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FOLD

A CALIBRATION PROGRAM FOR THE ANALYSIS OF QUASI-ELASTIC NEUTRON SCATTERING DATA

by

D.J. WINFIELD

1970

Joint Nuclear Research Center
Ispra Establishment - Italy

Reactor Physics Department
Experimental Neutron Physics

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ABSTRACT

A Fortran IV computer program has been written which gives a means of calibrating the quasi-elastic peaks obtained from the time-of-flight data of the ISPRA-1 Double Chopper Spectrometer in terms of the widths of Lorentzian distributions.

Plots of quasi-elastic peaks calculated by the numerical convolution of the instrumental resolution, which may be of any shape, with Lorentzian functions of various widths are produced by the program. These plots allow a comparison to be made with experimental quasi-elastic peak shapes. The validity of the assumption of a Lorentzian function for the quasi-elastic scattering may thus be tested.

KEYWORDS

FORTRAN
COMPUTERS
CALIBRATION
ELASTIC SCATTERING
PEAKS
SPECTROMETERS
TIME OF FLIGHT METHOD
CHOPPERS
LORENTZ LINE SHAPES

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1. Introduction

2. Theory

3. Program Description

4. The Calibration Curve.

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Appendix: Program Listing and Typical Output Data.

1. Introduction *)

Diffusive motions of hydrogen containing molecules or hydrogen atoms in samples such as hydrogenous liquids or metallic hydrides may be conveniently studied by the technique of inelastic neutron scattering. These motions generally result in a "quasi-elastic" broadening of the infinitely sharp elastic peak which would be observed in the case of a solid, provided that the thermal motions were zero and the intrumental resolution was perfect. From this broadening, information may be gained about the exact nature of the diffusive motions in the particular sample of interest.

Experimentally however, finite instrumental resolution always imposes a limit on the energy transfers which are observable. With present chopper time of flight spectrometers the smallest detectable energy transfers are about 0.05 meV. The largest quasi-elastic broadenings of interest are normally around 5 meV so that this energy transfer and the above lower limit cover a time scale from 1.3×10^{-13} sec to 1.3×10^{-11} sec. As typical incident energies are about 5 meV with resolutions $\sim$ 0.5 meV, it is therefore always necessary to correct the experimental quasi-elastic peak widths for instrumental resolution in order to extract the true widths of the quasi-elastic peaks, resulting from the broadening process alone.

For a given instrumental resolution function and assuming a scattering law /1/

$$S(\underline{K},\omega) = \frac{\Delta E_L/2}{(\Delta E_L/2)^2 + (\hbar\omega)^2} \qquad /1/$$

of Lorentzian form, the program calculates and plots theoretical quasi-elastic peak shapes for a series of

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*) Manuscript received on 16 June 1970

widths (*)ΔE_L of this Lorentzian function. Constants have been omitted from equation [1] as the absolute value of the scattering law is not required.

Depending upon the theoretical model used to describe the sample under observation, the Lorentzian width ΔE_L is usually a function of the momentum transfer and it is this $\Delta E_L(\underline{K})$ relationship which is normally desired from any quasi-elastic scattering experiment.

From the calculated quasi-elastic peak shapes generated by the program a calibration curve may be obtained, relating the widths of the calculated peaks ΔEcalc to the true Lorentzian width ΔE_L, for a given incident energy E_o.

If now the shape of a given experimental quasi-elastic peak, with width ΔE_{obs}, is represented accurately by the calculated quasi-elastic peak of identical width, i.e. $\Delta E_{obs} = \Delta E_{calc}$ then the true Lorentzian width ΔE_L, corresponding to ΔE_{obs}, may be obtained immediately from inspection of the relevant calibration curve. As the $\underline{K}$ value of each quasi-elastic peak is known from the particular scattering angle of the relevant detector, the $\Delta E_L(\underline{K})$ relationship may thus be determined for further analysis.

2. Theory

Most theories of quasi-elastic scattering predict a scattering law $S(\underline{K}, \omega)$ of Lorentzian form [2], [3], [4] independent of the type of sample being analysed. Hence it is assumed here that the experimental quasi-elastic peak shap may be represented by a Lorentzian line shape convoluted by the resolution function of the apparatus.

(*) All "widths" described in this report refer to the full width at half peak height.

The line shape of the resolution function is normally taken as the elastic peak of a vanadium time of flight spectrum obtained under identical conditions as the experimental sample spectra. After corrections for the filtering effect have been made the vanadium elastic peaks obtained for different counter angles should be identical since the scattering is incoherent and isotropic. The room temperature Debye-Waller factor of vanadium is given by exp $(-0.006\ K^2)$ and hence varies very little over the normal K^2 range covered, which is from zero to about 10 $Å^{-2}$, so that no correction is necessary for this effect.

Alternatively the elastic peak from one of the sample spectra may be used for the resolution function, provided that the spectra were obtained whilst the sample was kept at a temperature which rendered the broadenings of the elastic peaks effectively zero. The difficulty with this method of obtaining the resolution function is that the elastic peaks of the sample spectra may be distorted a) from finite coherent scattering of the sample, and b) from any remaining inelastic scattering. Hence the elastic peak shapes at different angles may not be identical, making the choice of the best shape for the resolution function difficult. As vanadium has a negligible coherent scattering cross-section and a region of inelastic scattering, well separated from the elastic peak for normal incident energies of interest, no difficulties arise in this case. However, if the above two effects are not important for the sample of interest, then the alternative method of obtaining the resolution function may be used. This then provides a useful check on the consistency of the apparatus, by comparison with the vanadium results.

With certain chopper-time of flight spectrometers it may be reasonable to represent the resolution function by a Gaussian distribution. In this case the Lorentzian width ΔE_L may be obtained directly from tables, (see section 4). In general, however, the resolution function is considerably distorted from a Gaussian shape, depending upon the chopper transmission function and the reactor spectrum, and hence varying according to the incident energy E_0. The advantage of the present program is that the shape of the resolution function of the instrument can take any form and still allow a ΔE_L value to be extracted.

The resolution function is now represented as a function of energy by N(E). Folding of this distribution with a Lorentzian energy distribution then gives an energy distribution:

$$T(E) = \int_{\infty}^{\infty} L(E-E') N(E') dE' \qquad [2]$$

where

$$L(E-E') = \frac{\Delta E_L/2}{(\Delta E_L/2)^2 + (E-E')^2} \qquad [3]$$

Putting equation [2] in a form suitable for computer calculation we have, as a time of flight distribution

$$T_j(E) = \sum_{i=NS}^{NF} \frac{(\Delta E_L/2) \times N_i(E)}{(\Delta E_L/2)^2 + (E_i - E_j)^2} \qquad [4]$$

where Ni(E) is the value of the resolution function as a time distribution in terms of counts/channel, for the time of flight channel number i and similarly for Tj(E) the function produced after Ni(E) has been convoluted with the Lorentzian. NS and NF are time of flight channel numbers, chosen symmetrically about i_o, the channel number corresponding to the incident energy E_o such that (NF-NS) $\geqslant 6\Delta E_R$ where ΔE_R is the resolution function width measured in terms of channel numbers. This criterion ensures that the Tj(E) values obtained from the above integration are sufficiently accurate, for all practical purposes, in representing the complete integration of equation [2].

The time of flight distribution Tj(E) is calculated and plotted by FOLD for a series of ΔE_L values, as a function of channel number j. In addition Tj(E) is converted into an energy distribution TEj(E) where

$$TE_j(E) = T_j(E) \times j^3 \qquad [5]$$

which is also plotted as a function of channel number j.

Strictly, the resolution function Ni(E) in equation [4] should first be converted to scattering law form by multiplication with $(i^4/io) \times \exp(-\beta i/2)$

where
$$\beta_i = (E_i - E_o)/kT \qquad [6]$$

is the energy transfer for channel i in units of kT. The final distribution Tj(E) will then be in scattering law form which has to be multiplied by $(io/j^4) \times \exp(-\beta i/2)$ for reconversion to a time of flight distribution.

Inclusion of the above factors however, leaves the widths of the functions unchanged and they have therefore been omitted. In addition the <u>K</u> dependence of the scattering law of the sample, through the Debye-Waller factor exp(-2W), is omitted in this program. For elastic peaks with wavelength resolutions better than 15% the variation of exp(-2W) over the peaks may be considered negligible.

3. Program Description.

The program is listed in the Appendix. Most of the variables have comment labels, and will not be discussed further. The data input, with the necessary format is as follows:

CARD 1: (TITLE (I), I = 1,18) (18A4)

This is the title card which is printed out on the first line of the output.

CARDS 2 - 20: (NG(I), I = 1,300) (16I5)

These integer values represent the resolution of the apparatus at the incident energy E_0, as a function of time of flight channel number i and correspond to the variable Ni(E) of equation /4/. Where the resolution function is zero, blanks may be used to fill in the data.

CARD 21: IBAR, CHWD, FPL (I5,2F10.6)

IBAR is the channel number io corresponding to the incident energy E_0. CHWD is the time analyser channel width in μsec. FPL is the sample-detector flight path length in metres.

CARD 22: NS, NF (2I5)

These are the channel numbers defining the limits of the numerical integration of equation /4/ discussed in section 2.

CARD 23: DELTAE (FIO.6)

DELTAE is the width of the Lorentzian function used in equation /4/ and is given in eV. As many DELTAE values as required may be fed in on subsequent cards.

CARD 23 + N: 0.2 (F10.6)

N is the total number of cards being used to feed in separate DELTAE values. This final data card acts only as a switch to stop the program.

On output the program prints all the above input parameters together with the incident neutron energy and the corresponding wavelength and reciprocal velocity. Using the plotting routine GRAPH, (5), plots are given of the resolution function and the final Lorentzian broadened function, as both time of flight and energy distributions, between channel numbers NS and NF, The plotted functions are all normalized to unity at maximum intensity and are also printed in a normalized format. The reciprocal velocity in μsec/m and energy in meV corresponding to the respective channel numbers are printed at the end of the program for reference.

The widths of the Lorentzian broadened functions are calculated, in channel numbers, by linear interpolation at the half height positions of the peaks, from the time of flight distributions. These widths, together with the corresponding values in meV, are listed in the print out.

Typical FOLD output for a single ΔE_L value is shown in the Appendix. This required 0.6 mins for execution.

4. The Calibration Curve.

A few typical Lorentzian broadened resolution curves computed by FOLD are given in Fig. 1 for three different ΔE_L values, on a time of flight scale. The input spectrum in this case was chosen to be a perfect Gaussian with an incident energy of 5.24 meV and a resolution of 5.25% in wavelength. The channel width and flight path taken were those currently used on the Double Chopper facility on ISPRA 1 and are 8 usec and 1.53 m respectively.

Fig. 2 shows a few points, calculated by FOLD, representing the widths ΔE_{calc} of a few typical broadened curves as a function of ΔE_L for this Gaussian resolution spectrum. To test the procedure, these points have been compared with a calibration curve, dashed line, obtained from tabulated convolutions of Lorentzian and Gaussian functions [6] using the same Gaussian width as above. Both scales on the graph are given in meV.

Agreement is seen to be good, over the range of broadenings ΔE_L shown, for this particular case of a Gaussian input function. Hence it can be taken that FOLD will enable reliable ΔE_L values to be obtained, using any arbitrary shaped resolution function.

Fig. 3 illustrates two typical calibration curves for the double chopper facility for two different incident energies of 8.6 meV and 5.2 meV, both with resolutions of 7% in wavelength. Both the Lorentzian and the calculated widths are quoted in meV. The actual resolution functions for these two energies were obtained from vanadium spectra.

Finally it should be noted that the FOLD program may be used quite generally to obtain calibration curves for quasi-elastic scattering from any time of flight apparatus. There is no upper limit on the incident energy which can be used by the program. The lower limit on the incident energy is determined by the number of channels available for the input resolution function. In the present program 300 channels are used but this number can easily be extended if required.

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   HENDRICKSON, J.K., WAPD. SR-506 (1954).

Fig. 1 - LORENTZIAN BROADENED RESOLUTION CURVES ON A TIME OF FLIGHT SCALE

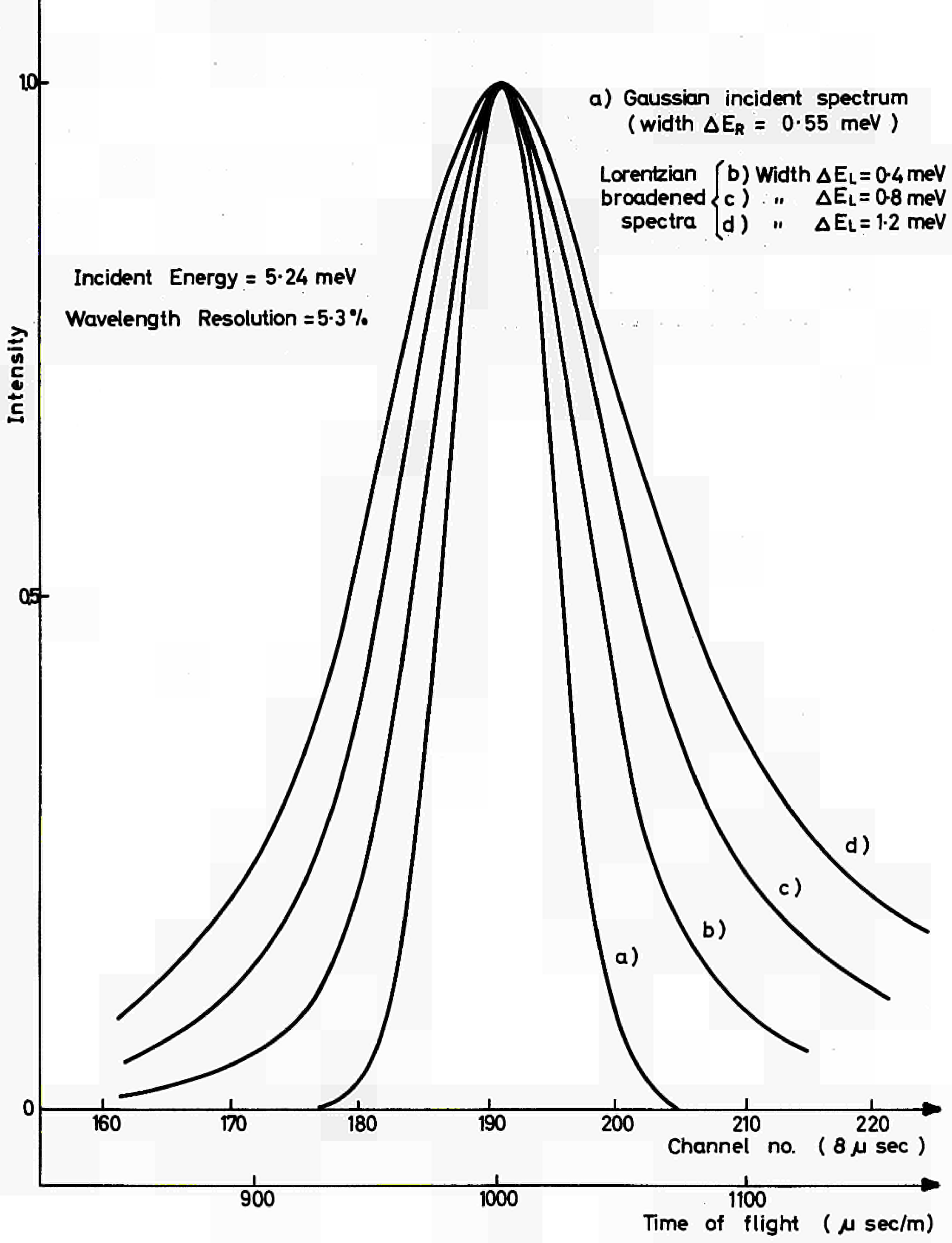


Fig. 2 – COMPARISON OF CALIBRATION OBTAINED FROM FOLD FOR A LORENTZIAN BROADENED GAUSSIAN WITH A TABULATED CALIBRATION CURVE

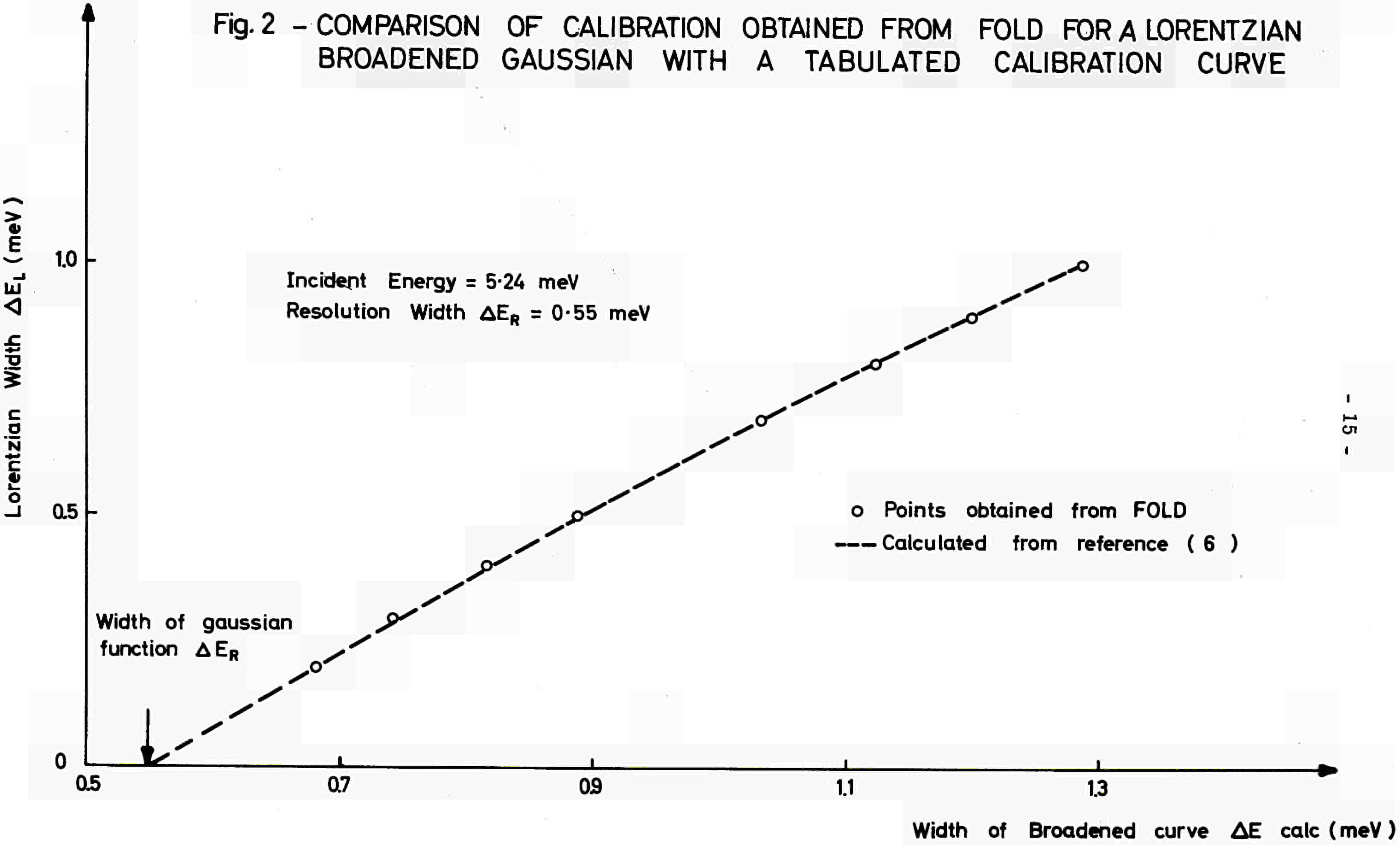
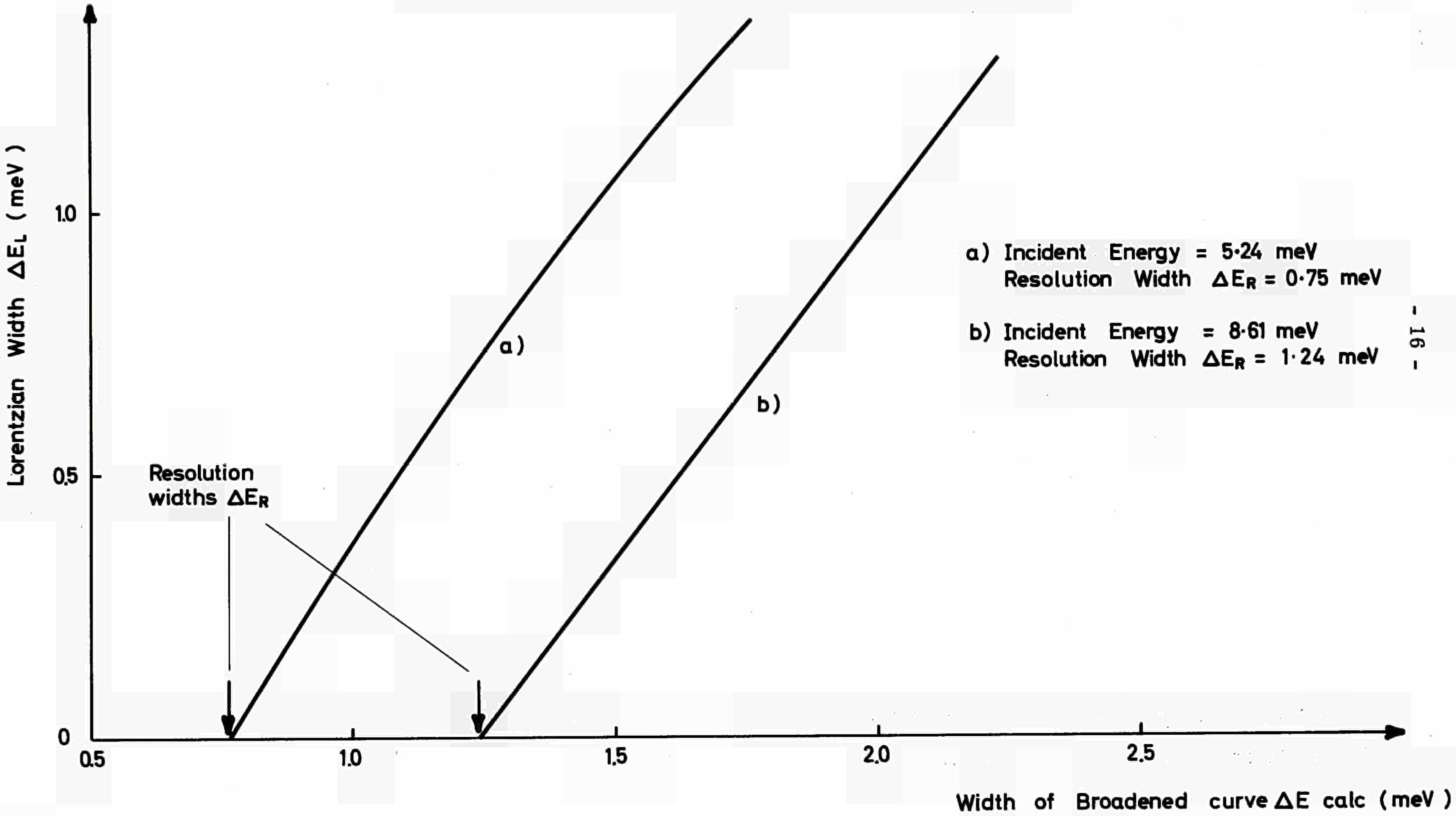


Fig. 3 - TYPICAL QUASI ELASTIC CALIBRATION CURVES FOR THE ISPRA 1 DOUBLE CHOPPER FACILITY



APPENDIX

PROGRAM LISTING AND TYPICAL OUTPUT DATA.

```
                 C      QUASI ELASTIC NEUTRON SCATTERING CALIBRATION PROGRAM
                 C
                 C      THIS PROGRAM CALCULATES THE BROADENING OF THE INCIDENT SPECTRUM
                 C      NG(I) WHEN CONVOLUTED WITH A LORENTZIAN SCATTERING LAW S(Q,W)  OF
                 C      ENERGY WIDTH AT HALF HEIGHT OF DELTAE (MEV)
                 C
0001                    DIMENSION NG(300),G(300),H(300),DEL(300,200),B(300),T(300),E(300),
                       1TITLE(18),TFMM(300),GE(300),TE(300)
0002                    CALL INTCTR (180)
                 C
0003                    READ (5,102)  (TITLE(I),I=1,18)
                 C      READ IN THE INCIDENT SPECTRUM AS A FUNCTION OF CHANNEL NUMBER
0004                    READ (5,107) (NG(I),I=1,300)
0005                    READ (5,106) IBAR,CHWD,FPL
                 C      IBAR IS THE MEAN CHANNEL NO. OF INCIDENT SPECTRUM
                 C      CHWD IS THE CHANNEL WIDTH (MICROSEC)
                 C      FPL  IS THE FLIGHT PATH LENGTH  IN  METRES
0006                    READ (5,132) NS,NF
0007                    READ (5,130) DELTAE
                 C      DELTAE IS THE FULL WIDTH AT HALF HEIGHT OF THE LORENTZIAN FUNCTION
                 C
0008                    XBAR=IBAR
0009
0010                    B1=10.0*FPL/(CHWD*XBAR)
0011                    TAUO=10.0/B1
                 C      TAUO  IS THE AVERAGE INCIDENT RECIPROCAL VELOCITY (MICROSEC/METRE)
0012                    WAVLO=0.03956/B1
                 C      WAVLO IS THE AVERAGE INCIDENT WAVELENGTH  (ANGSTROMS)
0013                    B1=B1**2
0014                    E0=52270.*B1
                 C      E0     IS THE AVERAGE INCIDENT ENERGY (MEV)
                 C
0015                    DO 3 I=1,300
0016                    XI=I
0017                    A=10.0*FPL/(CHWD*XI)
0018                    TFMM(I)=10./A
                 C      TFMM(I) IS THE RECIPROCAL VELOCITY OF A NEUTRON DETECTED IN CH NO
                 C       I  RELATIVE TO THE INCIDENT CHANNEL NUMBER IBAR
0019                    G(I)=NG(I)
0020                    GE(I)=G(I)*I**3
                 C      GE(I) IS THE INCIDENT SPECTRUM ON AN ENERGY SCALE
0021                    XMAT=NG(I)
0022                    H(I)=XMAT
0023                  3 CONTINUE
                 C
0024                    WRITE (6,103) (TITLE(I),I=1,18)
0025                    WRITE (6,106) IBAR,CHWD,E0,TAUO,WAVLO
0026                    WRITE (6,133) NS,NF
```

```
 0027                   WRITE (6,125)
 0028                   WRITE (6,136) (G(I),I=1,300)
             C
 0029                 6 DO 4 I=1,300
 0030                   XI=I
 0031                   XI=XI*0.1*CHND/FPL
 0032                   E1=52.25/XI**2
             C          E1 IS IN EV
 0033                   DO 5 J=NS,NF
 0034                   JJ=J-NS+1
 0035                   XJ=J
 0036                   XJ=XJ*0.1*CHND/FPL
 0037                   E2=52.25/XJ**2
             C          E2 IS IN EV
 0038                   DEL (I,JJ)=(E1-E2)**2
 0039                 5 CONTINUE
 0040                 4 CONTINUE
             C
 0041                   WRITE (6,104)  DELTAE
 0042                   DELTAE=DELTAE/2.0
             C
 0043                   DO 7 J=1,300
 0044                   DO 8 K=NS,NF
 0045                   KK=K-NS+1
 0046                   XK=K
 0047                   X=(DELTAE)/(DEL(J,KK)+(DELTAE)**2)
 0048                   X=X*H(K)
 0049                   DEL (J,KK)=X
 0050                 8 CONTINUE
 0051                 7 CONTINUE
             C
 0052                   DO 9 J=1,300
 0053                   B(J)=0.
 0054                   DO 10 K=NS,NF
 0055                   KK=K-NS+1
 0056                   B(J)=B(J)+DEL(J,KK)
 0057                10 CONTINUE
 0058                   XJ=J
 0059                   T(J)=B(J)
 0060                   TE(J)=T(J)*J**3
             C          TE(J) IS IS THE BROADENED SPECTRUM ON AN ENERGY SCALE
 0061                   E(J)=(52.25/XJ**2)
 0062                   E(J)=E(J)*(10.0*FPL/CHND)**2
 0063                 9 CONTINUE
             C
 0064                   SOE=0.
 0065                   TTE=0.
 0066                   SG=0.
```

```
 0067                 Y=0.
               C
 0068                 DO 11 I=1,300
 0069                 GGE=AMAX1(GGE,GE(I))
 0070                 TTE=AMAX1(TTE,TE(I))
 0071                 GG=AMAX1 (GG,G(I))
 0072                 Y=AMAX1 (Y,T(I))
 0073              11 CONTINUE
               C
 0074                 DO 12 I=1,300
 0075                 GE(I)=GE(I)/GGE
 0076                 TE(I)=TE(I)/TTE
 0077                 G(I)=G(I)/GG
 0078                 T(I)=T(I)/Y
 0079              12 CONTINUE
               C
 0080                 WRITE (6,125)
 0081                 WRITE (6,126) (T(I),I=1,300)
 0082                 WRITE (6,127)
 0083                 WRITE (6,126) (TE(I),I=1,300)
               C
 0084                 NP=NF-NS
               C      PLOT INCIDENT AND BROADENED SPECTRA ON TIME OF FLIGHT SCALE
               C      (ABSCISSAE IS IN MICROSEC/METRE)
 0085                 WRITE (6,140)
 0086                 CALL GRAPH (2,NP,0.,0,-1,-1,TFMM(NS),T(NS),G(NS),Y3)
               C      PLOT INCIDENT AND BROADENED SPECTRA ON ENERGY SCALE
               C      (ABSCISSAE IS IN  EV)
 0087                 WRITE (6,141)
 0088                 CALL GRAPH (2,NP,0.,0,-1,-1,E(NS),TE(NS),GE(NS),Y3)
               C
               C      LINEAR INTERPOLATION AT HALF HEIGHT POSITIONS OF FINAL PEAK
 0089                 DO 13 I=NS,IBAR
 0090                 IF (T(I).GT.0.5) GO TO 21
 0091              13 CONTINUE
               C
 0092              21 IMIL=I-1
               C
 0093                 IF ((T(I)-0.5).GT.(0.5-T(IMIL))) IMIDL=IMIL
 0094                 IF ((T(I)-0.5).LT.(0.5-T(IMIL))) IMIDL=I
               C
 0095                 IPLUSL=IMIDL+1
 0096                 IMINL=IMIDL-1
 0097                 TANGL=(T(IPLUSL)-T(IMINL))/2.0
 0098                 TMIDL=(0.5-T(IMINL))/TANGL
 0099                 FIMINL=IMINL
 0100                 TMIDL=TMIDL+FIMINL
               C
```

```
0101               DO 14 I=IBAR,NF
0102               IF (T(I).LT.0.5) GO TO 22
0103            14 CONTINUE
             C
0104            22 IM1R=I-1
             C
0105               IF ((0.5-T(I)).GT.(T(IM1R)-0.5)) IMIDR=IM1R
0106               IF ((0.5-T(I)).LT.(T(IM1R)-0.5)) IMIDR=I
             C
0107               IPLUSR=IMIDR+1
0108               IMINR=IMIDR-1
0109               TANGR=(T(IMINR)-T(IPLUSR))/2.0
0110               TMIDR=(T(IMINR)-0.5)/TANGR
0111               FIMINR=IMINR
0112               TMIDR=TMIDR+FIMINR
0113               WIDTH=TMIDR-TMIDL
             C     END OF LINEAR INTERPOLATION ROUTINE
             C
0114               EL=52.23/TMIDL**2
0115               EL=EL*(10.*FPL/CHWD)**2
0116               ER=52.23/TMIDR**2
0117               ER=ER*(10.*FPL/CHWD)**2
0118               EWIDTH=1000.*(EL-ER)
0119               DELTAE=DELTAE*2000.
             C
0120               WRITE (6,110) EWIDTH,DELTAE
             C     EWIDTH IS WIDTH OF BROADENED PEAK IN MEV
0121               WRITE (6,109) WIDTH
             C     WIDTH  IS WIDTH OF BROADENED PEAK IN CHANNEL NUMBERS
             C
             C     READ IN NEXT LORENTZIAN WIDTH DELTAE  (EV)
0122               READ (5,130) DELTAE
             C
0123               IF (DELTAE-2.) 6,23,23
0124            23 WRITE (6,142)
             C
0125               DO 15 J=1,300
0126               WRITE (6,143) (J,TFW(J),E(J))
0127            15 CONTINUE
             C
0128           102 FORMAT (18A4)
0129           103 FORMAT (1H1,18A4)
0130           104 FORMAT (1H1,10X,50H F.W.H.M. OF THE LORENTZIAN FUNCTION IS DELTAE
                  1 = ,F10.6,3X,4H(EV))
0131           106 FORMAT (I5,2F10.6)
0132           107 FORMAT (16I5)
0133           108 FORMAT (///10X,24HINCIDENT CHANNEL NUMBER=,I7,2X,14HCHANNEL WIDTH=
                  1,F4.1,2X,8HMICROSEC,3X,16HINCIDENT ENERGY=,F7.4,2X,3HMEV,//10X,15H
```

```
                      2TIME OF FLIGHT=,2X,F7.2,2X,10HMICROSEC/M,5X,11HWAVELENGTH=,F8.4,2X
                      3,9HANGSTROMS)
0134              109 FORMAT (///36H WIDTH OF THE BROADENED FUNCTION IS ,3X,F10.3,3X,15H
                      1CHANNEL NUMBERS///)
0135              110 FORMAT (///39H ENERGY WIDTH OF BROADENED FUNCTION IS ,F10.6,3X,3HM
                      1EV,3X,34HCORRESPONDING LORENTZIAN WIDTH WAS,3X,F10.6,3X,3HMEV////)
0136              125 FORMAT (///24X,18H INCIDENT SPECTRUM,//)
0137              126 FORMAT (10(3X,F7.4))
0138              127 FORMAT (///10X,27HENERGY SPECTRUM...BROADENED//)
0139              128 FORMAT (///10X,35HTIME OF FLIGHT SPECTRUM...BROADENED//)
0140              130 FORMAT (F10.6)
0141              132 FORMAT (2I5)
0142              136 FORMAT (10(2X,F8.2))
0143              138 FORMAT (/10X,40HTRUNCATION TAKEN BETWEEN CHANNEL NUMBERS,I7,2X,3HA
                      1ND,I7//)
0144              140 FORMAT (///10X,62HPLOT OF INCIDENT AND BROADENED SPECTRA ON TIME O
                      1F FLIGHT SCALE,//20X,32H(ABSCISSAE IS IN MICROSEC/METRE)//)
0145              141 FORMAT (///10X,57HPLOT OF INCIDENT AND BROADENED SPECTRA ON AN ENE
                      1RGY SCALE,//20X,21H(ABSCISSAE IS IN EV )//)
0146              142 FORMAT (1H1,15X,11HCHANNEL NO.,10X,27HTIME OF FLIGHT (MICROSEC/M),
                      111X,12HENERGY (EV) //)
0147              143 FORMAT (13X,I5,19X,F10.3,19X,F13.6)
                C
0148                  STOP
0149                  END
```

```
QUASI ELASTIC SCATTERING CALIBRATION FOR DOUBLE CHOPPER DATA

 INCIDENT CHANNEL NUMBER=    191  CHANNEL WIDTH= 8.0  MICROSEC   INCIDENT ENERGY= 5.2367  MEV
 TIME OF FLIGHT=   998.69  MICROSEC/M     WAVELENGTH=  3.9528  ANGSTROMS
 TRUNCATION TAKEN BETWEEN CHANNEL NUMBERS     151  AND    231


                  INCIDENT SPECTRUM

    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0         59.00        73.00       109.00       179.00       227.00       296.00       404.00       436.00       519.00
  730.00       907.00      1040.00      1190.00      1460.00      1790.00      1920.00      1980.00      2120.00      2160.00
 2170.00      2070.00      1950.00      1790.00      1520.00      1350.00      1120.00       852.00       655.00       489.00
  338.00       219.00       120.00        79.00        47.00        31.00         0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
    0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0          0.0
```

```
              F.W.H.M. OF THE LORENTZIAN FUNCTION IS DELTAE  =   0.000500   (EV)

       TIME OF FLIGHT SPECTRUM...BROADENED

 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0001     0.0001     0.0001     0.0001     0.0001     0.0001     0.0001     0.0001     0.0001     0.0001
 0.0001     0.0001     0.0001     0.0001     0.0001     0.0001     0.0002     0.0002     0.0002     0.0002
 0.0002     0.0002     0.0002     0.0002     0.0002     0.0003     0.0003     0.0003     0.0003     0.0003
 0.0004     0.0004     0.0004     0.0004     0.0004     0.0005     0.0005     0.0005     0.0006     0.0006
 0.0006     0.0007     0.0007     0.0007     0.0008     0.0008     0.0009     0.0009     0.0010     0.0010
 0.0011     0.0011     0.0012     0.0013     0.0013     0.0014     0.0015     0.0016     0.0017     0.0018
 0.0019     0.0020     0.0021     0.0022     0.0023     0.0025     0.0026     0.0028     0.0029     0.0031
 0.0033     0.0035     0.0037     0.0040     0.0042     0.0045     0.0048     0.0051     0.0054     0.0058
 0.0061     0.0066     0.0070     0.0075     0.0080     0.0086     0.0092     0.0099     0.0106     0.0114
 0.0123     0.0135     0.0144     0.0156     0.0159     0.0183     0.0200     0.0218     0.0239     0.0263
 0.0269     0.0320     0.0355     0.0396     0.0445     0.0502     0.0572     0.0656     0.0761     0.0892
 0.1056     0.1257     0.1496     0.1778     0.2104     0.2475     0.2898     0.3372     0.3902     0.4490
 0.5133     0.5816     0.6550     0.7249     0.7947     0.8589     0.9140     0.9576     0.9862     1.0000
 0.9979     0.9800     0.9475     0.9018     0.8459     0.7825     0.7145     0.6447     0.5757     0.5097
 0.4482     0.3926     0.3456     0.2997     0.2623     0.2304     0.2034     0.1806     0.1613     0.1451
 0.1513     0.1195     0.1094     0.1007     0.0931     0.0864     0.0805     0.0755     0.0707     0.0665
 0.0628     0.0594     0.0563     0.0535     0.0510     0.0486     0.0465     0.0445     0.0427     0.0410
 0.0394     0.0379     0.0366     0.0353     0.0341     0.0350     0.0319     0.0309     0.0300     0.0291
 0.0263     0.0275     0.0266     0.0261     0.0254     0.0248     0.0242     0.0236     0.0231     0.0225
 0.0220     0.0218     0.0211     0.0207     0.0203     0.0199     0.0195     0.0191     0.0187     0.0184
 0.0181     0.0178     0.0175     0.0172     0.0169     0.0166     0.0164     0.0161     0.0159     0.0156
 0.0154     0.0152     0.0150     0.0148     0.0140     0.0144     0.0142     0.0140     0.0138     0.0136
 0.0135     0.0133     0.0132     0.0130     0.0129     0.0127     0.0126     0.0124     0.0123     0.0122
 0.0120     0.0119     0.0118     0.0117     0.0116     0.0115     0.0113     0.0112     0.0111     0.0110

       ENERGY SPECTRUM...BROADENED

 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000     0.0000
 0.0000     0.0000     0.0000     0.0000     0.0001     0.0001     0.0001     0.0001     0.0001     0.0001
 0.0001     0.0001     0.0001     0.0001     0.0001     0.0001     0.0002     0.0002     0.0002     0.0002
 0.0002     0.0002     0.0002     0.0003     0.0003     0.0003     0.0003     0.0004     0.0004     0.0004
 0.0005     0.0005     0.0006     0.0006     0.0007     0.0007     0.0008     0.0008     0.0009     0.0010
 0.0011     0.0012     0.0013     0.0014     0.0015     0.0016     0.0018     0.0019     0.0021     0.0023
 0.0025     0.0027     0.0029     0.0032     0.0035     0.0036     0.0042     0.0046     0.0051     0.0055
 0.0061     0.0067     0.0074     0.0082     0.0090     0.0100     0.0111     0.0124     0.0138     0.0155
 0.0174     0.0193     0.0221     0.0251     0.0287     0.0330     0.0383     0.0447     0.0523     0.0630
 0.0759     0.0920     0.1114     0.1347     0.1621     0.1942     0.2311     0.2755     0.3219     0.3766
```

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  0.4377      0.5044      0.5756      0.6494      0.7237      0.7949      0.8596      0.9146      0.9575      0.9865
  1.0000      0.9976      0.9795      0.9470      0.9021      0.8474      0.7856      0.7197      0.6525      0.5865
  0.5236      0.4054      0.4127      0.3659      0.3250      0.2897      0.2595      0.2337      0.2118      0.1932
  0.1773      0.1636      0.1520      0.1419      0.1330      0.1252      0.1183      0.1122      0.1067      0.1018
  0.0974      0.0934      0.0898      0.0865      0.0835      0.0807      0.0782      0.0759      0.0737      0.0717
  0.0699      0.0681      0.0665      0.0650      0.0637      0.0624      0.0611      0.0600      0.0589      0.0579
  0.0570      0.0561      0.0553      0.0545      0.0538      0.0531      0.0524      0.0518      0.0512      0.0506
  0.0501      0.0496      0.0492      0.0487      0.0483      0.0479      0.0475      0.0472      0.0468      0.0465
  0.0462      0.0460      0.0457      0.0454      0.0452      0.0450      0.0448      0.0446      0.0444      0.0442
  0.0441      0.0439      0.0436      0.0437      0.0435      0.0434      0.0433      0.0432      0.0431      0.0431
  0.0430      0.0429      0.0429      0.0428      0.0428      0.0428      0.0427      0.0427      0.0427      0.0427
  0.0427      0.0427      0.0427      0.0427      0.0427      0.0427      0.0428      0.0428      0.0428      0.0429

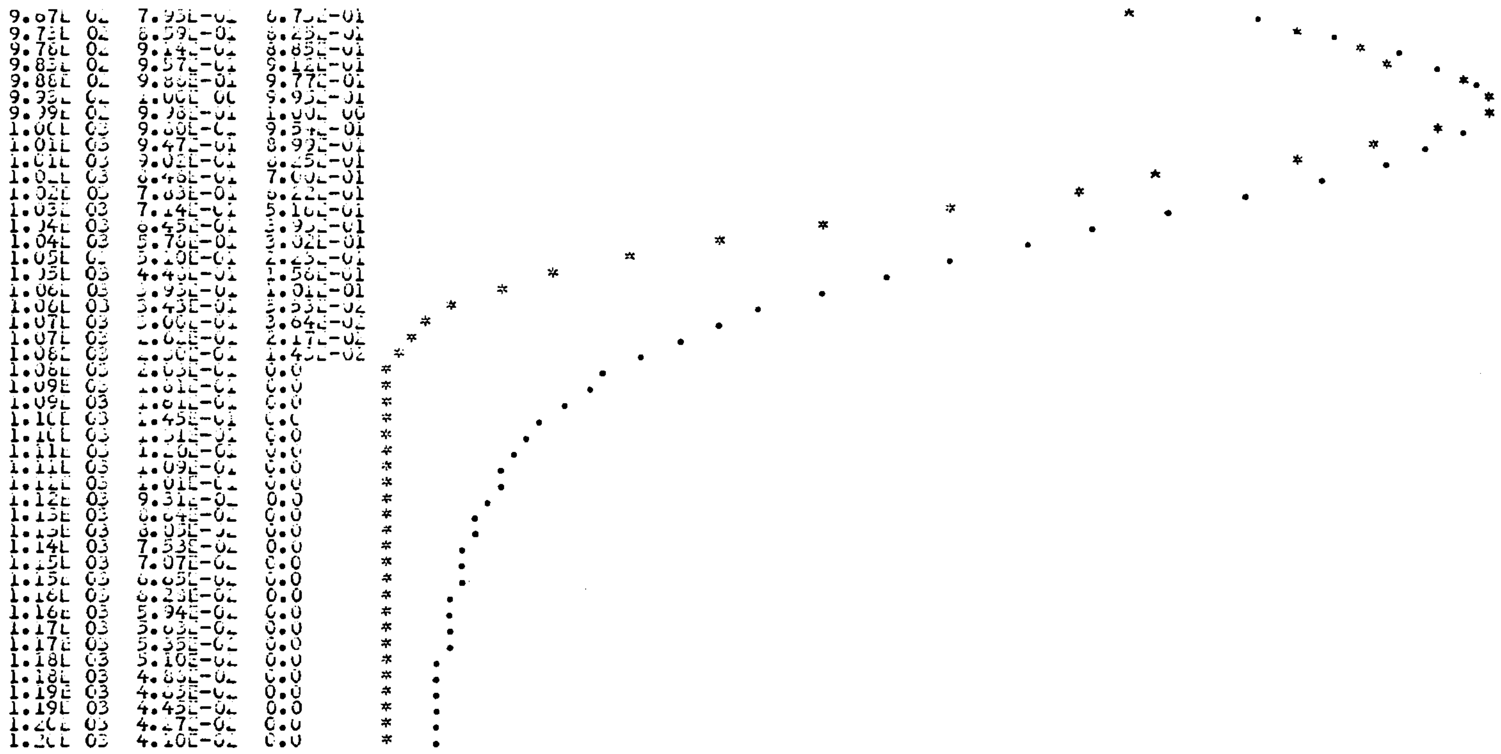

         PLOT OF INCIDENT AND BROADENED SPECTRA ON TIME OF FLIGHT SCALE
                     (ABSCISSAE IS IN MICROSEC/METRE)

NORMAL SCALE IN ABSCISSA

NORMAL SCALE IN ORDINATE

INFORMATIONS ON ORDINATE SCALE - LEFT SCALING POINT =    0.0       =INTERVAL BETWEEN SCALING POINTS=   1.000E-01
   X         Y1 = .     Y2 = *     .         .         .         .         .         .         .         .         .         .         .

 7.90E 02    1.23E-02   0.0        *.
 7.95E 02    1.33E-02   0.0        *.
 8.00E 02    1.44E-02   0.0        *.
 8.05E 02    1.56E-02   0.0        *.
 8.10E 02    1.69E-02   0.0        *.
 8.16E 02    1.83E-02   0.0        * .
 8.21E 02    2.00E-02   0.0        * .
 8.26E 02    2.18E-02   0.0        * .
 8.31E 02    2.39E-02   0.0        * .
 8.37E 02    2.63E-02   0.0        * .
 8.42E 02    2.89E-02   0.0        * .
 8.47E 02    3.20E-02   0.0        *  .
 8.52E 02    3.55E-02   0.0        *  .
 8.58E 02    3.96E-02   0.0        *  .
 8.63E 02    4.45E-02   0.0        *   .
 8.68E 02    5.02E-02   0.0        *   .
 8.73E 02    5.72E-02   0.0        *    .
 8.78E 02    6.56E-02   0.0        *     .
 8.84E 02    7.61E-02   0.0        *      .
 8.89E 02    8.92E-02   0.0        *       .
 8.94E 02    1.06E-01   0.0        *         .
 8.99E 02    1.26E-01   2.72E-02     *         .
 9.05E 02    1.50E-01   3.59E-02      *           .
 9.10E 02    1.78E-01   5.02E-02        *           .
 9.15E 02    2.10E-01   8.25E-02           *            .
 9.20E 02    2.48E-01   1.05E-01             *             .
 9.25E 02    2.90E-01   1.36E-01                *               .
 9.31E 02    3.37E-01   1.86E-01                     *              .
 9.36E 02    3.90E-01   2.01E-01                       *                  .
 9.41E 02    4.49E-01   2.39E-01                          *                    .
 9.46E 02    5.13E-01   3.36E-01                                    *                 .
 9.52E 02    5.82E-01   4.16E-01                                            *                .
 9.57E 02    6.55E-01   4.79E-01                                                  *                 .
 9.62E 02    7.25E-01   5.43E-01                                                         *                 .
```



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9.67E 02   7.95E-01   6.75E-01
9.73E 02   8.59E-01   8.25E-01
9.78E 02   9.14E-01   8.85E-01
9.83E 02   9.57E-01   9.12E-01
9.88E 02   9.88E-01   9.77E-01
9.93E 02   1.00E 00   9.93E-01
9.99E 02   9.98E-01   1.00E 00
1.00E 03   9.80E-01   9.54E-01
1.01E 03   9.47E-01   8.99E-01
1.01E 03   9.02E-01   8.25E-01
1.02E 03   8.46E-01   7.00E-01
1.02E 03   7.83E-01   6.22E-01
1.03E 03   7.14E-01   5.16E-01
1.04E 03   6.45E-01   3.93E-01
1.04E 03   5.76E-01   3.02E-01
1.05E 03   5.10E-01   2.25E-01
1.05E 03   4.46E-01   1.56E-01
1.06E 03   3.93E-01   1.01E-01
1.06E 03   3.43E-01   5.53E-02
1.07E 03   3.00E-01   3.64E-02
1.07E 03   2.62E-01   2.17E-02
1.08E 03   2.30E-01   1.43E-02
1.08E 03   2.03E-01   0.0
1.09E 03   1.81E-01   0.0
1.09E 03   1.61E-01   0.0
1.10E 03   1.45E-01   0.0
1.10E 03   1.31E-01   0.0
1.11E 03   1.20E-01   0.0
1.11E 03   1.09E-01   0.0
1.12E 03   1.01E-01   0.0
1.12E 03   9.31E-02   0.0
1.13E 03   8.64E-02   0.0
1.13E 03   8.05E-02   0.0
1.14E 03   7.53E-02   0.0
1.15E 03   7.07E-02   0.0
1.15E 03   6.65E-02   0.0
1.16E 03   6.23E-02   0.0
1.16E 03   5.94E-02   0.0
1.17E 03   5.63E-02   0.0
1.17E 03   5.35E-02   0.0
1.18E 03   5.10E-02   0.0
1.18E 03   4.85E-02   0.0
1.19E 03   4.65E-02   0.0
1.19E 03   4.45E-02   0.0
1.20E 03   4.27E-02   0.0
1.20E 03   4.10E-02   0.0
```
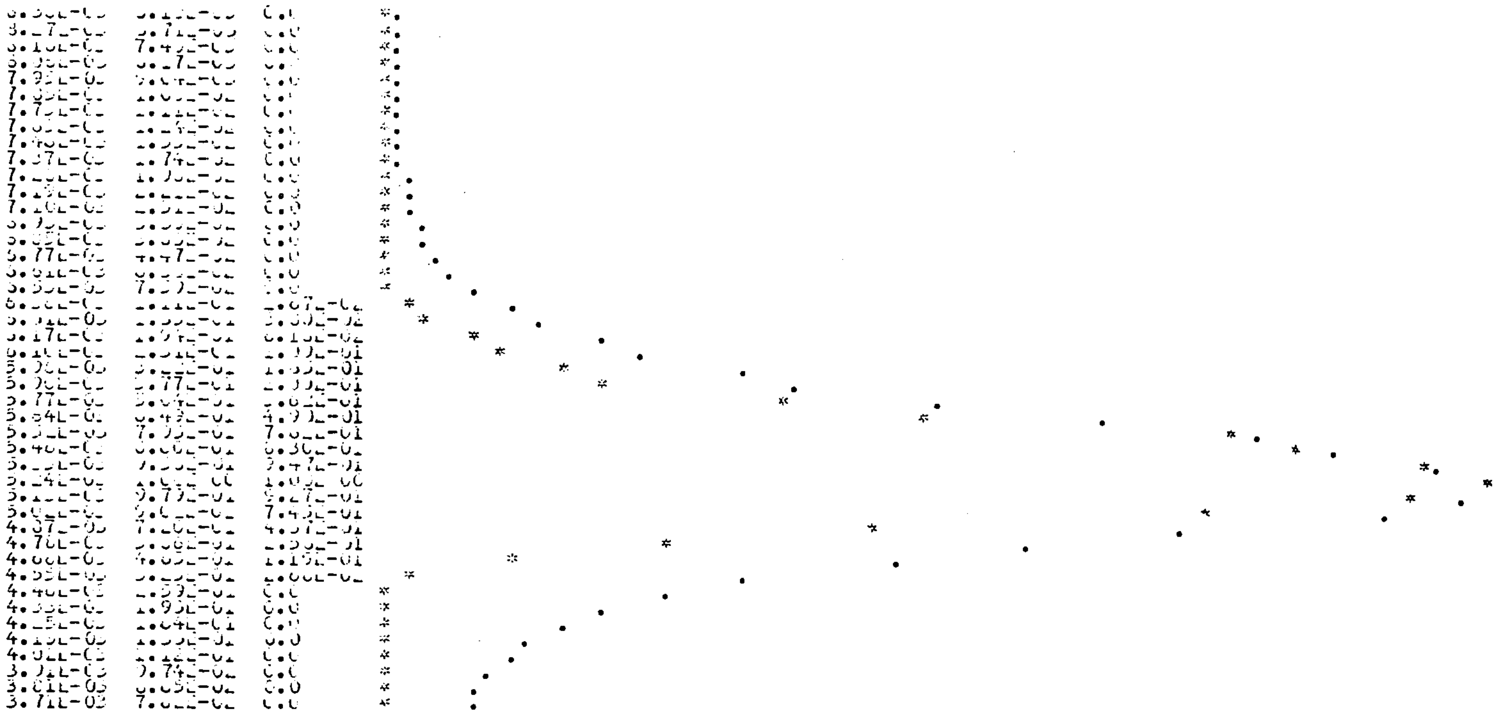

```
        PLOT OF INCIDENT AND BROADENED SPECTRA ON AN ENERGY SCALE
                 (ABSCISSAE IS IN EV )

NORMAL SCALE IN ABSCISSA
NORMAL SCALE IN ORDINATE
INFORMATION ON ORDINATE SCALE - LEFT SCALING POINT =    0.0       =INTERVAL BETWEEN SCALING POINTS=   1.000E-01
  X        Y1 = .    Y2 = *   .        .        .        .        .        .        .        .        .        .
```



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ENERGY WIDTH OF BROADENED FUNCTION IS    1.079267    MEV    CORRESPONDING LORENTZIAN WIDTH WAS      0.500009    MEV



WIDTH OF THE BROADENED FUNCTION IS          19.421    CHANNEL NUMBERS
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CHANNEL NO.          TIME OF FLIGHT (MICROSEC/M)          ENERGY (EV)

     1                        5.229                        191.039230
     2                       10.458                         47.759796
     3                       15.686                         21.226578
     4                       20.915                         11.939952
     5                       26.144                          7.641566
     6                       31.373                          5.306643
     7                       36.601                          3.898759
     8                       41.830                          2.984987
     9                       47.059                          2.358508
    10                       52.288                          1.910392
    11                       57.516                          1.578836
    12                       62.745                          1.326661
    13                       67.974                          1.130409
    14                       73.203                          0.974690
    15                       78.431                          0.849063
    16                       83.660                          0.746247
    17                       88.889                          0.661035
    18                       94.118                          0.589627
    19                       99.346                          0.529194
    20                      104.575                          0.477598
    21                      109.804                          0.433195
    22                      115.033                          0.394709
    23                      120.262                          0.361133
    24                      125.490                          0.331665
    25                      130.719                          0.305663
    26                      135.948                          0.282602
    27                      141.177                          0.262056
    28                      146.405                          0.243672
    29                      151.634                          0.227157
    30                      156.863                          0.212266
    31                      162.092                          0.198792
    32                      167.320                          0.186562
    33                      172.549                          0.175426
    34                      177.778                          0.165259
    35                      183.007                          0.155950
    36                      188.235                          0.147407
    37                      193.464                          0.139547
    38                      198.693                          0.132299
    39                      203.922                          0.125601
    40                      209.150                          0.119399
    41                      214.379                          0.113646
    42                      219.608                          0.108299
    43                      224.837                          0.103320
    44                      230.065                          0.098677
    45                      235.294                          0.094340
    46                      240.523                          0.090283
    47                      245.752                          0.086482
    48                      250.980                          0.082916
    49                      256.209                          0.079566
    50                      261.438                          0.076416
    51                      266.667                          0.073448
    52                      271.895                          0.070651
    53                      277.124                          0.068010
    54                      282.353                          0.065514
    55                      287.582                          0.063153
    56                      292.810                          0.060918
    57                      298.039                          0.058799
    58                      303.268                          0.056789
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 59        308.497        0.054881
 60        313.725        0.053066
 61        318.954        0.051341
 62        324.183        0.049698
 63        329.412        0.048133
 64        334.640        0.046640
 65        339.869        0.045216
 66        345.098        0.043857
 67        350.327        0.042557
 68        355.555        0.041315
 69        360.784        0.040126
 70        366.013        0.038988
 71        371.242        0.037897
 72        376.470        0.036852
 73        381.699        0.035849
 74        386.928        0.034887
 75        392.157        0.033963
 76        397.385        0.033075
 77        402.614        0.032221
 78        407.843        0.031400
 79        413.072        0.030610
 80        418.301        0.029850
 81        423.529        0.029117
 82        428.758        0.028412
 83        433.987        0.027731
 84        439.216        0.027075
 85        444.444        0.026441
 86        449.673        0.025830
 87        454.902        0.025240
 88        460.131        0.024669
 89        465.359        0.024118
 90        470.588        0.023585
 91        475.817        0.023070
 92        481.046        0.022571
 93        486.274        0.022088
 94        491.503        0.021621
 95        496.732        0.021168
 96        501.961        0.020729
 97        507.189        0.020304
 98        512.418        0.019892
 99        517.647        0.019492
100        522.876        0.019104
101        528.104        0.018727
102        533.333        0.018362
103        538.562        0.018007
104        543.791        0.017663
105        549.020        0.017328
106        554.248        0.017002
107        559.477        0.016686
108        564.706        0.016379
109        569.935        0.016079
110        575.164        0.015788
111        580.392        0.015505
112        585.621        0.015230
113        590.850        0.014961
114        596.078        0.014700
115        601.307        0.014445
116        606.536        0.014197
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118        616.993        0.013720
119        622.222        0.013491
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125        653.595        0.012227
126        658.823        0.012033
127        664.052        0.011844
128        669.281        0.011660
129        674.510        0.011480
130        679.739        0.011304
131        684.967        0.011132
132        690.196        0.010964
133        695.425        0.010800
134        700.654        0.010639
135        705.883        0.010482
136        711.111        0.010329
137        716.340        0.010178
138        721.569        0.010031
139        726.798        0.009888
140        732.026        0.009747
141        737.255        0.009609
142        742.484        0.009474
143        747.713        0.009342
144        752.941        0.009213
145        758.170        0.009086
146        763.399        0.008962
147        768.627        0.008841
148        773.856        0.008722
149        779.085        0.008605
150        784.314        0.008491
151        789.543        0.008379
152        794.771        0.008269
153        800.000        0.008161
154        805.229        0.008055
155        810.458        0.007952
156        815.687        0.007850
157        820.915        0.007750
158        826.144        0.007653
159        831.373        0.007557
160        836.601        0.007462
161        841.830        0.007370
162        847.059        0.007279
163        852.288        0.007190
164        857.517        0.007103
165        862.745        0.007017
166        867.974        0.006933
167        873.203        0.006850
168        878.432        0.006769
169        883.660        0.006689
170        888.889        0.006610
171        894.118        0.006533
172        899.346        0.006458
173        904.575        0.006383
174        909.804        0.006310
175        915.033        0.006238
176        920.261        0.006167
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178        930.719        0.006030
179        935.948        0.005962
180        941.177        0.005896
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186	972.549	0.005522
187	977.778	0.005463
188	983.007	0.005405
189	988.236	0.005348
190	993.464	0.005292
191	998.693	0.005237
192	1003.922	0.005182
193	1009.150	0.005129
194	1014.379	0.005076
195	1019.608	0.005024
196	1024.837	0.004973
197	1030.066	0.004923
198	1035.294	0.004873
199	1040.523	0.004824
200	1045.752	0.004776
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204	1066.667	0.004591
205	1071.896	0.004546
206	1077.124	0.004502
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210	1098.040	0.004332
211	1103.268	0.004291
212	1108.497	0.004251
213	1113.726	0.004211
214	1118.955	0.004172
215	1124.183	0.004133
216	1129.412	0.004095
217	1134.641	0.004057
218	1139.870	0.004020
219	1145.098	0.003983
220	1150.327	0.003947
221	1155.556	0.003911
222	1160.785	0.003876
223	1166.013	0.003842
224	1171.242	0.003807
225	1176.471	0.003774
226	1181.700	0.003740
227	1186.929	0.003707
228	1192.157	0.003675
229	1197.386	0.003643
230	1202.615	0.003611
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232	1213.072	0.003549
233	1218.301	0.003519
234	1223.530	0.003489
235	1228.759	0.003459
236	1233.987	0.003430
237	1239.216	0.003401
238	1244.445	0.003373
239	1249.674	0.003344
240	1254.902	0.003317
241	1260.131	0.003289

242	1265.360	0.003262
243	1270.588	0.003235
244	1275.817	0.003209
245	1281.046	0.003183
246	1286.275	0.003157
247	1291.504	0.003131
248	1296.732	0.003106
249	1301.961	0.003081
250	1307.190	0.003057
251	1312.419	0.003032
252	1317.647	0.003008
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254	1328.105	0.002961
255	1333.334	0.002938
256	1338.562	0.002915
257	1343.791	0.002892
258	1349.020	0.002870
259	1354.249	0.002848
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261	1364.706	0.002804
262	1369.935	0.002783
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264	1380.393	0.002741
265	1385.621	0.002720
266	1390.850	0.002700
267	1396.079	0.002680
268	1401.307	0.002660
269	1406.537	0.002640
270	1411.765	0.002621
271	1416.994	0.002601
272	1422.223	0.002582
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274	1432.680	0.002545
275	1437.909	0.002526
276	1443.138	0.002508
277	1448.366	0.002490
278	1453.595	0.002472
279	1458.824	0.002454
280	1464.053	0.002437
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282	1474.510	0.002402
283	1479.739	0.002385
284	1484.968	0.002369
285	1490.197	0.002352
286	1495.425	0.002336
287	1500.655	0.002319
288	1505.883	0.002303
289	1511.112	0.002287
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291	1521.569	0.002256
292	1526.798	0.002241
293	1532.027	0.002225
294	1537.256	0.002210
295	1542.484	0.002195
296	1547.713	0.002180
297	1552.942	0.002166
298	1558.171	0.002151
299	1563.399	0.002137
300	1568.628	0.002123

To disseminate knowledge is to disseminate prosperity — I mean general prosperity and not individual riches — and with prosperity disappears the greater part of the evil which is our heritage from darker times.

Alfred Nobel

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