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RFUNC - A Code to Analyze Differential Elastic-Scattering Data

F. G. Perey

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Engineering Physics and Mathematics Division

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F. G. Perey

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ABSTRACT

The code RFUNC is used at ORELA to analyze high resolution differential elastic scattering data from spin zero nuclides in the resonance energy region. This report presents the real R-Function formalism used in RFUNC and gives details of how the finite size corrections are currently made. Appendix A describes the input to the code RFUNC. Appendix B describes the input to a utility code MAKPA that transforms a resonance parameter file in SAMMY format into a resonance parameter file in RFUNC format. Appendix C describes the input to an adjunct code RFUNCXT that generates the contributions to the total cross section from resonances of different orbital and total angular momenta. The FORTRAN listing of the code RFUNC is given in Appendix D.

1. INTRODUCTION

The code RFUNC was written to analyze high resolution differential elastic scattering data obtained in the resonance energy region at ORELA. The purpose of these experiments is to assist in the determination of the orbital and total angular momenta of the resonances. These differential elastic scattering experiments are done in conjunction with transmission experiments that are analyzed using the code SAMMY, which uses an R-matrix formalism.

In practice, the transmission data are first analyzed, with the code SAMMY, using tentative values for the orbital momentum, l, and the total angular momentum, j, of each resonance. Because of finite energy resolution in the experiments, frequently one cannot determine unambiguously the l and j values of resonances from the analysis of the transmission data. The validity of the l and j values assigned to resonances in the transmission data analysis can then be tested by comparing predicted differential elastic scattering excitation functions at various angles, calculated with the code RFUNC, with the experimental data. The excitation functions at various angles, in particular the back angles, are usually very sensitive to the l assignment of resonances and to a lesser degree to the j value for a given l. No adjustment of the resonance parameters is performed in the code RFUNC. Since only resonances having neutron widths much larger than their capture widths are clearly observed in the differential scattering data, the code RFUNC is based upon the much simpler real R-function formalism which ignores the capture reaction channel. For resonances having neutron widths more than five times their capture widths the total cross sections calculated with RFUNC agree with those calculated with SAMMY to fractions of one per cent. Because so far scattering experiments have only been performed on spin zero nuclides, the code RFUNC only deals, at the moment, with scattering from such nuclides.

In Section 2 the real R-function formalism used in RFUNC is briefly given. In Section 3 the finite size effects currently incorporated in RFUNC are described. The input to the code RFUNC is presented in Appendix A. In Appendix B the description of the input to a utility code MAKPA, used to transform a resonance parameter file in SAMMY format to one in RFUNC format, is given. Appendix C describes the input to an adjunct code RFUNCXT which can be used to obtain the contributions of resonances of given l and j values to the total cross section. Appendices A, B and C are taken from the HELP files on the ORELA VAX computer system. Finally, the FORTRAN listing of the code RFUNC is given in Appendix D.

2. THE REAL R-FUNCTION FORMALISM

Let us consider a set of resonance parameters:

$$E^i_{l,j}, \Gamma^i_{l,j}$$

where $E^i_{l,j}$ is the resonance energy of the ith resonance having an orbital angular momentum l and a total angular momentum j and $\Gamma^i_{l,j}$ is the neutron width of this resonance. Since we are dealing with only spin zero nuclides, we have:

$$j = l \pm 1/2 \ .$$

If $P_l(E)$ stands for the neutron penetrability for orbital angular momentum l at the energy E, then the reduced neutron widths, $\gamma^{2i}_{l,j}$, are given by:

$$\gamma^{2i}_{l,j} = \Gamma^i_{l,j}/2P_l(E^i_{l,j}) \ .$$

At an energy E one can construct for each value of l, j a real R-function given by:

$$R_{l,j}(E) = \sum_i \gamma^{2i}_{l,j}/(E^i_{l,j} - E) \ .$$

From these R-functions one can obtain phase shifts $\delta_{l,j}(E)$:

$$\delta_{l,j}(E) = -\phi_l(E) + \arctan(P_l(E)R_{l,j}(E)/(1 - R_{l,j}(E)(S_l(E) - B_{l,j})) \ ,$$

where $\phi_l(E)$, $S_l(E)$ and $B_{l,j}$ are respectively the hard sphere phase shifts, the shift factors, and the boundary conditions. There is an option in the code to calculate $\delta_{l,j}$ in the approximation used in ENDF/B whereby $B_{l,j}$ is made energy dependent and equal to $S_l(E)$ at all energies.

From the phase shifts $\delta_{l,j}(E)$ one can construct the total cross section at energy E:

$$\sigma_T(E) = (4\pi/k^2) \sum_{l,j} g_j \sin^2(\delta_{l,j}(E)) \ ,$$

where g_j is the statistical factor $(2j+1)/2$.

Following Meier et al. (*Helv. Phys. Acta* **27** 577 (1954)), from the values of the phase shifts $\delta_{l,j}(E)$ the values of the coefficients of the Legendre expansion of the angular distributions are directly computed. This is done in RFUNC, rather than calculating the scattering amplitudes and squaring them which is the more usual procedure, because at one time the Legendre polynomial expansion coefficients were extracted from the experimental data which were also corrected for the finite size of the sample and detectors. In order to calculate the Legendre polynomial expansion coefficients from the phase shifts an auxiliary matrix $D(m,n)$ is calculated at each energy. The elements of this matrix are given by:

$$D(m,n) = sin(\delta_m)\sin(\delta_n)(\sin(\delta_m)\sin(\delta_n) + \cos(\delta_m)\cos(\delta_n)) \ ,$$

where the following convention for the labeling the rows m and the columns n of the matrix D is used:

$$\begin{aligned} n \text{ or } m &= 2, \text{ for } l = 0,\ j = 1/2, \\ &= 3, \text{ for } l = 1,\ j = 1/2, \\ &= 4, \text{ for } l = 1,\ j = 3/2, \\ &= 5, \text{ for } l = 2,\ j = 3/2, \\ &= 6, \text{ for } l = 2,\ j = 5/2, \\ &= 7, \text{ for } l = 3,\ j = 5/2, \\ &= 8, \text{ for } l = 3,\ j = 7/2. \end{aligned}$$

In terms of the elements of this matrix $D(n,m)$ the values of the Legendre coefficients B_L, where L is the order of the Legendre polynomial, are given by:

$$\begin{aligned} B_0 &= D(2,2) + D(3,3) + 2(D(4,4) + D(5,5)) + 3(D(6,6) + D(7,7)) \\ &\quad + 4D(8,8) \\ B_1 &= 2D(2,3) + 4(D(2,4) + D(3,5)) + (4D(4,5) + 36(D(4,6) \\ &\quad + D(5,7)))/5 + (18D(6,7) + 360D(6,8))/35 \\ B_2 &= 4(D(2,5) + D(3,4) + 6(D(2,6) + D(3,7)) + 2(D(4,4) + D(5,5) \\ &\quad + (12(D(4,7) + D(5,6)) + 24(D(6,6) + D(7,7)) + 72D(4,8) \\ &\quad + 8D(7,8) + 100D(8,8)/3)/7 \\ B_3 &= 6(D(2,7) + D(3,6) + 8(D(2,8) + D(6,8)) + 4.8(D(4,6) \\ &\quad + D(5,7)) + 7.2D(4,5) + 3.2D(6,7) + 16D(5,8)/6 \\ B_4 &= 8D(3,8) + (72(D(4,7) + D(5,6)) + 18(D(6,6) + D(7,7) \\ &\quad + 40D(4,8))/7 + (360D(7,8) + 324D(8,8))/77 \\ B_5 &= 40D(5,8)/3 + (100D(6,7) + 40D(6,8))/7 \\ B_6 &= (600D(7,8) + 100D(8,8))/33 \end{aligned}$$

Having obtained these Legendre coefficients B_L, the center of mass differential elastic scattering at the center of mass angle θ is given by:

$$\sigma(\theta) = (4\pi/k^2) \sum_L B_L P_L(\cos(\theta)) \ .$$

This Legendre expansion of the differential elastic scattering cross section is not the one used in the ENDF/B files. In RFUNC, having obtained the above values of B_L they are converted to the ENDF/B form, and then Doppler and resolution broadened.

3. FINITE SIZE CORRECTIONS

Since no adjustment of the resonance parameter values is performed in RFUNC and because relatively thin samples have been used so far in the scattering experiments at ORELA, the treatment of finite size effects is at the moment rather crude, but appears adequate to be able to assign unambiguously the l and j values of resonances clearly seen in the measured excitation functions. Should the geometry of these scattering experiments change in the future, the adequacy of the finite size corrections currently done in RFUNC should be investigated.

The finite size effects are accounted for in two distinct steps that will be referred to as: incident neutron attenuation and, for reasons that will shortly become apparent, scattered neutron attenuation.

A linear approximation is used in calculating the attenuation of the incident neutrons in the sample. That is to say, at all angles the calculated differential scattering cross sections are multiplied by the factor:

$$\exp(-n_i \sigma_T(E)) \ ,$$

where $\sigma_T(E)$ is the Doppler broadened total cross section at the laboratory energy E, and n_i is an input number of atoms/barn. Therefore, one should use for n_i a value which is half the mean scatterer thickness as seen from the incident beam direction. In the code this correction is applied to the B_0 Legendre polynomial expansion coefficients after these have been Doppler broadened.

The so-called scattered neutron attenuation is intended to account for three distinct effects. First, neutrons initially scattered in the direction of a detector may suffer a second scattering that causes them not to be detected in that detector. If the solid angles of the detectors were very small, this effect would be accounted for by an attenuation of the scattered neutrons in the direction of the detectors. The relevant cross sections for this attenuation would be the Doppler broadened total cross sections at the energies of the neutrons scattered through the appropriate laboratory angles. Second, neutrons may reach a detector after multiple scattering in the scatterer, whether initially scattered in the direction of that detector or not. This second effect is in the opposite direction to the first one since it will increase rather than decrease the yield of neutrons observed at any angle. Finally, we need to account for the rather large angular spread in the geometry due to the finite size of the scatterer and the detectors. The large angular spread of once scattered neutrons of a given incident energy that may reach a particular detector means that there is a large dispersion in the energies of such neutrons that are proceeding toward a detector, due to kinematic effects. Therefore, in accounting for the first finite size effect mentioned above, the attenuation of once scattered neutrons in the sample, we need to take into consideration the different energies of neutrons once scattered that are proceeding in the direction of a detector. This is accomplished by using, instead of the Doppler broadened total cross section at an energy corresponding to the mean angle of a detector, a total cross section that is in addition broadened by the distribution of energies of once scattered neutrons proceeding toward a detector. Currently, in the scattering experiments, all detectors have the same solid angle, but

the energy spread of neutrons once scattered that are proceeding toward a detector will be a function of the laboratory angle where this detector is located.

In RFUNC, at the moment, the above three effects are empirically accounted for by multiplying the calculated differential scattering cross section at the central angle θ of a detector, after it has been corrected for incident neutron attenuation in the sample, by the factor:

$$\exp(-n_o \sigma_T(E')) \ ,$$

where n_o is an input number of atoms/barn, not necessarily equal to n_i, and $\sigma_t(E')$ is the total cross section, at the laboratory energy E' of the neutrons of energy E scattered through the angle θ in the laboratory system of coordinates,that has been energy resolution broadened to account for kinematic energy losses of scattered neutrons due to the finite size of the scatterer and the detector. For the hollow cylinders so far used as the scatterer, the value of n_o should be the same as the value of n_i, since the mean scatterer thickness as seen from the direction of the detectors is the same as seen from the incident beam direction. However, multiple scattering effects can be crudely accounted for by using a value of n_o which is smaller than the value of n_i.

Currently a triangular representation of the resolution function is used to obtain the cross sections $\sigma_T(E')$. The energy width of this effective triangular resolution function is different for every detector and varies as a function of energy. For the detectors and the hollow cylindrical samples so far used at ORELA in the scattering experiments, if the half width of the angle subtended at the center of the sample by the detectors is denoted a and the half width of the angle subtended at the center of the detectors by the sample is denoted b, then the input angular spread for the detectors should be specified as:

$$\sqrt{2(a^2 + b^2)} \ ,$$

where a and b are in degrees. The reason for using a triangular representation for the resolution function is that the angles a and b are very close to each other. Even for the relatively thin scatterer so far used at ORELA, finite size effects can be observed in the experimental data for low energy s-waves. They show up as a dip in the scattering cross sections at energies above the resonance energy. How far above the resonance energy this dip occurs is a function of the scattering angle. The value of n_o can be adjusted empirically to reproduce these effects in the experimental data. For a relatively thick ^{56}Fe scatterer with $n_i = 0.034$ atom/barn, the thickest scattering sample used to date, the data from 39 degrees to 160 degrees could be reasonably well reproduced with a value of $n_o = 0.020$ atom/barn, as shown on Figures 1, 2 and 3, where the data are compared with calculations using three different values of n_o.

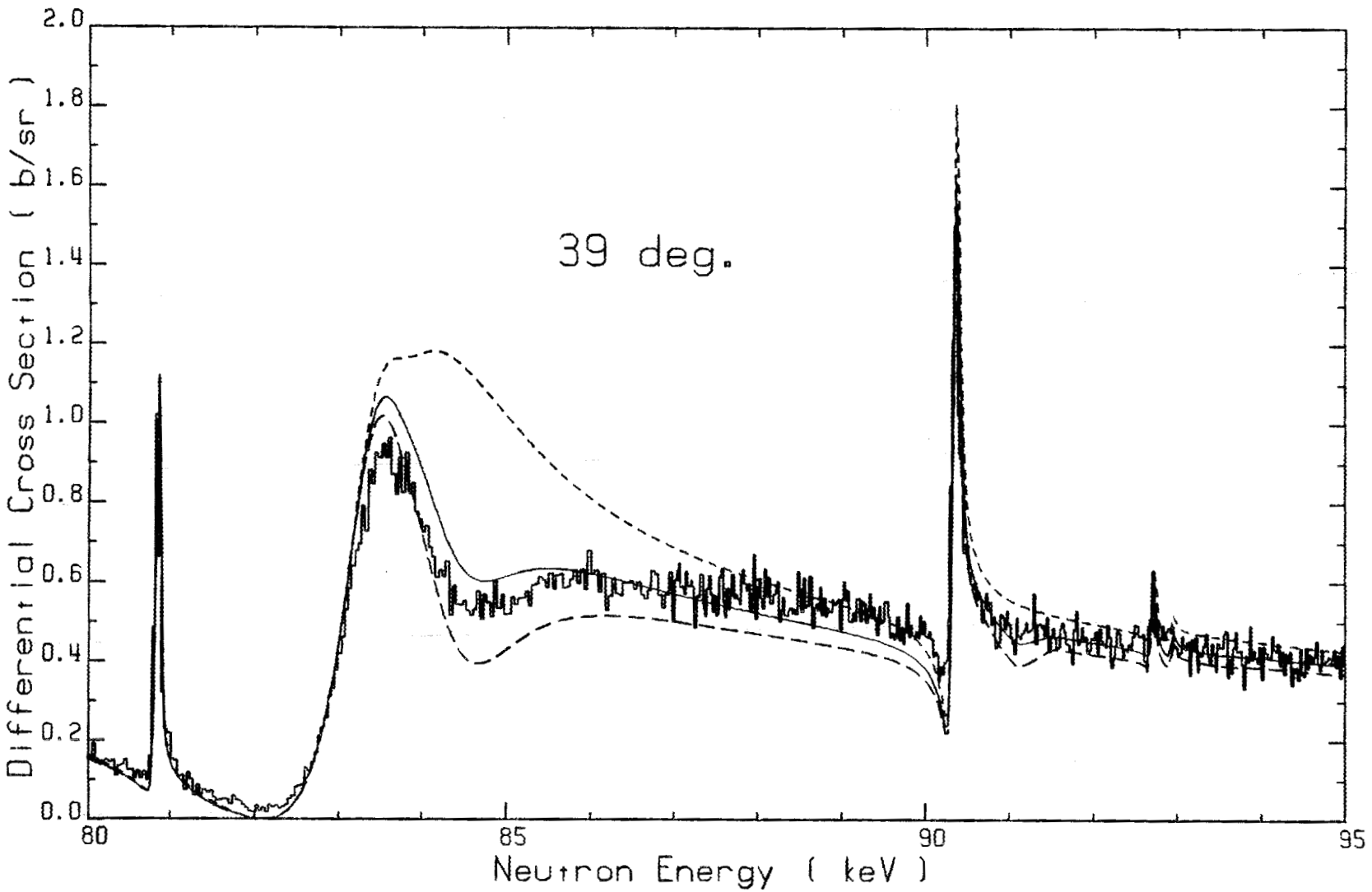

Fig. 1. Scattering of neutrons from ^{56}Fe. The full line was calculated with $n_0 = 0.02$ atom/barn, the short dash line with $n_0 = 0$, and the long dash line with $n_0 = 0.034$.

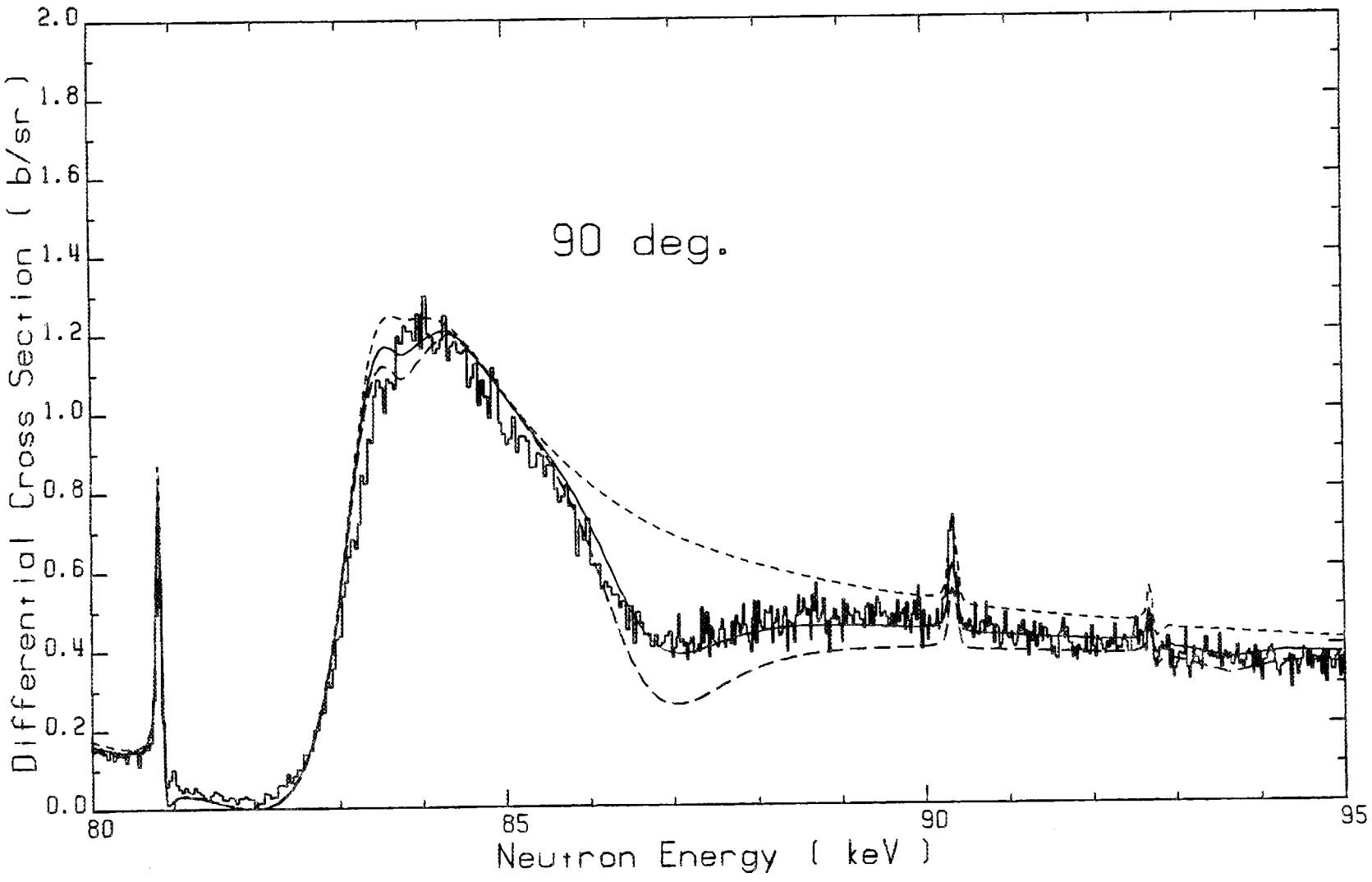

Fig. 2. Scattering of neutrons from ^{56}Fe. The full line was calculated with $n_0 = 0.02$ atom/barn, the short dash line with $n_0 = 0$, and the long dash line with $n_0 = 0.034$.

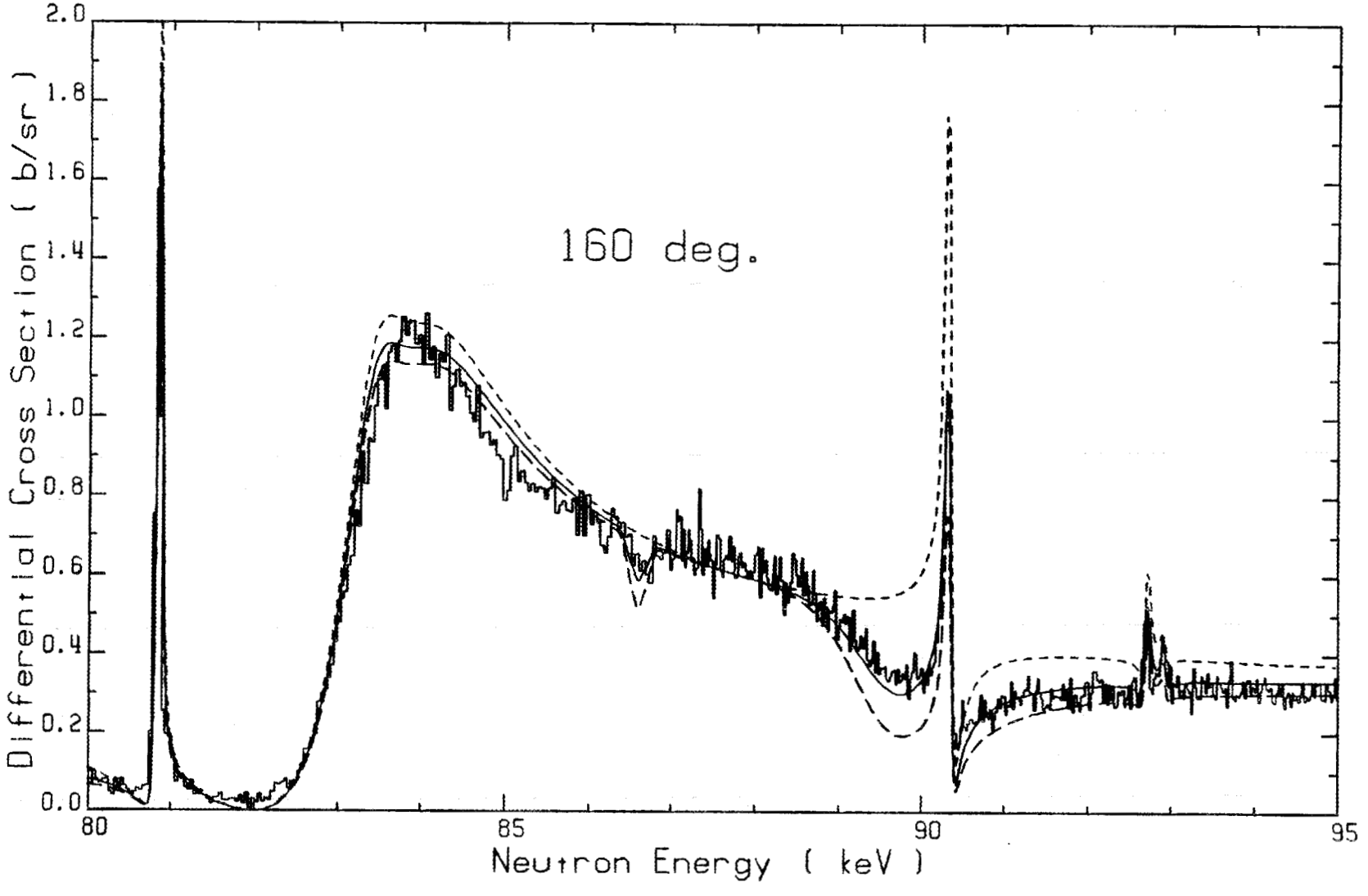

Fig. 3. Scattering of neutrons from ^{56}Fe. The full line was calculated with $n_0 = 0.02$ atom/barn, the short dash line with $n_0 = 0$, and the long dash line with $n_0 = 0.034$.

APPENDIX A

DESCRIPTION OF THE INPUT TO RFUNC

The code RFUNC was written to be run interactively with a prompt being issued for every line of input. It can be run with a command file in which each line of input appears. This appendix contains a brief description of the input to the code. All of the information contained in this appendix appears in the HELP file for RFUNC on the ORELA VAX system.

Line 1 prompt: #OF ANGLES (< 7) ?

List: IAN

Format: I

The number of angles must be less than or equal to 6.

Line 2 prompt: IAN ORDERED ANGLES ?

List: (ANG(I),I=1,IAN)

Format: 6F

The laboratory scattering angles, in degrees. They should be ordered with the smallest one given first.

Line 3 prompt: NORMALIZATIONS ?

List: (ANOR(I),I=1,IAN)

Format: 6F

If ANOR(I) = 0. then code sets it to 1. The calculations at ANG(I) will be multiplied by ANOR(I).

Line 4 prompt: BACKGROUNDS (B/SR) ?

List: (BAKG(I),I=1,IAN)

Format: 6F

BAKG(I) will be added to the renormalized calculations at ANG(I).

Line 5 prompt: E-SHIFT (EV) ?

List: ESHIFT

Format: F

ESHIFT will be added to the energies of calculations in the output ODF file.

Line 6 prompt: DELTA THETA, ISHIFT, IRES ?

List: DANG, ISHIFT, IR

Format: F,2I

DANG is the half width, in degrees, of the effective triangular resolution function for outgoing neutron attenuation. Let a be the half width of the angle subtended by the detectors at the sample and b be the half width of the angle subtended by the sample at the detectors, then :

$$DANG = \sqrt{2 * (a^2 + b^2)}.$$

If ISHIFT = 0 then no shift factors are used, as in ENDF/B. If ISHIFT = 1 then the boundary conditions are set to the values of the shift factors in the middle of the energy range calculated, or at EMIDL (see line 9 of the input).

Only every IRth calculated point is resolution broadened and written in the ODF output file. If IR = 0 then the code sets it equal to 1.

Line 7 prompt: RES. PAR. FILENAME ?

List: A

Format: A

The resonance parameter file can be obtained by processing a SAMMY parameter file using the code MAKPA (see Appendix B).

The format of the RFUNC resonance parameter file is as follows:

Line 1: AM (F12.5) The scattering nuclide atomic mass.

Line 2: (R(I),I=1,7) (7F12.5) 7 radii for the 7 SPIN-GROUPS.

If a single radius appears on this line, this radius will be used for all the SPIN-GROUPS.

In RFUNC the key to the SPIN-GROUP numbers are:

l	j	SPIN-GROUP number
0	1/2	1
1	1/2	2
1	3/2	3
2	3/2	4
2	5/2	5
3	5/2	6
3	7/2	7

Subsequent lines: ER(I), GAMMAN(I), LJ(I) (2E11.5,I5)

Where: ER(I) is the resonance energy, in KeV, in the laboratory coordinate system.

GAMMAN(I) is its neutron width in KeV.

LJ(I) is its SPIN-GROUP number.

The resonances energies should be in increasing order.

The highest energy resonance is followed by a blank line.

Up to 550 resonances may be used.

Line 8 prompt: A/B I, A/B O ?

List: APBI, APBO

Format: 2F

APBI is half the average value of the sample thickness in atoms/barn. It is the value used to calculate the average attenuation of the incident neutrons.

APBO is used to calculate the attenuation of outgoing neutrons. A value of APBO less than the value of APBI will simulate the effects of multiple scattering.

Line 9 prompt: ELO, EHI, DE, EMIDL (KEV) ?

List: ELO, EHI, DE, EMIDL

Format: 4F

The excitation functions at ANG(I) will be calculated from ELO to EHI.

DE is the energy mesh size used to calculate the excitation functions. DE should be not larger than half the Doppler width. Resonances whose widths are less than DE may not be properly described. If there are any such resonances in the energy range calculated the code will identify where they are and give their widths. If DE is set equal to zero in the input, then the code sets DE equal to the Doppler width in the center of the energy range divided by 2.5.

If ISHIFT = 1 and EMIDL is not zero then the boundary conditions are set to the values of the shift factors at EMIDL rather than at (ELO + EHI)/2.

NOTE: Due to the dimensions in the code (EHI - ELO)/DE must be less than 9750. If this condition is not met a message is printed and the code stops.

Line 10 prompt: FP-L, DELTA-L, DELTA-T ?

List: FPL, DELTAL, DELTAT

Format: 2F

FPL is the flight path length in meters.

DELTAL is the effective flight path length distribution width in meters.

DELTAT is the pulse width in microseconds.

FPL, DELTAL and DELTAT are used to construct two variables RESDL and RESDT:

$$RESDL = (0.8165 * DELTAL/FPL)^2$$

$$RESDT = (0.01661 * DELTAT/FPL)^2$$

The resolution, in eV, at energy E, in eV, is taken to be a Gaussian of width:

$$E\sqrt{RESDL + E * RESDT}$$

Line 11 prompt: ODF OUTPUT FILENAME ?

List: B

Format: A

The sections of the ODF file are:

Section 1: The lab energies, in eV.

Section 2 through section IAN+1: The excitation functions.

Section IAN+2: The Doppler and resolution broadened total cross section.

The following is an example of a command file used to run RFUNC on the ORELA VAX:

```
$SET VERIFY
$R RFUNC
 6
 39.,55.,90.,120.,140.,160.
 1.33,1.33,1.28,1.33,1.33,1.33
 0.03,0.03,0.03,0.02,0.02,0.02
 -25.
 11.15,0,2
 JAN89B.PAR
 0.034,0.020
 120.,135.,0.0
 200.191,0.085,0.006
 JAN89B.OD
```

APPENDIX B

THE UTILITY CODE MAKPA

MAKPA is a utility code on the ORELA VAX computer system used to convert a SAMMY parameter file into a parameter file for the codes RFUNC and RFUNCXT. This appendix contains information on the input to the code MAKPA. This information is available in the HELP file for MAKPA on the ORELA VAX. The code MAKPA was written to be run interactively, or via a command file, and a prompt is given by the code for every line of input. An example of command file to run MAKPA is given at the end of this appendix.

INPUT DESCRIPTION

Line 1 prompt: INPUT FILENAME ?

Give the name of the SAMMY parameter file to be converted into a RFUNC parameter file.

Line 2 prompt: OUTPUT FILENAME ?

Give the name for the output parameter file which will be the input parameter file for RFUNC or RFUNCXT.

Line 3 prompt: AM ?

List: AM

Format: F

AM is the atomic mass of the scattering nuclide in amu's.

Line 4 prompt: RADII (1s, 2p, 2d, 2f) ?

List: (R(I),I=1,7)

Format: 7F

Give 7 radii in Fermis. The first one for s-waves, the next 2 for p-waves the next 2 for d-waves and finally the last 2 for f-waves. If a single radius is given, it will be used for all angular momenta.

Line 5 prompt: IGNORE SPIN GROUPS K AND GREATER, K=?

List: K

Format: I

Spin groups, i.e. various combinations of orbital angular momentum l and total angular momentum j, having a value K and greater in the SAMMY parameter file will be ignored, i.e. they will not appear in the output parameter file.

CAUTION !!!!! It is assumed that in the SAMMY parameter file the spin groups less than this value of K have the following meaning:

l	j	SPIN-GROUP number
0	1/2	1
1	1/2	2
1	3/2	3
2	3/2	4
2	5/2	5
3	5/2	6
3	7/2	7

EXAMPLE OF COMMAND FILE

The following is a listing of a command file used to run MAKPA:

```
$SET VERIFY

$R MAKPA

 FE13.PAR

 JAN89B.PAR

 55.935

 5.43,4.89,4.89,5.43,5.43,5.43,5.43

 7
```

The following is a listing of the first few resonances in the file FE13.PAR, note that the resonance energies are in eV and the widths in meV:

```
-1.0000E+05 6.0000E+03 4.0169E+07        0 0 1   1
-3.7000E+04 2.0000E+03 1.2067E+07        0 0 1   7
-2.4982E+03 6.4600E+02 2.2069E+05        1 0 1   1
 3.9550E+03 1.1400E+03 2.2388E+05        0 0 0  10
 6.2666E+03 1.3200E+03 4.4149E+05        1 0 1  11
 7.7992E+03 2.1000E+03 1.1711E+06        1 0 1   7
 1.0434E+04 1.6000E+03 3.4045E+06        0 0 1  12
 2.0900E+04 5.0000E+02 9.3397E+05        0 0 0  13
 2.2801E+04 1.0000E+03 2.0117E+02        0 0 0   2
 2.7100E+04 5.0000E+02 4.1999E+05        0 0 0  14
```

The following is a listing of the beginning of file JAN89B.PAR, note that the resonance energies and the neutron widths are now all in keV:

```
 55.93500
  5.43000   4.89000   4.89000   5.43000   5.43000   ETC...
-1.0000E+02 4.0169E+01   1      -100.0000   40.1690
-2.4982E+00 2.2069E-01   1        -2.4982    0.2207
 2.2801E+01 2.0117E-04   2        22.8010    0.0002
 2.7775E+01 1.3960E+00   1        27.7750    1.3960
```

APPENDIX C

THE CODE RFUNCXT

RFUNCXT is a code that uses the same parameter file as the code RFUNC to calculate, also in the real R-function approximation, the contributions of the various SPIN-GROUPS (combinations of values of the orbital angular momentum l and total angular momentum j) to the total cross section. Such information has been found useful when analyzing transmission data in energy regions where many resonances overlap.

The output of RFUNCXT is an ODF file that contains the total cross section and the contributions to it from the various SPIN-GROUPS. The code RFUNCXT was written to be run interactively, or via a command file, and the code provides a prompt for each line of input. An example of a command file for RFUNCXT is given at the end of this appendix.

The code RFUNCXT is on the ORELA VAX computer system where it is called RFUNC_XT. The information in this appendix is available from the HELP file for RFUNC_XT on the ORELA VAX computer system.

DESCRIPTION OF THE INPUT

Line 1 prompt: ISHIFT, IRES ?

List: ISHIFT, IR

Format: 2I

If ISHIFT = 0 then no shift factors are used, as in ENDF/B. If ISHIFT = 1 then the boundary conditions are set to the values of the shift factors in the middle of the energy range calculated, or at EMIDL (see input line 3).

Only every IR^{th} calculated point is resolution broadened and written in the ODF output file. If IR = 0 then the code sets it equal to 1.

Line 2 prompt: RES. PAR. FILENAME ?

List: A

Format: A

The resonance parameter file can be obtained by processing a SAMMY parameter file using the code MAKPA, see Appendix C. The resonance parameter file for RFUNCXT is identical in format to the one used by RFUNC. See Appendix A for a description of its format.

Line 3 prompt: ELO, EHI, DE, EMIDL (KEV) ?

List: ELO, EHI, DE, EMIDL

Format: 4F

The total cross sections will be calculated from ELO to EHI.

DE is the energy mesh size used. DE should be not larger than half the Doppler width. Resonances whose widths are less than DE may not be properly described. If there are any such resonances in the energy range calculated the code will identify where they are and give their widths. If DE is set equal to zero in the input, then the code sets DE equal to the Doppler width in the center of the energy range divided by 2.5.

If ISHIFT = 1 and EMIDL is not zero then the boundary conditions are set to the values of the shift factors at EMIDL rather than at (ELO + EHI)/2.

NOTE: Due to the dimensions in the code (EHI - ELO)/DE must be less than 9750. If this condition is not met a message is printed and the code stops.

Line 4 prompt: FP-L, DELTA-L, DELTA-T ?

List: FPL, DELTAL, DELTAT

Format: 2F

FPL is the flight path length in meters.

DELTAL is the effective flight path length distribution width in meters.

DELTAT is the pulse width in microseconds.

FPL, DELTAL and DELTAT are used to construct two variables RESDL and RESDT:

$$RESDL = (0.8165 * DELTAL/FPL)^2$$
$$RESDT = (0.01661 * DELTAT/FPL)^2$$

The resolution, in eV, at energy E, in eV, is taken to be a Gaussian of width:

$$E\sqrt{RESDL + E * RESDT}$$

Line 5 prompt: ODF OUTPUT FILENAME ?

List: B

Format: A

The sections of the ODF file are:

Section 1: The lab energies, in eV.

Sections 2 through 8 contain the contributions to the total cross section from SPIN-GROUPS 1 through 7 respectively.

Section 9: The total cross section.

EXAMPLE OF COMMAND FILE USED TO RUN RFUNCXT

The following is a listing of a command file used to run RFUNCXT:

```
$SET VERIFY
$R RFUNC_XT
 0,2
 JAN89B.PAR
 120.,135.,0.0
 200.191,0.085,0.006
 JAN89B.ODF
```

APPENDIX D

LISTING OF THE FORTRAN CODING OF RFUNC

```
      PROGRAM RFUNC
       DIMENSION ER(550),LJ(550),GAM(550),GAMSQ(550),AO(8),
      * XSD(30000),ED(30000),X1(10000),X2(10000),ANOR(6),BAKG(6)
       COMMON/STUF/ D(8,8),DELT(8),SAN(8),CAS(8)

COMMON/JAZ/AM,AMRT,AR(8),AFAC,P(8),S(8),PHI(8),BC(8),B(8),R(8),WN
       COMMON /FGP/ XS(10000,7),COE(10000,7),EE(10000),XSM(7),
      1 JFAC,FAC(100),ANG(6)
CC
CC    A IS NAME OF PAR FILE, BBB IS NAME OF ODF FILE
CC
       CHARACTER*80 A,BBB
       PI2 = 3.14159/2.
CC
CC    GET NUMBER OF ANGLES, IAN, AND THEIR VALUES IN LAB.
CC
       TYPE 91
91     FORMAT (' # OF ANGLES ( < 7) ? ',$)
       ACCEPT 90, IAN
90     FORMAT (I)
       IF (IAN.GT.6) IAN = 6
       TYPE 89
89     FORMAT (' IAN ORDERED ANGLES ? ',$)
       ACCEPT 88, (ANG(I),I=1,IAN)
88     FORMAT (6F)
CC
CC   GET NORMALIZATIONS ANOR(I), BACKGROUNDS BAKG(I), ESHIFT
CC
       TYPE 95
95     FORMAT (' NORMALIZATIONS ? ',$)
       ACCEPT 94, (ANOR(I),I=1,IAN)
94     FORMAT (6F)
       DO I=1,IAN
       IF (ANOR(I).EQ.0.) ANOR(I) = 1.
       END DO
       TYPE 93
93     FORMAT (' BACKGROUNDS (B/SR) ? ',$)
       ACCEPT 94, (BAKG(I),I=1,IAN)
       TYPE 92
92     FORMAT (' E-SHIFT (EV) ? ',$)
       ACCEPT 94, ESHIFT
       TYPE 9007
9007   FORMAT (' NORMALIZATIONS, BACKGROUNDS AND ESHIFT USED')
       TYPE 9008, (ANOR(I),I=1,IAN)
9008   FORMAT (6F8.5)
       TYPE 9008, (BAKG(I),I=1,IAN)
```

```
      TYPE 9009, ESHIFT
9009  FORMAT (F8.1)
CC
CC GET DANG, OPTIONS FOR SHIFT AND RESOLUTION STEP
CC
CC   DANG IS HALF WIDTH IN DEG. OF EFFECTIVE TRIANGULAR RESOLUTION
CC   IF ISI = 0 NO SHIFT
CC   AFTER THE DOPPLER BROADENING, THE RESOLUTION BROAD. IS DONE
EVERY
CC   IRES POINTS IN THE ENERGY GRID
CC
      TYPE 97
97    FORMAT (' DELTA THETA, ISHIFT, IRES ? ',$)
      ACCEPT 96, DANG,ISI,IRES
96    FORMAT (F,2I)
      IF (IRES.EQ.0) IRES = 1
CC
CC  GET RESONANCE PARAMETERS FILENAME AND OPEN IT AS UNIT 1
CC   THIS PAR FILE IS A SAMMY PAR FILE PROCESSED BY MAKPA
CC
      TYPE 99
99    FORMAT (' RES. PAR. FILENAME ? ',$)
      ACCEPT 98, A
98    FORMAT (A)
      OPEN (UNIT=1,FILE=A,STATUS='OLD')
CC
CC READ MASS. THEN THE 8 RADII
CC
      READ (1,100) AM
      READ (1,100) (AR(I),I=2,8)
      AR(1) = AR(2)
      DO I=3,8
      IF (AR(I).EQ.0.) AR(I)=AR(1)
      END DO
 100  FORMAT (8F12.5)
      TYPE 87
87    FORMAT (' RADII USED')
      TYPE 86, (AR(I),I=2,8)
86    FORMAT (7F12.5)
CC
CC READ RES. ENERGIES (ER), GAMMA N (GAM) AND SPIN GROUP (LJ)
CC
      NR = 1
 1    READ (1,101,END=2) ER(NR),GAM(NR),LJ(NR)
 101  FORMAT (2E12.4,I5)
CC
CC MODIFIED 3/7/88 TO AGREE WITH SAMMY
CC
      LJ(NR) = LJ(NR) + 1
CC
      NR = NR + 1
```

```
      GO TO 1
CC
CC FINISHED READING RESONANCE PARAMETERS
CC
 2    NR = NR - 1
CC
CC  GET A/B, APBI FOR INCIDENT, APBO FOR OUTGOING
CC
      TYPE 104
104   FORMAT (' A/B I, A/B O ? ',$)
      ACCEPT 103, APBI, APBO
CC
CC  GET RANGE OF ENERGIES FOR CALCULATION
CC
      TYPE 102
102   FORMAT (' ELO, EHI, DE, EMIDL (KEV) ? ')
      ACCEPT 103,ELOI,EHII,DE,EMIDL
103   FORMAT (4E)
      EMID = (ELOI + EHII)/2.
CC
CC  GET RESOLUTION PARAMETERS IN CASE DE = 0.
CC
CC     USE SAMMY RECIPE FOR RESDL AND RESDT
CC
      TYPE 106
106   FORMAT (' FP-L, DELTA-L, DELTA-T ',$)
      ACCEPT 107, FPL, DELTAL, DELTAT
      RESDL = (.81650*DELTAL/FPL)**2
      RESDT = 1000.*(.01661*DELTAT/FPL)**2
107   FORMAT (3F)
CC
CC   CALCULATE DOPPLER AND RESOLUTION WIDTHS TO COMPARE WITH DE
CC       OR SET DE IF ZERO
CC
      SIGD = 0.0003178*SQRT(1000.*EMID/AM)
      SIGR = EMID*SQRT(RESDL + RESDT*EMID)
      IF (DE.EQ.0.) THEN
      DE = SIGD/2.5
      DEV = 1000.*DE
      TYPE 9010, DEV
9010  FORMAT (' DE SET TO : ',F10.2,' EV')
      ELSE
      END IF
      DODE = SIGD/DE
      RODE = SIGR/DE
      SIGD = 1000.*SIGD
      SIGR = 1000.*SIGR
      TYPE 9000, SIGD, DODE, SIGR, RODE
9000  FORMAT (' DOPPLER WIDTH (EV) ',F12.2,' RATIO TO DE ',F6.2,/
     * ,' RESOLU. WIDTH (EV) ',F12.2,' RATIO TO DE ',F6.2)
CC
```

```
CC  CHECK WHICH RES. MAY NOT BE CORRECTLY REPRESENTED
CC
      TYPE 9004
9004  FORMAT (' RESONANCES THAT MAY NOT BE CORRECTLY DESCRIBED')
      ICRES = 0
      DO I=1,NR
      IF ((ER(I).GE.ELOI).AND.(ER(I).LE.EHII)) THEN
      IF (GAM(I).LT.DE) THEN
      ICRES = 1
      JNK = LJ(I) - 1
      TYPE 9005, ER(I), GAM(I), JNK
9005  FORMAT (F12.4,F12.5,I5)
      ELSE
      END IF
      ELSE
      END IF
      END DO
      IF (ICRES.EQ.0) THEN
      TYPE 9006
9006  FORMAT (' NONE !!!')
      ELSE
      END IF
CC
      EHI = EHII + 125.*DE
CC  ANG(IAN) IS THE LARGEST ANGLE
      ANGR = (ANG(IAN) + DANG)*3.14159/180.
      CHI = COS(ANGR)
      SHI = SIN(ANGR)
      RAT = ((CHI + SQRT( AM**2 - SHI**2))/(AM + 1.))**2
      ELO = RAT*ELOI - 125.*DE
      ELOS = ELOI - 125.*DE
      AKPT = (EHI - ELO)/DE
      KPT = AKPT
      TYPE 9001, KPT, ELO, EHI
9001  FORMAT (' SIGT   (#,ELO,EHI) ',I6,2F9.3)
      IF (KPT.LT.30000) GO TO 31
      TYPE 105, KPT
105   FORMAT (I6,'  IS TOO MANY POINTS TRY AGAIN !!')
      STOP
31    CONTINUE
      JNK = (EHI - ELOS)/DE
      IF (JNK.GT.10000) THEN
      TYPE 105, JNK
      STOP
      ELSE
      END IF
CC
CC   X-TOT FROM ELO  TO EHI   KPT POINTS
CC   SCATT FROM ELOS TO EHI   JNK POINTS
CC
CC  GET OUTPUT FILE NAME
```

```
CC
      TYPE 108
108   FORMAT ('  ODF OUTPUT FILENAME ? ',$)
      ACCEPT 98, BBB
      AFAC = AM/(AM + 1.009)
      AMRT = SQRT(AFAC)
      IF ((ISI.EQ.1).AND.(EMIDL.NE.0.)) EMID=EMIDL
CC
CC CALCULATE SHIFT FACTORS (S) IN THE MIDDLE OF RANGE
CC    AND SET BOUNDARY COND. EQUAL TO THEM
CC    NEEDED IF ISI = 1
CC
      CALL PSPHI(EMID)
      DO I=2,8
      BC(I) = S(I)
      END DO
CC
CC   CONVERT NEUTRON WIDTHS ,GAM, TO REDUCED WIDTHS, GAMSQ.
CC
      DO I=1,NR
      CALL PSPHI(ABS(ER(I)))
      J = LJ(I)
      GAMSQ(I) = GAM(I)/(2.*P(J))
      END DO
CC
CC START OF BIG LOOP TO CALCULATE XSECTION'S FOR ATTENUATION OUT
CC
CC   SET UP E = ELO
CC
      E = ELO
      EB = E
CC
CC   JS IS COUNTER TO CALCULATE DIFF. ELASTIC
CC
      JS = 1
      DO 233 IKP=1,KPT
CC
CC  ZERO R FUNCTIONS
CC
      DO I=2,8
      R(I) = 0.0
      END DO
CC
CC CALCULATE THE R FUNCTIONS
CC
      DO 209 I=1,NR
      J = LJ(I)
      IF (E.EQ.ER(I)) GO TO 208
CC
CC C. OF M. ENERGY IS E*AFAC
CC
```

```
      T = GAMSQ(I)/(ER(I) - E)
      R(J) = R(J) + T
      GO TO 209
208   R(J) = 1.E20
209   CONTINUE
      CALL PSPHI (E)
CC
CC  CALCULATE THE PHASE SHIFTS DELT'S
CC   THEY ARE SET BETWEEN -PI AND + PI
CC
      DO 216 J=2,8
      IF (R(J).GE.1.E19) GO TO 210
      SS = P(J)*R(J)
CC
CC   A LA ENDF/B I.E. S(J) = BC(J) EVERYWHERE IF ISI = 0
CC
      CS = 1. - R(J)*(S(J) - BC(J))
      IF (ISI.EQ.0) CS = 1.
      GO TO 211
210   SS = P(J)
      CS = -(S(J) - BC(J))
      IF (ISI.EQ.0)  CS = 0.
211   IF (CS.EQ.0.) GO TO 212
      T = ATAN2(SS,CS)
      GO TO 213
212   T = PI2
      IF (SS.LT.0.)  T = -T
213   DELT(J) = - PHI(J) + T
214   TK = DELT(J)
      IF (ABS(TK).LE.PI2) GO TO 216
      IF (TK.LT.0.)  GO TO 215
      DELT(J) = DELT(J) - 3.14159
      GO TO 214
215   DELT(J) = DELT(J) + 3.14159
      GO TO 214
216   CONTINUE
CC
CC  TEST IF SIGT ONLY NEEDED E < ELOS
CC
      IF (E.LT.ELOS) THEN
CC
CC  CALCULATE LEGENDRE COEFF B(1) - NOT ENDF PRESCRIPTION
CC
      B(1) = SIN(DELT(2))**2 + SIN(DELT(3))**2 +
     * 2.*(SIN(DELT(4))**2 + SIN(DELT(5))**2) +
     * 3.*(SIN(DELT(6))**2 + SIN(DELT(7))**2) +
     * 4.*(SIN(DELT(8))**2)
CC
CC CONVERT TO ENDF FORM - B(1) IS TOTAL X-SEC.
CC
      B(1) = 40.*3.14159*B(1)/WN**2
```

```
CC
CC STORE TOTAL X-SECTION IN XSD AND ENERGY IN ED TO DO
CC  THE OUTGOING ATTENUATION LATER
CC
      XSD(IKP) = B(1)
      ED(IKP) = E
CC
CC SET NEW ENERGY FOR LOOP
CC
      AKP = IKP
      E = EB + AKP*DE
      ELSE
CC
CC  GET THE SIN AND COS'S FOR CALCULATING THE LEGENDRE COEFF
CC
      CALL SETBIG
CC
CC  CALCULATE LEGENDRE COEFF - NOT ENDF PRESCRIPTION
CC
      B(1) = D(2,2) + D(3,3) + 2.*(D(4,4) + D(5,5)) + 3.*(D(6,6)
     * + D(7,7)) + 4.*D(8,8)
      B(2) = 2.*D(2,3) + 4.*(D(2,4) + D(3,5)) + (4.*D(4,5)
     * + 36.*(D(4,6) + D(5,7)))/5. + (18.*D(6,7) + 360.*D(6,8))/35.
      B(3) = 4.*(D(2,5) + D(3,4)) + 6.*(D(2,6) + D(3,7))
     * + 2.*(D(4,4) + D(5,5)) + (12.*(D(4,7) + D(5,6))
     * + 24.*(D(6,6) + D(7,7)) + 72.*D(4,8) + 8.*D(7,8)
     * + 33.333*D(8,8))/7.
      B(4) = 6.*(D(2,7) + D(3,6)) + 8.*(D(2,8) + D(6,8))
     * + 4.8*(D(4,6) + D(5,7)) + 7.2*D(4,5) + 3.2*D(6,7)
     * + 2.66667*D(5,8)
      B(5) = 8.*D(3,8) + (72.*(D(4,7) + D(5,6)) + 18.*(D(6,6)
     * + D(7,7)) + 40.*D(4,8))/7. + (360.*D(7,8) + 324.*D(8,8))/77.
      B(6) = 40.*D(5,8)/3. + (100.*D(6,7) + 40.*D(6,8))/7.
      B(7) = (600.*D(7,8) + 100.*D(8,8))/33.
CC
CC CONVERT TO ENDF FORM - B(1) IS TOTAL X-SEC.
CC
      B0 = B(1)
      B(1) = 40.*3.14159*B(1)/WN**2
      DO I=2,7
      C0 = 2*I-1
      B(I) = B(I)/(C0*B0)
      END DO
CC
CC STORE LEGENDRE COEFF'S IN XS(NPT,I)
CC
      DO I=1,7
      XS(JS,I) = B(I)
      END DO
      EE(JS) = E
CC
```

```
CC    SAVE THE X-TOTAL IN XSD
CC
      XSD(IKP) = B(1)
      ED(IKP) = E
CC
CC   SET NEW ENERGY AND INCREMENT COUNTER
CC
      JS = JS + 1
      AKP = IKP
      E = EB + AKP*DE
CC
CC    END OF BIG LOOP
CC
      END IF
CC
CC    END OF BIG LOOP
CC
233   CONTINUE
CC
CC SAVE  KPTD FOR TOTAL AND SET KPT = JS - 1
CC
      KPTD = KPT
      KPT = JS - 1
CC
CC
CC DOPPLER SMEAR XS INTO COE AND DO INCOMING ATTENUATION
CC
      I1 = 25
      I2 = KPT - 25
      ITS = KPT - 50
      E = EE(25)
      EB = E
      JJ = 0
      DO 6 NCH=I1,I2
      JJ = JJ+1
CC   E IS IN KEV AND WE NEED SIG IN UNITS OF DE
      SIG = 0.0003178*SQRT(1000.*E/AM)
      CALL SETWT(DE,SIG,JFAC,FAC(1))
      DO K=1,7
      SUM = FAC(1)*XS(NCH,K)
      DO J=2,JFAC
      SUM = SUM + FAC(J)*(XS(NCH+J-1,K) + XS(NCH-J+1,K))
      END DO
      XSM(K) = SUM
      END DO
      EE(JJ) = E
      AJJ = JJ
      E = EB + AJJ*DE
CC
CC   DO THE INCOMING NEUTRON AVG. ATTENUATION
CC      SAVE DOP. BROADENED TOTAL IN X1
```

```
CC
      ATTI = EXP(-APBI*XSM(1)/1000.)
      X1(JJ) = XSM(1)
      XSM(1) = XSM(1)*ATTI
CC
CC   STORE RESULTS IN COE
CC
      DO J=1,7
      COE(JJ,J) = XSM(J)
      END DO
6     CONTINUE
CC
CC RESTORE KPT AND XS TO DO RES. SMEAR
CC
CC TEST IF RES IS NEEDED
CC
      IF ((RESDL.EQ.0.).AND.(RESDT.EQ.0.)) THEN
CC TRANSFER X1 INTO X2
      DO I=1,ITS
      X2(I) = X1(I)/1000.
      END DO
CC SKIP RESOLUTION BROADENING
CC
      ELSE
      KPT = ITS
      DO I=1,KPT
      DO J=1,7
      XS(I,J) = COE(I,J)
      END DO
      END DO
CC
CC RES SMEAR XS INTO COE
CC
CC ONLY FROM ELOI TO EHII
CC UPPER LIMIT IS OK
CC LOWER LIMIT IS MUCH TOO LOW
CC
CC  FIND  I1 THE INDEX OF LOWEST ENERGY NEEDED
CC
      I1 = 1
      DO I=1,10000
      IF (EE(I1).GT.ELOI) GO TO 20
      I1 = I1 + 1
      END DO
      STOP
20    IF (I1.LT.100)  I1 = 100
      I2 = KPT - 100
      ITS = (KPT - 100 -I1)/IRES
      ARES = IRES
      DEARES = ARES*DE
      TYPE 9003, ITS,EE(I1),EE(I2)
```

```
9003  FORMAT (' OUTPUT (#,ELO,EHI) ',I6,2F9.3)
      E = EE(I1)
      EB = E
      JJ = 0
      DO 37 NCH=I1,I2,IRES
      JJ = JJ+1
      SIG = E*SQRT(RESDL + RESDT*E)
      CALL SETWT(DE,SIG,JFAC,FAC(1))
      DO K=1,7
      SUM = FAC(1)*XS(NCH,K)
      DO J=2,JFAC
      SUM = SUM + FAC(J)*(XS(NCH+J-1,K) + XS(NCH-J+1,K))
      END DO
      XSM(K) = SUM
      END DO
CC
CC RES SMEAR TOTAL (X1) IN X2 FOR OUTPUT
CC
      SUM = FAC(1)*X1(NCH)
      DO J=2,JFAC
      SUM = SUM + FAC(J)*(X1(NCH+J-1) + X1(NCH-J+1))
      END DO
      X2(JJ) = SUM/1000.
CC DONE
      EE(JJ) = E
      AJJ = JJ
      E = EB + AJJ*DEARES
      DO J=1,7
      COE(JJ,J) = XSM(J)
      END DO
37    CONTINUE
      END IF
CC
CC CALCULATE CROSS SECTION INTO XS
CC
      P4 = 4.*3.14159*1000.
      DO 41 IJ=1,IAN
      ANGR = ANG(IJ)*3.14159/180.
      ANGL = (ANG(IJ) + DANG)*3.14159/180.
      ANGH = (ANG(IJ) - DANG)*3.14159/180.
      CHIL = COS(ANGL)
      CHIH = COS(ANGH)
      SHIL = SIN(ANGL)
      SHIH = SIN(ANGH)
      CHI = COS(ANGR)
      SHI = SIN(ANGR)
CC
CC  RAT IS RATIO OF E(OUT)/E(IN) AT ANGLE ANG(IJ)
CC
      RATL = ((CHIL + SQRT( AM**2 -SHIL**2))/(AM + 1.))**2
      RATH = ((CHIH + SQRT( AM**2 -SHIH**2))/(AM + 1.))**2
```

```
CC
      CHI2 = CHI*CHI
      T = SQRT(CHI2 + AM**2 - 1.)
CC
CC   FMU IS COSINE OF CM ANGLE CORRESPONDING TO ANG(IJ)
CC   DMU IS THE JACOBEAN OF CM TO LAB TRANSFORMATION
CC
      FMU = (CHI2-1. + CHI*T)/AM
      DMU = (2.*CHI + (CHI2 + T**2)/T)/AM
CC
CC   CALCULATE LEGENDRE POLY.
CC
      P(1) = 1.
      P(2) = FMU
      DO N=2,6
      FL = N - 1
      P(N+1) = (FMU*(2.*FL + 1.)*P(N) - FL*P(N-1))/(FL + 1.)
      END DO
CC
CC  CALCULATE THE EXCITATION FUNCTION
CC
      DO I=1,ITS
      SUM = 1.
      DO J=2,7
      FI = J - 1
      SUM = SUM + (2.*FI + 1.)*COE(I,J)*P(J)
      END DO
      XS(I,IJ) = SUM*DMU*COE(I,1)/P4
CC
CC  HERE WE MUST DO THE OUTGOING ATTENUATION
CC  THE INCIDENT LAB ENERGY IS IN EE(I) THE ANGLE IS ANG(IJ)
CC  FIND IS A BINARY SEARCH SUBROUTINE
CC
      EANGL = RATL*EE(I)
      EANGH = RATH*EE(I)
      CALL FIND(ED,XSD,KPTD,EANGL,XSANG,IOL)
      CALL FIND(ED,XSD,KPTD,EANGH,XSANG,IOH)
      IF ((IOH-IOL).LT.2) THEN
      ATTO = EXP(-APBO*XSANG/1000.)
      XS(I,IJ) = XS(I,IJ)*ATTO
      ELSE
CC AVERAGE CROSS SECTION, TRIANGULAR RESOL
      IOC = 1 + IOL + (IOH - IOL - 1)/2
      XSANG = 0.
      WEI = 0.
      WEIT = 0.
      DO IOK=IOL,IOC
      WEI = WEI + 1.
      WEIT = WEIT + WEI
      XSANG = XSANG + WEI*XSD(IOK)
      END DO
```

```
      DO IOK=IOC+1,IOH
      WEI = WEI - 1.
      WEIT = WEIT + WEI
      XSANG = XSANG + WEI*XSD(IOK)
      END DO
      XSANG = XSANG/WEIT
      ATTO = EXP(-APBO*XSANG/1000.)
      XS(I,IJ) = XS(I,IJ)*ATTO
      END IF
      END DO
41    CONTINUE
CC
CC DO NORMALIZATIONS, BACKGROUNDS AND ESHIFT
CC
      DO J=1,IAN
      IF ((ANOR(J).NE.1.).OR.(BAKG(J).NE.0.)) THEN
      DO I=1,ITS
      XS(I,J) = XS(I,J)*ANOR(J) + BAKG(J)
      END DO
      ELSE
      END IF
      END DO
      DO I=1,ITS
      EE(I) = EE(I)*1000. + ESHIFT
      END DO
CC
CC WRITE OUT THE ODF FILE
CC
      NDST = 0
      IFB = 3
      ISEC = IAN + 2
      CALL ODFIO(30,BBB,IFB,1,ISEC,ITS,3,NDST,-1,6)
      CALL OUTODF(30,IFB,ISEC,1,3,NDST,1,ITS,EE(1),1)
      DO M=1,IAN
      CALL OUTODF(30,IFB,ISEC,M+1,3,NDST,1,ITS,XS(1,M),1)
      END DO
      CALL OUTODF(30,IFB,ISEC,ISEC,3,NDST,1,ITS,X2(1),1)
      CALL EXIT
      END
CC  ****************************************
      SUBROUTINE SETBIG
CC
CC THE D(I,J)'S ARE COEFFICIENTS TO CALCULATE LEGENDRE COEFF
CC    FROM PHASE SHIFTS
CC
      COMMON/STUF/ D(8,8),DELT(8),SAN(8),CAS(8)
      DO I=2,8
      CAS(I) = COS(DELT(I))
      SAN(I) = SIN(DELT(I))
      END DO
      DO I=2,8
```

```
      DO J=I,8
      A = SAN(I)*SAN(J)
      D(I,J) = A*(A + CAS(I)*CAS(J))
      END DO
      END DO
      RETURN
      END
CC  ***********************************************
      SUBROUTINE PSPHI (E)
CC
CC  PSPHI CALCULATE AT ENERGY E, IN THE LAB SYSTEM,
CC   1-  WN THE WAVE NUMBER IN CM SYSTEM, I.E. K.
CC   2-  P(I) THE PENETRABILITIES
CC   3-  S(I) THE SHIFT FACTORS
CC   4-  PHI(I) THE HARD SPHERE PHASE SHIFTS
CC
CC      .00694689 = .21968/SQRT(1000.)
CC      THE CONSTANT .21968 IS THE SAMA AS IN SAMMY (1986)
CC

COMMON/JAZ/AM,AMRT,AR(8),AFAC,P(8),S(8),PHI(8),BC(8),B(8),R(8),WN
      WN=.00694689*AFAC*SQRT(E)
CC
CC   THE X'S ARE K*R
CC
CC   L=0, J=1/2
CC
      X = WN*AR(2)
      P(2) = X
      PHI(2) = X
      S(2) = 0.
CC
CC   L=1, J=1/2
CC
      X = WN*AR(3)
      P(3) = X**3/(1. + X*X)
      S(3) = -1./(1. + X*X)
      PHI(3) = X - ATAN(X)
CC
CC   L=1, J=3/2
CC
      X = WN*AR(4)
      T1 = 1. + X*X
      P(4) = X**3/T1
      S(4) = -1./T1
      PHI(4) = X - ATAN(X)
CC
CC   L=2, J=3/2
CC
      X = WN*AR(5)
      T2 = 9. + 3.*X*X + X**4
```

```
      P(5) = X**5/T2
      S(5) = -( 18. + 3.*X*X)/T2
      PHI(5) = X - ATAN2( 3.*X , 3.-X*X )
CC
CC   L=2,  J=5/2
CC
      X = WN*AR(6)
      T2 = 9. + 3.*X*X + X**4
      P(6) = X**5/T2
      S(6) = -( 18. + 3.*X*X)/T2
      PHI(6) = X - ATAN2( 3.*X , 3. - X*X )
CC
CC   L=3, J=5/2
CC
      X = WN*AR(7)
      T3 = 225. + 45.*X*X + 6.*X**4 + X**6
      P(7) = X**7/T3
      S(7) = -3.*(225. + 30.*X*X + 2.*X**4)/T3
      PHI(7) = X - ATAN2( X*(X*X -15.) , 6.*X*X - 15. )
CC
CC   L=3, J=7/2
CC
      X = WN*AR(8)
      T3 = 225. + 45.*X*X + 6.*X**4 + X**6
      P(8) = X**7/T3
      S(8) = -3.*(225. + 30.*X*X + 2.*X**4)/T3
      PHI(8) = X - ATAN2( X*(X*X - 15.) , 6.*X*X - 15. )
      RETURN
      END
CC  ***********************************************************
      SUBROUTINE FIND(X,Y,N,Z,R,IO)
CC
CC                THIS IS A BINARY SEARCH
CC
CC        X(I) AND Y(I) ARE 2 TABLES OF LENGTH N,  N > 2.
CC    IF  ( Z.GE.X(IO) ).AND.( Z.LT.X(IO+1) ) THEN R = Y(IO)
CC     IF Z.LT.X(2)  THEN R = Y(1)
CC     IF Z.GE.X(N)  THEN R = Y(N)
CC
      DIMENSION X(1),Y(1)
      IF (Z.LT.X(2)) THEN
      R = Y(1)
      IO = 1
      ELSE IF (Z.GE.X(N)) THEN
      R = Y(N)
      IO = N
      ELSE
      IO = 1
      ID = N/2
1     IO = IO + ID
      IF ( Z.GT.X(IO) ) GO TO 2
```

```
      IO = IO - ID
2     ID = ID/2
      IF ( ID.GT.0 ) GO TO 1
      IF ( Z.EQ.X(IO) ) GO TO 5
      IF ( Z.GT.X(IO) ) GO TO 4
3     IO = IO - 1
      IF ( Z.GE.X(IO) ) GO TO 5
      GO TO 3
4     IO = IO + 1
      IF ( Z.EQ.X(IO) ) GO TO 5
      IF ( Z.GT.X(IO) ) GO TO 4
      IO = IO -1
      R = Y(IO)
      GO TO 6
5     R = Y(IO)
6     CONTINUE
      END IF
      RETURN
      END
CC  ************************************************************
      SUBROUTINE SETWT(DE,SIG,JFAC,FAC)
CC
CC  CALCULATES JFAC WEIGHTS, FAC(1) TO FAC(JFAC), TO PERFORM
CC    THE CONVOLUTION OF A GAUSSIAN , EXP(-(E/SIG)**2), WITH A
CC    FUNCTION CALCULATED AT EQUALLY SPACED INTERVALS DE
CC
CC    LET THE FUNCTION VALUES BE F(I), THEN THE CONVOLUTION C(I) IS
CC    OBTAINED WITH:
CC
CC        C(I) = FAC(1)*F(I)
CC        DO J=2,JFAC
CC        C(I) = C(I) + FAC(J)*(F(I+J-1) + F(I-J+1))
CC        END DO
CC
      REAL*8 ERF,U
      DIMENSION FAC(1)
      DEL = - DE/2
      I = 1
      ERLST = 0.
1     DEL = DEL + DE
      U = DEL/SIG
      ER = ERF(U)
      FAC(I) = ER - ERLST
      ERLST = ER
      IF (ER.GT..99999) GO TO 2
      IF (I.EQ.100) GO TO 2
      I = I + 1
      GO TO 1
2     FAC(1) = 2.*FAC(1)
      JFAC = I
      SUM = FAC(1)
```

```
      DO I=2,JFAC
      SUM = SUM + 2.*FAC(I)
      END DO
      DO I=1,JFAC
      FAC(I) = FAC(I)/SUM
      END DO
      RETURN
      END
CC*********************************************************
      DOUBLE PRECISION FUNCTION ERF(XX)
      IMPLICIT REAL*8 (A-H,O-Z)
C
CC                          ERF(XX)
C
CC                 ABRAMOWITZ AND SEGUM 7.1.26
C
CC       APPROXIMATION GOOD TO BETTER THAN +/- 0.00000015
C
      DATA A1 /2.54829592D-1/
      DATA A2 /-2.84496736D-1/
      DATA A3 /1.421413741D0/
      DATA A4 /-1.453152027D0/
      DATA A5 /1.061405429D0/
      DATA P /3.275911D-1/
      X = XX
      IF (XX.LT.0.0D0) X = -X
      T=1.0D0/(1.0D0+P*X)
      ERF = 1.0D0 -T*((((A5*T+A4)*T+A3)*T+A2)*T+A1)*DEXP(-X*X)
      IF (XX.LT.0.0D0) ERF = -ERF
      RETURN
      END
```

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