
L. C. Leal
N. M. Larson
Computational Physics and Engineering Division

SAMDIST: A COMPUTER CODE FOR CALCULATING STATISTICAL DISTRIBUTIONS FOR R-MATRIX RESONANCE PARAMETERS

L. C. Leal
N. M. Larson

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ABSTRACT

The SAMDIST computer code has been developed to calculate distribution of resonance parameters of the Reich-Moore R-matrix type. The program assumes the parameters are in the format compatible with that of the multilevel R-matrix code SAMMY.

SAMDIST calculates the energy-level spacing distribution, the resonance width distribution, and the long-range correlation of the energy levels. Results of these calculations are presented in both graphic and tabular forms.
1. INTRODUCTION

The existence of statistical distributions for R-matrix resonance parameters has important implications for data analyses in both the resolved and the unresolved energy regions. In the resolved energy region, an evaluator may encounter difficulties in obtaining a set of resonance parameters that fit simultaneously various sets of experimental data. The most common source of these difficulties is the broadening of the data due to finite experimental resolution; this broadening may preclude the identification of some small-resonance levels. In such a case, the known statistical distributions of the resonance parameters can be used to provide guidance for the location and the magnitudes of missing levels in the resonance set. In the unresolved energy region, the statistical distributions of the resonance parameters can be used to generate average cross sections.

The purpose of this work is to describe a tool, the code SAMDIST, which can be used in conjunction with a cross-section evaluation code such as SAMMY\(^1\) to verify the consistency of a resonance parameter set with the predicted theoretical statistical distribution.

The SAMDIST code has been designed for calculating distributions of resonance parameters of the Reich-Moore R-matrix type. The program accommodates resonance parameters in a format compatible with that of the SAMMY code. SAMDIST calculates distributions of the resonance parameters and compares them with theoretical predictions; results of those calculations are given in graphic and tabular forms. Average values and standard deviations are also given. A listing of the SAMDIST program is given in Appendix A.

The following tasks can be performed with the SAMDIST code:
\begin{enumerate}
\item Level spacing distributions may be determined according to the Wigner distribution law.
\item Distributions may be calculated for all widths, including neutron width, radiation width, and fission width (usually two channels in the Reich-Moore formalism). Values for each of these widths are distributed according to a \(\chi^2\) distribution with the appropriate number of degrees of freedom.
\item Long-range correlations of the energies can be tested via the A, statistic test of Mehta-Dyson.
\end{enumerate}
2. BRIEF OVERVIEW OF THE THEORETICAL DISTRIBUTIONS OF THE RESONANCE PARAMETERS

2.1 LEVEL SPACING DISTRIBUTION LAW

The spacing between two consecutive resonance energies for the same total angular momentum and parity exhibits random behavior. For a set of \( n \) resonance energy levels, \( E_1, E_2, \ldots, E_n \), where the level spacing between two consecutive energies, \( E_k \) and \( E_{k+1} \), is \( D_k \), and the average level spacing is \( \langle D \rangle \), the probability distribution function predicted by the Wigner law is

\[
p(x) \, dx = \frac{\pi x}{2} \exp\left(-\frac{\pi x^2}{4}\right) \, dx,
\]

where \( x = D_k / \langle D \rangle \), and \( \langle D \rangle \) is the average level spacing. The Wigner probability distribution function has the following property:

\[
\int_0^\infty p(x) \, dx = \int_0^\infty x p(x) \, dx = 1.
\]

The second moment of the Wigner distribution is given by

\[
\overline{x^2} = \int_0^\infty x^2 p(x) \, dx = \frac{4}{\pi}.
\]

Equation (1) was the first mathematical prediction of the level spacing distribution to provide excellent agreement with experimental results; it has triggered a series of investigations on the subject of the statistical distribution of resonance parameters. Although other accurate level spacing distributions have been proposed, Wigner's law is the most widely used and is suitable for practical applications.

2.2 RESONANCE WIDTH DISTRIBUTION LAW

Systematic measurements of the resonance widths show strong fluctuations among resonances of the same angular momentum and parity. The definition of resonance width involves two other quantities, namely the reduced widths, \( \gamma_{\lambda e} \), and the penetration factor, \( P_e \), which are related according to the equation

\[
\Gamma_\lambda = \sum_e (2 P_e) \gamma_{\lambda e}^2,
\]
where $\lambda$ refers to the energy levels in the compound nucleus and $c$ refers to the particle channel. One should expect that the fluctuations are connected to either the reduced widths, $\gamma_{\lambda c}$, or to the penetration factors, $P_c$. However, it is improbable that the fluctuations are due to the penetration factors since they are smooth functions of energy. Therefore, the observed fluctuations are caused by the reduced widths, $\gamma_{\lambda c}$, these, in turn, are related to the projection of the eigenfunctions of the Hamiltonian of the compound nucleus on the nuclear surface. This projection involves an integration of many uncorrelated contributions, positive and negative, over the high-dimensional phase space of the compound nucleus. It then follows from the central limit theorem that the distributions of $\gamma_{\lambda c}^2$ have a Gaussian distribution with zero-mean. Therefore, the distribution function of the reduced widths can be written as

$$P(\gamma_{\lambda c}) \ d\gamma_{\lambda c} = \frac{1}{\sqrt{2\pi <\gamma_{\lambda c}^2>}} \exp(-\frac{\gamma_{\lambda c}^2}{2<\gamma_{\lambda c}^2>}) \ d\gamma_{\lambda c},$$

where $<\gamma_{\lambda c}^2>$ is the average value of $\gamma_{\lambda c}^2$.

The probability distribution function of the resonance widths, $\Gamma_{\lambda}$, can be derived from Eq. (3) as follows: The statistical theorem states that if $y$ is a variable that is the sum of squares of $v$ normally distributed zero-mean independent variables, then $y$ is distributed according to a $\chi^2$ distribution with $v$ degrees of freedom. Therefore, the distribution of $\Gamma_{\lambda}$ is

$$p_v(x) \ dx = \frac{v}{2G(v/2)} \left(\frac{x}{2}\right)^{v/2-1} \exp(-vx/2) \ dx,$$

where $x = \Gamma_{\lambda}/\langle\Gamma\rangle$, $G(v/2)$ is the mathematical gamma function, and $\langle\Gamma\rangle$ is the average value of the width taken over a given energy range. For $v = 1$, Eq. (6) is well known as the Porter-Thomas distribution law of the neutron width. It is generally accepted that fission is a few-channel process, and that there are only a limited number of effectively open channels; 2 or 3 degrees of freedom ($v = 2$ or $v = 3$) are usually assumed in the fission width distribution. In the neutron capture event, a large number of capture channels are opened; the gamma width distribution is represented by a $\chi^2$ distribution with a large number of degrees of freedom ($v-w$), which corresponds to a Dirac-delta function centered at $\Gamma_{\lambda} = \langle\Gamma\rangle$.

The $\chi^2$ distribution function has the following property:

$$\int_0^\infty p_v(x) \ dx = \int_0^\infty x p_v(x) \ dx = 1.$$
The second moment of a $\chi^2$ distribution with $v$ degrees of freedom is given as

$$x^2 = \int_0^\infty x^2 p_v(x) \, dx = \frac{2}{v} + 1. \quad (8)$$

2.3 DYSON AND MEHTA LONG-RANGE CORRELATION OF $\Delta_3$ STATISTICS TEST

Another useful tool for evaluating nuclear data is the $\Delta_3$ statistics test introduced by Dyson and Mehta.\textsuperscript{4} The $\Delta_3$ test provides a measure of the mean-square deviation between the number of observed energy levels in the energy interval $E_i$ to $E_f$ and the best fit to the straight line, as a function of energy, given as $aE + b$. Strictly speaking, the definition is

$$\Delta_3 = \text{Min}_{(a,b)} \left[ \frac{1}{2L} \int_{E_i}^{E_f} (N(E) - aE - b)^2 \, dE \right], \quad (9)$$

where $N(E)$ is the corresponding cumulative number of energy levels as a function of energy.

The Dyson and Mehta $\Delta_3$ test predicts that the theoretical average value $<\Delta_3>$ is given as

$$<\Delta_3> = \frac{1}{\pi^2} [\ln(n) - 0.06871], \quad (10)$$

with variance $V_{\Delta_3} = 1.169/\pi^4$. Here $n$ is the number of energy levels observed in the interval $E_i$ to $E_f$.

For practical applications, the coefficients $a$ and $b$ in Eq. (9) are determined according to the following conditions:

$$\frac{\partial \Delta_3}{\partial a} = 0, \quad (11)$$

and

$$\frac{\partial \Delta_3}{\partial b} = 0. \quad (12)$$
These conditions lead to the following equations:

\[
a \int_{E_i}^{E_f} E^2 \, dE + b \int_{E_i}^{E_f} E \, dE = \int_{E_i}^{E_f} N(E) \, dE, \tag{13}
\]

and

\[
a \int_{E_i}^{E_f} E \, dE + b \int_{E_i}^{E_f} dE = \int_{E_i}^{E_f} N(E) \, dE. \tag{14}
\]

The following identities will be used in evaluating \(a\) and \(b\):

\[
\int_{E_i}^{E_f} dE = E_f - E_i, \tag{15}
\]

\[
\int_{E_i}^{E_f} E \, dE = \frac{(E_f^2 - E_i^2)}{2}, \tag{16}
\]

and

\[
\int_{E_i}^{E_f} E^2 \, dE = \frac{(E_f^3 - E_i^3)}{3}. \tag{17}
\]

If the energy levels in the range \(E_i\) to \(E_f\) are numbered from \(l = -L\) to \(l = +L\), then the following relations also hold:

\[
\int_{E_i}^{E_f} N(E) \, dE = \sum_{l=-L}^{L} \int_{E_l}^{E_{l+1}} l \, dE = \sum_{l=-L}^{L} l (E_{l+1} - E_l), \tag{18}
\]
\[ \int_{E_i}^{E_f} N(E) E \, dE = \sum_{l=-L}^{L} \int_{E_i}^{E_{i+1}} l \, E \, dE = \sum_{l=-L}^{L} l \left( E_{i+1}^2 - E_i^2 \right) / 2, \] (19)

and

\[ \int_{E_i}^{E_f} N^2(E) E \, dE = \sum_{l=-L}^{L} l^2 \left( E_{i+1} - E_i \right). \] (20)

The system of Eqs. (13) and (14) can be written as

\[ \alpha_1 a + \beta_1 b = \gamma_1 \] (21)

and

\[ \alpha_2 a + \beta_2 b = \gamma_2, \] (22)

in which the Greek symbols are defined as

\[ \int_{E_i}^{E_f} E \, dE = \left( E_f^2 - E_i^2 \right) / 2, \] and

\[ \alpha_2 = \beta_1 = \left( E_f^2 - E_i^2 \right) / 2, \] (23)

\[ \beta_2 = E_f - E_i, \] (24)

\[ \gamma_1 = \sum_l l \left( E_{i+1}^2 - E_i^2 \right) / 2, \] (25)

\[ \gamma_2, \] (26)

and
\[ \gamma_n = \sum I(E_{i+1} - E_i) \]  \hspace{1cm} (27)

The solution for \( a \) and \( b \) is then

\[ a = \frac{\gamma_1 - \gamma_2 \beta_1 / \beta_2}{\alpha_1 - \alpha_2 \beta_1 / \beta_2}, \]  \hspace{1cm} (28)

and

\[ b = \frac{\gamma_2}{\beta_2} - \frac{\alpha_2 \gamma_1 - \gamma_2 \beta_1 / \beta_2}{\beta_2 \alpha_1 - \alpha_2 \beta_1 / \beta_2}. \]  \hspace{1cm} (29)

Substituting these definitions into Eq. (9) leads to the expression for the \( A \), test:

\[ \Delta_3 = \frac{1}{E_f - E_i} \left\{ \int_{E_i}^{E_f} N^2(E) \, dE - \gamma_1 a - \gamma_2 b \right\}, \]  \hspace{1cm} (30)

or

\[ \Delta_3 = \frac{1}{E_f - E_i} \left\{ \sum_{E_i}^{E_f} I^2(E_{i+1} - E_i) - \gamma_1 a - \gamma_2 b \right\}, \]  \hspace{1cm} (31)

where \( a \) and \( b \) are given by Eqs. (28) and (29), and \( \gamma_1 \) and \( \gamma_2 \) by Eqs. (26) and (27).
3. SAMPLING PROCEDURE

3.1. FIRST AND SECOND MOMENTS, VARIANCE AND STANDARD DEVIATION

The statistical sampling of the experimental data, such as the energy level spacing, the resonance width, etc., are carried out following the usual procedure applied in statistics. For a number \( n \) of random variables \((x_1, x_2, \ldots, x_n)\) selected according to a probability distribution function, \( f(x) \), the estimation of the first moment, \( \bar{x} \), also referred to as the mean, is given by

\[
\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i .
\]  

(32)

Similarly, the second moment is given by

\[
\bar{x}^2 = \frac{1}{n} \sum_{i=1}^{n} x_i^2 .
\]  

(33)

The dispersion of the \( x_i \) with respect to \( \bar{x} \) is defined as

\[
\sigma^2_{x_i} = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2 .
\]  

(34)

The variance of \( \bar{x} \) is given by

\[
\sigma^2_{\bar{x}} = \frac{1}{n} \sum_{i=1}^{n} \sigma^2_{x_i}
\]  

(35)

or

\[
\sigma^2_{\bar{x}} = \frac{1}{n(n-1)} \sum_{i=1}^{n} (x_i - \bar{x})^2 .
\]  

(36)

whereas the standard deviation, \( s \), is given by

\[
s = \sqrt{\sigma^2_{\bar{x}}} .
\]  

(37)
3.2. DATA HISTOGRAM REPRESENTATION

The histogram distribution of the $n$ samples are obtained according to the following steps:\n
1. The set of random variables $(x_1,x_2,\ldots,x_n)$ are ordered such that $x_i < x_{i+1}$.

2. For a user-defined bin width, $\delta x$, the number of intervals, $n_i$, is determined as

   $$n_i = \frac{y_n}{\delta x} \quad \quad (38)$$

3. The random variables $(x_1,x_2,\ldots,x_n)$ are sampled to determine the frequency in which $x_i$, for $i=1,\ldots,n$, falls in the interval between $(k-1)\delta x$ and $k\delta x$, where $k=1,\ldots,n_i$.

4. To calculate the probability $p_k$ of finding $x \in (x_1,x_2,\ldots,x_n)$ in the $k^{th}$ interval between $(k-1)\delta x$ and $k\delta x$, and the corresponding variance $\sigma_k^2$, and consequently the standard deviation $s$, we note that each event in the $k^{th}$ interval adds to a success, such as

   $$\xi_{ik} = \begin{cases} 
   1 & \text{event in the } k^{th} \text{ interval } (i \in k) \\
   0 & \text{otherwise } (i \notin k)
   \end{cases} \quad \quad (39)$$

Therefore, the probability, $p_k$, is

$$p_k = p((k-1)\delta x < x < k\delta x) = \frac{1}{n} \sum_{i=1}^{n} \xi_{ik}, \quad \quad (40)$$

or

$$p_k = \frac{k_i}{n}, \quad \quad (41)$$

where $k_i$ is the number of samples falling into the $k^{th}$ interval.

The variance $\sigma_k^2$ is given by

$$\sigma_k^2 = \frac{1}{n(n-1)} \sum_{i=1}^{n} (\xi_{ik} - p_k)^2 \quad \quad (42)$$

or
\[ \sigma_k^2 = \frac{1}{(n-1)} p_k (1 - p_k) , \]  

(43)

and the standard deviation, \( s \), is given as

\[ s = \sqrt{\frac{1}{(n-1)} p_k (1 - p_k)} . \]  

(44)
4. RUNNING SAMDIST

The SAMDIST program is written in FORTRAN77 on a RISC-6000 UNIX-based system. The input to SAMDIST is constructed by answering various prompts that ask for the type of the distribution, the name of the resonance parameters in the SAMMY format, the energy range in which the calculations are to be performed, etc. Two output files are produced as the result of a SAMDIST run: one of them is in ASCII format, named samdist.avg, while the other is in the FORODF format, named samdist.odf, which, in turn, can be displayed in graphic form. To illustrate the procedure to execute the SAMDIST program, the $^{235}\text{U}$ s-wave resonance parameters are used. These represent the cross sections in the energy range from 0 to 500 eV and are stored in the file Oto500.par. Two resonance spin groups are in the resonance parameter sets; these groups are specified by the numbers in the last columns of the file in the SAMMY format (for which a listing is displayed in Appendix B). In the following examples, the resonance parameter distributions are taken for the entire energy range from 0 to 500 eV. To distinguish program prompts from reply, the prompts are given in boldface letters.

a. **Level-spacing distribution for spin group 1**

samdist

**Type d (for spacing), w (for width), or d3 (for delta3)**

d

**Parameter file name**

Oto500.par

**Spin group, initial and final energies**

1,0,500.0

**Bin width for sampling**

0.2

b. **Level-spacing distribution for spin group 2**

samdist

**Type d (for spacing), w (for width), or d3 (for delta3)**

d

**Parameter file name**

Oto500.par

**Spin group, initial and final energies**

2,0,500.0

**Bin width for sampling**

0.2
c. Reduced neutron-width distribution for spin-group 1

samdist
Type d (for spacing), w (for width), or d3 (for delta3)

Parameter file name
0to500.par
Particle channel
neutron
Spin group, initial and final energies
1,0.0,500.0
Bin width for sampling
1.0
Degrees of freedom
1

d. Reduced neutron-width distribution for spin-group 2

samdist
Type d (for spacing), w (for width), or d3 (for delta3)

Parameter file name
0to500.par
Particle channel
neutron
Spin group, initial and final energies
2,0.0,500.0
Bin width for sampling
1.0
Degrees of freedom
1

e. Fission-width distribution for spin-group 1

samdist
Type d (for spacing), w (for width), or d3 (for delta3)

Parameter file name
0to500.par
Particle channel
fission
Spin group, initial and final energies
1,0.0,500.0
Bin width for sampling
1.0

Degrees of freedom
4

f. Fission-width distribution for spin group 2

samdist
Type d (for spacing), w (for width), or d3 (for delta3)

w
Parameter file name
Oto500.par

Particle channel
fission

Spin group, initial and final energies
2.0,0,500.0

Bin width for sampling
1.0

Degrees of freedom
4

  g. $\Delta_3$ statistic test for spin group 1

samdist
Type d (for spacing), w (for width), or d3 (for delta3)
d3

Parameter file name
Oto500.par

Spin group, initial and final energies
1.0,0,500.0

  h. $\Delta_3$ statistic test for spin group 2

samdist
Type d (for spacing), w (for width), or d3 (for delta3)
d3

Parameter file name
Oto500.par

Spin group, initial and final energies
2.0,0,500.0
5. SAMDIST OUTPUT

Two output files, named `samdist.avg` and `samdist.odf`, are generated by a SAMDIST run. The samdist.avg output is in the BCD format, whereas the samdist.odf file is the graphic form of the statistical distribution, both of which were originated with the FORODF program. Description of the FORODF program can be found in ref. However, for completeness the FORODF statements used to generate the graphics shown here will be presented. The ASCII output contains average values calculated over the statistical distribution of the resonance parameters along with the standard deviations. The results of the calculations for the theoretical prediction are also provided. In addition to the average values and the standard deviations, the sampling distribution of the sampled variables is also given. It is the sampling distribution that is given in graphical form in the samdist.odf file. To illustrate the results of a SAMDIST calculation, the output obtained for each of the inputs described in the previous section (inputs a to f) will be shown here. Recall that the data are $^{235}\text{U}$ s-wave resonance parameters of a SAMMY evaluation covering the energy range 0 to 500 eV.

a. Level-spacing distribution for spin group 1

The output created in this run is shown in Table 1, with the corresponding graphic output in Fig. 1. The FORODF sequence of statements used for generating the plot given in Fig. 1 is the following:

```
dvt/hist /err3 /nodash fl s2se0ee4,/noerr /dash 0.2 fl s4
```

A complete explanation of the previous command is given in the FORODF manual. However, a brief description of each switch used in this command is as follows:

- `dvt` is used to obtain the plot in the screen. It varies according to the kind of graphic device being used;
- `/hist` indicates to FORODF that the data will displayed in the form of histogram;
- `/err3` indicates that the standard deviations of the sampled variables, given by the vertical bars in the pictures, are in the position 3 in the FORODF file;
- `fl s2se0ee4` indicates that the x variable is stored in the position 1 and the theoretical distribution of x, $p(x)$ is in the position 2; `se0ee4` indicates that x will span from 0 to 4;
- `/noerr` indicates to turn off the `/err3` switch;
- `/dash 0.2` indicates that the line will be dashed for differentiation purposes. The user may need to trigger this switch off for the next plot;
- `fl s4` indicates that the x variable is stored in the position 1 and the experimental results is in the position 4.
Table 1. Nearest-neighbor-spacing distribution for J = 3

<table>
<thead>
<tr>
<th>Sampling Interval</th>
<th>Calculated</th>
<th>sdt</th>
<th>Theory</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0000E+00 - 0.2000E+00</td>
<td>0.3099E-01</td>
<td>0.9210E-02</td>
<td>0.3093E-01</td>
</tr>
<tr>
<td>0.2000E+00 - 0.4000E+00</td>
<td>0.7324E-01</td>
<td>0.1385E-01</td>
<td>0.8716E-01</td>
</tr>
<tr>
<td>0.4000E+00 - 0.6000E+00</td>
<td>0.1239E+00</td>
<td>0.1751E-01</td>
<td>0.1282E+00</td>
</tr>
<tr>
<td>0.6000E+00 - 0.8000E+00</td>
<td>0.1521E+00</td>
<td>0.1909E-01</td>
<td>0.1488E+00</td>
</tr>
<tr>
<td>0.8000E+00 - 0.1000E+01</td>
<td>0.1690E+00</td>
<td>0.1992E-01</td>
<td>0.1490E+00</td>
</tr>
<tr>
<td>0.1000E+01 - 0.1200E+01</td>
<td>0.1577E+00</td>
<td>0.1937E-01</td>
<td>0.1332E+00</td>
</tr>
<tr>
<td>0.1200E+01 - 0.1400E+01</td>
<td>0.9577E-01</td>
<td>0.1564E-01</td>
<td>0.1082E+00</td>
</tr>
<tr>
<td>0.1400E+01 - 0.1600E+01</td>
<td>0.5915E-01</td>
<td>0.1254E-01</td>
<td>0.8061E-01</td>
</tr>
<tr>
<td>0.1600E+01 - 0.1800E+01</td>
<td>0.5915E-01</td>
<td>0.1254E-01</td>
<td>0.554-13-01</td>
</tr>
<tr>
<td>0.1800E+01 - 0.2000E+01</td>
<td>0.3380E-01</td>
<td>0.9605E-02</td>
<td>0.3528E-01</td>
</tr>
<tr>
<td>0.2000E+01 - 0.2200E+01</td>
<td>0.1127E-01</td>
<td>0.5610E-02</td>
<td>0.2087E-01</td>
</tr>
<tr>
<td>0.2200E+01 - 0.2400E+01</td>
<td>0.1972E-01</td>
<td>0.7389E-02</td>
<td>0.1149E-01</td>
</tr>
<tr>
<td>0.2400E+01 - 0.2600E+01</td>
<td>0.1127E-01</td>
<td>0.5610E-02</td>
<td>0.5901E-02</td>
</tr>
</tbody>
</table>

Fig. 1. Level spacing distribution for J = 3. Calculations (solid line) compared with Wigner distribution (dashed line).
The FORODF switch for plotting the other results is very similar to the one just described, and, therefore, it will not be described. For users who do not have FORODF, it will be worthwhile to use the ASCII results given in the `samdist.avg` and construct the graphic output using any available plotting capability.

b. Level-spacing distribution for spin group 2

The output created in this run is shown in Table 2. The corresponding graphic output is given in Fig. 2. The FORODF sequence of statements used for generating the plot given in Fig. 2 is the following:

```
dvt /hist /err3 /nodash fl s2se0ee4,/noerr /dash 0.2 fl s4
```

Table 2. Nearest-neighbor-spacing distribution for J = 4

<table>
<thead>
<tr>
<th>Sampling interval</th>
<th>Calculated</th>
<th>sdt</th>
<th>Theory</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0000E+00 - 0.2000E+00</td>
<td>0.34673-01</td>
<td>0.78223-02</td>
<td>0.30933-01</td>
</tr>
<tr>
<td>0.2000E+00 - 0.4000E+00</td>
<td>0.47453-01</td>
<td>0.90903-02</td>
<td>0.87163-01</td>
</tr>
<tr>
<td>0.4000E+00 - 0.6000E+00</td>
<td>0.91243-01</td>
<td>0.1231E-01</td>
<td>0.1282E+00</td>
</tr>
<tr>
<td>0.6000E+00 - 0.8000E+00</td>
<td>0.1588E+00</td>
<td>0.15633-01</td>
<td>0.1488E+00</td>
</tr>
<tr>
<td>0.8000E+00 - 0.1000E+01</td>
<td>0.1807E+00</td>
<td>0.16453-01</td>
<td>0.1490E+00</td>
</tr>
<tr>
<td>0.1000E+01 - 0.1200E+01</td>
<td>0.2135E+00</td>
<td>0.17523-01</td>
<td>0.1332E+00</td>
</tr>
<tr>
<td>0.1200E+01 - 0.1400E+01</td>
<td>0.1204E+00</td>
<td>0.13923-01</td>
<td>0.1082E+00</td>
</tr>
<tr>
<td>0.1400E+01 - 0.1600E+01</td>
<td>0.67523-01</td>
<td>0.1073E-01</td>
<td>0.8061E-01</td>
</tr>
<tr>
<td>0.1600E+01 - 0.1800E+01</td>
<td>0.36503-01</td>
<td>0.80183-02</td>
<td>0.55413-01</td>
</tr>
<tr>
<td>0.1800E+01 - 0.2000E+01</td>
<td>0.2007E-01</td>
<td>0.5997E-02</td>
<td>0.35283-01</td>
</tr>
<tr>
<td>0.2000E+01 - 0.2200E+01</td>
<td>0.16423-01</td>
<td>0.54343-02</td>
<td>0.20873-01</td>
</tr>
<tr>
<td>0.2200E+01 - 0.2400E+01</td>
<td>0.36503-02</td>
<td>0.25783-02</td>
<td>0.1149E-01</td>
</tr>
<tr>
<td>0.2400E+01 - 0.2600E+01</td>
<td>0.54743-02</td>
<td>0.31553-02</td>
<td>0.59013-02</td>
</tr>
<tr>
<td>0.2600E+01 - 0.2800E+01</td>
<td>0.18253-02</td>
<td>0.18253-02</td>
<td>0.28283-02</td>
</tr>
<tr>
<td>0.2800E+01 - 0.3000E+01</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.12663-02</td>
</tr>
<tr>
<td>0.3000E+01 - 0.3200E+01</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.52993-03</td>
</tr>
<tr>
<td>0.3200E+01 - 0.3400E+01</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.20753-03</td>
</tr>
</tbody>
</table>
Fig. 2. **Level** spacing distribution for $J = 4$. Calculations (solid line) compared with Wigner distribution (dashed line).

c. Reduced neutron-width distribution for **spin group** $J$

The output created in this run is shown in Table 3. The corresponding graphic output is given in Fig. 3. The FORODF sequence of statements used for generating the plot given in Fig. 3 is the following:

```
dvt hist/err3/nodash fls2se0ee8/noerr/dash 0.2 fls4
```
Table 3. Reduced neutron-width distribution for \( J = 3 \)

\[
\langle g.n \rangle = 1.2401E-01 \quad \text{std} = 8.58193-03
\]

number of levels = 355

no. of levels in each interval of \( 0.1000E+01 \)

<table>
<thead>
<tr>
<th>Sampling interval</th>
<th>Calculated std</th>
<th>Theory</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0000E+00 - 0.1000E+01</td>
<td>0.6648E+00</td>
<td>0.25093-01, 0.6363E+00</td>
</tr>
<tr>
<td>0.1000E+01 - 0.2000E+01</td>
<td>0.1887E+00</td>
<td>0.1600E+00</td>
</tr>
<tr>
<td>0.2000E+01 - 0.3000E+01</td>
<td>0.73243-01</td>
<td>0.74033-01</td>
</tr>
<tr>
<td>0.3000E+01 - 0.4000E+01</td>
<td>0-36623-01</td>
<td>0.37763-01</td>
</tr>
<tr>
<td>0.4000E+01 - 0.5000E+01</td>
<td>0.1127E-01</td>
<td>0.2015E-01</td>
</tr>
<tr>
<td>0.5000E+01 - 0.6000E+01</td>
<td>0.1408E-01</td>
<td>0.1104E-01</td>
</tr>
<tr>
<td>0.6000E+01 - 0.7000E+01</td>
<td>0.84513-02</td>
<td>0.06155-02</td>
</tr>
<tr>
<td>0.7000E+01 - 0.8000E+01</td>
<td>0.0000E+00</td>
<td>0.03473-02</td>
</tr>
<tr>
<td>0.8000E+01 - 0.9000E+01</td>
<td>0.0000E+00</td>
<td>0.19783-02</td>
</tr>
<tr>
<td>0.9000E+01 - 1.0000E+02</td>
<td>0.0000E+00</td>
<td>0.11343-02</td>
</tr>
</tbody>
</table>

Fig. 3. Reduced neutron-width distribution for \( J = 3 \). Calculations (solid line) compared with Porter-Thomas distribution (dashed line).
d. Reduced neutron-width distribution for spin group 2

The output created in this run is shown in Table 4. The corresponding graphic output is given in Fig. 4. The FORODF sequence of statements used for generating the plot given in Fig. 4 is the following:

```
dvt /hist /err3 /nodash f1s2se0ee8 /noerr /dash 0.2 f1s4
```

Table 4. Reduced neutron-width distribution for J = 4

<table>
<thead>
<tr>
<th>Spin Slot</th>
<th>J = 4</th>
<th>Calculated</th>
<th>std</th>
<th>Theory</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0000E+00</td>
<td>0.1000E+01</td>
<td>0.6776E+00</td>
<td>0.19973-01</td>
<td>0.6363E+00</td>
</tr>
<tr>
<td>0.1000E+01</td>
<td>0.2000E+01</td>
<td>0.1403E+00</td>
<td>0.14833-01</td>
<td>0.1600E+00</td>
</tr>
<tr>
<td>0.3000E+01</td>
<td>0.4000E+01</td>
<td>0.6011E-01</td>
<td>0.1015E-01</td>
<td>0.37763-01</td>
</tr>
<tr>
<td>0.4000E+01</td>
<td>0.5000E+01</td>
<td>0.2550E-01</td>
<td>0.2015E-01</td>
<td>0.2015E-01</td>
</tr>
<tr>
<td>0.6000E+01</td>
<td>0.7000E+01</td>
<td>0.5464E-02</td>
<td>0.4441E-02</td>
<td>0.1104E-01</td>
</tr>
<tr>
<td>0.7000E+01</td>
<td>0.8000E+01</td>
<td>0.3643E-02</td>
<td>0.3149E-02</td>
<td>0.61553-02</td>
</tr>
<tr>
<td>0.8000E+01</td>
<td>0.9000E+01</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.1978E-02</td>
</tr>
<tr>
<td>0.9000E+01</td>
<td>0.1000E+02</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.11343-02</td>
</tr>
</tbody>
</table>

Fig. 4. Reduced neutron-width distribution for J = 4. Calculations (solid line) compared with Porter-Thomas distribution (dashed line).
e. Fission-width distribution for spin group 1

The output created in this run is shown in Table 5. The corresponding graphic output is given in Fig. 5. The FORODF sequence of statements used for generating the plot given in Fig. 5 is the following:

```
dvt /hist /err3 /nodash fls2se0ee8 /noerr /dash 0.2 fls4
```

Table 5. Fission-width distribution with 4 degrees of freedom for J = 3

<table>
<thead>
<tr>
<th>Sampling interval</th>
<th>Calculated</th>
<th>std</th>
<th>Theory</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0000E+00 - 0.1000E+01</td>
<td>0.6282E+00</td>
<td>0.25693-01</td>
<td>0.5940E+00</td>
</tr>
<tr>
<td>0.1000E+01 - 0.2000E+01</td>
<td>0.2394E+00</td>
<td>0.22683-01</td>
<td>0.3144E+00</td>
</tr>
<tr>
<td>0.2000E+01 - 0.3000E+01</td>
<td>0.1014E+00</td>
<td>0.1604E-01</td>
<td>0.74233-01</td>
</tr>
<tr>
<td>0.3000E+01 - 0.4000E+01</td>
<td>0.19723-01</td>
<td>0.73893-02</td>
<td>0.14333-01</td>
</tr>
<tr>
<td>0.4000E+01 - 0.5000E+01</td>
<td>0.84513-02</td>
<td>0.48653-02</td>
<td>0.25203-02</td>
</tr>
<tr>
<td>0.5000E+01 - 0.6000E+01</td>
<td>0.0000E+00</td>
<td>0.0000E+00</td>
<td>0.41953-03</td>
</tr>
</tbody>
</table>

Fig. 5. Fission-width distribution for J = 3. Calculations (solid line) compared with $\chi^2$ distribution with 4 degrees of freedom (dashed line).
Fission-width distribution for spin group 2

The output created in this run is shown in Table 6. The corresponding graphic output is given in Fig. 6. The FORODF sequence of statements used for generating the plot given in Fig. 6 is the following:

```
dvt /hist/err3 /nodash fl s2 se0 ee8 ./noerr /dash 0.2 fl s4
```

Table 6. Fission-width distribution with 4 degrees of freedom for J = 4

<table>
<thead>
<tr>
<th>Sampling Interval</th>
<th>'Calculated'</th>
<th>std</th>
<th>Theory</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0000E+00 - 0.1000E+01</td>
<td>0.6393E+00</td>
<td>0.2051E-01</td>
<td>0.5940E+00</td>
</tr>
<tr>
<td>0.1000E+01 - 0.2000E+01</td>
<td>0.2131E+00</td>
<td>0.1749E-01</td>
<td>0.3144E+00</td>
</tr>
<tr>
<td>0.2000E+01 - 0.3000E+01</td>
<td>0.9290E-01</td>
<td>0.1240E-01</td>
<td>0.7423E-01</td>
</tr>
<tr>
<td>0.3000E+01 - 0.4000E+01</td>
<td>0.3825E-01</td>
<td>0.8193E-02</td>
<td>0.1433E-01</td>
</tr>
<tr>
<td>0.4000E+01 - 0.5000E+01</td>
<td>0.1275E-01</td>
<td>0.4793E-02</td>
<td>0.2520E-02</td>
</tr>
</tbody>
</table>

Fig. 6. Fission-width distribution for J = 4. Calculations (solid line) compared with $\chi^2$ distribution with 4 degrees of freedom (dashed line).
g. A statistic test for spin group 1

The output created in this run is shown in Table 7. The corresponding graphic output is given in Fig. 7. The FORODF sequence of statements used for generating the plot given in Fig. 7 is the following:

dvt /nohist fl s2ese500./hist fl s3

Table 7. The A, results for J = 3 (only the first 30 $^{235}$U s-wave resonances are shown)

<table>
<thead>
<tr>
<th>Coefficients</th>
<th>5.88297433-01 ± 1.09548773-01</th>
<th>5.20125813-01</th>
</tr>
</thead>
<tbody>
<tr>
<td>a = 7.16210073-01</td>
<td>b = -2.02650653-01</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Energy</th>
<th>N(E)</th>
<th>a*E+b</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2775E+00</td>
<td>0.1000E+01</td>
<td>-0.38883-02</td>
</tr>
<tr>
<td>0.2034E+01</td>
<td>0.2000E+01</td>
<td>0.1254E+01</td>
</tr>
<tr>
<td>0.3139E+01</td>
<td>0.3000E+01</td>
<td>0.2046E+01</td>
</tr>
<tr>
<td>0.6189E+01</td>
<td>0.4000E+01</td>
<td>0.4230E+01</td>
</tr>
<tr>
<td>0.7698E+01</td>
<td>0.5000E+01</td>
<td>0.5311E+01</td>
</tr>
<tr>
<td>0.8942E+01</td>
<td>0.6000E+01</td>
<td>0.6202E+01</td>
</tr>
<tr>
<td>0.9754E+01</td>
<td>0.7000E+01</td>
<td>0.6784E+01</td>
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<tr>
<td>0.1071E+02</td>
<td>0.8000E+01</td>
<td>0.7466E+01</td>
</tr>
<tr>
<td>0.1240E+02</td>
<td>0.9000E+01</td>
<td>0.8676E+01</td>
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<tr>
<td>0.1368E+02</td>
<td>0.1000E+02</td>
<td>0.9597E+01</td>
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<td>0.1392E+02</td>
<td>0.1100E+02</td>
<td>0.9767E+01</td>
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<tr>
<td>0.1455E+02</td>
<td>0.1200E+02</td>
<td>0.1022E+02</td>
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<td>0.1802E+02</td>
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<td>0.1270E+02</td>
</tr>
<tr>
<td>0.1909E+02</td>
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<td>0.1347E+02</td>
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<tr>
<td>0.2017E+02</td>
<td>0.1500E+02</td>
<td>0.1424E+02</td>
</tr>
<tr>
<td>0.2358E+02</td>
<td>0.1600E+02</td>
<td>0.1669E+02</td>
</tr>
<tr>
<td>0.2422E+02</td>
<td>0.1700E+02</td>
<td>0.1714E+02</td>
</tr>
<tr>
<td>0.2553E+02</td>
<td>0.1800E+02</td>
<td>0.1808E+02</td>
</tr>
<tr>
<td>0.2644E+02</td>
<td>0.1900E+02</td>
<td>0.1873E+02</td>
</tr>
<tr>
<td>0.2716E+02</td>
<td>0.2000E+02</td>
<td>0.1925E+02</td>
</tr>
<tr>
<td>0.2833E+02</td>
<td>0.2100E+02</td>
<td>0.2009E+02</td>
</tr>
<tr>
<td>0.3059E+02</td>
<td>0.2200E+02</td>
<td>0.2171E+02</td>
</tr>
<tr>
<td>0.3203E+02</td>
<td>0.2300E+02</td>
<td>0.2273E+02</td>
</tr>
<tr>
<td>0.3457E+02</td>
<td>0.2400E+02</td>
<td>0.2456E+02</td>
</tr>
<tr>
<td>0.3487E+02</td>
<td>0.2500E+02</td>
<td>0.2477E+02</td>
</tr>
<tr>
<td>0.3517E+02</td>
<td>0.2600E+02</td>
<td>0.2499E+02</td>
</tr>
<tr>
<td>0.3840E+02</td>
<td>0.2700E+02</td>
<td>0.2730E+02</td>
</tr>
<tr>
<td>0.3988E+02</td>
<td>0.2800E+02</td>
<td>0.2836E+02</td>
</tr>
<tr>
<td>0.4152E+02</td>
<td>0.2900E+02</td>
<td>0.2953E+02</td>
</tr>
<tr>
<td>0.4186E+02</td>
<td>0.3000E+02</td>
<td>0.2978E+02</td>
</tr>
</tbody>
</table>
h. $\Delta_3$ statistic test for spin group 2

The output created in this run is shown in Table 8. The corresponding graphic output is given in Fig. 8. The FORODF sequence of statements used for generating the plot given in Fig. 8 is the following:

```
dvt /nohist fl s2s0ee500, /hist fl s3
```
Table 8. The A, results for J = 4 (only the first 30 $^{235}\text{U}$ s-wave resonances are shown)

<table>
<thead>
<tr>
<th>Energy</th>
<th>N(E)</th>
<th>a*E+b</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.113E+01</td>
<td>0.100E+01</td>
<td>0.166E+00</td>
</tr>
<tr>
<td>0.2777E+01</td>
<td>0.200E+01</td>
<td>0.1978E+01</td>
</tr>
<tr>
<td>0.3614E+01</td>
<td>0.300E+01</td>
<td>0.2900E+01</td>
</tr>
<tr>
<td>0.4852E+01</td>
<td>0.400E+01</td>
<td>0.4264E+01</td>
</tr>
<tr>
<td>0.5438E+01</td>
<td>0.500E+01</td>
<td>0.4910E+01</td>
</tr>
<tr>
<td>0.6393E+01</td>
<td>0.600E+01</td>
<td>0.5962E+01</td>
</tr>
<tr>
<td>0.7079E+01</td>
<td>0.700E+01</td>
<td>0.6718E+01</td>
</tr>
<tr>
<td>0.8767E+01</td>
<td>0.800E+01</td>
<td>0.8578E+01</td>
</tr>
<tr>
<td>0.9277E+01</td>
<td>0.900E+01</td>
<td>0.9140E+01</td>
</tr>
<tr>
<td>0.1016E+02</td>
<td>0.100E+02</td>
<td>0.1012E+02</td>
</tr>
<tr>
<td>0.1167E+02</td>
<td>0.110E+02</td>
<td>0.1177E+02</td>
</tr>
<tr>
<td>0.1240E+02</td>
<td>0.120E+02</td>
<td>0.1258E+02</td>
</tr>
<tr>
<td>0.1286E+02</td>
<td>0.130E+02</td>
<td>0.1309E+02</td>
</tr>
<tr>
<td>0.1327E+02</td>
<td>0.140E+02</td>
<td>0.1354E+02</td>
</tr>
<tr>
<td>0.1411E+02</td>
<td>0.150E+02</td>
<td>0.1447E+02</td>
</tr>
<tr>
<td>0.1541E+02</td>
<td>0.160E+02</td>
<td>0.1590E+02</td>
</tr>
<tr>
<td>0.1609E+02</td>
<td>0.170E+02</td>
<td>0.1664E+02</td>
</tr>
<tr>
<td>0.1664E+02</td>
<td>0.180E+02</td>
<td>0.1725E+02</td>
</tr>
<tr>
<td>0.1803E+02</td>
<td>0.190E+02</td>
<td>0.1878E+02</td>
</tr>
<tr>
<td>0.1900E+02</td>
<td>0.200E+02</td>
<td>0.1985E+02</td>
</tr>
<tr>
<td>0.1929E+02</td>
<td>0.210E+02</td>
<td>0.2018E+02</td>
</tr>
<tr>
<td>0.2063E+02</td>
<td>0.220E+02</td>
<td>0.2165E+02</td>
</tr>
<tr>
<td>0.2107E+02</td>
<td>0.230E+02</td>
<td>0.2213E+02</td>
</tr>
<tr>
<td>0.2293E+02</td>
<td>0.240E+02</td>
<td>0.2418E+02</td>
</tr>
<tr>
<td>0.2341E+02</td>
<td>0.250E+02</td>
<td>0.2472E+02</td>
</tr>
<tr>
<td>0.2435E+02</td>
<td>0.260E+02</td>
<td>0.2575E+02</td>
</tr>
<tr>
<td>0.2499E+02</td>
<td>0.270E+02</td>
<td>0.2645E+02</td>
</tr>
<tr>
<td>0.2649E+02</td>
<td>0.280E+02</td>
<td>0.2810E+02</td>
</tr>
<tr>
<td>0.2778E+02</td>
<td>0.290E+02</td>
<td>0.2953E+02</td>
</tr>
<tr>
<td>0.2813E+02</td>
<td>0.300E+02</td>
<td>0.2992E+02</td>
</tr>
</tbody>
</table>
Fig. 8. Cumulative number of energy levels vs energy for $J = 4$. 
6. REFERENCES


5. Dennis Wolfe, Computer Science and Mathematics Division, ORNL, personal communication, August 1995.


APPENDIX A

Listing of the SAMDIST code written in FORTRAN 77 language on the IBM RISC6000 platform.

```fortran
program samdist
  character char*2
  write(6, *)' Type d (for spacing), w (for width), or d3 (for delta *3)'
  read(5, '(a)') char
  if( char .eq. 'd' .or. char .eq. 'd') call space
  if( char .eq. 'w' .or. char .eq. 'w') call width
  if( char .eq. 'd3' .or. char .eq. 'd3') call delta3'
  stop
end

---_--------------------------------------------
C
C
C
subroutine 'space

C
character*20 file
dimension e(5000), d(5000), ak(5000), akk(5000), std(5000),
*y(5000)
write(6, *)' Parameter file name'
read(S, '(a)') file
open(unit=1, file=file, status='old')
open(unit=2, file='samdist.avg', status='unknown')
write(6, '*') jspi, ei, ef
k = 0
sum1 = 0.0
sum2 = 0.0
1    read(1, 1000) er, gg, gn, gfl, gf2, il, i2, i3, i4, i5, i6
    if( er .lt. ei) go to 1
    if( er .le. ef .and. i6. eq. jspi) then
        k = k + 1
        e(k) = er
        go to 1
    else if( er .gt. ef) then
        go to 2
    else
        go to 1
    endif
2    num = k - 1
    do 3 i = 1, num
        d(i) = e(i + 1) - e(i)
    continue
    sum1 = sum1 + d(i)
    sum2 = sum2 + d(i) * d(i)
3    continue
    dav = sum1/num
    nuns = num * (num - 1)
    temp = num * sum2 - sum1 * sum1
    varil = temp/nuns
    vari2 = vari1 / num
```

27
subroutine wigdis(y)

dimension y(5000)

common/al,delt,num

C program to calculate Wigner spacing distribution for one population

sum=0.
xl = 0.0

do 1 i = 1, num + 1
   x = i * delt - delt
   pon1 = 0.7854 * xl * xl
   pon2 = 0.7854 * x * x
   if(pon1 .ge. 20.0) pon1 = 20.0
   if(pon2 .ge. 20.0) pon2 = 20.0
   expl = exp(- pon1)
   exp2 = exp(- pon2)
   y(i) = (expl - exp2)
   xl = x
1 continue
return
end

subroutine width

character*20 file, word, char, chwid(3)
dimension ak(5000), akk(5000), std(5000), y(5000)
dimension x(5000), ggam(5000)

C data chwid/'< gn >', '< gf >', '< gg >/write(6,*)' Parameter file name'
read(5,'(a)') file
open(unit=1, file=file,status='old')
open(unit=2, file='samdist.avg',status='unknown')
write(6,*)' enter particle channel'
read(5,'(a)') word
write(6,*)' Spin state, initial and final energy '
read(5,*) jspi, ei, ef
k = 0
sum1 = 0.0
sum2 = 0.0
read(1,1000) er, gg, gn, gf1, gf2, il, i2, i3, i4, i5, i6
if( er .lt. ei ) then
go to 1
else if( i6 .eq. jspi ) then
  k = k + 1
  if( word .eq. 'gamma' ) then
    sum1 = sum1 + gg
    sum2 = sum2 + gg * gg
    wid = gg
  else if( word .eq. 'neutron' ) then
    sum1 = sum1 + gn/sqrt(er)
    sum2 = sum2 + gn * gn / er
    wid = gn/sqrt(er)
  else if( word .eq. 'fission' ) then
    sum1 = sum1 + abs(gf1) + abs(gf2)
    sum2 = sum2 + (abs(gf1) + abs(gf2)) *
     (abs(gf1) + abs(gf2))
    wid = abs(gf1) + abs(gf2)
  end if
  ggam(k) = wid
  go to 1
else if( er .lt. ef ) then
  go to 1
end if
num = k - 1
if( word .eq. 'neutron' ) then
  char = chwid(1)
else if( word .eq. 'fission' ) then
  char = chwid(2)
else if( word .eq. 'gamma' ) then
  char = chwid(3)
endif
avegam = sum1/num
do 3 i = 1, num
  x(i) = ggam(i)/avegam
3  continue
nuns = num * ( num - 1)
temp = num* sum2 - sum1 * sum1
varil = temp/nuns
vari2 = varil / num
astd = sqrt(vari2)
call order(num, x)
call sample(num, x, ak, akk, std)
call chisq(y)
call order(num, y)
call sample(num, y, ak, akk, std)
call chisq(y)
write(2,1003) char, avegam, astd, num
write(2,1004) ( ak(i), ak(i+1), akk(i+1), std(i+1), y(i+1),
               i = 1, num - 1)
write(6, *)'Average and sampling values are in file *** samdist.av
.
***!
call plot(ak, akk, std, y, num)
return
1000 format(5e11.4, 6i2)
1002 format(1lx, lp, a6, '= ', ell.4, ' std=', ell.4//
  * number of levels = ', 14)
1003 format(///6x,'Sampling Interval', 6x,'Calculated', 5x,'std', 8x,
  'Theory')
1004 format(///6x, 'Sampling Interval', 6x, 'Calculated', 5x, 'std', 8x,
  'Theory')
end
--------------------------------------------
C
C
C

subroutine sample(num, x, ak, akk, std)
dimension ak(5000), k(5000), akk(5000), x(5000), std(5000)
common/al/delt, nnum
write(6,*),'Bin width for sampling'
read(5,*) delt
nnum = x(num) / delt
if( nnum * delt .lt. x(num) ) nnum = nnum + 1
do 2 j = 1, num
  gn = x(j)
i = 1
tdelt = delt
  if ( gn .le. tdelt ) then
    k(i) = k(i) + 1
  else
    i = i + 1
    tdelt = tdelt + delt
    go to 1
endif
2 continue
num= nnum
ak(1) = 0.0000
do 3 i = 1, num
  ak(i+1) = ak(i) + delt
3 continue
aksum = 0
do 4 i = 1, num
  aksum = aksum + k(i)
4 continue
akk(1) = 0.0
do 5 i = 2, num
  akk(i) = k(i-1)/aksum
  pk = akk(i)
  ains = pk * ( 1.0 - pk )
  if( akk(i), ne. 0.0 ) std(i) = sqrt(ains/(aksum - 1.0))
5 continue
knum= num
if ( knum .ge. 50 ) knum = 50
write(2, 100) delt, ( k(i), i = 1, knum )
return
100 format(///' no. of levels in each interval of ',
  * ell.4 // 10i4 // 10i4 // 10i4 // 10i4 // 10i4)
end
subroutine chisq(yy)

dimension yy(5000)
common/rq/xf
common/al/del, n

external chipdf

write(6,*)' Degrees of freedom:'
read(5,*) df
xf=df
delz=del
zl=0.0
yy(1) = 0.0
do 10 i=1,n
   zu=delz*float(i)
   call rqg7(zl,zu,chipdf,y)
   yy(i+1) = y
   zl=zu
10 continue
return
end

function chipdf(z)

c==------------------------------------------------------------------------
common/rq/df,p1,p2,p3

z = df * z
dfh=df/2.0
edfh=dfh-1.0
call gamma(df, gam)
c=dh/(2.0**edfh)*gam
chipdf=c*(z**edfh)*exp(-z/2.0)
return
end

c==------------------------------------------------------------------------

subroutine rqg7(xl,xu,fct,y)

c==------------------------------------------------------------------------
common/rq/parml,parm2,parm3,parm4,parm5

a=.5*(xl+xu)
b=xu-xl
c=.4745540*b
d=.06474248*(fct(a+c)+fct(a-c))
e=.3707656*b
f=.1398527*(fct(a+c)+fct(a-c))
g=.2029226*b
h=.1905150*(fct(a+c)+fct(a-c))
y=b*(y+.2089796*fct(a))
return
eend

subroutine gamma(df, gam)
ad = amod(df, 2.0)
if ( ad .eq. 0.0 ) then
  gam = 1.0
  i = df/2.0 - 1.0
  akey = 0.0
else
  gam = -7724539
  i = df/2.0
  akey = 0.5
endif
if( df .eq. 1.0 .or. df .eq. 2.0 ) return
do i = 1, 1
  dn = float(i) - akey
  gam = dn * gam
1 continue
return
eend

subroutine delta3
character*30 file
dimension e(5000), akp(5000), yp(5000)
write(6,*)' Parameter file name'
read(5,'(a)') file
open(unit=1, file=file, status='old')
write(6,*)' Spin group, intial and final energies'
read(S,*)
jspin, el, eh
open(unit=2, file='samdist.avg', status='unknown')
pi = 3.141592654
last=1
1 read(1, 1000, end=2) etmp, j
if(etmp .eq. 0.0) go to 2
if(etmp .lt. el) go to 1
if(etmp .gt. eh) go to 1
if(j .ne. jspin) go to 1
e(last) = etmp
last = last + 1
2 continue
last = last - 1
if (last.gt.4000) stop 5
do m = 1, last
  if(l .eq. last) go to 5
  ml = l + 1
4 do m = ml, last
    if(e(l) .le. e(m)) go to 4
  do j = 1, 5
    tmp = e(1)
```fortran
e(l) = e(m)
e(m) = tmp
continue
c
continue
alast = last
s0 = (eh - e(last)) * alast
s1 = s0 * (eh + e(last))
sn2 = s0 * alast
lml = last - 1
do 6 1 = 1, lml
al = 1
tmp = al * (e(l+1) - e(l))
so = so + tmp
s1 = s1 + tmp * (e(l+1) + e(l))
sn2 = sn2 + tmp * al
continue
sl = 0.5 * sl
t0 = eh - el	eml = 0.5 * (eh + el)	em2 = (eh * eh + eh * el + el * el)/3.0
t1 = em1 * t0
t2 = em2 * to
tmp = 12.0 / to**3
a = tmp * (s1 - em1 * s0)
b = tmp * (em2 * s0 - em1 * s1)
del13 = (sn2 - b * s0 - a * s1) / t0
del = 0.10132 * (log(alast) - 0.0686)
fr = sqrt(1.169 / pi ** 4)
write(2, 1001) del, fr, del13, a, b
write(2, 1002)
ak = 0.0
do 7 i = 1, last
    ak = ak + 1.0
akp(i) = ak
    y = a * e(i) + b
yp(i) = y
write(2, 1003) e(i), akp, yp
continue
write(6, 1000) 'Average and sampling values are in file *** samdist.av'
call plot(e, akp, yp, yp, last)
return
1000 format(ell.4, 54x, i2)
1001 format(/20x,'Delta3 Results'//10x,'theory',14x,'std',
    *12x,' measured',// 5x, 1p,e14.7, '+'- ',e14.7,5x,e14.7///
    *20x,' Coefficients',//
    *'
    a=',e14.7,' b=',e14.7)
1002 format(////20x,'Energy Levels in the (-L,+L) Interval'
    *//' Energy    N(E)    a*E+b ')
1003 format(10x, e11.4, 4x, e11.4, 4x, e11.4)
end

subroutine order(n, x)
dimension x(n)
```
dimension sig1(3000), sig2(3000), sig3(3000), sig4(3000)
nl=n-1

do 2 i = 1, nl
   il = i + 1
   do 1 j = il, n
      if(x(i) .le. x(j)) go to 2
      temp = x(i)
      x(i) = x(j)
      x(j) = temp
   1 continue
2 continue
return
end

-------------------------------------------------------------------

subroutine plot(energy, data, unc, theory, ndat)

*** purpose -- make odf file containing four segments

dimension energy(ndat), data(ndat), unc(ndat), theory(ndat)
character*11 odffilen
data odffilen /'samdist.odf'/

if (ndat.eq.0) stop 'no points to be plotted'
nbl = 3
nsect = 4
nch = ndat
mode = 3
ndstrt = 0
iener = -1
irun = 1

   call odfio(14, odffilen, nbl, 1, nsect, nch, mode, ndstrt, iener, irun)
   call outodf(14, nbl, nsect, 1, mode, ndstrt, 1, nch, energy, 1)
   call outodf(14, nbl, nsect, 2, mode, ndstrt, 1, nch, data, 1)
   call outodf(14, nbl, nsect, 3, mode, ndstrt, 1, nch, unc, 1)
   call outodf(14, nbl, nsect, 4, mode, ndstrt, 1, nch, theory, 1)

close (unit=14)

return
end
subroutine odfio(iu,file,ifb,new,ins,inc,mode,strt,iener,irun)
implicit none
include '/users/craven/forodf/odfhed.unv'
integer*4 odfhed(126)
0=18 bit integer 1=32 bit integer 3=floating point
integer*4 ndmode(1)
equivalence(odfhed(l),ndmode(1))
c 0=sel data 1=csisrs 2=endf/b
integer*4 nsorce(1)
equivalence(odfhed(2),nsorce(1))
c numerical id
integer*4 ndrun(1)
c equivalence(odfhed(3),ndrun(1))
c starting block number of comment section
integer*4 ncblds(1)
equivalence(odfhed(4),ncblks(l))
c number of bytes in comment section
integer*4 ncwrds(1)
equivalence(odfhed(5),ncwrds(1))
c starting block of scaler section
integer*4 nsblks(1)
equivalence(odfhed(6),nsblks(1))
c number of words in scaler section
integer*4 nswrds(1)
equivalence(odfhed(7),nswrds(1))
c starting word in scaler section of sel scaler/count section
integer*4 ncstrt(l)
equivalence(odfhed(8),ncstrt(l))
c number words in sel scaler/counter section
integer*4 ncntrs(1)
equivalence(odfhed(9),ncntrs(l))
c starting word in scaler section of sel variable section
integer*4 nxstrt(l)
equivalence(odfhed(10),nxstrt(l))
c number of words in sel variable section
integer*4 nxwrds(1)
equivalence(odfhed(11),nxwrds(l))
c starting block of parameter section
integer*4 npblks(1)
equivalence(odfhed(12),npblks(1))
c number words in parameter section
integer*4 npwrds(1)
equivalence(odfhed(13),npwrds(1))
c =0 data described by parameter section =1 data corresponds to sect 1
integer*4 ndtype(1)
equivalence(odfhed(14),ndtype(1))
c number of datasets in data section
integer*4 ndvars(l)

equivalence(odfhed(15), ndvars(1))
c starting block of data section
  integer*4 ndblks(1)
equivalence(odfhed(16), ndblks(1))
c number of words in each dataset
  integer*4 ndwrds(1)
equivalence(odfhed(17), ndwrds(1))
c endf/b designation (charge, mass)
  integer*4 ndzan(1)
equivalence(odfhed(18), ndzan(1))
c endf/b ratio nuclear mass to neutron
  integer*4 ndawr(1)
equivalence(odfhed(19), ndawr(1))
c endf/b number assigned by national neutron cross section center
  integer*4 ndmat(1)
equivalence(odfhed(20), ndmat(1))
c endf/b file number
  integer*4 ndmf(1)
equivalence(odfhed(21), ndmf(1))
c endf/b reaction type number
  integer*4 ndmt(1)
equivalence(odfhed(22), ndmt(1))
c if ndtype=1 then ndvswt =0 energy decreases, =1 increases
  integer*4 ndvswt(1)
equivalence(odfhed(23), ndvswt(1))
c =1 data dead time created, =0 not
  integer*4 nddswt(1)
equivalence(odfhed(24), nddswt(1))
c starting word of data from mode 0
  integer*4 ndstrt(1)
equivalence(odfhed(25), ndstrt(1))
c last word written of parameter section
  integer*4 ndwend
  equivalence (odfhed(26), ndwend)
  C words 27 through 126 is energy index table,
c largest energy for each n blocks, n=(ndwrds/125)+1
  real*4 ndtabl(100)
equivalence(odfhed(27), ndtabl(1))
c starting block number of comment section
  integer iu, ifb, new, ins, inc, mode, strt, iener, irun, iarray(l)
  integer ibuf4(126)
  integer*4 i,j,k, l, zero, iblk, ibc, ilc, isn, index, junk, iword4
  integer*4 iii, system
  integer*2 ibuf2(252), xword4(2), iword2
  logical*4 ex
  character*(*) file
  character commd*3, fcommd*252
  equivalence (xword4(1), iword4), (xword4(1), iword2)
equivalence (ibuf2(1), odfhed), (ibuf4(1), odfhed)
data commd/"rm '/
data zero/0/
c  if(new.eq.0) then
    open(unit=iu,
    file=file,
    status='old',
    access='direct',
    reacl=512)
else
    inquire(file=file, exist=ex)
    if(ex) then
        fcommd=commd//file//char(0)
        iii = system(fcommd)
        endif
        open(unit=iu, file=file,
        status='unknown',
        access='direct',
        recl=512)
        go to 12
    endif
endif

read(iu, rec=1) odfhed
ins=ndvars(l)
ifb=ndblks(1)
inc=ndwrds(1)
mode=ndmode(1)
strt=ndstrt(l)
ier=0
if(ndtype(l).ne.0) iener=-1
irun=ndrun(l)
j=125
if(mode.eq.0) j=250
i=(inc-1)/j
if(i*j.ne.inc) i=i+l
iblk=ifb+(i*ins)-1
read(iu, rec=iblk, err=1) odfhed
return
1 write(iu, rec=iblk) odfhed
return
entry outodf(iu, ifb, ins, isn, mode, strt, isc, inc, iarray, index)
if(ins.le.0) go to 14
if(ins.le.0) go to 14
if(isn.gt.ins) go to 14
if(isc.le.0) go to 14
if(inc.le.0) go to 14
ibc=l
ilc=inc
if(mode.eq.0) go to 23
iblk=(isc-1)/125
i=isc-(iblk*125)
iblk=(iblk*ins)+ifb+isn-1
if(i.eq.1) go to 3
read(iu, rec=iblk) ibuf4
l=i+ilc-1
if(l.gt.125) l=125
do 2 j=i+1, l+1
ibuf4(j)=iarray(ibc)
iibs+index
write(iu, rec=iblk) odfhed
ibl=iblk+ins
2 if(ilc.eq.0) return
1 iblk=iblk+ins
3 i=i+ilc/125
if(i.eq.0) go to 5
  do 4 j=ibc,ibc-1+(i*125*index),125*index
  write(iu,rec=iblk) zero,(iarray(k),k=j,j+(125*index),index)
  iblk=iblk+ins
  ibc=ibc+(i*125*index)
  ilc=ilc-(i*125)
  if(ilc.eq.0) return
  read(iu,rec=iblk)ibuf4
  do 6 j=2,ilc+1
    ibuf4(j)=iarray(ibc)
    ibc=ibc+index
  write(iu,rec=iblk)ibuf4
  return
entry inodf(iu,ifb,ins,isn,mode,strt,isc,inc,iarray,index)
  if(ins.le.0) go to 16
  if(isn.le.0) go to 16
  if(isn.gt.ins) go to 16
  if(isc.le.0) go to 16
  if(inc.le.0) go to 16
  ibc=1
  ilc=inc
  if(mode.eq.0) go to 20
  iblk=(isc-1)/125
  i=isc-(iblk*125)
  ilc=(iblk*ins)+ifb+isn-1
  if(i.eq.1) go to 8
  read(iu,rec=iblk)ibuf4
  iblk=iblk+ins
  l=i+ilc-1
  if(l.gt.125) l=125
  do 7 j=i+1,l+1
    iarray(ibc)=ibuf4(j)
    ibc=ibc+index
  ilc=ilc-(l-i+1)
  if(ilc.eq.0) return
  i=ilc/125
  if(i.eq.0) go to 10
  do 9 j=ibc,ibc-1+(i*125*index),125*index
    read(iu,rec=iblk) junk, (iarray(k), k=j, j-1+(125*index), index)
  iblk=iblk+ins
  ibc=ibc+(i*125*index)
  ilc=ilc-(i*125)
  if(ilc.eq.0) return
  read(iu,rec=iblk)ibuf4
  do 11 j=2,ilc+1
    iarray(ibc)=ibuf4(j)
  ibc=ibc+index
  return
  do 13 i=1,126
    odfhed(i)=0
    if(mode.eq.0 .and. i.equiv.0) go to 28
    if(mode.eq.0 .and. ins.ne.1) go to 28
    if(mode.ne.0 .and. strt.ne.0) go to 28
    if(strt.lt.0) go to 28
    ndmode(l)=mode
    ndrun(l)=irun
    ndwrds(l)=inc
    ndvars(l)=ins
ndtype(1)=0
if(iener.ne.0)ndtype(1)=-1
ndstrt(1)=strt
ncblks(1)=2
nsblks(1)=3
npwrd(1)=128
if(ndmode(1).eq.0)ndtype(1)=0
ncwrd(1)=1*126
ncstrt(1)=32+1
nxstrt(1)=ncstrt(1)+ncntrs(1)
nswrd(1)=nxstrt(1)+nwxrd(1)
nsblks(1)=ncblks(1)+ncwrd(1)/126
if(ncwrd(1)-((ncwrd(1)/126)*126).ne.0)nsblks(1)=nsblks(1)+1
npblks(1)=nsblks(1)+nswrd(1)/126
if(nswrd(1)-((nswrd(1)/126)*126).ne.0)npblks(1)=npblks(1)+1
ndblks(1)=npblks(1)+npwrd(1)/126
if(npwrd(1)-((npwrd(1)/126)*126).ne.0)ndblks(1)=ndblks(1)+1
ifb=ndblks(1)
write(iu,rec=1)odfhed
do 131 i=1,126
  odfhed(i)=0
  do 132 i=2,ifb-1
    write(iu,rec=i)odfhed
  enddo
  j=125
  if(mode.eq.0)j=250
  i=(inc-1)/j
  if(i*j.ne.inc)i=i+1
  iblk=ifb+(i*ins)-1
  write(iu,rec=iblk)odfhed
  return
format('bad calling parameters to outodf')
go to 18
print 17
format('bad calling parameters to inodf')
print 19,iu,ifb,ins,isan,isc,inc,index
format(1x,'iu=',i5,
   1   //,ix,'ifb=',i5,
   2   //,ix,'ins=',i5,
   3   //,ix,'isan=',i5,
   4   //,ix,'isc=',i5,
   5   //,ix,'inc=',i5,
   6   //,ix,'index=',i5)
return

c mode 0 inodf
iwrd=0
iblk=(isan-1+strt)/250+ifb
i=isan+strt-(((isan-1+strt)/250)*250)+2+250
do 22 j=ibc,ilc
   if(i.le.252)goto 21
read(iu,rec=iblk)ibuf2
iblk=iblk+1
i=i-250
21 iword2=ibuf2(i)
array(j)=iword4
22 i=i+1
return

c mode 0 outodf
iblk=(isc-1+strt)/250+ifb
read(iu, rec=iblk, err=24) ibuf2
i=isc+strt-(((isc-1+strt)/250)*250)+2
    do 27 j=1bc,1lc
      if(i.le.252)goto 26
      write(iu, rec=iblk) ibuf2
      iblk=iblk+1
    read(iu, rec=iblk, err=25) ibuf2
 25 i=i-250
 26 iword4=iarray(j)
    ibuf2(i)=iword2
 27 i=i+1
    write(iu, rec=iblk) ibuf2
return
print 29, iu, file, ifb, new, ins, inc, mode, strt, iener, irun
format('bad calling parameters to odfio',
    'iu=',i5,
    'file=',a10,
    'ifb=',i5,
    'new=',i5,
    'ins=',i5,
    'inc=',i5,
    'mode=',i5,
    'strt=',i5,
    'iener=',i5,
    'irun=',i5)
return end
### APPENDIX B

Listing of the $^{235}$U s-wave resonance parameters. File `0to500.par`

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<th>Energy (MeV)</th>
<th>Real Part</th>
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1. O. Bouland
2. H. Derrien
3. F. DiCillo
4. R. H. Fowler
5. N. M. Greene
6. J. A. Harvey
7. D. M. Hetrick
8. P. E. Koehler
9. M. A. Kulisha
10. D. C. Larson
11-15. N. M. Larson
16-20. L. C. Leal
21. L. F. Norris
22. C. V. Parks
23. S. Raman

24. R. W. Roussin
25. C. H. Shappert
26. M. S. Smith
27. R. R. Spencer
28. R. C. Ward
29. R. M. Westfall
30. J. E. White
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32. RSIC
33-34. Laboratory Records Dept.
35. Laboratory Records, ORNL-RC
36. Y-12 Technical Library
37. Central Research Library
38. Document Reference Section
39-40. Laboratory Records Dept.
41. J. Burke, Rensselaer Polytechnic Institute, Troy, NY 12180-3590
42. D. E. Carlson, Reactor and Plant System Branch, Division of System Research, Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission, MS T-10 G6, RM T-10, 17, Washington, DC 20555-0001
43. R. C. Carlton, Box 407, Middle Tennessee State University, Murfreesboro, TN 37132
45. C. Dunford, Bldg 197D, National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973
46. J. R. Felty, DynCorp, Advanced Technology Services, 4401 Ford Avenue, Suite 300, Alexandria, VA 22302-1432
47. P. Finck, DER/SPRC/LEPH, Batiment 230, Centre d’Etudes de CADARACHE, 13 108 Saint Paul-lez-Durance, France
48. C. M. Frankle, Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, NM 87544
49. F. Froener, Kernforschungszentrum Karlsruhe, Institut fuer Neutronenphysik und Reactortechnik, Postfach 336 40, D-76021 Karlsruhe, Germany
50. R. N. Hwang, Argonne National Laboratory, Reactor Analysis Division, Bldg 208, Argonne, IL 60439
51. Y. Kikuchi, Nuclear Data Center, Japan Atomic Energy Research Institute, Tokaimura, Naka-gun, Ibaraki-ken 3 19-11, Japan
52. C. Lubitz, Knolls Atomic Power Laboratory, P. 0. Box 1072, Schenectady, NY 12301
53. R E. MacFarlane, Los Alamos National Laboratory, T2, MS342, Los Alamos, NM 87545
54. B. Moretti, Rensselaer Polytechnic Institute, Troy, NY 12180-3590
55. C. Nordborg, OECD/NEA, Le Seine St-Germain 12, Boulevard Iles, 92130 Issy-les-Moulineaux, France
58. Office of the ORNL Site Manager, Department of Energy, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831
59. M. Salvatores, DRN/P, Batiment 707, C. E. CADARACHE, 13 108 Saint Paul-lez-Durance, France
60. C. Werner, Rensselaer Polytechnic Institute, Troy, NY 12180-3590
61. Roger White, Lawrence Livermore National Laboratory, P. 0. Box 8.08, Livermore, CA 94550
62. M. Williams, Nuclear Science Center, Louisiana State University; Baton Rouge, LA 70803
63. R. R. Winters, Denison University, Physics Department, Granville, Ohio 43023