000+00		.000000+00		not used		

Cards 3 +  $\lambda$  for Parameters of Each Resonance

$\Gamma^\lambda$ (ev)	$E^\lambda$	$(f/g\Gamma_n^0)^\lambda$ (ev)	...	80				
1	12	13	24	25	36	37	...	80
.100000+00	.617257+01	.134408-03	not used					
.100000+00	.526592+01	.769157-04						
.100000+00	.482369+01	.230876-04						
.100000+00	.438405+01	.580115-04						

Fig. 5. Input Data for Shape-Analysis Program.

INPUT PARAMETERS FOR SHAPE ANALYSIS (CONTINUED) JOB 1910

Cards for Fixed Parameters

Potential Scattering Radius ( $10^{-12}$ cm)	Sample Thickness (atoms/barn)	Atomic Weight	Effective Nuclear Radius ( $10^{-12}$ cm)	Flight Path (meters)	Channel Width ( $\mu$ sec)		
1	12	13 24	25 36	37 48	49 60	61 72	73 ... 80
.730000+00	.449200-02	.176000+03	.730000+00	.453080+02	.200000+01	not used	
Delay ( $\mu$ sec)	Doppler Constant, $D_0$	$B_0$	$B_1$	PSA			
1	12	13 24	25 36	37 48	49 60	61 72	73 ... 80
.441500+03	.318000+00	.284140-02	.112530-01	.138000+01	not used		

Output

The program gives two forms of output at the end of an analysis. The printed sheet consists of the run identification, the computed estimates of the parameters for each resonance for each iteration, and the standard deviation of the last estimate of each parameter, as well as the input data. In order to assess the accuracy of the parameters, the effects of uncertainties in the resolution function, the Doppler broadening, and the base line must be considered in addition to the standard deviation of the parameters. Curve plots (from the Oracle) consist of a plot of the experimental transmission represented by  $x$ , a plot of the calculated transmission represented by  $\bullet$ , and a plot of the base-line polynomial  $P(E_i)$  times  $\exp(-N\sigma_p)$  represented by  $\circ$ . Examples of the two forms of output are shown in Figs. 6 and 7.

Estimate of Cost

The running time for the shape analysis of a region of experimental transmissions depends upon the number of channels and the number of resonances in the region of analysis, as well as the number of iterations required.

The sample problem in Figs. 4-7 is a region of experimental transmissions for 355 channels with four resonances. The fixed parameters  $K_0$ ,  $K_1$ , and  $K_2$  for  $P(E_i)$ ,  $B_0$  and  $B_1$  for  $R(E_i)$ , and the initial parameters for each resonance were obtained by running the problem in the area analysis program. This run cost \$5.25. Using these parameters in the shape-analysis program five iterations were required to meet the convergence criterion. The running time on the IBM 7090 computer was 0.09 hr, which cost \$15.75.

Fig. 6. Printed Output for Shape-Analysis Program.

SHAPE ANALYSIS OF TRANSMISSION DATA      JOB 1910

RUN 169S

ELEMENT LUI76

ED	GAMMA	FGXGAMMA N 0				
NUMBER OF ITERATIONS 0						
0.617257E 01	1.000000E-01	0.134408E-03				
0.526592E 01	1.000000E-01	0.769157E-04				
0.482369E 01	1.000000E-01	0.230876E-04				
0.438405E 01	1.000000E-01	0.580115E-04				
NUMBER OF ITERATIONS 1						
0.618196E 01	0.747965E-01	0.161797E-03				
0.526698E 01	0.660973E-01	0.906228E-04				
0.482878E 01	0.362936E-01	0.232107E-04				
0.438227E 01	0.542946E-01	0.702490E-04				
NUMBER OF ITERATIONS 2						
0.618135E 01	0.686398E-01	0.181723E-03				
0.526714E 01	0.654731E-01	0.989452E-04				
0.482713E 01	0.516653E-01	0.243928E-04				
0.438227E 01	0.544172E-01	0.812476E-04				
NUMBER OF ITERATIONS 3						
0.618124E 01	0.671724E-01	0.186919E-03				
0.526706E 01	0.647470E-01	0.100056E-03				
0.482717E 01	0.514954E-01	0.245586E-04				
0.438211E 01	0.530373E-01	0.833135E-04				
NUMBER OF ITERATIONS 4						
0.618122E 01	0.670200E-01	0.187386E-03				
0.526706E 01	0.647571E-01	0.100074E-03				
0.482717E 01	0.514671E-01	0.245577E-04				
0.438211E 01	0.530878E-01	0.833294E-04				
NUMBER OF ITERATIONS 5						
ED	STD. DEV. ED	GAMMA	STD. DEV. G	FG GAMMA N 0	S.D. FG GN 0	COV.(G,GN 0)
0.618122E 01	0.915500E-03	0.670148E-01	0.499192E-02	0.187399E-03	0.109737E-04	-0.537913E-07
0.526706E 01	0.780252E-03	0.647565E-01	0.339011E-02	0.100074E-03	0.292085E-05	-0.903867E-08
0.482717E 01	0.105137E-02	0.514687E-01	0.364712E-02	0.245578E-04	0.323372E-06	0.350185E-09
0.438211E 01	0.600065E-03	0.530866E-01	0.231609E-02	0.833303E-04	0.219238E-05	-0.463279E-08
A# 0.73000E 00	T DELAY# 0.44150E 03	CL# 600				
N# 0.44920E-02	DO# 0.31800E-00	ND# 4				
AW# 0.17600E 03	BO# 0.28414E-02	IF# 1				
R# 0.73000E 00	B1# 0.11253E-01	IM# 8				
DIST# 0.45308E 02	CN#1023	CHI SQUARE# 0.273329E 03				
T# 0.20000E 01	CF# 400	DEGREES OF FREEDOM# 188				

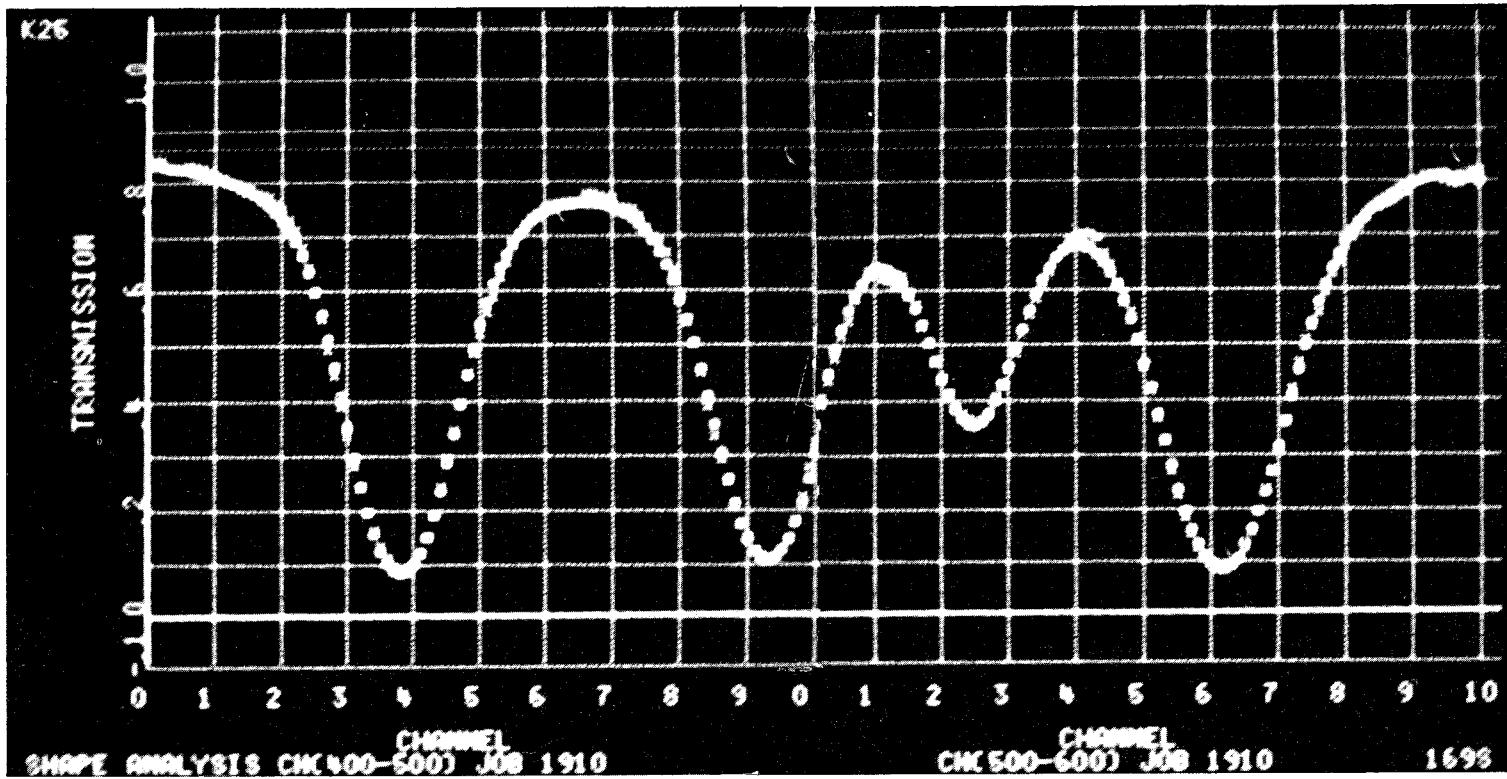


Fig. 7. Curve-Plotter Output for Shape-Analysis Program.

- x represents experimental transmissions;
- represents calculated transmissions;
- represents  $P(E_i) \exp(-NO_p)$ .

## AREA ANALYSIS PROGRAM

### Input

The area-analysis program requires the following input data on IBM cards.

The first card, format (I6, 2A6), is for the problem identification. It requires the problem identification number, the IBM 7090 run identification number, and the element and isotope identification.

The second card, format (7I5), is for the problem control data. It requires the number of channels of experimental transmission data, the numbers for the first and the last channels of the region to be analyzed, the number of resonances in the region, the multiplication factor for determining the number of partitions to be used in the evaluation of the integral of Eq. (6), the maximum number of iterations to be run, and the IC factor for designating the coefficients to be determined for the polynomial  $P(E_i)$ .

If IC equals zero, the next card, format (3E12.6), is for the coefficients of  $P(E_i)$ . It requires the coefficients  $K_0$ ,  $K_1$ , and  $K_2$ . If IC does not equal zero, this card is omitted.

The next group of cards, format (2I5, 3E12.6), is for the parameters of the resonances, with one card for each resonance. Each card requires the first and the last channel numbers for the resonance  $\lambda$ ,  $\Gamma_n^\lambda$ , the resonant channel number, and  $(/g\Gamma_n^0)^\lambda$ .

The next two cards, format (6E12.6), are for the fixed parameters of the problem. They require the potential scattering radius in  $10^{-12}$  centimeters, the sample thickness in atoms of the element per barn, the atomic weight, the effective nuclear radius in  $10^{-12}$  centimeters, the flight path in meters, the channel width in microseconds, the delay in microseconds, the Doppler constant,  $R_0$  and  $R_1$  for computing the resolution width, and the per cent statistical accuracy.

The last group of cards, format (6I12), require the experimental transmission data.

If other regions of the data are to be included in a run on the computer, then for each additional region the experimental transmission data are followed by the input-parameter cards numbered one through three plus the cards for the parameters of the resonances. The last two cards for the fixed parameters and the experimental transmissions are omitted.

If other sets of transmission data are to be included in a run, then cards for the input parameters and the experimental transmissions follow in the order described above.

A blank card should be placed at the end of the deck to indicate the end of a run.

An example of an input-data sheet is shown in Figs. 8 and 9.

Fig. 8. Input Data for Area-Analysis Program.

INPUT PARAMETERS FOR AREA ANALYSIS JOB 1910

Card 1 for Problem Identification

Problem Number	7090 Run Number	Element and Isotope					80	
1	6	7	12	13	18	19	...	80
189		189S		LU176		not used		

Card 2 for Program Control Data

For Input Data	Channel Numbers					Number of Resonances	Interval Factor for Integration	Maximum Number of Iterations	IC Coefficients for $P(E_i)$	
	For Analysis		First	Last	15					
	1	5	6	10	11					
511			8		320	17	1	8	1	not used

Card 3 for Coefficients of  $P(E_i)$  if IC = 0

$K_0$	$K_1$	$K_2$	80					
1	12	13	24	25	36	37	...	80
					not used			

Cards 3 +  $\lambda$  for Parameters of Each Resonance

Resonance $\lambda$	$\Gamma^\lambda$ (ev)	Resonant Channel Number	$(fg\Gamma_n^0)^\lambda$ (ev)	80				
First Channel	Last Channel	23	34	35	46	47	...	80
8	.600000-01	.145000+02	.000000+00	not used				
20	.600000-01	.235000+02	.509062-03					
34	.600000-01	.400000+02	.000000+00					
44	.600000-01	.505000+02	.649291-03					
72	.600000-01	.785000+02	.000000+00					
85	.600000-01	.910000+02	.000000+00					
96	.600000-01	.985000+02	.540000-04					
103	.600000-01	.107500+03	.227644-03					

Fig. 9. Input Data for Area-Analysis Program.

INPUT PARAMETERS FOR AREA ANALYSIS (CONTINUED) JOB 1910

First Channel		Resonance $\lambda$	$\Gamma^\lambda$ (ev)	Resonant Channel Number	$(fg\Gamma_n^0)^\lambda$ (ev)					80	
1	5	6	10	11	22	23	34	35	46	47	...
		110		124	.600000-01	.114000+03		.117237-02		not used	
		125		132	.600000-01	.130500+03		.000000+00			
		133		152	.600000-01	.139500+03		.000000+00			
		167		179	.600000-01	.173000+03		.000000+00			
		180		198	.600000-01	.186500+03		.000000+00			
		205		224	.600000-01	.213500+03		.000000+00			
		225		239	.600000-01	.234000+03		.000000+00			
		240		250	.600000-01	.244500+03		.000000+00			
		256		269	.600000-01	.263000+03		.810000-05			

Cards for Fixed Parameters

Potential Scattering Radius $(10^{-12}$ cm)		Sample Thickness (atoms/barn)		Atomic Weight		Effective Nuclear Radius $(10^{-12}$ cm)		Flight Path (meters)		Channel Width ( $\mu$ sec)		
1	12	13	24	25	36	37	48	49	60	61	72	73 ... 80
		.730000+00		.449200-02		.176000+03		.730000+00		.453080+02		.100000+01

Delay ( $\mu$ sec)		Doppler Constant		$R_0$ (channels)		$R_1$ (channels)		Per Cent Statistical Accuracy				
1	12	13	24	25	36	37	48	49	60	61	...	80
		.487500+03		.318000+00		.480000+01		.000000+00		.100000+01		not used

### Output

The program gives two forms of output at the end of an analysis. The printed sheet consists of the run identification, the computed estimates of the  $(fg\Gamma_n^0)$  for each resonance, a computed number for assessing the accuracy of  $(fg\Gamma_n^0)^{\lambda}$ , as well as the input data. In order to assess the accuracy of the parameters, the effect of the uncertainty in the base line must be considered. Curve plots (from the Oracle) consist of a plot of the experimental data represented by x, a plot of the calculated data represented by •, and a plot of the base-line polynomial  $P(E_i)$  times  $\exp(-N\sigma_p)$  represented by .. Examples of the two forms of output are shown in Figs. 10, 11, and 12.

AREA ANALYSIS OF TRANSMISSION DATA                    JOB 1910

RUN 189S

ELEMENT LU176

NUMBER OF ITERATIONS 3

C1	C2	GAMMA	CO	EO	FGXGAMMA N 0	SA	FGXGAMMA N 0
8	19	0.600000E-01	0.145000E 02	0.425813E 02	0.646939E-03	0.223459E-04	
20	33	0.600000E-01	0.235000E 02	0.410946E 02	0.103755E-02	0.385369E-04	
34	43	0.600000E-01	0.400000E 02	0.385639E 02	0.586215E-04	0.295958E-05	
44	61	0.600000E-01	0.505000E 02	0.370733E 02	0.145727E-02	0.429550E-04	
72	84	0.600000E-01	0.785000E 02	0.334960E 02	0.192060E-03	0.511501E-05	
85	95	0.600000E-01	0.910000E 02	0.320641E 02	0.226557E-03	0.559858E-05	
96	102	0.600000E-01	0.985000E 02	0.312486E 02	0.939579E-04	0.257184E-05	
103	109	0.600000E-01	0.107500E 03	0.303105E 02	0.272895E-03	0.788986E-05	
110	124	0.600000E-01	0.114000E 03	0.296589E 02	0.127358E-02	0.369257E-04	
125	132	0.600000E-01	0.130500E 03	0.280963E 02	0.592025E-04	0.198411E-05	
133	152	0.600000E-01	0.139500E 03	0.272955E 02	0.989560E-03	0.233728E-04	
167	179	0.600000E-01	0.173000E 03	0.245969E 02	0.259422E-03	0.519084E-05	
180	198	0.600000E-01	0.186500E 03	0.236214E 02	0.261979E-03	0.564605E-05	
205	224	0.600000E-01	0.213500E 03	0.218369E 02	0.113208E-03	0.228255E-05	
225	239	0.600000E-01	0.234000E 03	0.206136E 02	0.812228E-04	0.151599E-05	
240	250	0.600000E-01	0.244500E 03	0.200265E 02	0.340861E-04	0.847280E-06	
256	269	0.600000E-01	0.263000E 03	0.190513E 02	0.106199E-04	0.641696E-06	
A# 0.73000E 00	T# 0.10000E 01		CN# 511	IM# 8	K0# 0.870465E 00		
N# 0.44920E-02	T DELAY# 0.48750E 03		CF# 8	K# 1	K1# 0.		
AW# 0.17600E 03	DO# 0.31800E-00		CL# 320	RO# 0.48000E 01	K2# 0.		
R# 0.73000E 00	BO# 0.17601E-02		NO# 17	R1#-0.			
DIST# 0.45308E 02	B1#-0.		IF# 1	PSA# 0.10000E 01			

Fig. 10. Printed Output for Area-Analysis Program.

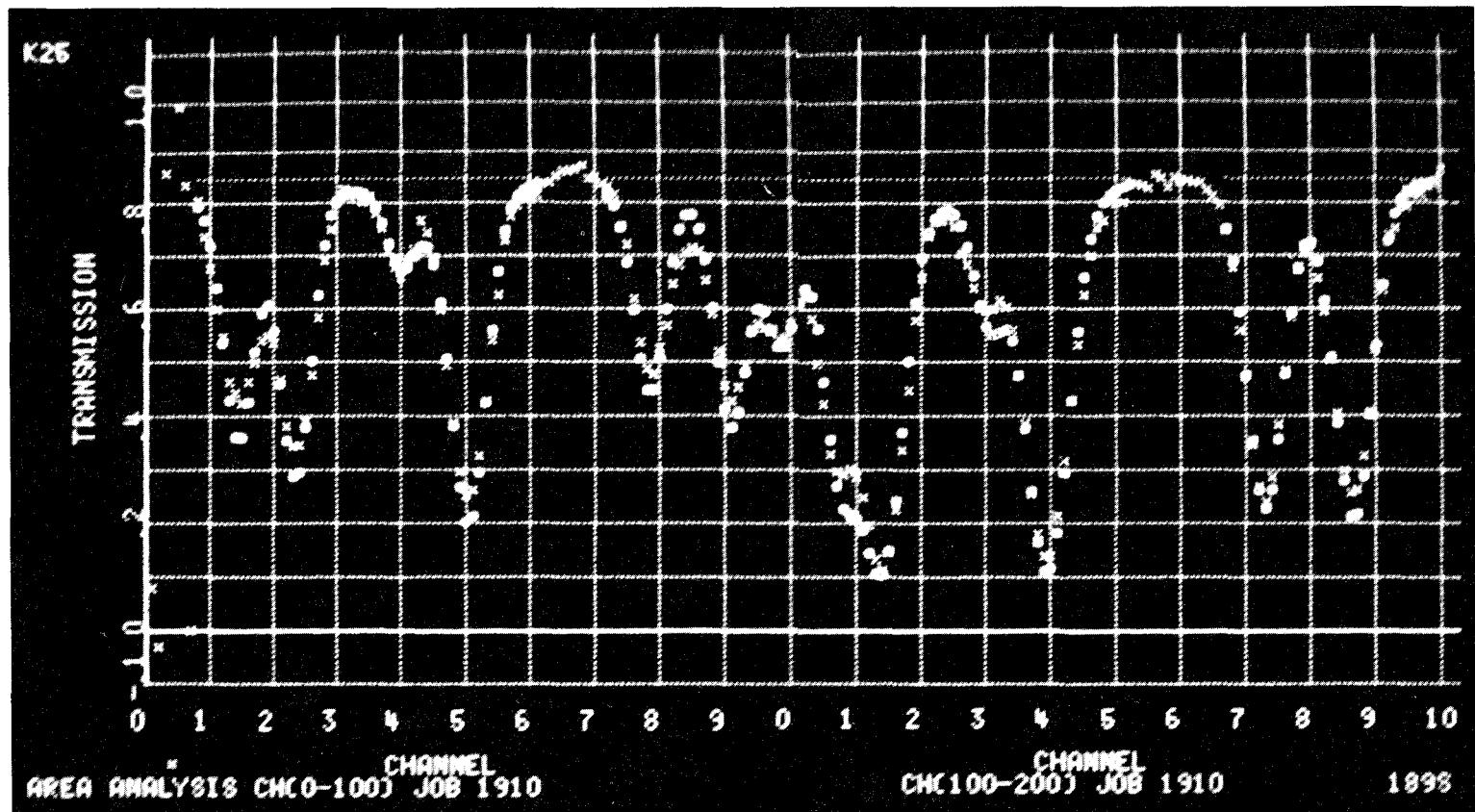


Fig. 11. Curve-Plotter Output for Area-Analysis Program.

- represents experimental transmissions;
- represents calculated transmissions;
- represents  $P(E_i) \exp(-N\sigma_p)$ .

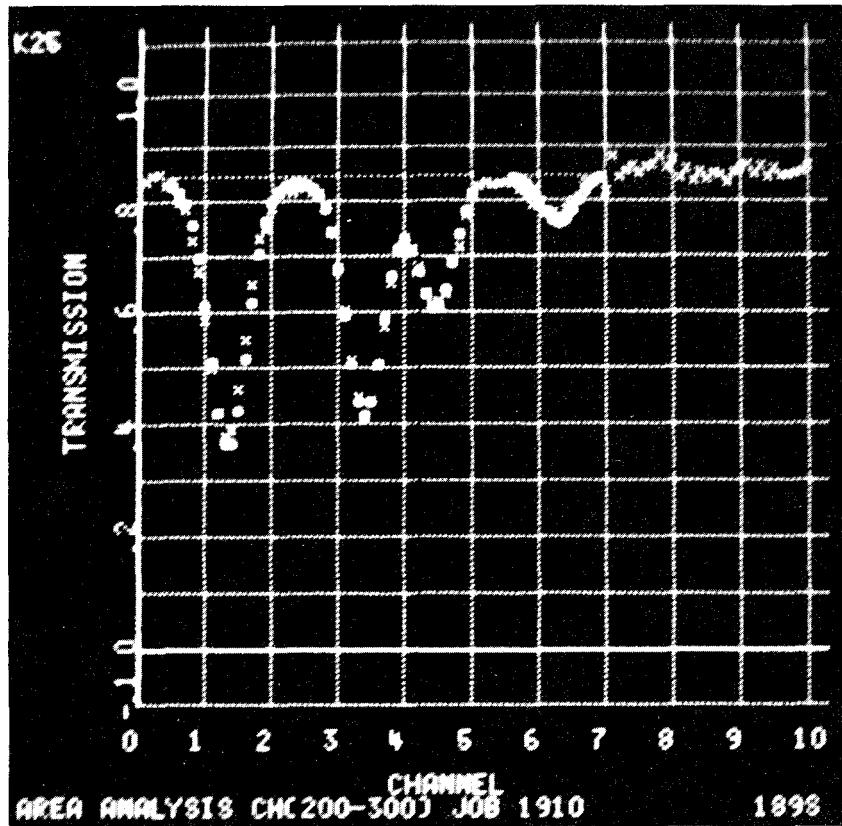


Fig. 12. Curve-Plotter Output for Area-Analysis Program.

- represents experimental transmissions;
- represents calculated transmissions;
- represents  $P(E_i) \exp(-N\sigma_p)$ .

#### Estimate of Cost

The running time for the area analysis of a region of experimental transmissions depends upon the number of channels and the number of resonances in the region of analysis, as well as the number of iterations required.

The sample problem in Figs. 8-12 is a region of experimental transmissions for 313 channels and 17 resonances. Using the initial parameters given on the input parameter sheet three iterations were required to meet the convergence criterion. The running time on the IBM 7090 was 0.10 hr, which cost \$17.50.

Appendix B.  
FORTRAN LISTINGS

**FORTRAN LISTING FOR SHAPE-ANALYSIS PROGRAM**

```
C      SEA 1910 SHAPE ANALYSIS OF TRANSMISSION DATA
COMMONSXI,ETA,U,V,GN,EN,G,IO,IM,T,ZTZ,ZTT,J,I,
1A,ON,AW,R,DIST,T1,DELAY,H0,ONSIGP,TM1,AM,IT,B0,B1,C0,C1,C2,
2F1,F2,F3,SIGTC,SIGT1,SIGT2,SIGT3,TA,AC
DIMENSIONGN(6),EN(6),G(6),T(2048),
1ZTZ(18,18),ZTT(18,19),AM(18),F1(6),F2(6),F3(6),TA(2048),AC(2048),
2SIGTC(600),SIGT1(6,600),SIGT2(6,600),SIGT3(6,600)
1 FORMAT(50H1SHAPE ANALYSIS OF TRANSMISSION DATA          JOB 1910/
14HORUN1A6)
2 FORMAT(I6,2A6)
L2=0
3 FORMAT(43H0      E0      GAMMA      FGXGAMMA N 0)
4 FORMAT(I6)
X=FPTRPF(0,-1)
5 READINPUTTAPE10,2,L1,L1A,LE
IF(L1)6,6,7
6 CALL NOPLOT
CALL EXIT
7 WRITEOUTPUTTAPE9,1,L1A
8 FORMAT(6I5)
9 FORMAT(3E12.6)
10 FORMAT(6E12.6)
READINPUTTAPE10,8,IMN,IO,IM,M,KI,ITMAX
READINPUTTAPE10,9,C0,C1,C2
READINPUTTAPE10,9,(G(J),EN(J),GN(J),J=1,M)
IT=0
IF(L1-L2)12,13,12
```

**FORTRAN LISTING FOR SHAPE-ANALYSIS PROGRAM (continued)**

```
11 FORMAT(6012)

12 READINPUTTAPE10,10,A,ON,AW,R,DIST,T1,DELAY,H0,B0,B1,PSA
    READINPUTTAPE10,11,(T(I),I=1,IMN)

15 FORMAT(8H0ELEMENT1A6)

13 WRITEOUTPUTTAPE9,15,LE

    WRITEOUTPUTTAPE9,3
    SIGP=12.566368*R*R
    ONSIGP=EXP(-ON*SIGP)
    COM1=SQRTF(AW)/H0
    COM4=A*2.86239E3
    SIG=(-2.0*ON*1.7724538)
    VI=(72.3*DIST)**2
    SIO=IO
    EIRO=VI/(SIO*T1+DELAY)**2
    SIO=IM
    EIRM=VI/(SIO*T1+DELAY)**2
    EIRO=EIRO+(3.0*(B1*EIRO+B0*(EIRO**1.5)))
    EIRM=EIRM-(3.0*(B1*EIRM+B0*(EIRM**1.5)))
    INT=((SQRTF(VI/EIRM)-SQRTF(VI/EIRO))/T1)
    INT=INT*KI
    IF((INT/2)*2-INT)77,78,76

76 CALLERROR

77 INT=INT+1

78 EINT=INT
    H=(EIRO-EIRM)/EINT
    HH=H*H
    HH2=HH+HH
```

FORTRAN LISTING FOR SHAPE-ANALYSIS PROGRAM (continued)

```
H31=(H/2.0)
H32=H
INT1=INT+1
M3=3*M
M31=1+M3
17 DO18J=1,M3
    DO19JJ=1,M3
        ZTZ(J,JJ)=0.0
        IF(J-JJ)40,41,40
41 ZTT(J,JJ)=1.0
    GO TO 19
40 ZTT(J,JJ)=0.0
19 CONTINUE
ZTT(J,M31)=0.0
18 CONTINUE
Y=EIRM
DO80IJ=1,INT1
CON=1.0/SQRTF(Y)
COM2=1.0/(COM1*2.0*Y)
COM3=COM1*CON
SIGMA=SIG*COM3
CON=6.52E5*CON
COM2=6.52E5*COM2
SUMJ=0.0
DO84JY=1,M
SXI=COM3*(Y-EN(JY))
ETA=COM3*G(JY)/2.0
```

FORTRAN LISTING FOR SHAPE-ANALYSIS PROGRAM (continued)

```
CALLPFCN  
HG=CON+COM2*SXI  
HK=COM2*ETA-COM4  
SOM=SIGMA*(HG*U-HK*V)  
SUMJ=SUMJ+GN(JY)*SOM  
SXIU=2.0*(ETA*V-SXI*U)  
ETAU=2.0*(0.56418958-SXI*V-ETA*U)  
GNCOM3=GN(JY)*COM3*SIGMA  
F1(JY)=SOM  
F2(JY)=-GNCOM3*(COM2*U+(HG*SXIU)-(HK*ETAU))  
F3(JY)=(GNCOM3/2.0)*(HG*(-ETAU)-(COM2*V+(HK*SXIU)))  
84 CONTINUE  
ONE=EXP(F(SUMJ))  
67 SIGTC(IJ)=ONE  
DO30JM=1,M  
SIGT1(JM,IJ)=ONE*F1(JM)  
SIGT2(JM,IJ)=ONE*F2(JM)  
SIGT3(JM,IJ)=ONE*F3(JM)  
30 CONTINUE  
Y=Y+H  
80 CONTINUE  
SUSQ=0.0  
SSQ=0.0  
DO90I=IO,IM  
SIO=I  
EI=VI/(SIO*T1+DELAY)**2  
BI=B1*EI+B0*(EI**1.5)
```

FORTRAN LISTING FOR SHAPE-ANALYSIS PROGRAM (continued)

```
BI2=BI*BI
CI=C0+(C1/(SQRTF(EI)))+(C2/EI)
CI=CI*ONSIGP
ACI=CI/(BI*1.772454)
EIKO=4.0*BI
EIKN=EI-EIKO
EIKO=EI+EIKO
IN=(EIRO-EIKN)/H
SIN=IN
EIKN=EIRO-SIN*H
INT=(EIKO-EIKN)/H
IF((INT/2)*2-INT)401,402,400
400 CALLERROR
401 INT=INT-1
402 IJS=INT1-IN
IJM=IJS+INT
EA=EXP(-(EI-EIKN)/BI)**2
EAH=EXP((2.0*(EI-EIKN)*H-HH)/BI2)
EHH2=EXP(-HH2/BI2)
KJ=0
TM1=0.0
DO81J=1,M
KJ=KJ+J
AM(KJ)=0.0
KJ=KJ+1
AM(KJ)=0.0
KJ=KJ+1
```

FORTRAN LISTING FOR SHAPE-ANALYSIS PROGRAM (continued)

```
AM(KJ)=0.0
KJ=KJ-J
81 CONTINUE
DO 95 IJ=IJS,IJM
IF(IJS-IJ)68,64,86
86 CALL ERROR
64 ONE=EA*H31
GO TO 407
68 IF(IJ-IJM)406,64,86
406 ONE=EA*H32
407 TM1=TM1+SIGTC(IJ)*ONE
KJ=0
DO91J=1,M
KJ=KJ+J
AM(KJ)=AM(KJ)+SIGT1(J,IJ)*ONE
KJ=KJ+1
AM(KJ)=AM(KJ)+SIGT2(J,IJ)*ONE
KJ=KJ+1
AM(KJ)=AM(KJ)+SIGT3(J,IJ)*ONE
KJ=KJ-J
91 CONTINUE
EA=EA*EAH
EAH=EAH*EHH2
95 CONTINUE
TM1=TM1*ACI
DIF=T(I)-TM1
SUSQ=SUSQ+((DIF*DIF)/TM1)
```

**FORTRAN LISTING FOR SHAPE-ANALYSIS PROGRAM (continued)**

```
SSQ=SSQ+(DIF*DIF)
IDF=IM-IO-(3*M)
KJ=0
DO96 J=1,M
KJ=KJ+J
AM(KJ)=AM(KJ)*ACI
KJ=KJ+1
AM(KJ)=AM(KJ)*ACI
KJ=KJ+1
AM(KJ)=AM(KJ)*ACI
KJ=KJ-J
96 CONTINUE
DO97 J=1,M3
DO98 JJ=J,M3
ZTZ(J,JJ)=ZTZ(J,JJ)+AM(J)*AM(JJ)
98 CONTINUE
ZTT(J,M31)=ZTT(J,M31)+AM(J)*DIF
97 CONTINUE
DO31 J=2,M3
J1=J-1
DO32 JJ=1,J1
ZTZ(J,JJ)=ZTZ(JJ,J)
32 CONTINUE
31 CONTINUE
TA(I)=TM1
AC(I)=CI
90 CONTINUE
```

FORTRAN LISTING FOR SHAPE-ANALYSIS PROGRAM (continued)

```
      WRITEOUTPUTTAPE9,111,IT
19 FORMAT(1H03E14.6)
      WRITEOUTPUTTAPE9,79,(EN(J),G(J),GN(J),J=1,M)
      IT=IT+1
      LA=XLOCF(ZTZ(1,1))
      LB=XLOCF(ZTT(1,1))
      IA=XLOCF(ZTZ(1,1))-XLOCF(ZTZ(1,2))
      IB=XLOCF(ZTT(1,1))-XLOCF(ZTT(1,2))
      DET=MATEQF(LA,LB,M3,M31,IA,IB)
      KJ=0
      DO110 J=1,M
      KJ=KJ+J
      GN(J)=GN(J)+ZTT(KJ,M31)
      KJ=KJ+1
      EN(J)=EN(J)+ZTT(KJ,M31)
      KJ=KJ+1
      G(J)=G(J)+ZTT(KJ,M31)
      KJ=KJ-J
110 CONTINUE
      KJ=0
      DO106 J=1,M
      KJ=KJ+J
      IF(ABSF(ZTT(KJ,M31)/GN(J))-0.0020)107,107,109
107 KJ=KJ+1
      IF(ABSF(ZTT(KJ,M31)/EN(J))-0.0001)108,108,109
108 KJ=KJ+1
      IF(ABSF(ZTT(KJ,M31)/G(J))-0.009)306,306,109
```

**FORTRAN LISTING FOR SHAPE-ANALYSIS PROGRAM (continued)**

```
306 KJ=KJ-J
106 CONTINUE
GOTO504
109 IF(IT>ITMAX)105,501,501
105 GOTO17
500 FORMAT(41H0 STOPPED ON MAXIMUM NUMBER OF ITERATIONS)
501 WRITE OUTPUT TAPE 9,500
GO TO 504
504 ICP=(I0/100)
IROJ=I0
IRNJ=IM
DO506I=IROJ,IRNJ
IF(I-(ICP*100))224,224,200
200 ICP=ICP+1
264 CALL CALCNH(L1A)
259 GO TO(201,202,203,204,205,206,207,208,209,210,211,212,213,214,
1215,216,217,218,219,220,221),ICP
201 ICON=0
CALL TITLE(48HSHAPE ANALYSIS CH(0-100) JOB 1910 )
GOTO222
202 ICON=100
CALL TITLE(48HSHAPE ANALYSIS CH(100-200) JOB 1910 )
GOTO222
203 ICON=200
CALL TITLE(48HSHAPE ANALYSIS CH(200-300) JOB 1910 )
GOTO222
204 ICON=300
```

FORTRAN LISTING FOR SHAPE-ANALYSIS PROGRAM (continued)

```
CALL TITLE(48HSHAPE ANALYSIS CH(300-400) JOB 1910 )
GOTO222

205 ICON=400
CALL TITLE(48HSHAPE ANALYSIS CH(400-500) JOB 1910 )
GOTO222

206 ICON=500
CALL TITLE(48HSHAPE ANALYSIS CH(500-600) JOB 1910 )
GOTO222

207 ICON=600
CALL TITLE(48HSHAPE ANALYSIS CH(600-700) JOB 1910 )
GOTO222

208 ICON=700
CALL TITLE(48HSHAPE ANALYSIS CH(700-800) JOB 1910 )
GOTO222

209 ICON=800
CALL TITLE(48HSHAPE ANALYSIS CH(800-900) JOB 1910 )
GOTO222

210 ICON=900
CALL TITLE(48HSHAPE ANALYSIS CH(900-1000) JOB 1910 )
GOTO222

211 ICON=1000
CALL TITLE(48HSHAPE ANALYSIS CH(1000-1100) JOB 1910 )
GOTO222

212 ICON=1100
CALL TITLE(48HSHAPE ANALYSIS CH(1100-1200) JOB 1910 )
GO TO 222

213 ICON=1200
```

FORTRAN LISTING FOR SHAPE-ANALYSIS PROGRAM (continued)

```
CALL TITLE(48HSHAPE ANALYSIS CH(1200-1300) JOB 1910 )
GO TO 222

214 ICON=1300

CALL TITLE(48HSHAPE ANALYSIS CH(1300-1400) JOB 1910 )
GO TO 222

215 ICON=1400

CALL TITLE(48HSHAPE ANALYSIS CH(1400-1500) JOB 1910 )
GO TO 222

216 ICON=1500

CALL TITLE(48HSHAPE ANALYSIS CH(1500-1600) JOB 1910 )
GO TO 222

217 ICON=1600

CALL TITLE(48HSHAPE ANALYSIS CH(1600-1700) JOB 1910 )
GO TO 222

218 ICON=1700

CALL TITLE(48HSHAPE ANALYSIS CH(1700-1800) JOB 1910 )
GO TO 222

219 ICON=1800

CALL TITLE(48HSHAPE ANALYSIS CH(1800-1900) JOB 1910 )
GO TO 222

220 ICON=1900

CALL TITLE(48HSHAPE ANALYSIS CH(1900-2000) JOB 1910 )
GO TO 222

221 ICON=2000

CALL TITLE(48HSHAPE ANALYSIS CH(2000-2100) JOB 1910 )
222 CALL CRT(100.0,0.0,10.0,1.1,-1,0.1,
142H0   1   2   3   4   5   6   7   8   9   10,
```

FORTRAN LISTING FOR SHAPE-ANALYSIS PROGRAM (continued)

```
242H-.1 0     .2     .4     .6     .8     1.0   ,
348HWRONG TITLE
412HCHANNEL   ,
512HTRANSMISSION)
ICP1=(ICP-1)*100+1
ICP2=ICP*100
DO223ICT=ICP1,ICP2
AICT=ICT-ICON
241 CALL PLOT(AICT,T(ICT),4)
223 CONTINUE
224 AI=I-ICON
243 CALL PLOT(AI,TA(I),5)
    CALL PLOT (AI,AC(I),1)
506 CONTINUE
    GOTO103
111 FORMAT(24HO NUMBER OF ITERATIONS I2)
103 WRITEOUTPUTTAPE9,111,IT
    SN=IDF+1
    SSQ=SSQ/SN
    KJ=0
    DO 16 J=1,M
        KJ=KJ+J
        ZTT(KJ,KJ+2)=SSQ*ZTT(KJ,KJ+2)
        ZTT(KJ,M31)=SQRTF(SSQ*ZTT(KJ,KJ))
        KJ=KJ+1
        ZTT(KJ,M31)=SQRTF(SSQ*ZTT(KJ,KJ))
        KJ=KJ+1
```

FORTRAN LISTING FOR SHAPE-ANALYSIS PROGRAM (continued)

```
ZTT(KJ,M31)=SQRTF(SSQ*ZTT(KJ,KJ))

KJ=KJ-J

16 CONTINUE

SUSQ=SUSQ*((100.0/PSA)**2)

14 FORMAT(99H0      E0          STD. DEV. E0      GAMMA          STD. DEV. G
1   FG GAMMA N 0  S.D. FG GN 0  COV.(G,GN 0))

WRITEOUTPUTTAPE9,14

24 FORMAT(1H07E14.6)

KJ=1

DO20 J=1,M

WRITE OUTPUT TAPE 9,24,EN(J),ZTT(KJ+1,M31),G(J),ZTT(KJ+2,M31),GN(J
1),ZTT(KJ,M31),ZTT(KJ,KJ+2)

KJ=KJ+3

20 CONTINUE

113 FORMAT(3H0A=E12.5,23H                                     K0=E14.6/3H N=E12.5,
123H                                         K1=E14.6/4H AW=E12.5,22H
2K2=E14.6/3H R=E12.5/6H DIST=E12.5/
33H T=12.5/9H T DELAY=E12.5/4H D0=E12.5/4H B0=E12.5/
44H B1=E12.5/4H CN=I4/4H CF=I4/4H CL=I4/4H NO=I4/
54H IF=I4/4H IM=I4/12H CHI SQUARE=E14.6/20H DEGREES OF FREEDOM=I4/
65H PSA=E14.6)

WRITEOUTPUTTAPE9,113,A,C0,ON,C1,AW,C2,R,DIST,T1,
1DELAY,H0,B0,B1,IMN,IO,IM,M,KI,ITMAX,SUSQ,IDF,PSA

L2=L1

GOTO5

END
```

FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM

```
C      SEA 1910  AREA ANALYSIS OF TRANSMISSION DATA
COMMONSXI,ETA,U,V,GN,EN,G,EL,IO,IM,SIGMAT,T,ZTZ,ZTT,IRO,IRN,J,I,
1SIGMAE,A,ON,AW,R,DIST,T1,DELAY,H0,ONSIGP,TM,AM,IT,
2SIGTC,SIGT1,SIGT2,SIGT3,B0,B1,R0,R1,PSA,TA,AC
DIMENSIONGN(20),EN(20),G(20),EL(20),IRO(21),IRN(20),SIGMAT(20),T(2
1048),ZTZ(3,3),ZTT(3),SIGMAE(5),TM(20),AM(20,20),
2SIGTC(500),SIGT1(500),SIGT2(500),SIGT3(500),TA(2048),AC(2048)
1 FORMAT(50H1AREA ANALYSIS OF TRANSMISSION DATA          JOB 1910 /
14HORUN1A6)

23 FORMAT(85H0  C1      C2      GAMMA      CO      EO
1 FGXGAMMA N 0 SA FGXGAMMA N 0)
2 FORMAT(I6,2A6)
L2=0
X=FPTRPF(0,-1)
3 READ INPUT TAPE 10,2,L1,L1A,LE
IF(L1)4,4,5
4 CALL NOPLOT
CALL EXIT
5 WRITEOUTPUTTAPE9,1,L1A
6 FORMAT(7I5)
7 FORMAT(2I5,3E12.6)
8 FORMAT(6E12.6)
READ INPUT TAPE 10,6,IMN,IO,IM,M,KI,ITMAX,IC
IF(IC)46,45,46
47 FORMAT(3E12.6)
45 READ INPUT TAPE 10,47,(ZTT(K),K=1,3)
46 READ INPUT TAPE 10,7,(IRU(J),IRN(J),G(J),EL(J),GN(J),J=1,M)
IT=0
```

FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)

```
IF(L1-L2)251,252,251
251 READ INPUT TAPE 10,8,A,UN,AW,R,DIST,T1,DELAY,H0,R0,R1,PSA
      B0=(R0*T1-R1*DELAY)/(72.3*DIST*.8325)
      B1=R1/.8325
      9 FORMAT(6012)
      READ INPUT TAPE 10,9,(T(I),I=1,IMN)
252 VI=(72.3*DIST)**2
260 FORMAT(8H0ELEMENT1A6)
      WRITE OUTPUT TAPE 9,260,LE
      DO15J=1,M
      SIGMAT(J)=0.0
      S10=EL(J)
      EN(J)=VI/(S10*T1+DELAY)**2
      IROJ=IRO(J)
      IRNJ=IRN(J)
      DO10I=IROJ,IRNJ
      SIGMAT(J)=T(I)+SIGMAT(J)
10 CONTINUE
      IF(GN(J))12,11,15
12 CALL ERROR
11 ILJ=EL(J)
      EI=EN(J)
      BI=B1*EI+B0*(EI**1.5)
      DELTA=H0*SQRTF(EI/AW)
      GNJ=.62+.66*SQRTF(DELTA*A*DELTA+BI*BI)/G(J))
      TIROJ=T(IROJ)
      TIRNJ=T(IRNJ)
      IF(TIROJ-TIRNJ)17,17,18
```

FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)

```
18 TIRNJ=TIROJ  
17 TILJ=T(ILJ)  
    IF(TILJ)13,13,14  
13 TILJ=0.001  
    GO TO 16  
14 IF(TILJ-0.001)13,16,16  
16 GN(J)=-((SQRTF(EN(J)))*G(J)*(LOGF(TILJ)-LOGF(TIRNJ))/(ON*  
12.608E6))*(GNJ)  
15 CONTINUE  
SIGP=12.566368*R*R  
ONSIGP=EXP(-ON*SIGP)  
COM1=SQRTF(AW)/HO  
COM4=A*2.86239E3  
SIG=(-2.0*ON*1.7724538)  
DO20K=1,5  
SIGMAE(K)=0.0  
20 CONTINUE  
IRO(M+1)=IM  
M1=M+1  
IF(IC)21,48,21  
21 DO25J=1,M1  
    IF(J-1)26,27,28  
26 CALL ERROR  
27 IRNJ1=IO  
    GOTO29  
28 IRNJ1=IRN(J-1)  
    M2=J-1  
    DO 36 J1=1,M2
```

FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)

```
IF( IRNJ1-IRN(J1))35,36,36
35 IRNJ1=IRN(J1)
36 CONTINUE
29 IROJ=IRO(J)
IF( IROJ-IRNJ1-1)25,25,30
30 DO33I=IRNJ1,IROJ
S10=I
SE=(S10*T1+DELAY)/(72.3*DIST)
SIGMAE(1)=SIGMAE(1)+1.0
E=SE**2
SIGMAE(2)=SIGMAE(2)+SE
SIGMAE(3)=SIGMAE(3)+E
SIGMAE(4)=SIGMAE(4)+SE*E
SIGMAE(5)=SIGMAE(5)+E*E
33 CONTINUE
25 CONTINUE
DETNEI=((SIGMAE(3))**IC)*1.0E-6
19 DO40L=1,IC
DO40N=1,IC
K=L+N-1
ZTZ(L,N)=SIGMAE(K)
40 CONTINUE
DO41L=1,3
ZTT(L)=0.0
41 CONTINUE
DO50J=1,M1
IF( J-1)51,52,53
51 CALL ERROR
```

FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)

```
52 IRNJ1=I0
      GOTO54
53 IRNJ1=IRN(J-1)
      M2=J-1
      DO 34 J1=1,M2
      IF(IRNJ1-IRN(J1))37,34,34
37 IRNJ1=IRN(J1)
34 CONTINUE
54 IROJ=IRO(J)
      IF(IROJ-IRNJ1-1)50,50,55
55 D057I=IRNJ1,IROJ
      S10=I
      SE=(S10*T1+DELAY)/(72.3*DIST)
      E=VI/(S10*T1+DELAY)**2
      EI=6.52E5*SE
      GE=0.0
      D056K=1,M
      ENE=EN(K)-E
      GE=GE+(GN(K)*(EI*G(K)-5.72478E3*ENE*A)/(ENE**2+(G(K)/2.0)**2))
56 CONTINUE
      TE=T(I)*EXP(ON*(SIGP+GE))
      ZTT(1)=ZTT(1)+TE
      IF(IC-1)702,57,700
700 ZTT(2)=ZTT(2)+(TE*SE)
      IF(IC-2)702,57,701
702 CALL ERROR
701 ZTT(3)=ZTT(3)+(TE/E)
57 CONTINUE
```

FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)

```
50 CONTINUE  
IF(IC-1)93,301,300  
301 ZTT(1)=ZTT(1)/ZTZ(1,1)  
GO TO 48  
300 LA=XLOCF(ZTZ(1,1))  
LB=XLOCF(ZTT(1))  
IA=XLOCF(ZTZ(1,1))-XLOCF(ZTZ(1,2))  
IB=XLOCF(ZTT(1))-XLOCF(ZTT(2))  
DET=MATEQDF(LA,LB,IC,1,IA,IB)  
IF(DET)514,514,715  
715 IF(DET-DETNEI)514,514,48  
513 FORMAT(6H0 DET=E14.6)  
514 WRITE OUTPUT TAPE 9,513,DET  
GO TO 106  
48 DIF=0.0  
IMAX=0  
D070 J=1,M  
IROJ=IRO(J)  
IRNJ=IRN(J)  
TM(J)=0.0  
D075 JJ=1,M  
AM(J,JJ)=0.0  
75 CONTINUE  
S10=IROJ  
EIROJ=VI/(S10*T1+DELAY)**2  
S10=IRNJ  
EIRNJ=VI/(S10*T1+DELAY)**2  
EIROJ=EIROJ+(4.0*(B1*EIROJ+B0*(EIROJ**1.5)))
```

FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)

```
EIRNJ=EIRNJ-(4.0*(B1*EIRNJ+B0*(EIRNJ**1.5)))

INT=((SQRTF(VI/EIRNJ)-SQRTF(VI/EIROJ))/T1)

INT=INT*KI

IF((INT/2)*2-INT)77,78,76

76 CALL ERROR

77 INT=INT+1

78 EINT=INT

H=(EIROJ-EIRNJ)/EINT

Y=EIRNJ

HH=H*H

HH2=HH+HH

H31=(H/2.0)

H32=H

INT1=INT+1

DO80IJ=1,INT1

CON=1.0/SQRTF(Y)

COM2=1.0/(COM1*2.0*Y)

COM3=COM1*CON

SIGMA=SIG*COM3

CON=6.52E5*CON

COM2=6.52E5*COM2

SUMJ=0.0

DO84JY=1,M

SXI=COM3*(Y-EN(JY))

ETA=COM3*G(JY)/2.0

CALLPFCN

SOM=(CON+COM2*SXI)*U-(COM2*ETA-COM4)*V

SUMJ=SUMJ+GN(JY)*SOM
```

FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)

```
IF(J-1)81,82,83
 81 CALL ERROR
 83 IF(JY-(J-1))84,85,82
 85 F1=SIGMA*SOM
    GOTO84
 82 IF(JY-J)84,88,89
 88 F2=SIGMA*SOM
    GOTO84
 89 IF(JY-(J+1))84,87,84
 87 F3=SIGMA*SOM
 84 CONTINUE
    ONE=EXPF(SIGMA*SUMJ)
 67 SIGTC(IJ)=ONE
    SIGT1(IJ)=ONE*F1
    SIGT2(IJ)=ONE*F2
    SIGT3(IJ)=ONE*F3
    Y=Y+H
 80 CONTINUE
    IMAX=IMAX+IRNJ-IR0J+1
    DO90I=IR0J,IRNJ
      S10=I
      EI=VI/(S10*T1+DELAY)**2
      BI=B1*EI+B0*(EI**1.5)
      BI2=BI*BI
      CI=ZTT(1)
      IF(IC-1)303,304,303
 303 CI=CI+(ZTT(2)/(SQRTF(EI)))
      IF(IC-2)305,304,305
```

FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)

```
305 CI=CI+(ZTT(3)/EI)
304 ACI=CI*ONSIGP
    CI=CI/(BI*1.772454)
    EIRO=4.0*BI
    EIRN=EI-EIRO
    EIRO=EI+EIRO
    IN=(EIROJ-EIRN)/H
    SIN=IN
    EIRN=EIROJ-SIN*H
    INT=(EIRO-EIRN)/H
    IF((INT/2)*2-INT)401,402,400
400 CALLERROR
401 INT=INT-1
402 IJS=INT1-IN
    IJM=IJS+INT
    EA=EXP(-(EI-EIRN)/BI)**2)
    EAH=EXP((2.0*(EI-EIRN)*H-HH)/BI2)
    EHH2=EXP(-HH2/BI2)
    TM1=0.0
    AM1=0.0
    AM2=0.0
    AM3=0.0
    DO 95 IJ=IJS,IJM
    IF(IJS-IJ)68,64,86
86 CALL ERROR
64 ONE=EA*H31
    GO TO 407
68 IF(IJ-IJM)406,64,86
```

FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)

```
406 ONE=EA*H32
407 TM1=TM1+SIGTC(IJ)*ONE
IF(J-1)93,92,91
91 AM1=AM1+SIGT1(IJ)*ONE
92 AM2=AM2+SIGT2(IJ)*ONE
AM3=AM3+SIGT3(IJ)*ONE
EA=EA*EAH
EAH=EAH*EHH2
95 CONTINUE
TM(J)=TM(J)+TM1*CI
TM1=TM1*CI*ONSIGP
IF(J-1)93,96,97
97 AM(J,J-1)=AM(J,J-1)+AM1*CI
96 AM(J,J)=AM(J,J)+AM2*CI
IF(J+1-M)110,110,112
110 AM(J,J+1)=AM(J,J+1)+AM3*CI
112 TA(I)=TM1
AC(I)=ACI
90 CONTINUE
TM(J)=SIGMAT(J)-ONSIGP*TM(J)
IF(J-1)93,98,99
99 AM(J,J-1)=ONSIGP*AM(J,J-1)
98 AM(J,J)=ONSIGP*AM(J,J)
IF(J+1-M)111,111,70
111 AM(J,J+1)=ONSIGP*AM(J,J+1)
70 CONTINUE
DO 800 JR=1,M
SRJ=IRN(JR)-IRO(JR)+1
```

FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)

```
SRJ=SQRTF(SRJ)
IF(ABSF(TM(JR))-0.005*PSA*SRJ)800,800,100
93 CALL ERROR
800 CONTINUE
GO TO 504
100 IF(IT>ITMAX)101,501,501
101 IT=IT+1
IF(M>1)93,107,108
107 TM(1)=TM(1)/AM(1,1)
GOTO109
108 LA=XLOCF(AM(1,1))
LB=XLOCF(TM(1))
IA=XLOCF(AM(1,1))-XLOCF(AM(1,2))
IB=XLOCF(TM(1))-XLOCF(TM(2))
DET=MATEQF(LA,LB,M,1,IA,IB)
109 DO102J=1,M
GN(J)=GN(J)+TM(J)
102 CONTINUE
DO 270 J=1,M
IF(GN(J))271,270,270
270 CONTINUE
IF(IC)19,48,19
271 DO 272 J=1,M
GN(J)=GN(J)-TM(J)
272 CONTINUE
IT=IT-1
273 FORMAT(17H0 DELTA GAMMA N 0)
274 FORMAT(31H0 STOPPED ON NEGATIVE GAMMA N 0)
```

FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)

```
275 WRITE OUTPUT TAPE 9,274
276 WRITE OUTPUT TAPE 9,273
277 WRITE OUTPUT TAPE 9,278,(TM(J),J=1,M)
278 FORMAT(1E14.6)

      GO TO 504

500 FORMAT(41HU STOPPED ON MAXIMUM NUMBER OF ITERATIONS)

501 WRITE OUTPUT TAPE 9,500

      GO TO 504

504 ICP=(I0/100)

      DO505J=1,M
      IROJ=IRO(J)
      IRNJ=IRN(J)
      DO506I=IROJ,IRNJ
      IF(I-(ICP*100))224,224,200
200 ICP=ICP+1
264 CALL CALCNH(L1A)

259 GO TO(201,202,203,204,205,206,207,208,209,210,211,212,213,214,
1215,216,217,218,219,220,221),ICP

201 ICON=0
      CALL TITLE(48HAREA ANALYSIS CH(0-100) JOB 1910 )
      GO TO 222

202 ICON=100
      CALL TITLE(48HAREA ANALYSIS CH(100-200) JOB 1910 )
      GO TO 222

203 ICON=200
      CALL TITLE(48HAREA ANALYSIS CH(200-300) JOB 1910 )
      GO TO 222

204 ICON=300
```

**FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)**

```
CALL TITLE(48HAREA ANALYSIS CH(300-400) JOB 1910 )
GO TO 222

205 ICON=400

CALL TITLE(48HAREA ANALYSIS CH(400-500) JOB 1910 )
GO TO 222

206 ICON=500

CALL TITLE(48HAREA ANALYSIS CH(500-600) JOB 1910 )
GO TO 222

207 ICON=600

CALL TITLE(48HAREA ANALYSIS CH(600-700) JOB 1910 )
GO TO 222

208 ICON=700

CALL TITLE(48HAREA ANALYSIS CH(700-800) JOB 1910 )
GO TO 222

209 ICON=800

CALL TITLE(48HAREA ANALYSIS CH(800-900) JOB 1910 )
GO TO 222

210 ICON=900

CALL TITLE(48HAREA ANALYSIS CH(900-1000) JOB 1910 )
GO TO 222

211 ICON=1000

CALL TITLE(48HAREA ANALYSIS CH(1000-1100) JOB 1910 )
GO TO 222

212 ICON=1100

CALL TITLE(48HAREA ANALYSIS CH(1100-1200) JOB 1910 )
GO TO 222

213 ICON=1200

CALL TITLE(48HAREA ANALYSIS CH(1200-1300) JOB 1910 )
```

FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)

GO TO 222

214 ICON=1300

CALL TITLE(48HAREA ANALYSIS CH(1300-1400) JOB 1910 )

GO TO 222

215 ICON=1400

CALL TITLE(48HAREA ANALYSIS CH(1400-1500) JOB 1910 )

GO TO 222

216 ICON=1500

CALL TITLE(48HAREA ANALYSIS CH(1500-1600) JOB 1910 )

GO TO 222

217 ICON=1600

CALL TITLE(48HAREA ANALYSIS CH(1600-1700) JOB 1910 )

GO TO 222

218 ICON=1700

CALL TITLE(48HAREA ANALYSIS CH(1700-1800) JOB 1910 )

GO TO 222

219 ICON=1800

CALL TITLE(48HAREA ANALYSIS CH(1800-1900) JOB 1910 )

GO TO 222

220 ICON=1900

CALL TITLE(48HAREA ANALYSIS CH(1900-2000) JOB 1910 )

GO TO 222

221 ICON=2000

CALL TITLE(48HAREA ANALYSIS CH(2000-2100) JOB 1910 )

222 CALL CRT(100.0,0.0,10.0,1.1,-.1,0.1,

142H0 1 2 3 4 5 6 7 8 9 10,

242H-.1 0 .2 .4 .6 .8 1.0 ,

348HWRONG TITLE ,

FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)

```
412HCHANNEL      ,
512HTRANSMISSION)
ICP1=(ICP-1)*100+1
ICP2=ICP*100
DO223ICT=ICP1,ICP2
AICT=ICT-ICON
241 CALL PLOT(AICT,T(ICT),4)
223 CONTINUE
224 AI=I-ICON
243 CALL PLOT(AI,TA(I),5)
CALL PLOT (AI,AC(I),1)
506 CONTINUE
505 CONTINUE
DO 750J=1,M
C2C1=IRN(J)-IRO(J)+1
SIGMAT(J)=(PSA*(.01))*(SQRTF(C2C1))/ABSF(AM(J,J))
750 CONTINUE
GO TO 106
105 FORMAT(24HO NUMBER OF ITERATIONS I2)
106 WRITEOUTPUTTAPE9,105,IT
WRITEOUTPUTTAPE9,23
24 FORMAT(1H02I6,5E14.6)
WRITEOUTPUTTAPE9,24,(IRO(J),IRN(J),G(J),EL(J),EN(J),GN(J),SIGMAT
1),J=1,M)
113 FORMAT(3HOA=E12.5,23H          KO=E14.6/3H N=E12.5,
123H           K1=E14.6/4H AW=E12.5,22H
2K2=E14.6/3H R=E12.5/6H DIST=E12.5/
33H T=12.5/9H T DELAY=E12.5/4H D0=E12.5/4H B0=E12.5/
```

**FORTRAN LISTING FOR AREA-ANALYSIS PROGRAM (continued)**

```
44H B1=E12.5/4H CN=I4/4H CF=I4/4H CL=I4/4H NO=I4/
54H IF=I4/4H IM=I4/3H K=I4/4H R0=E12.5/4H R1=E12.5/5H PSA=E12.5)
      WRITE OUTPUT TAPE 9,113,A,ZTT(1),ON,ZTT(2),AW,ZTT(3),R,DIST,T1,
      IDELAY,HU,B0,B1,IMN,IO,IM,M,KI,ITMAX,IC,R0,R1,PSA
      L2=L1
      GO TO 3
      END
```



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