THE EVALUATION OF MINIMA IN TOTAL NEUTRON CROSS-SECTION
BY TRANSMISSION OF FISSION SPECTRA THROUGH THICK SAMPLES

by 6-9/

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Major Professor
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1.0 INTRODUCTION

Total neutron cross-section data is available from many sources and reasonable agreement is found between independently determined cross-section tables. However, small discrepancies in the minima of integral cross-section data lead to large errors in transport calculations involving deep penetration. An error of a few percent in the cross-section data can approach an order of magnitude error in transmitted spectrum through a thick sample (ten or more mean free paths). To determine the reliability of literature data the neutron cross-section has been experimentally evaluated by measuring the uncollided neutron spectra transmitted through thick samples. Experimental data were compared to a calculated transmitted spectrum determined as a function of the spectrum, the resolution of the detector, and the particular cross-section data being tested. Since thick samples (three or more mean free paths) were used, the experimental versus calculated analysis is very sensitive to minima in the cross-section.

In this work, total neutron cross-sections were evaluated for iron, lead, liquid oxygen, solid sodium and liquid sodium. The incident neutron spectra for these measurements were obtained from the fast (northeast) beam port of the K.S.U. Triga Mark II reactor and the transmitted neutron spectra were detected with an NE-213 fast neutron spectrometer system. Data were collected with a TMC 4096 Multiparameter Analyzer and the results were unfolded with a suitable computer code.
THIS BOOK CONTAINS NUMEROUS PAGES WITH DIAGRAMS THAT ARE CROOKED COMPARED TO THE REST OF THE INFORMATION ON THE PAGE. THIS IS AS RECEIVED FROM CUSTOMER.
2.0 THEORY

The theoretical basis for this experiment is similar to that applied in the transmission method of cross-section determination. A collimated beam of neutrons striking, perpendicularly, a specified area of a material of thickness \( x \) will be attenuated. Considering a thin layer of thickness \( dx \) parallel to the surface and recalling the definition of cross-section, it follows that \( \Sigma T dx \) is the fraction of neutrons that will interact with the material. This fraction may be set equal to \(-dI/I\) which is the fractional decrease in the neutron beam as the result of passing through thickness \( dx \).

Thus,

\[
- \frac{dI}{I} = \Sigma T dx
\]

Integration over the thickness \( x \) of the material gives,

\[
I_x = I_0 \exp(-\Sigma T x)
\]

where \( I_0 \) = number of incident neutrons/cm\(^2\)

\( I_x \) = number of neutrons/cm\(^2\) left at thickness \( x \)

\( \Sigma T \) = total neutron cross-section
Recalling that this experiment dealt with neutron fluxes as a function of energy, equation 2 can be rewritten as:

\[
\phi_{\text{trans}}(E) = \phi_I(E) \exp[-\Sigma_t(E)t]
\]  

(3)

where \(\phi_I\) = incident flux \((n/cm^2\cdot\text{min} \cdot \text{MeV})\)

\(\phi_{\text{trans}}\) = transmitted flux \((n/cm^2\cdot\text{min} \cdot \text{MeV})\)

\(\Sigma_t\) = total cross-section

The quantities \(\phi\) and \(\Sigma_t\) are now functions of energy.

In this experiment very large thicknesses (three or more mean free paths) were used causing the argument of the exponential term in equation 3 to be large. Any variation in the total cross-section, \(\Sigma_t\), would produce an exponential variation in the transmitted flux. This becomes especially apparent for minima in the cross-section. For a given material of thickness \(t\) and some mean cross-section \(\overline{\Sigma}_t\), equation 3 becomes:

\[
\frac{\phi_{\text{trans}}}{\phi_I} = \exp(-\overline{\Sigma}_t t)
\]  

(4)

Now, if there is a minima in the cross-section at some energy such that the cross-section is reduced by some fraction \(k\) \((k<1)\) of the mean value, then:

\[
[\frac{\phi_{\text{trans}}}{\phi_I}]_{\text{minima}} = \exp[-(1-k)\overline{\Sigma}_t t]
\]  

(5)

Likewise, for a maxima in the cross-section resulting in an increase in the cross-section by the same fraction \(k\) of the mean value, then:

\[
[\frac{\phi_{\text{trans}}}{\phi_I}]_{\text{maxima}} = \exp[-(1+k)\overline{\Sigma}_t t]
\]  

(6)

The fractional change in the transmitted flux, obtained by dividing equation 5 and equation 6 by equation 4, is given by:
fractional change for minima = \( \exp(k\Sigma t) \) \( (7) \)

fractional change for maxima = \( \exp(-k\Sigma t) \)

These two functions are plotted in Fig. 2 and, as can be seen, the resultant change in the transmitted flux at a minima increases greatly for large thicknesses whereas the corresponding change in the transmitted flux at a maxima is small. Therefore, by using large thicknesses in the experiment, the sensitivity to minima becomes great. When the experimental results are compared to the corresponding calculated results, large errors in the transmitted spectrum will appear for small errors in the minima of total cross-section.

If a detection system with infinite resolution was used, the experimentally measured transmitted spectrum could be directly compared to the transmitted spectrum calculated by equation 3. However, the actual resolution of the spectrometer system must be included to "smooth" the calculated spectrum as the experimentally measured spectrum is "smoothed" by the measuring system. The transmitted spectrum can be calculated as:

\[ \phi_{\text{trans}}(E) = \int_0^\infty \phi_I(E') \exp[-E_t(E')t]R(E,E')dE' \] \( (8) \)
where $\phi_1(E')$ = incident flux at energy $E'$

$$\Sigma_t = \text{total neutron cross-section at } E'$$

$R(E,E') = \text{probability of a neutron of energy } E' \text{ being detected at energy } E.$

Based upon the unfolded responses of the detection system to mono-energetic neutrons, it can be seen that the resolution function $R(E,E')$ is of the form of a gaussian:

$$R(E,E') = \gamma_o(E) \exp\left[-\frac{(E-E')^2}{b_o(E)}\right]$$

(9)

where $\gamma_o = \frac{1}{\sqrt{b_o \pi}}$, which normalizes the function $R(E,E')$

such that $\int R(E,E') \, dE' = 1$

$E = \text{neutron energy detected}$

$E' = \text{actual neutron energy}$

$b_o = (\text{FWHM})^2/4 \cdot \ln(2)$, where FWHM is the full width at half maximum of the gaussian.

Experimental measurements$^1,23$ have been made to determine $R(E,E')$ at several energies $E$. These measurements actually give the probability of neutrons of energy $E$ being detected at $E'$, but since the detection system cannot discriminate between neutrons of energy $E$ and $E'$ (within the probability given by this function) it is assumed that neutrons of $E'$ have an equal probability of being detected at $E$.

If it is assumed that $\phi_1(E')$ and $\Sigma_t(E')$ have values at discrete energy points $E_i$, then the integral of equation 8 can be integrated piecewise from $E_i$ to $E_{i+1}$, from $E_{i+1}$ to $E_{i+2}$, etc. If it is also assumed that the log ($\phi_1$) is linear between energy points and that $\Sigma_t(E')$ is linear between energy points, then equation 8 can be integrated into the exact form:
\[ \phi_{\text{trans}}(E) = \sum_{i=1}^{\infty} \left\{ \frac{1}{2} \exp \left[ \text{erf} \left( \frac{\Sigma_{i+1} - \Sigma_i}{E_{i+1} - E_i} \right) \right] \right. \\
\left. \left[ \text{erf} \left( \frac{\Sigma_{i+1} - \Sigma_i}{E_{i+1} - E_i} \right) + \text{erf} \left( \frac{\Sigma_i - \Sigma_i}{E_{i+1} - E_i} \right) \exp \left[ \frac{\ln \phi_{i+1}^i - \ln \phi_i^i}{E_{i+1} - E_i} \right] \right] \right\} \right\}

\]

\[ \left\{ \phi_{i}^i \left[ \text{erf} \left( y_{i+1} \right) - \text{erf} \left( y_i \right) \right] + \left[ \text{erf} \left( z_{i+1} \right) - \text{erf} \left( z_i \right) \right] \exp \left[ \frac{\ln \phi_{i+1}^i - \ln \phi_i^i}{E_{i+1} - E_i} \right] \right\} \]

where \( \phi_i^i \) is the incident flux at \( E_i \)

\( E_i \) = cross-section at \( E_i \)

\[ y_i = \frac{1}{\sqrt{b_o}} \left| E_i - E + \frac{b_o \left( \Sigma_{i+1} - \Sigma_i \right)}{2 \left( E_{i+1} - E_i \right)} \right| \]

\[ z_i = \frac{1}{\sqrt{b_o}} \left| E_i - E + \frac{b_o \left( \Sigma_{i+1} - \Sigma_i \right)}{2 \left( E_{i+1} - E_i \right)} - \frac{b_o \left( \ln \phi_{i+1}^i - \ln \phi_i^i \right)}{2 \left( E_{i+1} - E_i \right)} \right| \]

The experiment was performed using several different experimental geometries. For the first condition the detector was placed as far from the beam port as possible (approximately 128 inches). In this case it was assumed that any interaction of a neutron with the sample would either result in absorption or in scattering at an angle larger than the solid angle subtended by the detector. If this assumption is true, only those neutrons that are uncollided will be detected resulting in a true measure of the total cross-section. However, two phenomenon can occur which will cause an error in this measurement. If there is a large probability for forward scattering in the sample, it is possible that neutrons scattering at small angles will reach the detector. To reduce this error a collimator was used directly in front of the detector to reduce its effective area. Thus, those neutrons scattered at shallow angles (solid angles greater than \( 7.5 \times 10^{-4} \) steradians) were removed by the collimator. Neutrons scattered
at 0° to the solid angle subtended between sample and detector could be present. Finally, there is a probability that neutrons will be scattered several times in a thick sample and some of these will be scattered back into the solid angle subtended by the detector. In this case, the end of the sample nearest the detector will be fully "illuminated" with neutrons, some of which will be scattered toward the detector. To study this effect, the collimator was placed against the sample, with the detector in the same position as before. With this latter geometry the area of the end of the sample viewed by the detector was smaller than that viewed with the collimator positioned next to the detector and thus a smaller number of multiple scattered neutrons would be expected to be detected.
3.0 EXPERIMENTAL FACILITIES AND EQUIPMENT

3.1 Neutron Source

The northeast fast beam port ("C") of the 250 kW K.S.U. Triga Mark II reactor was used as the source of fast neutrons. This radial beam port is aligned with a cylindrical void in the core reflector graphite as shown in Fig. 3, and is nominally 8 inches in diameter at the reactor face. It is fitted with a lead and borated paraffin 1-1/4 inch square collimator (Fig. 4). The neutron beam from this beam port diverges slightly to approximately five inches by five inches at the reactor bay wall 146 inches from the face of the beam port and is well defined even at this distance. Since there is little material in the path of neutrons coming from the core, the spectrum is essentially a fission spectrum with sufficient neutrons for experimental measurement up to 12 MeV. A 2 inch long bismuth plug inserted in the end of the collimator reduces the gamma background while leaving the neutron spectrum essentially unaffected.

3.2 Neutron Detection System

Neutrons were detected with a proton recoil NE-213 liquid scintillator spectrometer. Fast neutrons produce both neutron-hydrogen and neutron-carbon interactions which are subsequently detected and amplified by a photomultiplier tube. Unfortunately NE-213 responses are not limited to neutron interactions; gamma rays produce electrons in the scintillator which are also detected and amplified. It is possible, however, to electronically distinguish between pulses caused by neutron and gamma ray interactions.

The K.S.U. NE-213 detector and tube base Forte gamma ray discrimination circuit are shown in Fig. 5. The pulse shape discrimination (PSD) output from the Forte circuit is a timing pulse which makes it possible to eliminate the gamma ray pulses. After additional pulse shaping this pulse
Figure 3  KSU TRIGA reactor core, reflector and beam port assembly.
Figure 4  Internal construction of KSU TRIGA beam port collimator.
Figure 5  KSU Gamma Ray Pulse Shape Discrimination Circuit
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is used in coincidence with the linear signal as shown in a block diagram of the NE-213 fast neutron spectrometer electronics in Fig. 6. (A description of the design and operating characteristics of the K.S.U. NE-213 fast neutron spectrometer system can be found in a report by Meyer, "Intercalibration of the K.S.U. Fast-Neutron Spectrometer System."\textsuperscript{16})

The resolution of the K.S.U. NE-213 system has been measured by Simons.\textsuperscript{23} Verbinski made similar measurements on another NE-213 detection system at ORNL.\textsuperscript{1} Both of these measurements were analyzed by unfolding the measured monoenergetic neutron response functions with the ORNL FERDOR code. The width of the approximately gaussian peak in the unfolded spectrum gave a measure of the resolution for that particular energy. This resolution was actually the resolution of the combined detection and unfolding processes at that energy.

3.3 Multiparameter Analyzer

A TMC-4096 Multiparameter Analyzer was used to measure the signals coming from the detection system with the resultant data stored in the memory. Readout options included paper tape, magnetic tape and omnigraphic plotter. The magnetic tape was converted directly to cards at the K.S.U. IBM 360-50 facility.

3.4 Sample Containers

For the experimental measurements involving liquid oxygen and sodium, special sample containers were fabricated in K.S.U. shops. The aluminum liquid oxygen container is shown in Fig. 7. It was of double-walled construction with the space between the inner and outer boxes filled with vermiculite insulation. Vermiculite is known for its inert, as well as insulating, properties. During an experiment the container was filled from the top to replace oxygen lost by evaporation.
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THIS IS THE BEST COPY AVAILABLE
Figure 6  Block Diagram of the KSU NE-213 Fast-Neutron Spectrometer System
The container for solid sodium was fabricated from stainless steel. The sodium was cast into this container under an inert atmosphere and then the container was sealed. After sealing there was no problem in handling the sodium. The liquid sodium container (Fig. 8) like the oxygen container was also double walled but in this case fabricated from stainless steel. The inner box was wrapped with resistance heating wire to permit heating the sodium sample above the melting point during an experiment. Thermocouples were welded to the container wall to monitor the sodium temperature. Vermiculite was again used as insulation. The inner box was vented into the outer container to allow for the expansion of the sodium during heating. When heated, an inert gas (nitrogen) was constantly passed through the container to reduce oxidation at the sodium-air interface.

3.5 Collimator and Shadow Shield

The neutron collimator was made of methyl methacrylate and was 3 inches by 3 inches by 24 inches long with a .318 inch square hole lengthwise through the center. By placing this collimator directly in front of the detector, the effective area of the detector was reduced to .101 square inches. This particularly sized collimator was used to duplicate the geometry used by Straker in a similar experiment at ORNL.26 By using the collimator the solid angle subtended by the effective detector area was the same as the solid angle subtended by Straker's detector which was placed 50 feet from the sample.

When the collimator was not used directly in front of the detector, a shadow shield was used for background measurements. This shield is an aluminum cylinder approximately 2.5 inches I.D. and 24 inches long and is filled with water. For background measurements in experiments where the collimator was used, the ends were sealed and the void was filled with water.
4.0 EXPERIMENTAL PROCEDURE

4.1 Equipment Calibration

The basic procedure for obtaining a neutron spectrum was the same for all experimental runs. This basic procedure established the detection system parameters, the maximum reactor power and the integrated reactor flux.

4.1.1 Calibration of the detection system - After a twelve hour warm-up period for the NE-213 system, several parameters were checked and adjusted to insure proper response. First, a $^{60}$Co gamma-ray spectrum was taken and the extrapolated Compton tail was used to set the energy gain. The gamma rejection ratio was set at >150:1 using the $^{60}$Co source; that is, less than one gamma-ray in 150 was counted. The efficiency of the system was also checked using the $^{60}$Co source. A one hour PuBe spectrum was measured with the gamma rejection circuit operative. This test spectrum was compared to a standard complex PuBe spectrum to insure that the system was working properly. A $^{60}$Co spectrum was again taken immediately before or after each experimental spectrum to reestablish the gain and gamma rejection ratio.

4.1.2 Maximum total flux at the detector. - Due to the sensitivity of the Forte circuit and photomultiplier tube to radiation, the total radiation at the detector was kept below 3 mrem/hr. When the detection system is operative in the anticoincidence mode a 10% dead time on the TMC 4096 corresponds roughly to 3 mrem/hr at the detector. Thus, the 10% dead time was used to establish the maximum reactor power for all experimental runs.

4.1.3 Integrated flux monitor - Nickel foils were activated in the central thimble of the Triga to monitor the integrated flux during an experimental run. Nickel-neutron interactions produce $^{58}$Co which decays,
emitting gamma-rays:

\[ \text{Ni} + n \rightarrow p + ^{58}\text{Co} \]

\[ ^{58}\text{Co} \xrightarrow{72\text{ day}} \gamma + \beta^+ + ^{58}\text{Fe} \]

The total number of counts in the 0.811 MeV photoelectric peak of the \(^{58}\text{Co}\) is directly proportional to the integrated flux. (It should be noted that one set of data reported in this work used sulfur as a flux monitor. However, all other experiments used nickel since it has proven to be a more accurate monitor.)

4.2 Neutron Spectrum Measurements

For all spectral measurements the detector, sample, shadow shield and collimator were placed on the centerline of the neutron beam. The detector was placed as far from the reactor as possible, or approximately 136 inches from the face of the beam port. All samples were placed so that the leading edge was flush with the beam port face except for the Pb sample which, because of its shape, could be placed inside the lip of the beam port collimator. When the shadow shield or collimator was used, it was placed as close to the detector as possible.

The experimental arrangement for collecting data without the collimator is shown in Fig. 9. To measure incident spectra the sample was removed or the empty sample container was placed in the beam. The background measurement for an incident spectrum measurement was obtained by placing the shadow shield directly in front of the detector. Foreground and background penetration (transmitted) spectra were collected in a manner similar to that described above except the sample was in place.

Figure 10 shows the geometry of the experimental measurements involving the use of the collimator at the detector. A surveyor's transit was used to insure proper alignment of the collimator and detector with the neutron
FIGURE 9
Experimental Geometry
No Collimator

Concrete Block Wall
(4 feet thick)

Detector

Borated Parafin Blocks
(6" thick)

Scale
0 1' 2'

Beam Port
Sample
Reactor
FIGURE 10
Experimental Geometry Collimated at Detector

Concrete Block Wall (4 feet thick)

Detector

Collimator

Borated Parafin Blocks (6" thick)

Sample

Beam Port

Reactor

Scale

0 1' 2'
beam. Again both foreground and background measurements were made for both incident and penetration spectra, the background being obtained by sealing the end of the collimator and filling the collimator void with water.

One additional measurement was taken with the collimator next to the sample as shown in Fig. 11. The shadow shield was again used in front of the detector for background measurements.
FIGURE 11
Experimental Geometry
Collimated at Sample

Concrete Block Wall
(4 feet thick)

Detector

Borated Parafin Blocks
(6" thick)

Collimator

Iron Sample

Beam Port

Reactor

Scale

0 1' 2'
5.0 DATA ANALYSIS

5.1 Data Handling

After several spectra were measured, the raw data in the memory of the TMC 4096 were read onto magnetic tape; the tape was subsequently processed to obtain punched cards. A computer code, NUDASBIN, compiled this raw data using the $^{60}$Co spectrum, the Ni foil data, and the foreground and background measurements. NUDASBIN treated the raw data using the $^{60}$Co data to normalize the raw data with respect to energy. Background subtraction was performed after an integrated flux normalization of the background to the foreground using the Ni foil measurement. The resultant complex spectrum was binned for use by the unfolding code. For this work, the complex spectrum was unfolded with the ORNL code FERDOR.

5.2 Calculated Transmitted Spectra

A computer code, CALFLUX, was written to calculate the transmitted spectra using the measured incident spectra, cross-section data and the resolution of the detector as given in equation 8. Input to the code included the normalization factor between the incident and transmitted measurements based on the Ni data.

5.3 System Resolution Analysis

As stated earlier, the resolution of the detector system had been previously measured by two separate experimenters. To use this data in equation 8, the unfolded results of the mono-energetic neutron spectrum measurements of Verbinski were fitted to a gaussian curve by a KSU computer code, NE213RES. The NE213RES results gave the full width at one-half the maximum (FWHM) for each experimental energy. Simons' data had previously been analysed by a similar procedure. Both sets of resolution data were
then fitted to an nth order polynomial by another computer code, POLYFIT. This formulation gave resolution (FWHM) versus energy (MeV) for the entire system (which included both the detector and unfolding resolution).
6.0 RESULTS

The plots of resolution versus energy for the NE-213 spectrometer system are shown in Fig. 12, along with the polynomial fit for this data. Simons' data set is fitted to a 6th order polynomial and Verbinski's data set is fitted to a 7th order polynomial.

All neutron spectra taken for this work are shown in table 1. Table 2 lists some of the sample constants used.

Figure 13 demonstrates the effect of the resolution function on the transmitted spectra. The "unsmoothed" spectrum was calculated at discrete energies by Equation 3 and the "smoothed" spectrum was calculated at the same energies by Equation 8. The data set used was that for an oxygen penetration run. Figure 14 shows a comparison between two different resolution functions for the same oxygen data. In one case Verbinski's data set is used as the resolution function, and in the other case Verbinski's resolution is increased by 25%. The modified resolution function (the one with FWHM decreased by 25%) shows better agreement with the experimental measurements and was therefore used for all subsequent calculations.

A plot of all the incident spectra taken is shown in Fig. 15. Figures 16 and 17 show the comparison between experimental and calculated transmitted (penetration) spectra for Fe and O₂ measured without the collimator present. Figures 18, 19, 20, and 21 show experimental and calculated results for Fe, Pb, O₂ and Na, respectively, measured with the collimator. For the Fe measurement the collimator was placed next to the sample while for all other measurements the collimator was placed next to the detector. Finally, Fig. 22 shows a comparison between the collimated and uncollimated experimental Fe penetration spectra.
<table>
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<td>.94199 x 10⁵</td>
</tr>
<tr>
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<td>&quot;</td>
<td>750 W</td>
<td>.2563 x 10⁵</td>
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<td>O₂ Pene</td>
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<td>20 kW</td>
<td>.242035 x 10⁷</td>
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<td>Collimator at Sample</td>
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<td>.55465 x 10⁵</td>
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<tr>
<td>3-16-71-6</td>
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<td>1.25 kW</td>
<td>.16989 x 10⁶</td>
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<td>3-16-71-9</td>
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<td>Uncollimated</td>
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<td>Collimator at Detector</td>
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<td>&quot;</td>
<td>1.2 kW</td>
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Table 2
Sample Descriptions

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<tr>
<th>Sample</th>
<th>Nominal Size (inches)</th>
<th>Thickness (cm)</th>
<th>$N$ (atom density) (atoms/cm$^3$)</th>
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<tr>
<td>Oxygen</td>
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<td>91.28</td>
<td>0.0403 x 10$^{24}$ *</td>
</tr>
<tr>
<td>Fe</td>
<td>2 x 2 x 6</td>
<td>15.24</td>
<td>0.0849 x 10$^{24}$</td>
</tr>
<tr>
<td>Pb</td>
<td>3 1/2 dia x 9 1/4</td>
<td>23.49</td>
<td>0.033 x 10$^{24}$</td>
</tr>
<tr>
<td>Na (solid)</td>
<td>2 1/2 x 2 1/2 x 36</td>
<td>91.60</td>
<td>0.02541 x 10$^{24}$</td>
</tr>
<tr>
<td>Na (liquid)</td>
<td>2 1/2 x 2 1/2 x 36</td>
<td>91.60</td>
<td>0.02389 x 10$^{24}$ **</td>
</tr>
</tbody>
</table>

*Corrected to account for void space caused by boiling

**At 165°C (taken from Smithalls$^{25}$)
FIGURE 14
VARYING CALCULATED SPECTRA
BY CHANGING RESOLUTION FUNCTION.

- EXPERIMENTAL
- 100\% - FWHM
- 75\% - FWHM
Figure 15
Incident Spectra

Magnitudes are not absolute

Neutron Flux (n/cm² sec MeV)
FIGURE 18
IRON EXPERIMENTAL & CALCULATED PENETRATED SPECTRA COLLIMATOR NEXT TO SAMPLE.

- EXPERIMENTAL
- CALCULATED KFK-1000
- DCL-2
- BNL-325

NEUTRON FLUX (n/cm² min. MeV)

ENERGY (MeV)
FIGURE 20

OXYGEN EXPERIMENTAL &
CALCULATED PENETRATION
SPECTRA (COLLIMATED)

- EXPERIMENTAL
  - CALCULATED (KFK 1000)
  - " (UNC-539)
  - " (DLC-9)
  - " (FOSTER)

NEUTRON FLUX [n/cm² min MeV]

ENERGY (MeV)
FIGURE 21
LIQUID & SOLID SODIUM EXPERIMENTAL & CALCULATED PENETRATED SPECTRA

- EXPERIMENTAL
- CALCULATED KFK 1000
- " BNL - 325
- " HARWELL

NEUTRON FLUX \( \text{[n/cm}^2 \cdot \text{min} \cdot \text{MeV}] \)

ENERGY (MeV)

10^3

10^2

10^1

1
7.0 CONCLUSIONS

7.1 Detector Resolution

As can be seen from Fig. 12, there is reasonable agreement between the two experimental resolution data. Simons' data set shows an unusual effect in that the resolution begins to decrease at approximately 7.5 MeV. This is considered to be an error in his data since there would seem to be no physical phenomenon which would produce this effect. Verbinski's data set does not show this effect in this region and is probably more representative of the actual resolution of the NE-213 detector. However, there is an inflection point in Verbinski's data at 3 MeV which is questionable. The point at 2.3 MeV seems to be in error, causing the resolution in this region to be poorer than that reported by Simons.

In order to check the resolution of the detector system, oxygen was chosen for a penetration measurement. The large minima in the cross-section at 2.35 MeV produces an almost mono-energetic peak at this energy. Therefore, the width of this peak is a good measure of the resolution of the detector. Figure 14 shows a comparison between the experimentally measured and the calculated transmitted spectra for oxygen using the KFK-1000² cross-section data (since this data set seems to best predict the transmitted spectrum in the 2.35 MeV region as shown in Fig. 20) and the Verbinski resolution data. Figure 14 also shows the comparison between the two spectra when the Verbinski resolution was improved by 25% (multiplying the FWHM by 75%). This latter calculation was used for the following reasons:

1) Verbinski's resolution data were taken on another NE-213 detector system at ORNL which does not necessarily have the same resolution as the KSU NE-213 detector, but should have a similar shape as a function of energy.

2) Simons' data show a better resolution in the 2.35 MeV region although the resolution at higher energies is in question.
3) Measurements of Na$^{22}$ and Co$^{60}$ spectra taken at ORNL and Kansas State University show that the KSU system appears to have at least as good, if not better, resolution.

4) The use of Verbinski's resolution data (unchanged) in the calculated transmitted spectrum shows poorer resolution in the 2.35 MeV region than does the experimental measurement. Furthermore, by improving the resolution by 25%, good agreement is found between the experimental and calculated results.

It was concluded that, although the calculated transmitted spectrum is not extremely sensitive to the resolution, improving Verbinski's resolution by 25% best describes the KSU NE-213 system resolution for this calculation and was therefore used on all subsequent calculations. The comparison between the calculated and experimental transmitted spectra for the other materials used in this experiment supports this assumption.

7.2 Energy Calibration

The 2.35 MeV peak in the transmitted oxygen spectrum also provides a check on the energy calibration. As can be seen, all of the calculated and experimental peaks fall between 2.35 and 2.40 MeV indicating that the energy calibration of the system is very accurate.

7.3 Consistency of Experimental Results

Figure 17 shows two experimentally determined transmitted spectra for oxygen. These runs were made to test the consistency of the experimental results, except for a normalization error, the two runs are identical. The normalization error occurred on this run because sulfur was used as a flux monitor. All subsequent runs used the more reliable nickel foils.

7.4 Forward Scattering Assumptions

As was stated in the theory, the first geometry condition (uncollimated) assumed that any forward scattering at shallow angles would miss the solid
angle subtended by the detector. Figure 17 shows such a run for oxygen. Even though there was a small normalization problem, there was a large discrepancy between the experimental and calculated results throughout the energy range. This discrepancy indicates that the experimental measured cross-section was much less than the published data. This result indicates that many neutrons scattered at shallow angles were reaching the detector. This would cause an increase in the experimental result, as shown, and would therefore make the actual cross-section appear too large. Figure 20 shows the same comparison between experimental and calculated results using the second geometry condition (with the collimator placed in front of the detector). The forward scattering problem was virtually eliminated and good agreement was found between the experimental and calculated results.

The total neutron cross-section predicted by the uncollimated case was about 25% lower than the published data. This error is due to forward scattered neutrons which were reaching the detector, but this forward scattering contribution seems very large. Therefore, a mathematical model was used to predict this discrepancy. DLC-2⁴ angular dependent cross-section data set was used with the following assumptions:

1: Any neutron that was scattered at an angle less than the solid angle subtended by the detector was assumed to be unscattered, and therefore, part of the original beam.

2: Any neutron that was scattered at an angle larger than the solid angle subtended by the detector was assumed to be lost from the beam and would not be scattered back into the detector.

3: The probability of neutrons scattering into the solid angle of the detector was equal to the probability of zero angle scattering integrated over the detector solid angle.

Neither of the first two assumptions were entirely valid. Neutrons that were scattered at small angles could be scattered again and miss the detector.
Also, neutrons scattered at large angles could be scattered again back into the solid angle of the detector. However, the discrepancies in these two assumptions tend to cancel each other. Thus, it is possible to predict the transmitted spectrum by:

\[ \phi_{\text{trans}} = \phi_I \exp[-(\Sigma_t - \Sigma_{fs})t] \]  

(11)

where \( \Sigma_{fs} \) is the correction in the total neutron cross-section from forward scattered neutrons which reach the detector. \( \Sigma_{fs} \) was calculated using the DLC-2 data and the solid angle of the detector, and the results are shown in Fig. 23. This calculation did not even start to describe the experimentally measured forward scattering contribution. The calculation gave a \( \Sigma_t \) correction of about .01% (see Fig. 23) compared to 25% in the experiment. It is realized that the assumptions made were not completely accurate; however, several orders of magnitude difference between the experimentally measured deviation and the calculated correction are involved. It appears unlikely that refinement of the assumptions would lead to significant improvement of the calculation. Therefore one is led to the conclusion that significant errors may exist in the DLC-2 shallow angle scattering data.

The DLC-2 cross-section data set was first checked against a theoretical minimum cross-section based on the optical model. The Wick's Limit gives the minimum zero angle scattering probability by the following equation:

\[ \frac{d\sigma}{d(\cos \phi)} \bigg|_{0^o} \geq \frac{k^2}{8\pi} \sigma_{\text{TOT}}^2 \]  

(12)

where \( k^2 = \frac{2\mu E}{\hbar^2} \)

\( \theta = \) scattering angle in center of mass system

and \( \mu = \frac{m \cdot M}{m + M} \)

and \( m, M = \) masses of the neutron and oxygen atom
FIGURE 23
CROSS SECTION FORWARD SCATTERING CORRECTION
DLC - 2
OXYGEN
This equation was used to check the DLC-2 data at several energies, and the data do indeed satisfy the theoretical minimum. However, this does not indicate that the actual forward scattering probability is not much greater than indicated by the Wick's minimum limit.

If it is assumed that the data taken in this experiment are correct, then there must be an explanation for the large errors in published forward scattering data. It is noted in looking at published data that the differential angular cross-section as a function on angle is not reported between 0° and approximately 30°. For example, the following figure shows such a plot for oxygen at 3.91 MeV taken from BNL-400.10

![Graph showing differential angular cross-section](image)

Experimental cross section data cannot be taken any closer to the zero angle than 30° because of interference between the neutrons scattered at small angles and the uncollided, transmitted flux. Therefore, the zero angle forward scattering probability is determined by exponential extrapolation of the data from 30° back to 0°. The measurements made in this report indicate that the actual forward scattering probability approaches a δ function, i.e., it is very sharply peaked at the zero angle. The error found in published data
is due to a lack of experimental data in this region. Forward scattering probability at small angles is rarely measured. For many materials the error between the extrapolated zero angle scattering probability and the actual may be small, but for oxygen it appears that the extrapolated data are in serious error.

7.5 Multiple Scattering Assumptions

Figure 22 shows a comparison between two iron penetration spectra, one uncollimated and one collimated at the sample. In this example, the effect of multiple scattered neutrons on the penetration data can be seen. A fraction of the incident neutrons were apparently scattered several times in the sample and emerged from the sample in a direction that would intercept the detector. This effect can be seen by the smoothing of the data and in the buildup in the low energy end for the uncollimated case (see Fig. 22). However, the magnitude of the discrepancy caused by multiple scattering of neutrons is much less than that caused by shallow angle scattering of neutrons as can be seen by comparison of Figs. 16 and 18. The uncollimated data points were slightly above the calculated and the collimated were slightly below, but the difference is small. Again, if a true measure of the total neutron cross-section was to be made, the collimator would be used.

7.6 Evaluation of Published Data

The cross section data sets used to obtain the calculated transmitted spectra to be compared with the measurements came from a variety of sources and methods. The KFK-1000 data and the data of Foster and Langsford were taken using an accelerator and time light measurements. The BNL-325 data set is a compilation of data from many sources and the best line is drawn through all of the combined data. The UNC-5139 data set is a
combination of experimental data and theoretical calculations. The DLC\textsuperscript{5} data set is grouped cross-section data from the ENDF/B\textsuperscript{6} file compiled with the ORNL code SUPERTOG\textsuperscript{29} using 1/E spectrum weighting.

7.6.1 Iron (Fig. 18) - All data show good agreement except for energies at about 1.7 MeV or below. Errors in the cross-section compared to the measurements range from approximately 10\% to 15\% at 1.3 MeV. The DLC-2 data set shows the best agreement with the experimental result (except in the low energy region), although the errors are small for all three data sets. The error above 9.5 MeV is probably due to poor statistics in the experimental spectrum.

7.6.2 Lead (Fig. 19) - Good agreement is found with both data sets. The largest error at 5.7 MeV is only about 4\% which is probably within the statistics of the experiment. The BNL data set seems to be best up to 6 MeV, after which both data sets differ from the experimental.

7.6.3 Oxygen (Fig. 20) - In general, much of the data do not adequately describe the depth of the minima at 2.35 MeV. At this point, the calculation based on the Foster data is within 8\% of the experimentally measured cross-section data while UNC-5139 is in error by 40\%. There is also some problem with most of the data at 4.7 MeV. The best data set over the entire spectrum is the DLC-9 data, except in the 2.35 MeV region. The discrepancy in this region would be expected since the cross-section has been averaged over some energy width and therefore underestimates the depth of the minima.

7.6.4 Sodium (Fig. 21) - Good agreement is found for most of the data for both samples. The experimental data points for the liquid sample tend to be slightly above the calculated as compared to the solid sample. However, the two experimental spectra agree within 3\% and the error is probably due to an error in the density calculation for the liquid sample. The comparison
between these two sets of data shows that the experiment is sensitive to density changes as should be noted. The change in the density from the solid to the liquid sample was 6.4% which resulted in an increase in the calculated transmitted flux by approximately 45% at 3 MeV. As can be seen in Fig. 21 this change in the calculated transmitted spectrum due to the density change in the sample was also measured in the experimental transmitted flux since the experimental and calculated results show good agreement.

The BNL data sets show large errors from 5 MeV down, with a cross-section error of 10% at 1.8 MeV. Langsford shows a discrepancy at 7.3 MeV which does not appear in other data nor in the experimental result. An unfolding problem occurred with the solid sample below about 1.6 MeV and the data below this point are in error. The fluctuations in the experimental results in the higher energy region are probably statistical in nature and should be disregarded.
8.0 SUGGESTIONS FOR FURTHER STUDY

Now that the experimental procedure has been established, the evaluation of total neutron cross-sections for many materials can be quickly and accurately completed. Possibly the most accurate results would be obtained by using two collimators; one at the sample and one at the detector. This would eliminate both multiple and shallow angle scatters. However, it would be difficult to align both collimators with the equipment now available and single collimation at the detector or at the sample does give adequate results.

In order to study the forward scattering vs. multiple scattering phenomenon several penetration spectra could be taken with varying sample thicknesses and without collimation. If the measured result produced the same error in the total cross-section for all thicknesses, then it could be concluded that forward scattering was contributing a great deal to the measured transmitted spectra. However, if the total cross-section error increased with increasing thicknesses it could be concluded that multiple scattering was contributing to the measured spectra. In this experiment the contribution from forward scattered neutrons would always be present, however, it would be constant for all thicknesses. The contribution from multiple scattering, on the other hand, would increase with increasing thickness. The larger thicknesses would have a greater probability for multiple scattering and some of these neutrons would reach the detector. For small thicknesses (approximately 1 mean free path) the probability of multiple scattering is small, and any contribution to the uncollided flux would be from forward scattering only.

If the experiment outlined in the previous paragraph proves conclusively that there is a large contribution to the uncollided flux from
forward scattering neutrons in the uncollimated geometry, as has been indicated by the data taken at this time, then additional measurements of the actual forward scattering probability should be made. First, a more exact formulation of the actual contribution to the uncollided flux from shallow angle scattering near 0° should be derived based on available angular dependent cross section data. This would be a more precise analysis than was used in deriving equation 11, and would take into account the effects of multiple shallow angle scatters in thicker samples, the physical size of the sample, etc. Measurements could then be made, possibly using several different sized collimators. The use of several collimators would make it possible to check the reliability of the experiment and to gain knowledge of the variation in differential scattering probability with angle for angles very close to the 0° angle. As the solid angle subtended by the detector is increased, the number of neutrons detected is a measure of the forward scattering probability over that particular solid angle. The resultant total cross-section discrepancies would be due to forward scattering and could be used to calculate the differential scattering probability near the 0° angle using the formulation derived.
9.0 ACKNOWLEDGEMENTS

The author wishes to express his sincerest gratitude to Dr. Walter Meyer for all of his help and advice throughout the course of this study. Special thanks must be extended to the Department of Nuclear Engineering, the Atomic Energy Commission Fellowship program, and the Atomic Energy Commission Division of Research for their financial support. Also, a note of thanks is extended to Dr. Hermann J. Donnert, Dr. J. K. Shultis, J. W. Thiesing and all others of the Department of Nuclear Engineering who gave their assistance. Finally, a special thank you is given to my wife, Kaye, for her encouragement and support.
10.0 REFERENCES


5. DLC-9, Code Name: FARS Data 122 Group (104 Neutron, 18 Gamma), Radiation Shielding Institute Center (June 11, 1969).

6. Evaluated Nuclear Data File of the National Neutron Cross Section Center, Brookhaven National Laboratory.


APPENDIX A

COMPUTER PROGRAMS

CALFLUX
NE213RES
POLYFIT
APPENDIX A

COMPUTER PROGRAMS

CALFLUX

This program calculates the transmitted neutron spectrum through samples and smooths the results with the NE-213 resolution function as given by Equation 10 on page 6. After reading all of the input data, the program establishes a cross-section data point or incident spectrum data point for each energy that appears in either the cross-section or incident spectrum library by calling subroutine ENGRID. The program then begins to calculate the transmitted flux at given energies starting with 0.8 MeV in 0.1 MeV intervals to 3.0 MeV, and then in 0.2 MeV intervals (same energy intervals as the FERDOR output). For each energy the FWHM of the resolution function is calculated, and the actual integration is carried out over some energy width calculated by multiplying constant (FWHM) times the FWHM. (The contribution to the area under a gaussian curve is small past approximately two times the FWHM from the center of the peak.) The contribution to the transmitted flux from each energy interval over the width of the integration is calculated and summed. The energy intervals are for each $E_i$ to $E_{i+1}$ as established by the subroutine ENGRID.

Only one problem was encountered with this procedure. When large positive slopes were present in the cross-section data, the arguments of Equation 10 became such that the value of the error function (erf) was very close to 1.0. Thus, when the difference between two error functions were taken, the result was set equal to zero by the computer. At the same time, the constants that were being multiplied by this difference became very large; however, the product calculated by the computer was always zero. To overcome this problem, the program tests the value of the difference term,
and if it becomes very small the program calls the subroutine ROMBRG which numerically finds the value of the integral between these two energy points.

Output from CALFLUX includes the physical constants for the sample used and a plot of the input cross-section library and incident spectrum library. The resultant calculated flux is listed and also plotted along with the experimentally measured transmitted flux.

**INPUT**

<table>
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<th>Card</th>
<th>Format</th>
<th>Description</th>
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</thead>
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<tr>
<td>1</td>
<td>8F10.4</td>
<td>1) T = Sample thickness (cm)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2) RHO = Molecular Density (atom/cc) \times 10^{24}</td>
</tr>
<tr>
<td>2</td>
<td>8F10.4</td>
<td>1) WIDTH = A multiplication constant times the FWHM at which the resolution gaussian will be truncated</td>
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<tr>
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<td>8F10.4</td>
<td>1) XNORM = normalization factor between the incident and penetration integrated flux</td>
</tr>
<tr>
<td>4</td>
<td>8F10.4</td>
<td>1) PFHW = the percentage of calculated FWHM used for the resolution function</td>
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<td>8F10.4</td>
<td>1) EMAX = Maximum energy to which the program will calculate the transmitted spectrum</td>
</tr>
<tr>
<td>6</td>
<td>I3</td>
<td>1) NXSECT = number of points in the cross-section library</td>
</tr>
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<td>1) EX(I) = energy of the \textit{i}th cross-section data point (MeV)</td>
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<td></td>
<td>2) XSECT(I) = the \textit{i}th cross-section (barns)</td>
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<td>8) XSECT(I+3) = cross-section...</td>
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</tbody>
</table>

**NOTE:**

1) The library cross-section must extend from .01 to 15 MeV and must exceed the incident spectrum library at both lower and upper energies.

2) The maximum energy in the incident and penetration spectrum library must exceed EMAX.
CALFLUX Listing

FORTAN IV G LEVEL 18 MAIN DATE = 71/09 22/14/21

C THIS PROGRAM CALCULATES TRANSMITTED NEUTRON SPECTRUM
C THROUGH SAMPLES AND SPECIFIES THE RESULTS WITH THE
C NL 213 RESOLUTION FUNCTION

C THE LIBRARY CROSS-SECTION MUST EXTEND FROM 0.1 TO 15 MEV
C AND MUST EXCEED THE SPECTRUM LIBRARY AT BOTH LOW AND UPPER ENERGIES

C T = THICKNESS OF SAMPLE (CM)
C RHO = MOLECULAR DENSITY (ATOMS/CC) X 10**24
C XFORM = NORMALIZATION FACTOR BETWEEN REACTOR POWER LEVELS FOR
C INCIDET AND TRANSMITTED SPECTRA MEASUREMENTS
C NSECT = NUMBER OF ENTRIES IN LIBRARY CROSS-SECTION
C EXIT1,IX**(1) = ENERGY AND CORRESPONDING CROSS-SECTION IN
C CROSS-SECTION LIBRARY (MEV, BARN)
C WIDTH = A MULTIPLICATION CONSTANT TIMES THE FWHM AT WHICH THE
C RESOLUTION GAUSSIAN WILL BE TRUNCATED
C FWHM = THE PERCENTAGE OF CALCULATED FWHM USED FOR RESOLUTION FUNCTION
C E(N),W(N) = ENERGY AND CORRESPONDING INCIDENT SPECTRUM FROM
C FERMIOR CODE AND MUST EXCEED EMAX
C E(N),W(N) = ENERGY AND CORRESPONDING EXPERIMENTAL
C SPECTRUM FROM FERMIOR CODE AND MUST EXCEED EMAX
C EMAX = MAXIMUM ENERGY TO WHICH THE PROGRAM WILL CALCULATE THE
C TRANSMITTED FLUX

IMPICLIT REAL*4 (A-H,O-Z,V,X-Z)

DOUBLE PRECISION DLOG,CERF,DECP,LBAPS

EXTERNAL FCN

DIMENSION SPCT(75),EV(75),SPECT(75),X(150),P(150),ENE(75),FL(75)

COMMON /HOLD2/ EX(150),X(150),SPECT(75)

COMMON /HOLD3/ EN(150),NLO

CALL ERSET (208,50,146,0,0)

0001 0009 900 FORMAT (9(1X,4I4))
0010 901 FORMAT (8F14.4)
0011 902 FORMAT (8X,E10.3,3X,E10.3)
0012 910 FORMAT (1H1,* THIS PROGRAM CALCULATES A SMOOTHED TRANSMITTED SPECTRUM
0013 FROM TABULATED DATA USING THE RESOLUTION FUNCTION OF THE NL 213
0014 1.04*10**(X+USING THE FOLLOWING PARAMETERS:*,*,*,*)
0015 911 FORMAT (*. THE RESOLUTION HAS BEEN TRUNCATED AT *.06.3,TIMES THE
0016 1FWHM OF THE GAUSSIAN)
0017 913 FORMAT (*. THE SAMPLE THICKNESS IS T = *F10.3,10**24 MOL
0018 1S*, THE MOLECULAR DENSITY IS RHO = *D3.3,10**24 MOLECULES/CC*,*,*)
0019 914 FORMAT (*. THE CALCULATED, SMOOTHED TRANSMITTED SPECTRA IS: *,*F10.3,*)
0020 915 FORMAT (5X,F5.1,10X,E12.5)
0021 916 FORMAT (5X,F5.1,10X,E12.5,* POSSIBLE ERROR BECAUSE GAUSSIAN RESOLU-
0022 1ITION CURVE IS BEING TRUNCATED AT *.1 AND PEV*)
0023 917 FORMAT (*. THE PROGRAM HAS BEEN EXCITED BECAUSE UPPER LIMIT OF IN-
0024 1TEGRATION EXCEEDS CROSS-SECTION LIBRARY)
0025 918 FORMAT (*,*)
0026 919 FORMAT (*. THE INPUT SPECTRUM IS AS FOLLOWS: *,*,*)
0027 920 FORMAT (*,*)
0028 921 FORMAT (*. THE INPUT SPECTRUM IS AS FOLLOWS: *,*,*)
FORTRAN IV LEVEL 18

MAIN

DATE = 711/20

22/14/21

0022 922 FORMAT (*0 THE FWHM HAS BEEN MULTIPLIED BY 1.0*3)
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0024
0025  PI = 3.141592653
0026  READ 401,F,HU
0027  READ 401,WIDTH
0028  READ 931,XNORM
0029  READ 931,PFHWM
0030  READ 931,EEX
0031  READ 931,EX(1),EX(I+1),EX(1+1),EX(I+2),EX(I+2),EX(I+3),EX(I+3)
0032  13)
0033  READ 900,NA
0034  DI = 20,1,NA
0035  READ 902,ES(I),SC(ES(I))
0036  ES(I) = ES(I)/.00-0D0
0037  20 SPCTE(I) = DLG(SPECT(I))
0038  READ 900,NE
0039  DU 42 = 1,NE
0040  42 READ 902,EE(I),SPCTE(I)
0041  DU 44 = 1,NE
0042  IF (SPCTE(I) .LE. 0.00D0) SPCTE(I) = SPCTE(NE)
0043  PRINT 910
0044  PPRINT 913,1,RHU,XNORM
0045  PRINT 911,WIDTH
0046  PRINT 902,PFHWM
0047  CALL ENGRID (NXSECT,NA,NG)
0048  CD 2 = 1,NG
0049  2 XSFCT(I) = XSECT(I)*PFHWM
0050  PRINT 920
0051  CALL PLATZ (EX,XS,NXSECT)
0052  PRINT 921
0053  CALL PLATZ (ES,SC(XS),NA)
0054  PRINT 914
0055  NMG1 = NG-1
0056  DU 3G = 1,NGM1
0057  DF = E(I+1)-E(I)
0058  XI(I) = (XSECT(I)+XSECT(I))/DF
0059  30 PII(I) = FLU(L+1)-FLU(L))/DF
0060  XMAX = (XMAX-3.00D0)/.23010D2
0061  MAX = IFIX(XMAX)
0062  CD 3 = 1,MAXE
0063  FLUX = 0.00D0
0064  NNM = 0
0065  IF (I,GT,22) GO TO 5
0066  4 ENERGY = I+.1*I
0067  GO TO 6
0068  5 ENERGY = 3.0+.2*(I-23)
0069  6 FWHM = .8153627120D1*ENERGY+.139923190D1*ENERGY**2-
0070  1.52943720D0*ENERGY**3+.5932513932*ENERGY**4-.103817137D0*ENE-
0071  RGY**5+.5126641/5120*ENERGY**6-.184207720D2*ENERGY**7
0072  7 FWHM = FWHM*PFHWM
0073  8 EUP = ENERGY+FWHM*WIDTH
0074  IF (ELO<.001) 7,7,8
0075  IF (ELO<.001) 7,7,8
0076  8 EUP = ENERGY+FWHM*WIDTH
0077 IF (IEXP=ENG) 9,9,10
0078 9 CONTINUE
0079 GO TO 22 J=1,NG
0080 IF (JLO .LT. E(J)) GO TO 23
0081 22 CONTINUE
0082 23 K = 0
0083 AB = E(J-1)
0084 E(J-1) = ELO
0085 24 K = K+1
0086 K1 = K-1
0087 NLO = J-1+K1
0088 NUP = J+K1
0089 IF (E(NUP) .LT. EUP) GC TO 27
0090 AUC = E(NUP)
0091 E(NUP) = EUP
0092 AUC1 = 1
0093 27 YLO = (E(NLD)-ENERGY+0.5&0*(X(NLO)-dO))/AL
0094 LYLO = DCERF(YLO)
0095 YUP = (E(NUP)-ENERGY+0.5&0*(X(NLD)-dO))/AL
0096 NYUP = DCERF(YUP)
0097 ZLO = YLO-PH(LAL)/AL/0.2001
0098 ZLZ = DCERF(ZLO)
0099 ZUP = YUP-PH(LAL)/AL/0.2001
0100 ZUP = DCERF(ZUP)
0101 CONST = X(NLD)*(E(NLO)-ENERGY-XSECT(NLO))*0.25*X(NLD)-2*BO
0102 IDY = NYUP-DCLO
0103 IF (_IDX<100) .LT. 0.1C-13) GO TO 40
0104 FLUX1 = DEXP(CONST*P(NLO))*(CONST)*IDY
0105 IDZ = ZUP-DCLZ
0106 IF (IDX>100) .LT. 0.1C-13) GO TO 40
0107 FLUX2 = DEXP(CONST*P(NLO))*(E(NLO)+ENERGY-E(NLO)-XSECT(NLO))*P(NLO)*BO/E/0.1D31-
0108 IF(P(NLO)*P(NLO)*BO/N/1.48)*BO
0109 GO TO 52
0110 52 FLUX1 = 0.0000
0111 E11 = E(NLO)
0112 E22 = E(NLO+1)
0113 EPS = .10-01
0114 MPN = 5
0115 MPN = 0
0116 FLUX2 = 2D01*ROUWRG(E11,E22,EPS,ROUN,FRN,FCN1)/(BDIPI)**5
0116 52 FLUX = FLUXC*S&0*(FLUX1+FLUX2)
0117 IF (K .LT. EQ, 1) E(NLO) = AB
0118 IF (NUP .EQ. 1) GO TO 31
0119 GO TO 24
0120 31 E(NUP) = AUC
0121 FLUX = FLUX *KROM
0122 VMAT = ENERGY
0123 FL = INCLUD(FLUX)
0124 IF (FL .LE. 0.1) GO TO 12
0125 PRINT 15,ENERGY,FLUX
0126 GO TO 31
0127 12 PRINT 916,ENERGY,FLUX
0128 3 CONTINUE
0129 PRINT 919
0130 CALL PLATF ((ENE,FL,SPC,E,MAX))
0131 GO TO 11
0132 10 PRINT 917
0133 11 STOP
SUBROUTINE EGRID (NXSECT,R,NA,NG)
  IMPLICIT REAL*8 (A-H,O-Z)
  DOUBLE PRECISION D_LU,DLU,D_LU,D_LU
  COMMON /HLCIN/ EX(I),X(I,J),ES(I,J),SPECTL(I,J)
  COMMON /HLCIN/ H(I,J),XSCT(I,J),FLUL(I,J)
  FLUL(I) = D_LU(1-(SPECTL(I,J)**2)*2*W)
  E(J) = EX(1)
  XSCT(I,J) = XS(I,J)
  K = 1
  J = 1
  I = 1
  J = 1
  K = K+1
  IF (E(I,J)-ES(I,J)) .GT. 0.1D-05 GO TO 10
  IF (ES(I,J)-E(I,J)) .LT. 0.1D-05 GO TO 11
  E(I,J) = EX(1)
  J = 1
  I = 1
  XSCT(I,J) = XS(I,J)
  FLUL(I) = (SPECTL(I,J)-FLUL(I-1))*(E(I,J)-E(I-1))/ES(I,J)-E(I-1))
  10 GO TO 12
  11 E(I,J) = ES(I,J)
  J = 1
  I = 0
  XSCT(I,J) = SPECTL(I,J)
  XSECT(I,J) = XSECT(I-1)*(1.0-E(K-1))/E(K-1)
  12 GO TO 12
  13 K = K+1
  I = I+1
  E(K) = EX(1)
  XSCT(K) = XS(I,J)
  FLUL(K) = SPECTL(I,J)
  CONTINUE
  IF (I .GE. NA) GO TO 13
  GO TO 1
  CONTINUE
  IF (I .GE. NXSECT) GO TO 15
  GO TO 13
  K = K+1
  RETURN
END
FUNCTION RUMB RUG (X, Rel, EPS, M, N, FCN)

IMPLICIT REAL*8 (A-H, O-Z)

CRUMB EK, INTEGRATION

DIMENSION F (L)

!H(Y,0.1GU TO 2.0)

!F(N,GT.31GO TO 2.0)

!IFM-29997,99,98

!99 X=90

!99 X=M

!99 X=N

!99 EP=FCN(X)

!99 X=FCN(X)

!2001 SUM=X*EP*0.500

!201 A=N-2

!2007 AEP=OAHS(EP)

!2008 AX=OAHS(X)

!2009 ASUM=AP+AX*0.500

!2010 FMAX=AEP

!2011 IF(FMAX.GE.AEP)GO TO 100

!2010 FMAX=AX

!100 I=1

!101 NC=1

!102 M=90-9

!104 S1=SUM

!105 P(I)=S1

!105 ASUM=SUM*0.500

!2002 X=4.990.500

!2002 GO TO 102 X=1, NC

!2029 X=X+H

!2030 N=N+1

!2031 EP=FCN(X)

!2032 2010 AEP=OAHS(EP)

!2033 IF(FMAX.GE.AEP)GO TO 101

!2034 FMAX=AEP

!2035 101 SUM=SUM+EP

!2036 ASUM=SUM*0.500

!2037 2003 S2=M*SUM*0.500

!2038 2011 AS2=M*SUM*0.500

!2039 K=1

!2040 GO TO 105

!2040 2012 (P=OAHS(S2-S1))

!2042 2013 AX=OAHS(S2)

!2043 GO TO (110,2004,111,112), VN

!110 CEP=AX

!110 GO TO 113

!111 CEP=A52

!112 CEP=A52

!113 IF(FP>EP)EP

!110 IF(F1107.107,103


!110 H=M+0.500

!110 S1=52

!110 AS1=52

!110 PK=A52

!1530.34
OC58    I=I+1
OC59    NC=2*NC
OC60    GO TO 2002
OC61    105 IF(K.GT.1) GO TO 2012
OC62    J=J+1
OC63    E=2**I
OC64    T=52
OC65    2)06 S2=(#S2-P(X))/[U-1.00C]
OC66    P(I)=T
OC67    K=K+1
OC68    GO TO 105
OC69    108 PRINT L+1
OC70    1 FORMAT(* H EXCEEDED I= *,12)
OC71    107 KUMURLG=S2
OC72    EPS=EPS/N
OC73    GO TO 120
OC74    200 PRINT 2,N
OC75    2 FORMAT(* ERROR RETURN N= *,12)
OC76    120 RETURN
OC77    END
FUNCTION FCN(X) 

IMPLICIT REAL*8 (A-H,O-Z) 
COMMON /HILDA/ E(NLO),XSECT(NLO),FLUXL(NLO) 
COMMON /HILDA/ ENERGY,BO,VL 

FLUXL = FLUXL(NLO)*((FLUXL(NLO+1)-FLUXL(NLO))*((E-E(NLO))+ (E(NLO)+1)- 
E(NLO)))/ 

X = XSECT(NLO)*((XSECT(NLO+1)-XSECT(NLO))*((E-E(NLO))+ (E(NLO)+1)- 
E(NLO))) 

FCN = DEXP(FLUXL-XS)*DEXP(-ENERGY-2/80) 

RETURN 

END
SUBROUTINE PLAT(2, Y, N)

C PLOTTING SUBROUTINE PLAT2

IMPLICIT REAL*8 (A-H, O-U, Y-Z)
INTEGER XX
DIMENSION XX(120), Z(1), Y(1), N(2)
DATA N(2)/0.0,
YMAX = -1.50
YMIN = 1.50
DO 3 I=1, N
3 IF (Y(I) = YMAX) 5, 5
4 YMAX = Y(I)
5 IF (YMIN = Y(I)) 3, 3, 6
6 YMIN = Y(I)
CONTINUE
C RANGE = YMAX - YMIN
DIV = RANGE/100.
PRINT 30, DIV
30 FORMAT(3H THE SCALE OF THIS GRAPH IS 1 DIVISION =', 1, 12, 5H U)
1 INCHES/29X, F12.6, F12.6, F12.6, F12.6, F12.6, F12.6, F12.6, F12.6, F12.6)
120
DO 1 J=1, 120
1 XX(J) = N(J)
IX = 1
EO 2 I=1, N
XX(I) = N(J)
X = 1.04*(290/RANGE)*(Y(I)-YMIN)
IX = IFIX(X)
XX(IX) = N(J)
GO TO 8
2 IF (J .LE. EO) GO TO 8
3 IF (XX(J) .LE. Z(I-1)) GT 15000 GO TO 7
8 PRINT 20, Z(I), Y(I), XX(J), J=1, 101
20 FORMAT(1H 20124, *-----', ', 101A1)
30 GO TO 2
31 IF (2 .LE. Z(I-1)) GT 25 GO TO 9
32 PRINT 10, Z(I), Y(I), XX(J), J=1, 101
10 FORMAT (1H 10214, *-----', ', 101A1)
33 GO TO 2
34 PRINT 40, Z(I), Y(I), XX(J), J=1, 101
40 FORMAT (1H 40124, *-----', ', 101A1)
CONTINUE
RETURN
END
SUBROUTINE PLT3(Z,Y,W,N)

DIMENSION XX(120),XY(120),Z(I),Y(I),W(I),X(120),Y(120)

IF (X(1) = X(2)) THEN
    WRITE(*,*) 'X1 = X2, SIDES NOT CONNECTED.'
    RETURN
END

DO I = 1, N
    IF (Y(I) .GT. YMAX) YMAX = Y(I)
    IF (Y(I) .LT. YMIN) YMIN = Y(I)
END DO

DO I = 1, N
    IF (Z(I) .GT. ZMAX) ZMAX = Z(I)
    IF (Z(I) .LT. ZMIN) ZMIN = Z(I)
END DO

RANGE = ZMAX - ZMIN

DO I = 1, N
    X(I) = X(I) * RANGE
    Y(I) = (Y(I) - YMIN) * RANGE
    Z(I) = (Z(I) - ZMIN) * RANGE
END DO

RETURN
END
### Sample Input Data - CALFLUX

<table>
<thead>
<tr>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
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<td>0.0000</td>
<td>0.7751</td>
<td>0.0000</td>
<td>0.8116</td>
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</table>

---

The table above shows sample input data for CALFLUX, with each row representing a different input value. The data is presented in a tabular format with columns labeled 1 to 8.
CALFLUX Sample Output

This program calculates a smoothed paraboloid spectrum from resolution data using the resolution function of the form $f(x) = \frac{1}{1 + (x/b)^2}$ for $x > 0$. The resolution has been truncated at 1.5 times the FWHM of the Gaussian.

The sample thickness is $T = 91.200$ cm, and the molecular density is $R = 0.400$ g cm$^{-3}$. The FWHM has been multiplied by 0.750.
<table>
<thead>
<tr>
<th>ENERGY</th>
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<td>0.254610 01</td>
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<td>0.9</td>
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<tr>
<td>1.0</td>
<td>0.145410 01</td>
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<tr>
<td>1.1</td>
<td>0.716730 00</td>
</tr>
<tr>
<td>1.2</td>
<td>0.490500 00</td>
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<tr>
<td>1.3</td>
<td>0.377750 01</td>
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<tr>
<td>1.4</td>
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<tr>
<td>1.5</td>
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<tr>
<td>1.6</td>
<td>0.562290 02</td>
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<tr>
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</tr>
<tr>
<td>1.9</td>
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</tr>
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<tr>
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<tr>
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<tr>
<td>2.4</td>
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<tr>
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<td>0.326480 04</td>
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<tr>
<td>2.6</td>
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</table>
NE213RES

This program determines the resolution of the NE-213 detection system from the measured and unfolded responses to the monoenergetic neutrons. The code is based upon the expressions derived in Appendix B for gaussian resolution fitting using weighted least squares. Input to the program includes the upper and lower bounds of each point in the unfolded spectrum over which the gaussian is to be fit. Output includes the FWHM and the standard deviation on this value along with the comparison between the actual data and the calculated data based on the gaussian fit. The matrix inversion required in the calculation is done by the subroutine MATINV.

**INPUT**

<table>
<thead>
<tr>
<th>Card</th>
<th>Format</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>I10</td>
<td>1) NDS = Number of data sets to be analyzed</td>
</tr>
</tbody>
</table>
| 2    | F10.0,I10 | 1) ENEUT = Nominal energy of the monoenergetic neutrons  
          2) NDP = Number of data points in this set to be fit to the gaussian |
| 3 (Deck) | 8F10.0 | 1) EN(I) = Energies in the unfolded spectrum (MeV)  
          : |
| 4 (Deck) | 8F10.0 | 1) FLO(I) = Lower bound of each point in the unfolded spectrum  
          : |
| 5 (Deck) | 8F10.0 | 1) FUP(I) = Upper bound of each point in the unfolded spectrum  
          : |
NE213RES Listing

**FORTRAN IV Level 18 MAIN DATE = 71109 22/12/23**

C**** THIS PROGRAM DETERMINES THE RESOLUTION OF A DETECTION SYSTEM FROM
C**** THE MEASUREMENTS OF THE UNFOLDED RESPONSES TO THE MONOENERGETIC NEUTRONS

C001 IMPLICIT REAL*8 (A-H,O-Z)
C002 DIMENSION YE(25),PL(25),Q(1,1),B(3,1),VAR(25),PL(I25),PUP(I25)
C003 1,1,1,1
C004 FORMAT(15,3(5,F10.0))
C005 2 FORMAT(110)
C006 3 FORMAT(15,3(5,I10))
C007 4 FORMAT(4X,27,EXP,3E13,P,2,2X,3HMEV)
C008 5 FORMAT(4X,17,EXP,3E13,P,2,2X,3HMEV)
C009 6 FORMAT(4X,12,EXP,3E13,P,2,2X,3HMEV)
C010 7 FORMAT(4X,16,EXP,3E13,P,2,2X,3HMEV)
C011 8 FORMAT(4X,9,EXP,3E13,P,2,2X,3HMEV)
C012 9 FORMAT(4X,2,PEAK ENERGIES=F5.2,2X,3HMEV,3X,4HMEV,F5.2,4HMEV)
C013 10 FORMAT(4X,2,PEAK HT=,X5,2X,3HMEV,3X,4HMEV,F5.3,2X,3HMEV)
C014 11 FORMAT(4X,2,PEAK HT=,4HMEV,3X,4HMEV,3X,4HMEV,3X,4HMEV)
C015 556 FORMAT(15,2,EXP,3E13,P,2,2X,3HMEV)
C016 557 FORMAT(15,2,EXP,3E13,P,2,2X,3HMEV)
C017 MS IS THE NUMBER OF DATA SETS TO BE ANALYZED
C018 READ(1,2)MS
C019 EU 160 K=1,MS
C**** ENEU IS THE MAXIMAL ENERGY OF THE MONOENERGETIC NEUTRONS
C**** NPD IS THE NUMBER OF DATA POINTS IN THIS SET
C020 READ(1,3)(ENEU,NPD)
C021 EU 20 II=1,NPD,8
C022 20 READ(1,1)(ENEU,NPD,8)
C**** ENEU(II) ARE THE ENERGIES IN MEV TO THE UNFOLDED SPECTRUM
C023 EU 21 II=1,NPD,8
C024 READ(1,1)(ENEU,NPD,8)
C025 22 READ(1,1)(PUP(I),I=1,NPD,8)
C026 EU 321 I=1,NPD
C027 PL(I)=(PL(I)+PUP(I))/2.0.
C028 321 PL(I)=PL(I)+100.0.
C**** PL(I) AND PUP(I) ARE THE LOWER AND UPPER BOUNDS OF EACH POINT ON THE
C**** UNFOLDED SPECTRUM
C029 EU 200 I=1,NPD
C030 Y(I)=(PL(I)+PUP(I))/2.
C031 200 VAR(I)=((PUP(I)-PL(I))/2.0)**2
C032 DIVG I=1,3
C033 Y(I)=0.
C034 EU 101 J=1,3
C035 101 AI(J)=0.
C036 EU J=1,3
C037 RATIO=Y(I)**2*VAR(I)
C038 AI(J)=AI(J)+RATIO*X(I)
C039 AI(J)=AI(J)+RATIO*X(I)**2
C040 AI(J)=AI(J)+RATIO*X(I)**3
C041 AI(J)=AI(J)+RATIO*X(I)**4
FORTRAN IV LEVEL 18

MAIN

DATE = 71129
22/12/23

0043      B(1) = B(1)+ATI0*DLG0(Y(11))**LUM0(EV(I))
0044         B(I) = B(I)+ATI0*DLG0(Y(I))**LUM0(EEV(I))
0045   102      B(1) = B(1)+ATI0*DLG0(Y(11))**LUM0(EV(I))
0046         A(3,1)=A(2,3)
0047         A(3,1)=A(2,2)
0048         A(1,3)=A(2,3)
0049         A(1,2)=A(2,1)
0050       DO 176 I=1,3
0051     176      BUM(1,1) = B(1)
0052
0053         N1 = 1
0054         N3 = 3
0055         CALL MATNV(A,3,BNUM,A1,DETERM,N3)
0056
0057 DO 177 I=1,3
0058     177         BUM(I,1) = B(1)
0059         BB(I) = B(I)
0060         E(I) = BB(I)*H(I)**2/2.
0061         YC = 1/EXP(B(I)+E(I)/HO/HC)
0062         DUM = DLOG1+20011
0063         FWHM = 2.*(BUM(I)**.5
0064         VARBU = A(I)**.5
0065         VARBO = VARBU**.5
0066         VAREU = VAREU**.5
0067         VARYO = VARYO**.5
0068         VARFW = VARFW**.5
0069         SDVF = SDVF**.5
0070         PI = 3.1415927
0071         YNORM = 1./HO**PI**.5
0072      WRITE(1,4)ENUT
0073      WRITE(1,5)
0074      WRITE(1,6)(EV(I),I=1,NEM)
0075      WRITE(1,7)
0076      WRITE(3,8)
0077      WRITE(1,9)(EV(I),I=1,NEM)
0078      WRITE(1,9)ENOT,SDVFW
0079      WRITE(1,4)ENUT
0080      WRITE(1,5)
0081      WRITE(1,6)(EV(I),I=1,NEM)
0082      WRITE(1,7)
0083      WRITE(3,11)FWHM,SDVF
0084      STOP
0085      END
SUBROUTINE MATINV (A,N,B,M,DETERM,NMAX)
C
MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS
C
A INPUT-COEFFICIENT MATRIX
C
RETURN-INVSESE MATRIX
C
N NUMBER OF EQUATIONS
C
B INPUT-RIGHT HAND SIDE VECTOR(S)
C
RETURN-SOLUTION VECTOR(S)
C
M NUMBER OF RIGHT HAND SIDE VECTOR(S)
C
DETERM RETURN-DETERMINATE OF A
C
NMAX MAXIMUM NUMBER OF EQUATIONS AS DIMENSIONED IN MAIN PROGRAM
C
C**** REMOVE NEXT STATEMENT IN SINGLE PRECISION VERSION
0002 IMPLICIT REAL*8 (A-H,O-Z)
0003 REAL*4 PIVOT
0004 DOUBLE PRECISION DABS
0005 DIMENSION A(NMAX,NMAX),B(NMAX,NMAX)
0006 COMMON /F402/ PIVOT(100), I-HEX(100)
C
C INITIALIZE DETERMINANT AND PIVOT ELEMENT ARRAY
0007 DETERM=1.0
0008 DO 20 I=1,N
0009 PIVOT(I)=0.0
0010 20 CONTINUE
C
C PERFORM SUCCESSIVE PIVOT OPERATIONS (GRAND LUOP)
C
DU 550 E=1,N
C
C SEARCH FOR PIVOT ELEMENT AND EXTEND DETERMINANT PARTIAL PRODUCT
C
AMAX=0.0
0012 DO 105 J=1,N
0013 IF (PIVOT(J),NE.,0.0) GO TO 105
0014 R=10C K=1,N
0015 IF (PIVOT(K),NE.,0.0) GO TO 100
0016 TEMP=ABS(A(J,K))
0017 IF (TEMP,LT.,AMAX) GO TO 100
0019 ICOLUMN=J
0020 ICOLUMN=K
0021 AMAX=TEMP
0022 100 CONTINUE
0023 105 CONTINUE
C
RETURN IF MATRIX IS SINGULAR (ZERO PIVOT) AFTER COLUMN INTERCHANGE
C
0028 IF (DETERM,EQ.,0.0) GO TO 603
C
C PIVOT(ICOLUMN)=AMAX
C
C INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL
C
0030 IF (IROW,EQ.,ICOLUMN) GO TO 260
0011 DETERM=-DETERM
0012 INI 200 K=1,N
0013 SWAP=A(J,J,K)
0014 A(J,J,K)=A(I,COLUMN,K)
0015 A(I,COLUMN,K)=SWAP
0026 200 CONTINUE
0027 IF (M.LE.0) GO TO 200
0028 DO 250 K=1,N
0029 SWAP=A(J,J,K)
0030 B(J,J,K)=B(I,COLUMN,K)
0031 B(I,COLUMN,K)=SWAP
0032 250 CONTINUE
C
0042 C
0043 C
0044 C
0045 C
0046 C
0047 C
0048 C
0049 C
0050 C
0051 C
0052 C
0053 IF (J.EQ.I) GO TO 550
0054 T=AF(J,I,COLUMN)
0055 AF(J,I,COLUMN)=0,0
0056 DO 450 K=1,N
0057 AF(J,K)=AF(J,K)-AF(I,COLUMN,K)*T
0058 450 CONTINUE
0059 IF (M.LE.0) GO TO 550
0060 DO 500 K=1,M
0061 AF(J,K)=AF(J,K)-AF(I,COLUMN,K)*T
0062 500 CONTINUE
0063 C
0064 C
0065 C
0066 C
0067 C
0068 IF (K.EQ.I) GO TO 710
0069 DO 700 J=1,N
0070 SWAP=A(J,J,K)
0071 A(I,J,K)=A(I,I,COLUMN)
0072 A(I,I,COLUMN)=SWAP
0073 705 CONTINUE
0074 710 CONTINUE
C
0075 C
0076 C
### Sample Input Data - NE213RES

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POLYFIT

This program fits a given resolution function to a polynomial of degree \( m \) by a weighted least squares procedure. The program was written to perform the calculations derived in Appendix B on polynomial fitting. Input to the program includes the upper and lower bounds on the resolution data to be fitted. Output includes the variance of the \( m \)th order polynomial fit, the coefficients of the fit, and a comparison between the input values and the values calculated by the polynomial. Again, the matrix inversion required by the calculation is done by the subroutine MATINV.

INPUT

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POLYFIT Listing

FORTRAN IV LEVEL 18 MAIN DATE = 7/11/64 22/07/41

C**** THIS PROGRAM FITS A GIVEN FUNCTION TO A POLYNOMIAL OF
C**** DEGREE M BY A WEIGHTED LEAST SQUARES PROCEDURE.

C**** DIMENSION: X(100), Y(100), W(100), SPECT(200), VAR(200), SDEV(200),
C**** SUM(100), N(100), B(100), C(100), SDEVG(100)

C 0001 1 FORMAT(11)
C 0002 2 FORMAT(1)
C 0003 3 FORMAT(1,10)
C 0004 4 FORMAT(1,10)
C 0005 5 FORMAT(1,10)
C 0006 6 FORMAT(1,10)
C 0007 7 FORMAT(1,10)
C 0008 8 FORMAT(1,10)
C 0009 9 FORMAT(1,10)
C 0010 10 FORMAT(1,10)
C 0011 11 FORMAT(1,10)
C 0012 12 FORMAT(1,10)
C 0013 13 FORMAT(1,10)
C 0014 14 FORMAT(1,10)
C 0015 15 FORMAT(1,10)
C
C**** N=NUMBER OF DATA POINTS
C**** M=NUMBER OF APPROXIMATIONS USED
C**** PLO=PLO=LOWER AND UPPER BOUNDS OF THE SPECTRUM
C**** E=ENERGY

C 0016 READ 2,N
C 0017 DO 10 I=1,N
C 0018 READ 3,(X(I),Y(I),W(I))
C 0019 READ 2,NA
C 0020 DO 10 I=1,NA
C 0021 READ 1, M
C 0022 IF(N(N+1)) GO TO 102
C 0023 P(I)=M+1
C 0024 DO 103 I=1,M
C 0025 D(I,J)=0.
C 0026 DO 104 J=1,M
C 0027 103 A(I,J)=0.
C 0028 DO 105 J=1,M
C 0029 104 A(I,J)=A(I,J)*E(I)*W(I)/VAR(I)
C 0030 DO 105 J=1,M
C 0031 DO 105 J=1,M
C 0032 105 A(I,J)=A(I,J)*E(I)*W(I)/VAR(I)
C 0033 DO 105 J=1,M
C 0034 DO 105 J=1,M
C 0035 DO 105 J=1,M
C 0036 DO 105 J=1,M
C 0037 DO 105 J=1,M
C 0038 DO 105 J=1,M
C 0039 DO 105 J=1,M
C 0040 DO 105 J=1,M
C 0041 DO 105 J=1,M
C 0042 DO 105 J=1,M
C 0043 DO 105 J=1,M
C 0044 CALL MTH1/2, M, W,1,DETERM,15
C 0045 DO 105 J=1,M
C 0046 C(1)=C(1)
FORTRAN IV LEVEL 1B

MAIN

DATE = 71/09
22/07/41

0647  108  SDEVCI(I) = DSUM1(A(I,I))
0648  109  CSPCT(I,J) = 0.
0649  110  DO 110 J = 1, N
0650    110  DSUM1(A(I,J)) = CSPCT(I,J) + G(I)*E(J)**(I-1)
0651  110  CONTINUE
0652  111  DLX = DLX + ((CSPCT(I,I) - SPCT(I,I))**2)/NFLUAT(N-M-I)
0653  112  PRINT 5, M
0654  113  PRINT 9
0655  114  PRINT 9
0656  115  PRINT 101
0657  116  STOP
0658  117  END
0659  118

0650  109  CSPCT(I,J) = 0.
0650  110  DO 110 J = 1, N
0651  110  DSUM1(A(I,J)) = CSPCT(I,J) + G(I)*E(J)**(I-1)
0652  111  DLX = DLX + ((CSPCT(I,I) - SPCT(I,I))**2)/NFLUAT(N-M-I)
0653  112  PRINT 5, M
0654  113  PRINT 9
0655  114  PRINT 9
0656  115  PRINT 101
0657  116  STOP
0658  117  END
0659  118
SUBROUTINE MATINV (A,N,R,M,DETERM,NMAX)

MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS
A INPUT-LEFT COEFFICIENT MATRIX
RETURN-INVERSE MATRIX
N NUMBER OF EQUATIONS
B INPUT-RIGHT HAND SIDE VECTOR(S)
RETURN-SOLUTION VECTOR(S)
M NUMBER OF RIGHT HAND SIDE VECTOR(S)
DETERM RETURN-DETERMINATE OF A
NMAX MAXIMUM NUMBER OF EQUATIONS AS DIMENSIONED IN MAIN PROGRAM

C**** REMOVE NEXT STATEMENT IN SINGLE PRECISION VERSION

IMPLICIT REAL*8 (A-H,O-Z)
REAL*4 PIVOT
DIMENSION A(NMAX,NMAX),B(NMAX,1)
COMMON /FA02/ PIVOT(100), INDEX(100)

C INITIALIZE DETERMINANT AND PIVOT ELEMENT ARRAY

DETERM=1.0
DU 20 I=1,N
PIVOT(I)=0.0
20 CONTINUE

C PERFORM SUCCESSIVE PIVOT OPERATIONS (GRAND LOOP)

DO 550 I=1,N
C SEARCH FOR PIVOT ELEMENT AND EXTEND DETERMINANT PARTIAL PRODUCT

AMAX=0.0
DU 105 J=1,N
IF (PIVOT(J)) .NE. 0.0) GO TO 105
DU 106 K=1,N
IF (PIVOT(K)) .NE. 0.0) GO TO 106
TEMP=MAGABS(A(J,J))
101 IF (TEMP .GT. AMAX) GO TO 100
100 IROW=J
ICOLUMN=K
AMAX=TEMP
105 CONTINUE
100 CONTINUE
105 CONTINUE
EMP(1)=4996*IROW+ICOLUMN
J=IROW
DU 25 I=1,N
AMAX=AMAX+J+ICOLUMN
DETERM=DETERM*DETERM

C RETURN IF MATRIX IS SINGULAR (ZERO PIVOT) AFTER COLUMN INTERCHANGE

C IF (DETERM.EQ.0.0) GO TO 500
C PIVOT(ICOLUMN)=AMAX

C INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL

IF (IROW.EQ.ICOLUMN) GO TO 260
DETERM=-DETERM

500 STOP
C
DIVIDE PIVOT ROW BY PIVOT ELEMENT
C
260 K=ICOLUM
0043 ICOLUM,K]=1.0
0044 DO 350 K=1,N
0045 ICOLUM,K]=A(ICOLUM,K)/AMAX
0046 350 CONTINUE
0047 IF (M.LE.O) GO TO 380
0048 DO 370 K=1,M
0049 ICOLUM,K]=BICOLUMN,K)/AMAX
0050 370 CONTINUE
C
REDUCE NON-PIVOT ROWS
C
380 DU 550 J=1,N
0052 IF (J.EQ.ICOLUM) GO TO 550
0053 I=I(J,ICOLUM)
0054 A(J,ICOLUM)=0.0
0055 DU 350 K=1,N
0057 350 CONTINUE
0058 IF (K.LE.O) GO TO 550
0059 DU 500 K=1,M
0060 AT J,K]=B(J,K)-BICOLUMN,K)*T
0061 500 CONTINUE
0062 550 CONTINUE
C
INTERCHANGE COLUMNS AFTER ALL PIVOT OPERATIONS HAVE BEEN PERFORMED
C
600 DU 710 I=1,N
0063 II=I(I)-1
0064 ICOLUM=INDEX(I)-4096
0065 ICOLUM=INDEX(I)-4096*K
0066 IF (K.EQ.ICOLUM) GO TO 710
0067 DU 705 J=1,N
0068 DU 705 J=1,N
0069 SWAP = A(J,K)
0070 AT J,K]=A(I,K)
0071 AT I,K]=SWAP
0072 705 CONTINUE
0073 710 CONTINUE
C
RETURN
0074 END
Sample Input Data - POLYFIT

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APPENDIX B

DERIVATIONS

TRANSMITTED FLUX INTEGRAL

GAUSSIAN RESOLUTION FITTING

POLYNOMIAL FITTING
APPENDIX B

DERIVATIONS

TRANSMITTED FLUX INTEGRAL

\[ \phi_{\text{trans}}(E) = \int_{0}^{\infty} \phi_{I}(E') e^{-\Sigma(E')t} R(E, E') \, dE' \]  
(1)

where \( R(E, E') = y_{o}(E) \exp\left(\frac{-(E' - E)^{2}}{b_{o}(E)}\right) \)  
(2)

\[ \therefore \phi_{\text{trans}}(E) = \int_{0}^{\infty} \phi_{I}(E') \exp(-\Sigma(E')t) y_{o}(E) \exp\left(\frac{(E' - E)^{2}}{b_{o}(E)}\right) \, dE' \]  
(3)

Assume \( \log(\phi_{I}(E')) \) is linear between discrete energy points; between \( E_{i} \) and \( E_{i+1} \):

\[ \phi_{I}(E') = \phi_{I}^{i} + \exp\left(\frac{1n\phi_{I}^{i+1} - 1n\phi_{I}^{i}}{E_{i+1} - E_{i}}\right)(E' - E_{i}) \]

where \( \phi_{I}^{i} \) = incident flux at \( E_{i} \)

now let \( P_{i} = \left(\frac{1n\phi_{I}^{i+1} - 1n\phi_{I}^{i}}{E_{i+1} - E_{i}}\right) \)

\[ \therefore \phi_{I}(E') = \phi_{I}^{i} + \exp(\{P_{i}\}(E' - E_{i})) \]

\[ = \phi_{I}^{i} + \exp(\{P_{i}\}E') \exp(-P_{i}E_{i}) \]  
(4)

Assume \( \Sigma(E') \) is linear between discrete energy points; between \( E_{i} \) and \( E_{i+1} \):

\[ \Sigma(E')t = \Sigma_{i} t + \left(\frac{E_{i+1} - E_{i}}{E_{i+1} - E_{i}}\right)(E' - E_{i})t \]

where \( \Sigma_{i} \) = cross-section at \( E_{i} \)

now let \( X_{i} = \left(\frac{E_{i+1} - E_{i}}{E_{i+1} - E_{i}}\right)t \)

and \( S_{i} = \Sigma_{i} t \)
\[ \Sigma(E')t = S_i - X_i(E' - E_i) \]
\[ \exp[-\Sigma(E')t] = \exp(-S_i + X_i E_i) \exp(-X_i E') \]
(5)

Also,
\[ \exp\left[\frac{-(E' - E)^2}{b_o}\right] = \exp\left[\frac{E^2}{b_o}\right] \exp\left[-\frac{E'^2}{b_o} + \frac{2E'E}{b_o}\right] \]
(6)

\[ y_o = \frac{1}{\sqrt{b_o \pi}} = \text{normalization factor for gaussian} \]
(7)

Now, if there exists a \( \phi_i^I \) and \( \Sigma_i \) for each \( E_i \), the integral of equation (3) can be integrated piecewise:

\[ \phi_{\text{trans}}(E) = \int_{E_0}^{E_1} \left[ \right] \, dE' + \int_{E_1}^{E_2} \left[ \right] \, dE' + \ldots + \int_{E_{i+1}}^{E_{i+1}} \left[ \right] \, dE' \]

\[ + \ldots + \int_{E_n}^{\infty} \left[ \right] \, dE' \]
(8)

or
\[ \phi_{\text{trans}}(E) = \sum_{i=0}^{\infty} \int_{E_i}^{E_{i+1}} \left[ \right] \, dE' \]
(9)

where \( \left[ \right] = \phi_i^I(E') \exp[-\Sigma(E')t] y_o(E) \exp[-\frac{(E' - E)^2}{b_o E}] \)
(10)

Now, substituting equation (4), (5), (6), and (7) into (10), each term of equation (9) will be:

\[ \int_{E_i}^{E_{i+1}} \left\{ \phi_i^I + \exp(P_i E') \exp(-P_i E_i) \right\} \left\{ \exp(-S_i + X_i E_i) \exp(-X_i E') \right\} \left( \frac{1}{\sqrt{b_o \pi}} \right) \]

\[ \cdot \left( \exp\left(-\frac{E^2}{b_o}\right) \exp\left(-\frac{E'^2}{b_o} + \frac{2E'E}{b_o}\right) \right) \, dE' \]

\[ = \frac{1}{\sqrt{b_o \pi}} \exp(-S_i + X_i E_i - \frac{E^2}{b_o}) \int_{E_i}^{E_{i+1}} \left\{ \phi_i^I + \exp(P_i E') \exp(-P_i E_i) \right\} \]

\[ \cdot \left( \exp\left(-\frac{E'^2}{b_o} + \frac{2E'E}{b_o} - X_i E' \right) \right) \, dE' \]
(11)
let \( C_1 = \frac{1}{\sqrt{b_o \pi}} \exp(-S_i + X_i E_i - \frac{E_i^2}{b_o}) \)  
\( = C_1 \frac{\phi_i}{E_i} \int_{E_i}^{E_{i+1}} \exp(-\frac{E_i^2}{b_o} + \frac{2E_i E_i'}{b_o} - X_i E_i') \, dE' \)

\( + C_1 \exp(-P_i E_i) \int_{E_i}^{E_{i+1}} \exp(-\frac{E_i^2}{b_o} + \frac{2E_i E_i'}{b_o} - X_i E_i' + P_i E_i') \, dE' \)

These two integrals are of the form:

\[
\int_{x_1}^{x_2} e^{-ax^2 + 2bx + c} \, dx = \frac{1}{\sqrt{a}} \left( b^2 - ac \right)^{1/2} \int_{y_1}^{y_2} e^{-y^2} \, dy 
\]

where \( y = \sqrt{a}(x + \frac{b}{a}) \)

Note \( \int_{y_1}^{y_2} e^{-y^2} \, dy = \sqrt{\frac{\pi}{2}} [\text{erf}(y_2) - \text{erf}(y_1)] \)

For first integral \( a = \frac{1}{b_o}, b = \left( \frac{X_i}{2} - \frac{E}{b_o} \right), c = 0, y_i = \frac{1}{\sqrt{b_o}} \left( E_i - E + \frac{X_i b_o}{2} \right) \)

Now, substituting these constants into (14), and combining (13) and (14)

\[
\text{first integral} = \frac{\phi_i}{2} \exp \left( \frac{X_i^2 b_o}{4} + X_i (E_i - E) - S_i \right) [\text{erf}(y_{i+1}) - \text{erf}(y_i)] \]

For second integral

\[
a = \frac{1}{b_o}, b = \frac{X_i}{2} - \frac{E}{b_o} - \frac{P_i}{2}, c = 0, z_i = \frac{1}{\sqrt{b_o}} \left( E_i - E + \frac{X_i b_o}{2} - \frac{P_i b_o}{2} \right) \]

Substituting these constants into (14) and combining (13) and (14)

second integral =  
\[
\frac{1}{2} \exp \left( \frac{X_i^2}{4} b_o + X_i (E_i - E) + P_i (E - E_i) - \frac{X_i P_i b_o}{2} - \frac{P_i^2}{4} b_o - S_i \right) 
\]
Adding (15) and (16), equation (11) is now equal to:

\[
\left[\frac{1}{2} \exp\left(\frac{X_1^2}{4} b_o + X_1 (E_1 - E) - S_1\right)\right] I^{i+1}_1(\text{erf}(y_{i+1}) - \text{erf}(y_i)) \\
+ \exp\left[\frac{P_i}{E - E_1} \frac{X_1 P_i b_o}{2} - \frac{P_i^2}{4} b_o\right] (\text{erf}(Z_{i+1}) - \text{erf}(Z_i))
\]

(17)

\[\therefore \phi_{\text{trans}}(E) = \]

\[
\sum_{i=1}^{\infty} \left\{ \left[\frac{1}{2} \exp\left(\frac{X_1^2}{4} b_o + X_1 (E_1 - E) - S_1\right)\right] I^{i+1}_1(\text{erf}(y_{i+1}) - \text{erf}(y_i)) \\
+ \exp\left(P_i (E - E_1) \frac{X_1 P_i b_o}{2} - \frac{P_i^2}{4} b_o\right) (\text{erf}(Z_{i+1}) - \text{erf}(Z_i)) \right\}
\]

(18)

where \( \phi^i_1 \) = incident flux at \( E_1 \)

\( \Sigma_1 = \) cross-section at \( E_1 \)

\( S_1 = \Sigma_1 t \)

\( X_1 = (\Sigma_{i+1} - \Sigma_1)/(E_{i+1} - E_1) \)

\( P_i = (\ln \phi^{i+1}_1 - \ln \phi^i_1)/(E_{i+1} - E_1) \)

\( y_i = \frac{1}{\sqrt{b_o}} (E_1 - E + \frac{X_1 b_o}{2}) \)

\( Z_i = \frac{1}{\sqrt{b_o}} (E_1 - E + \frac{X_1 b_o}{2} - \frac{P_i b_o}{2}) \)

\( b_o = \) function of the resolution = \( \frac{(\text{FEP/R})^2}{4 \cdot \ln 2} \)
GAUSSIAN RESOLUTION FITTING

Using Weighted Least Squares

Gaussian:

\[ y_i = y_o e^{-\frac{(x_i - x_o)^2}{b_o}} \]

(1)

Definition: FWHM

\[ \frac{1}{2} y_o = y_o \exp\left\{ -\frac{(x - x_o)^2}{b_o} \right\} \]

\[ \ln y_o = \ln 2 = \ln y_o - \frac{(x - x_o)^2}{b_o} \]

\[ \ln 2 = \frac{(x - x_o)^2}{b_o} \]

\[ (x - x_o)^2 = b_o \cdot \ln 2 \]

\[ x - x_o = (b_o \ln 2)^{\frac{1}{2}} \]

Now,

\[ \text{FWHM} = 2(x - x_o) = 2(b_o \ln 2)^{\frac{1}{2}} \]

(2)

also,

\[ b_o = \frac{(\text{FWHM})^2}{4 \ln 2} \]

(3)

Determine \( y_o \) so total area under Gaussian is equal to 1

\[ 1 = \int_{0}^{\infty} y_o \exp\left\{ -\frac{(x_i - x_o)^2}{b_o} \right\} dx_i = y_o \int_{-\infty}^{\infty} \exp\left\{ -\frac{(x_i - x_o)^2}{b_o} \right\} dx_i \]

(4)

since the gaussian curves are on the positive real axis, and at some distance from the origin.

Let \( z = x_i - x_o \), \( dx_i = dz \)

\[ \therefore = y_o \int_{-\infty}^{\infty} e^{-\frac{z^2}{b_o}} dz = y_o \left\{ 2 \int_{0}^{\infty} e^{-\frac{z^2}{b_o}} dz \right\} \]

(5)
\[ \int_{0}^{\infty} e^{-z^2/b_o} dz = \sqrt{b_o} \int_{0}^{\infty} e^{-z^2} dz = \sqrt{b_o} \frac{\pi}{2} [\text{erf}(z)]_{0}^{\infty} \]

\[ \therefore \int_{0}^{\infty} e^{-z^2/b_o} dz = \frac{\sqrt{b_o} \pi}{2} (1 - 0) = \frac{\sqrt{b_o} \pi}{2} \] (6)

\[ \therefore 1 = 2y_o \frac{\sqrt{b_o} \pi}{2} \]

or

\[ y_o = \frac{1}{\sqrt{b_o} \pi} \text{ Normalized} \] (7)

Using Weighted Least Squares

Taking the ln( ) of equation 1.

\[ \ln y_i = \ln y_o - \frac{(x_i - x_o)^2}{b_o} \] (8)

let \( z_i = \ln y_i \)

\[ \therefore \sigma_{z_i}^2 = \left( \frac{\delta z_i}{\delta y_i} \right)^2 \sigma_{y_i}^2 = \left( \frac{1}{y_i} \right)^2 \sigma_{y_i}^2 = \frac{\delta y_i}{y_i^2} \]

Thus, weight the function \( z_i \) by \( \frac{1}{\sigma_{z_i}^2} = \frac{y_i^2}{\sigma_{y_i}^2} \)

\[ W = \begin{pmatrix} \frac{y_1^2}{\sigma_{z_1}^2} & 0 & 0 & \cdots \\ 0 & \frac{y_2^2}{\sigma_{z_2}^2} & \cdots \\ 0 & 0 & \ddots & \frac{y_n^2}{\sigma_{z_n}^2} \end{pmatrix} \] (9)

Now, using equation 8

\[ \ln y_i = \ln y_o - \frac{x_i^2}{b_o} + \frac{2x_i x_o}{b_o} - \frac{x_o^2}{b_o} \] (10)
Let
\[ \ln y_o - \frac{x_o^2}{b_o} = S_3 \] (11)
\[ \frac{2x_o}{b_o} = S_2 \] (12)
\[ -\frac{1}{b_o} = S_1 \] (13)

Thus
\[
\begin{pmatrix}
  x_1^2 & x_1 & 1 \\
  x_2^2 & x_2 & 1 \\
  \vdots & \vdots & \vdots \\
  x_n^2 & x_n & 1
\end{pmatrix}
\begin{pmatrix}
  S_1 \\
  S_2 \\
  \vdots \\
  S_3
\end{pmatrix}
= 
\begin{pmatrix}
  z_1 \\
  z_2 \\
  \vdots \\
  z_n
\end{pmatrix}
\] (14)

This is of the form: \[ A \cdot X = B \]

For least square solution: \[ A^T A \cdot X = A^T B \]

Now, applying weighting function:
\[ W A^T A \cdot X = W A^T B \] (15)

Since \( W \) is a diagonal matrix, equation 15 can be written as:
\[ A^T W A X = A^T W B \]

or
\[ X = (A^T W A)^{-1} A^T W B \] (16)

Defining the term of equation 16:
\[ A^T = \begin{bmatrix}
  x_1^2 & x_2^2 & \cdots & x_n^2 \\
  x_1 & x_2 & \cdots & x_n \\
  1 & 1 & \cdots & 1
\end{bmatrix} \]
\[
W A = \begin{pmatrix}
\frac{x_1 y_1^2}{\sigma y_1^2} & \frac{x_1 y_2^2}{\sigma y_1^2} & \frac{y_1^2}{\sigma y_1^2} \\
\frac{x_2 y_1^2}{\sigma y_2^2} & \frac{x_2 y_2^2}{\sigma y_2^2} & \frac{y_2^2}{\sigma y_2^2} \\
\vdots & \vdots & \vdots \\
\frac{x_n y_1^2}{\sigma y_n^2} & \frac{x_n y_2^2}{\sigma y_n^2} & \frac{y_1^2}{\sigma y_n^2}
\end{pmatrix}
\]

\[
A^T W A = \begin{pmatrix}
\sum_{i=1}^{n} \frac{x_i^4 y_i^2}{\sigma y_i^2} & \sum_{i=1}^{n} \frac{x_i^3 y_i^2}{\sigma y_i^2} & \sum_{i=1}^{n} \frac{x_i^2 y_i^2}{\sigma y_i^2} \\
\sum_{i=1}^{n} \frac{x_i^3 y_i^2}{\sigma y_i^2} & \sum_{i=1}^{n} \frac{x_i^2 y_i^2}{\sigma y_i^2} & \sum_{i=1}^{n} \frac{y_i^2}{\sigma y_i^2} \\
\sum_{i=1}^{n} \frac{x_i^2 y_i^2}{\sigma y_i^2} & \sum_{i=1}^{n} \frac{x_i y_i^2}{\sigma y_i^2} & \sum_{i=1}^{n} \frac{y_i^2}{\sigma y_i^2}
\end{pmatrix}
\]

\[
W B = \begin{pmatrix}
\frac{y_1^2}{\sigma y_1^2} & z_1 \\
\frac{y_2^2}{\sigma y_2^2} & z_2 \\
\vdots & \vdots \\
\frac{y_n^2}{\sigma y_n^2} & z_n
\end{pmatrix}
\]

\[
A^T W B = \begin{pmatrix}
\sum_{i=1}^{n} \frac{x_i y_i^2}{\sigma y_i^2} & z_1 \\
\sum_{i=1}^{n} \frac{x_i y_i^2}{\sigma y_i^2} & z_2 \\
\sum_{i=1}^{n} \frac{x_i y_i^2}{\sigma y_i^2} & z_3
\end{pmatrix}
\]

Substituting these quantities into equation 16, get solution of the form:

\[
X = \begin{pmatrix}
S_1 \\
S_2 \\
S_3
\end{pmatrix}
\]
where $S_1$, $S_2$ and $S_3$ are given by equations 11, 12, and 13.

Also

$$\sigma_{S_1}^2 = (A^TA)^{-1}_{11}$$

$$\sigma_{S_2}^2 = (A^TWA)^{-1}_{22}$$

$$\sigma_{S_3}^2 = (A^TWA)^{-1}_{33}$$

Therefore:

$$b_o = -\frac{1}{S_1}$$

and $\sigma_{b_o}^2 = \left(\frac{\partial b_o}{\partial S_1}\right)^2 \sigma_{S_1}^2 = \frac{1}{S_1^2} \sigma_{S_1}^2$

$$x_o = \frac{b_o S_2}{2}$$

and $\sigma_{x_o}^2 = \left(\frac{\partial x_o}{\partial b_o}\right)^2 \sigma_{b_o}^2 + \left(\frac{\partial x_o}{\partial S_2}\right)^2 \sigma_{S_2}^2 = \frac{S_2^2}{4} \sigma_{b_o}^2 + \frac{b_o^2}{4} \sigma_{S_2}^2$

$$\ln y_o = S_3 + \frac{x_o^2}{b_o}$$

$$\sigma_{y_o}^2 = \left(\frac{\partial y_o}{\partial S_3}\right)^2 \sigma_{S_3}^2 + \left(\frac{\partial y_o}{\partial x_o}\right)^2 \sigma_{x_o}^2 + \left(\frac{\partial y_o}{\partial b_o}\right)^2 \sigma_{b_o}^2$$

$$= \left[\begin{array}{c}
S_3 + \frac{x_o^2}{b_o} \\
s^2 + \frac{x_o^2}{b_o}
\end{array}\right] \sigma_{s^2}^2 + \left[\begin{array}{c}
2x_o S_3 + \frac{x_o^2}{b_o} \\
- \frac{x_o^2}{b_o} e - \frac{x_o^2}{b_o}
\end{array}\right] \sigma_{x_o}^2 + \frac{x_o^2}{b_o} \sigma_{b_o}^2$$

Note, exponentials may get large, causing overflows on the computer.

Therefore, let $z = \ln y_o = S_3 + \frac{x_o^2}{b_o}$
$$\sigma_3^2 = \left(\frac{1}{y_o}\right)^2 \quad \sigma_{y_o}^2 = \left(\frac{33}{\sigma_3}\right)^2 \sigma_{S_3}^2 + \left(\frac{33}{\sigma_x o}\right)^2 \sigma_{x o}^2 + \left(\frac{33}{\sigma_b o}\right)^2 \sigma_{b o}^2$$

$$= \sigma_{S_3}^2 + \left(\frac{2x_o}{b_o}\right)^2 \sigma_{x o}^2 + \left(-\frac{x_o^2}{b_o}\right)^2 \sigma_{b o}^2$$

$$\therefore \sigma_{y_o}^2 = y_o^2 \left(\frac{4x^2}{b_o^2} \sigma_{x o}^2 + \frac{x_i^2}{b_o^4} \sigma_{b o}^2\right)$$
POLYNOMIAL FITTING

Using Weighted Least Squares

The method used for this problem is the same as that used for the gaussian fitting problem. In this case, data is fit to a polynomial of degrees m:

\[ y_1 = a_0 + a_1 x_1 + a_2 x_1^2 + a_3 x_1^3 + \ldots + a_m x_1^m \]  \hspace{1cm} (1)

For this function, the weighting function \( W \) is the variance of \( y_1 \), that is:

\[
W = \begin{bmatrix}
\frac{1}{\sigma_{y_1}^2} & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & \frac{1}{\sigma_{y_n}^2}
\end{bmatrix}
\]  \hspace{1cm} (2)

Rewriting equation 1:

\[
\begin{bmatrix}
1 & x_1 & x_1^2 & \cdots & x_1^m \\
1 & x_2 & x_2^2 & \cdots & x_2^m \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & x_n & x_n^2 & \cdots & x_n^m
\end{bmatrix}
\begin{bmatrix}
a_0 \\
a_1 \\
a_2 \\
\vdots \\
a_m
\end{bmatrix} =
\begin{bmatrix}
y_1 \\
y_2 \\
y_3 \\
\vdots \\
y_n
\end{bmatrix}
\]  \hspace{1cm} (3)

This is of the form \( A \cdot X = B \)

If \( n > m \), which is normally the case, the set of equations in equation 3 is over determined, and the least squares solution is:

\[
A^T A X = A^T B
\]

Now, applying the weighting function \( W \) and rearranging as before:

\[
X = (A^T W A)^{-1} A^T W B
\]  \hspace{1cm} (4)

This is the same equation as used in the gaussian fitting problem, where \( A \) and \( B \) are defined by equation 3, and
\[
A^T = \begin{pmatrix}
1 & 1 & \cdots & 1 \\
x_1 & x_2 & \cdots & x_n \\
x_1^2 & x_2^2 & \cdots & x_n^2 \\
\vdots & \vdots & \ddots & \vdots \\
x_1^m & x_2^m & \cdots & x_n^m
\end{pmatrix}
\]

\[
WA = \begin{pmatrix}
\frac{1}{\sigma z} & \frac{x_1}{\sigma y_1} & \cdots & \frac{x_m}{\sigma y_1} \\
\frac{1}{\sigma y_1} & \frac{x_1}{\sigma y_1} & \cdots & \frac{x_m}{\sigma y_1} \\
\frac{1}{\sigma y_2} & \frac{x_2}{\sigma y_2} & \cdots & \frac{x_m}{\sigma y_2} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{1}{\sigma y_n} & \frac{x_n}{\sigma y_n} & \cdots & \frac{x_m}{\sigma y_n}
\end{pmatrix}
\]

\[
A_{\text{WA}}^T = \begin{pmatrix}
\sum_{i=1}^{n} \frac{1}{\sigma y_i} & \sum_{i=1}^{n} \frac{x_i}{\sigma y_i} & \cdots & \sum_{i=1}^{n} \frac{x_m}{\sigma y_i} \\
\sum_{i=1}^{n} \frac{x_i}{\sigma y_i} & \sum_{i=1}^{n} \frac{x_i^2}{\sigma y_i^2} & \cdots & \sum_{i=1}^{n} \frac{x_{m+1}}{\sigma y_i^2} \\
\vdots & \vdots & \ddots & \vdots \\
\sum_{i=1}^{n} \frac{x_i^m}{\sigma y_i^m} & \sum_{i=1}^{n} \frac{x_i^{m+1}}{\sigma y_i^{m+1}} & \cdots & \sum_{i=1}^{n} \frac{x_{m+m}}{\sigma y_i^{m+m}}
\end{pmatrix}
\]
\[
 WB = 
 \begin{pmatrix}
 \frac{y_1}{\sigma y_1} \\
 \frac{y_2}{\sigma y_2} \\
 \vdots \\
 \frac{y_n}{\sigma y_n}
 \end{pmatrix}
\]

\[
 A^T WB = 
 \begin{pmatrix}
 \frac{n}{\sigma y_1} \\
 \frac{n}{\sigma y_1} \\
 \vdots \\
 \frac{n}{\sigma y_1}
 \end{pmatrix}
\]

Substituting these quantities into equation (4), the solution is of the term

\[
 X = \begin{pmatrix}
 a_0 \\
 a_1 \\
 a_2 \\
 \vdots \\
 a_m
 \end{pmatrix}
\]

where the \( a_1 \)'s are the coefficients of the polynomial of degree \( m \).
APPENDIX C

SAMPLE CONTAINERS

OXYGEN SAMPLE CONTAINER DESIGN

LIQUID SODIUM SAMPLE CONTAINER DESIGN
APPENDIX C

SAMPLE CONTAINERS

OXYGEN SAMPLE CONTAINER DESIGN

A rectangular tank was the sample (liquid oxygen) vessel and had an inner box of 2" x 2" x 36", an outer box of 4" x 4" x 40", and the void in between was filled with Vermiculite insulating material. A double walled cylinder (1 1/2" I.D., 3 1/2" O.D., 8" high) acted as a vent at the top of the oxygen reservoir. The inner pipe extended 12" beyond the double walled cylinder for venting purposes. The entire insulating chamber was sealed to prevent exposure to the liquid oxygen.

Due to the flammable and sometimes explosive nature of materials in the presence of high concentrations of oxygen, several precautions were necessary. The sample tank was cleaned several times both inside and out during construction with trichlorethylene to remove any contamination, especially oil, and was checked using a black light. The insulating material, Vermiculite, is known for its inert properties, but a further check was made to determine if oxygen is absorbed to a great extent by the material. The Vermiculite was also "outgassed" at 600°F for several hours to remove contaminants. All equipment was grounded so that static electricity would not cause a spark. The venting tube on top of the sample tank had a "goose-neck" shape to prevent foreign material from falling into the oxygen reservoir. The venting tube was large enough to reduce the number of fillings necessary during an experiment. Evaporation of $O_2$ was estimated to be ~500 liters/hr of gas (~6 liters/hr liquid) which was dispersed into the volume of the reactor bay. This created a rise of .005%/hour in oxygen concentration in the bay. Total increase in oxygen concentration during a single experiment was less than .01% since the initial filling of the sample
was carried out outside the reactor bay; thus, the large evolution of
gaseous oxygen associated with "cooling down" of the sample tank took
place out of doors.

As a final precaution, before any large volumes of oxygen were intro-
duced into the bay, a small sample (≈.5 liter) of liquid oxygen in an
aluminum dewar was placed in the neutron beam from the reactor to insure
that no unforeseen reactions would take place.
LIQUID SODIUM SAMPLE CONTAINER DESIGN

Due to the high chemical reactivity of sodium, especially with water, several precautions were taken to insure that the sodium was kept under an inert atmosphere. To achieve this, a double walled stainless steel container of 1/16" stock was used. The inner container, 2" x 2" x 36" long, held the sodium and was heated with resistance heating wire. A funnel shaped reservoir provided an expansion chamber for the sodium as it was heated. The outer container was 4" x 6" x 40", with the void between the inner and outer chamber being filled with Vermiculite for insulation to a depth of 4". The top two inches of the void were filled with an inert gas (nitrogen) which was constantly passed over the sodium, and maintained at a pressure of approximately 2 psi gage. Directly over the sodium expansion chamber, the outer chamber had a removable section so that calcium carbonate could be added in case of fire at the sodium interface. Exposure of the sodium to the neutron beam resulted in a radiation hazard with the formation of ≈15 millicuries of Na²⁴, which resulted in a dose rate of ≈15 mr/hr. at 1 foot. Therefore, the sample had to be stored in a dry, shielded area until the Na²⁴ decayed.
THE EVALUATION OF MINIMA IN TOTAL NEUTRON CROSS-SECTION
BY TRANSMISSION OF FISSION SPECTRA THROUGH THICK SAMPLES

by

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ABSTRACT

An evaluation of minima in total neutron cross-sections was performed for several materials by comparing an experimentally measured transmitted spectrum with the corresponding calculated result. Published cross-section data were evaluated for iron, lead, liquid oxygen, and solid and liquid sodium. Since thick samples (three or more mean free paths thick) were used, the analysis was very sensitive to minima in the cross-section.

The incident neutron spectrum was obtained from the Triga Mark II reactor and was detected using an NE-213 liquid scintillator spectrometer system. Computer codes were used to unfold the raw data and to calculate the transmitted spectrum (which was a function of published cross-section data, the measured incident flux on the sample and the resolution of the detector). The results of this study demonstrate the usefulness of this technique in evaluating total neutron cross-section.

Several experimental geometry conditions were used in this work to obtain valid results and to study the effects of forward scattering and multiple scattering in the thick samples. The results showed that there is a question as to the accuracy of published angular cross-section data near the zero scattering angle.