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A Least-Structure Unfolding Code

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A LEAST-STRUCTURE UNFOLDING CODE

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A. A. Robba and L. R. Veesser

ABSTRACT

A computer code has been written to solve integral equations of the first kind, subject to constraints on the structure of the solution. The code has been tested by unfolding measured neutron and gamma-ray spectra. The unfolding method, least-structure analysis, is described briefly, and a listing of the computer program is given.

I. INTRODUCTION

Many kinds of spectrometers have been used to detect neutrons in the energy range from a few hundred keV to several MeV. For neutrons that cannot be pulsed to allow time-of-flight measurements, one of the most useful is the proton recoil spectrometer. Extensive work has been done to determine the responses of organic scintillators to monoenergetic neutrons.^{1,2} However, to make such detectors useful as spectrometers, one must also solve the mathematical problem of unfolding the spectrum from the response functions and the measured detector yield. Although several computer programs have been written to unfold spectra, some of them are intended primarily for the relatively complicated problem of unfolding spectra with discrete components.^{3,4} Others do not give the spectrum directly, but

instead give uncertainty limits arising from a least-squares fit to the data, with the constraints that neither the spectrum nor the response functions can have negative components.^{5,6} The program described here was written to unfold smooth, continuous spectra using a method called "least-structure analysis."⁷⁻⁹

II. RESPONSE FUNCTIONS

In measuring a quantity which is a function of a single variable, the response observed for a given value of the variable is broadened by the resolution (often assumed to be Gaussian shaped) of the measuring instrument. In less direct experiments, such as the measurement of a neutron spectrum, the situation is even more complicated. The ideal spectrum of recoil protons from monoenergetic neutrons striking an

organic scintillator is rectangular; all proton energies below the neutron energy are equally likely. The output of a real detector is very nonideal because of edge effects, multiple scattering, nonelastic interactions and scattering from carbon nuclei, nonlinear light output vs proton energy, and several other effects. Consequently, it is difficult to determine the detector response functions from calculations alone; some measurements are usually required in addition to any calculations.

Because the unfolding results are quite sensitive to small changes in the response functions used, it is important that the responses be determined accurately. A thorough discussion of the techniques for finding the detector response functions is given in Ref. 1. The remainder of this paper is concerned with unfolding a spectrum when the response functions are accurately known.

III. UNFOLDING

The equation describing the measurement of a neutron spectrum $S(E)$ is the integral equation of the first kind⁷

$$Y(\xi) = \int_{E_1}^{E_2} dE R(\xi, E) S(E) \quad (1)$$

Here $Y(\xi)$ is the detector yield, given as a function of the pulse height, ξ , and $R(\xi, E)$ is the detector response function for neutrons of energy E . In practice, Y is measured for only a finite number of discrete intervals, or ranges of the variable ξ ;

$$Y_i = \int_{\xi_i}^{\xi_{i+1}} d\xi Y(\xi), \quad i = 1, 2, \dots, N. \quad (2)$$

The subscript i might indicate, for example, the channel numbers for a measurement made with an N -channel pulse-height analyzer. Alternatively, the spectrum might

be regrouped into bins or channels of varying width to take advantage of the variation of detector resolution with changing pulse height to minimize the number of bins.^{1,5} In this case, the subscripts would represent the bin numbers.

Substituting Eq. (1) into Eq. (2) gives

$$Y_i = \int_{\xi_i}^{\xi_{i+1}} d\xi \int_{E_{\min}}^{E_{\max}} dE R(\xi, E) S(E) \quad .$$

Thus

$$Y_i = \int_{E_{\min}}^{E_{\max}} dE S(E) R_i(E), \quad i = 1, 2, \dots, N, \quad (3)$$

where

$$R_i(E) = \int_{\xi_i}^{\xi_{i+1}} d\xi R(\xi, E) \quad .$$

Equation (3) can be solved by approximating $S(E)$ and $R_i(E)$ by analytic functions so that the integrations are possible. Another way to solve Eq. (3) involves defining discrete intervals of the variable E to obtain a set of linear equations. The second method is more appropriate here because of the complexity of the response functions. The intervals $\Delta E_j = E_{j+1} - E_j$ are chosen such that the approximations $\rho_{ij} \simeq R_i(E)$ and $S_j \simeq S(E)$ are valid over each interval. For simplicity, the derivation assumes that the ΔE_j are all equal. Defining $R_{ij} = \rho_{ij} \Delta E_j$ gives

$$Y_i = \sum_{j=1}^M R_{ij} S_j \quad i = 1, 2, \dots, N \quad (4)$$

In matrix notation, $\vec{Y} = \vec{R}\vec{S}$.

The most obvious solution to Eq. (4) is $\vec{S} = \vec{R}^{-1}\vec{Y}$. Unfortunately it is known⁷ that the solution to Eq. (1) is unstable for small errors in $\vec{Y}$; such errors produce

unbounded oscillations in $\vec{S}$. The instability is also present in the solution to Eq. (4), which is, after all, only an approximation to Eq. (1) and cannot be expected to be more stable. Because a measurement of the Y_i produces numbers which are statistically distributed around the "true" yield, errors are always present. Because the resulting oscillations are unphysical, it is desirable to remove or damp them, if possible, without seriously affecting the accuracy of the spectrum determination.

Least-structure analysis⁷⁻⁹ is a method of introducing a controlled amount of smoothing to damp the oscillations in the solution by finding the "smoothest" of all the solutions that are consistent with the measured data. It is expected that least-structure will work best for smooth, continuous spectra, although attempts have been made to modify it to better calculate discrete spectra.^{3,4}

Changing the calculated spectrum by smoothing will invalidate Eq. (4). However, since the changes in the Y_i are small, Eq. (4) can be rewritten as

$$\sum_{j=1}^M R_{ij} S_j = Y_i + \epsilon_i \quad i = 1, 2, \dots, N, \quad (5)$$

where the ϵ_i are unknowns which depend on the amount of smoothing in the spectrum. They represent the difference between the measured detector yield and the yield that is calculated by refolding -- multiplying the response matrix times the calculated, smooth spectrum.

The quantity $\chi^2 = \sum_{i=1}^N (\epsilon_i / \sigma_i)^2$ is in-

troduced in analogy to the χ^2 used in least-squares fitting of a parameter to a set of data. Here σ_i is the uncertainty in the measurement of Y_i . The most probable value of χ^2 is N , the number of data channels. If $\chi^2 < N$, the solution is under-smoothed; more smoothing can be used without

making the refolded calculated yield inconsistent with the measurement. If $\chi^2 > N$, the solution is oversmoothed.

To find the "smoothest" of the spectra which satisfy Eq. (5) within the constraint that $\chi^2 = N$, one defines a structure function, $F(\vec{S})$, which is to be minimized.

$$F(\vec{S}) = \sum_{j=2}^{M-1} (S_{j+1} - 2S_j + S_{j-1})^2. \quad (6)$$

Note that $F(\vec{S})$ in this case is simply a numerical approximation to the second derivative of the solution with respect to energy. Other structure functions have been defined,^{3,7-9} but for unfolding a smooth spectrum, Eq. (6) should be relatively good. If the general shape and magnitude of the spectrum are known, however, it might be better to construct a trial solution and minimize the squares of the departures of the spectrum from the trial solution than to use a structure function.⁸

Minimizing $F(\vec{S})$ with the constraint that $\chi^2 = N$ is done by introducing a Lagrangian multiplier, λ , and minimizing the quantity $[F(\vec{S}) + \lambda^{-1} \chi^2]$. Setting $\partial/\partial S_k (F + \lambda^{-1} \chi^2) = 0$ gives

$$\lambda(S_{k+2} - 4S_{k+1} + 6S_{k-1} + S_{k-2}) + \sum_{i=1}^N R_{ik} \frac{1}{\sigma_i^2} \epsilon_i = 0. \quad (7)$$

This can be changed to matrix notation by defining the matrices

$$G = \begin{matrix} & 1 & -2 & 1 & 0 & 0 & 0 & . & . & . \\ -2 & 5 & -4 & 1 & 0 & 0 & . & . & . \\ 1 & -4 & 6 & 1 & 0 & 0 & . & . & . \\ 0 & 0 & -4 & 6 & -4 & 1 & . & . & . \\ 0 & 0 & 1 & -4 & 6 & -4 & . & . & . \\ . & . & . & . & . & . & . & . & . \end{matrix} \quad (8)$$

and W where $W_{ij} = (1/\sigma_i^2)\delta_{ij}$. Then Eq. (7)

is written $\lambda \vec{G} \vec{S} + \tilde{R} \vec{W} \vec{c} = 0$, where $\tilde{R}$ is the transpose of the response matrix R . Using Eq. (5) to eliminate c gives

$$(\lambda G + \tilde{R} W R) \vec{S} = \tilde{R} \vec{W} \vec{Y}.$$

Now, inverting the matrix $(\lambda G + \tilde{R} W R)$ gives the spectrum

$$\vec{S} = (\lambda G + \tilde{R} W R)^{-1} \tilde{R} \vec{W} \vec{Y}.$$

Note that if $\lambda = 0$, the least-structure solution reduces to the simple matrix inversion solution with no smoothing.

The structure function can be made slightly more general by using weighting factors to emphasize the smoothing of part of the spectrum.

$$F(S) = \sum_{j=2}^{M-1} q_j (S_{j+1} - 2S_j + S_{j-1})^2.$$

One case for which the weighting factors, q_j , might be useful is that in which the spectrum changes greatly with energy. If the values of σ_i/y_i do not depend strongly on i , then the smallest values of S_j contribute relatively little to $F(S)$ unless they are weighted more heavily than the larger ones. Alternatively, if the spectrum is known to have a peak at some energy and one wishes to damp out oscillations near the peak but not necessarily far from it, then increased weighting of the values of S_j near the peak might be useful.³

Another generalization that can be considered is the case in which the S_j are not evenly spaced (that is, where ΔE_j varies with j). To keep the smoothing proportional to the second derivative of $S(E)$, it is necessary to change the matrix G , Eq. (8), somewhat.

The program is written to include both weighting factors and nonuniform energy intervals, although the necessary changes are not derived here. The structure function used is

$$F(\vec{S}) = \sum_{j=2}^{M-1} q_j \left(\frac{S_{j+1} - S_j}{E_{j+1} - E_j} - \frac{S_j - S_{j-1}}{E_j - E_{j-1}} \right)$$

$$\times \left(\frac{2}{E_{j+1} - E_{j-1}} \right).$$

To find the uncertainties in the spectrum, let $H = (\lambda G + \tilde{R} W R)^{-1}$ and calculate the quantity

$$\Delta S_j = \left[\sum_{i=1}^N \left(\frac{\partial S_j}{\partial Y_i} \sigma_i \right)^2 \right]^{1/2}.$$

$$\begin{aligned} \frac{\partial S_j}{\partial Y_i} &= \sum_{\ell=1}^N \sum_{k=1}^M H_{jk} R_{\ell k} W_{\ell i} \\ &= \sum_{k=1}^M H_{jk} R_{ik} \frac{1}{\sigma_i^2} \end{aligned}$$

$$\Delta S_j = \left[\sum_{i=1}^N \left(\sum_{k=1}^M H_{jk} R_{ik} \frac{1}{\sigma_i^2} \right)^2 \right]^{1/2}.$$

In the foregoing form, ΔS_j does not include the uncertainties arising from errors or uncertainties in the response matrix. It is assumed that those uncertainties will be included by increasing appropriately the values of σ_i , the uncertainties in Y_i .

Uncertainties of the form

$$\frac{\partial S_j}{\partial Y_i} \quad \frac{\partial S_j}{\partial Y_l} \quad \sigma_i \quad \sigma_l$$

have likewise not been included in the calculation. If there is a scale-factor uncertainty in the yield measurement, it can be included as a scale-factor uncertainty in the spectrum.

IV. USING THE CODE

Following is a description of the data required to run the code.

Card No.	Description
1	TITLE CARD
2	NC, the number, N of bins or channels. NE, the number, M, of energies. NZL, the number of channels of data to be zeroed at the low-pulse-height end. NZE, the number of energies to be zeroed at the low-energy end. NZH, the number of channels of data to be zeroed at the high-energy end. IFTRS, set to 1 if using a trial solution, 0 if not. IFWTD, set to 1 if reading smoothing weight factors, 0 if no weight factors are to be used, -1 to reset weight factors to inverse of solution from IFWTF = 0 case.
3	AMAT(I,J), the response matrix, R_{ij} . Read in the response functions in the order of increasing energy.
4	E(J), the energies at which response functions are given.
5	DVEC(I), the detector yield data to be unfolded. The data should be grouped into the same pulse-height bins as the response functions.
6	SIG(I), the uncertainties in the yield data expressed as a percentage.
7	RESIG, a normalization factor to multiply times each value of SIG(I). REDATA, a normalization factor to multiply times each value of DVEC(I).
8	QVEC(J), the trial solution. Read only if IFTRS $\neq$ 0.
9	WT(J), the smoothing weight factors. Read only if IFWTF > 0.

We have used the response functions, pulse-height bins, and energies given by Verbinski¹ to unfold data. The bin widths are not of equal size, and the response functions have been divided by the bin widths. To make our yield data compatible, we group them into the same bins and divide each value by the bin width. Because the response functions are given in units of

counts

(neutrons on detector) x (pulse height width)

we renormalize our data by dividing by 4π times the number of neutrons hitting the detector during a run. The spectrum output is then in units of

neutrons

sr MeV

Running requires about 13,000 words of storage on the CDC 6600 for our cases with 156 pulse-height channels and 21 response functions, and running times are typically a few seconds.

We find that most problems in running the code have resulted either from using the wrong uncertainties for the data or from using inaccurate response functions. Either mistake can cause χ^2 to be larger than N, even for $\lambda = 0$, and, because χ^2 increases with λ , the problem will not converge. Even if $\chi^2 < N$, the proper smoothing will not be included unless χ^2 is calculated accurately.

Because no provision is made for including uncertainties in the response functions, it is important to determine how such uncertainties affect the unfolding and then to include them in the uncertainties assigned to the data. A set of upper bounds, τ_i , for the effects of response-function uncertainties can be estimated by assuming that the uncertainties are completely correlated to get

$$\tau_i = \sum_{j=1}^M \left| \Delta R_{ij} \right| S_j .$$

Here S_j is an estimate of the spectrum.
The τ_i should be combined quadratically
with the σ_i to get the uncertainties to be
used in the run.

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APPENDIX

PROGRAM LISTING

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PROGRAM CONFOLD(INPUT,OUTPUT,TAPE10)
  DIMENSION E(21), DE(21), WT(21)
  COMMON AMAT(156,21),HMAT(21,21),PVEC(21),DVEC(156),EVEC(156),SUMA,
  1GMAT(21,21),QVEC(21),SIG(156),CVEC(156),SCOL(21),DET(21),TITLE(8)
  C 2-ND PARAMETER IN CALL MATINV AND 5-TH PARAMETER IN CALL MATMPY
  C MUST EQUAL 2-ND DIMENSION OF AMAT.
  1 READ 52, TITLE
    IF (TITLE.EQ.10H ) STOP
    PRINT 53, TITLE
    READ 40, NC,NE,NZL,NZE,NZH,IFTRS,IFWTF
    IF (NC.EQ.3) STOP
    PRINT 40, NC,NE,NZL,NZE,NZH,IFTRS,IFWTF
    DO 2 J=1,NE
      QVEC(J)=0.
  2 READ (10,41)(AMAT(I,J),I=1,NC)
    READ 43, (E(I),I=1,NE)
    READ 43, (DVEC(I),I=1,NC)
    READ 54, (SIG(I),I=1,NC)
    READ 43, RESIG,REDATA
    IF (RESIG.EQ.0.) RESIG=1.
    IF (IFTRS.EQ.0) GO TO 3
    READ 43, (QVEC(J),J=1,NE)
  3 DO 4 I=1,NE
  4 WT(I)=1.
    IF (IFWTF.LE.0) GO TO 5
    READ 43, (WT(I),I=1,NE)
  5 IF (REDATA.EQ.0.) GO TO 7
    DO 6 I=1,NC
  6 DVEC(I)=DVEC(I)*REDATA
  7 NFM=NE-1
    DE=E(2)-E
    DO 8 I=2,NEM

```

8	DE(I)=.5*(E(I+1)-E(I-1))	A	33
	DE(NE)=E(NE)-E(NEM)	A	34
	DC 9 I=1,NE	A	35
	DC 9 J=1,NC	A	36
9	AMAT(J,I)=AMAT(J,I)*DE(I)	A	37
	NC=NC-NZL-NZH	A	38
	NE=NE-NZE	A	39
	NEM=NEM-1	A	40
	ANC=NC	A	41
	DC 10 I=1,NC	A	42
	DVEC(I)=DVEC(I+NZL)	A	43
	SIG(I)=SIG(I+NZL)	A	44
	DC 10 J=1,NE	A	45
10	AMAT(I,J)=AMAT(I+NZL,J+NZE)	A	46
	DC 11 I=1,NE	A	47
	WT(I)=ABS(WT(I+NZE))	A	48
	QVEC(I)=QVEC(I+NZE)	A	49
11	E(I)=E(I+NZE)	A	50
	DC 12 I=1,NE	A	51
	DC 12 J=1,NE	A	52
12	GMAT(I,J)=0.	A	53
13	IF (IFTRS.GT.0) GO TO 16	A	54
	NEMM=NEM-1	A	55
	NEM3=NEMM-1	A	56
	DC 14 I=1,NEM	A	57
14	DE(I)=E(I+1)-E(I)	A	58
	DC 15 I=3,NEMM	A	59
	GMAT(I,I-2)=4./((DE(I-1)+DE(I-2))*2/DE(I-1)/DE(I-2)*WT(I-1)	A	60
	GMAT(I,I-1)=-4./((DE(I-1)+DE(I-2))/DE(I-2)*WT(I-1)+4./((DE(I)+DE(I-1))	A	61
	11))/DE(I)*WT(I))/DE(I-1)**2	A	62
	GMAT(I,I)=4./((DE(I-1)+DE(I-2))*2/DE(I-1)**2*WT(I-1)+4./DE(I)**2/D	A	63
	1E(I-1)**2*WT(I)+4./((DE(I)+DE(I+1))*2/DE(I)**2*WT(I+1)	A	64
	GMAT(I,I+1)=-4./((DE(I)+DE(I-1))/DE(I-1)*WT(I)+4./((DE(I)+DE(I+1))/	A	65
	1DE(I+1)*WT(I+1))/DE(I)**2	A	66
15	GMAT(I,I+2)=4./((DE(I+1)+DE(I))*2/DE(I)/DE(I+1)*WT(I+1)	A	67
	GMAT=4./((DE+DE(2))*2/DE**2*WT(2)	A	68
	GMAT(1,2)=-4./((DE+DE(2))/DE**2/DE(2)*WT(2)	A	69
	GMAT(1,3)=GMAT(3,1)	A	70
	GMAT(2,1)=GMAT(1,2)	A	71
	GMAT(2,2)=(4./DE**2*WT(2)+4./((DE(2)+DE(3))*2*WT(3))/DE(2)**2	A	72
	GMAT(2,3)=GMAT(3,2)	A	73
	GMAT(2,4)=GMAT(4,2)	A	74
	D=DE(NEM)	A	75
	DM=DE(NEMM)	A	76
	GMAT(NE,NE)=4./((D+DM)**2/D**2*WT(NEM)	A	77
	GMAT(NE,NEM)=-4./((D+DM)/DM/D**2*WT(NEM)	A	78
	GMAT(NE,NEMM)=GMAT(NEMM,NE)	A	79
	GMAT(NEM,NE)=GMAT(NE,NEM)	A	80
	GMAT(NEM,NEM)=(4./D**2*WT(NEM)+4./((DM+DE(NEM?))*2*WT(NEMM))/DM**2	A	81
	GMAT(NEM,NEMM)=GMAT(NEMM,NEM)	A	82
	GMAT(NEM,NEM3)=GMAT(NEM3,NEM)	A	83
	GO TO 18	A	84
16	DC 17 I=1,NE	A	85
17	GMAT(I,I)=WT(I)	A	86
18	IF (IFWTF.NE.163) GO TO 19	A	87
	IFWTF=1	A	88
	GO TO 22	A	89
19	DC 20 I=1,NC	A	90
	SIG(I)=SIG(I)*DVEC(I)/100.*RESIG	A	91
	IF (SIG(I).EQ.0.) SIG(I)=1.	A	92
20	CCNTINUE	A	93
	PRINT 42	A	94
	PRINT 39, (DVEC(I),I=1,NC)	A	95
	PRINT 44	A	96
	PRINT 39, (SIG(I),I=1,NC)	A	97
	DC 21 I=1,NC	A	98
21	SIG(I)=1./SIG(I)**2	A	99
	GAM=0.	A	100
22	DC 23 I=1,NE	A	101
	DC 23 J=1,NE	A	102
	HMAT(I,J)=GAM*GMAT(I,J)	A	103
	DC 23 K=1,NC	A	104

23	HMAT(I,J)=HMAT(I,J)+AMAT(I,I)*SIG(I)*AMAT(K,J)	A	105
	CALL MATINV (HMAT,21,NE,PVEC,DET)	A	106
	DC 24 I=1,NE	A	107
	SCOL(I)=0.	A	108
	DC 24 J=1,NC	A	109
24	SCOL(I)=SCOL(I)+AMAT(J,I)*SIG(J)*DVEC(J)	A	110
	DC 25 I=1,NE	A	111
25	SCOL(I)=SCOL(I)+GAM*QVEC(I)*WT(I)	A	112
	CALL MATMPY (NE,NE,1,HMAT,21,SCOL,21,PVEC,21)	A	113
	PRINT 46	A	114
	PRINT 39, (PVEC(J),J=1,NE)	A	115
	CHISQ=0.	A	116
	DC 26 I=1,NC	A	117
	EVEC(I)=0.	A	118
	DC 26 J=1,NE	A	119
26	EVEC(I)=EVEC(I)+AMAT(I,J)*PVEC(J)	A	120
	DC 27 I=1,NC	A	121
27	CHISQ=CHISQ+(EVEC(I)-DVEC(I))**2*SIG(I)	A	122
	PRINT 48, CHISQ,GAM	A	123
	IF (GAM.EQ.0.) GO TO 28	A	124
	IF (CHISQ.EQ.CHISQB) GO TO 30	A	125
	GAMA=GAM+(GAM-GAMB)*(1.-CHISQ/ANC)/(CHISQ-CHISQB)*ANC	A	126
	IF (GAMA.LE.0.) GAMA=GAM*ANC/CHISQ	A	127
	GO TO 31	A	128
28	IF (CHISQ.LE.ANC) GO TO 29	A	129
	PRINT 57	A	130
	GO TO 32	A	131
29	GAMA=1./DVEC	A	132
	PRINT 45	A	133
	PRINT 39, (EVEC(I),I=1,NC)	A	134
	GO TO 31	A	135
30	GAMA=2.*GAM-GAMB	A	136
31	GAMB=GAM	A	137
	GAM=GAMA	A	138
	IF (ABS(GAM-GAMB)/GAM.LE..001) GO TO 32	A	139
	IF (GAM.LE.1.E-12) GO TO 32	A	140
	CHISQB=CHISQ	A	141
	IF (IFWTF.EQ.163) GO TO 13	A	142
	GO TO 22	A	143
32	IF (IFWTF.GE.0) GO TO 34	A	144
	DC 33 I=1,NE	A	145
33	WT(I)=1./PVEC(I)**2	A	146
	PRINT 58	A	147
	IFWTF=163	A	148
	GAM=GAM/2.	A	149
	CHISQB=3.*CHISQB	A	150
	GO TO 13	A	151
34	PRINT 47	A	152
	PRINT 48, CHISQ,GAMB	A	153
	PRINT 46	A	154
	PRINT 39, (PVEC(I),I=1,NE)	A	155
	PRINT 49	A	156
	PRINT 50, (E(I),I=1,NE)	A	157
	DC 36 I=1,NE	A	158
	PVEC(I)=0.	A	159
	DC 35 J=1,NE	A	160
	DC 35 K=1,NC	A	161
35	PVEC(I)=PVEC(I)+(HMAT(I,J)*AMAT(K,J)*SQRT(SIG(K)))*2	A	162
36	PVEC(I)=SQRT(PVEC(I))	A	163
	PRINT 51	A	164
	PRINT 39, (PVEC(I),I=1,NE)	A	165
	IF (IFTRS.EQ.0) GO TO 37	A	166
	PRINT 56	A	167
	PRINT 39, (QVEC(I),I=1,NE)	A	168
37	IF (IFWTF.EQ.0) GO TO 38	A	169
	PRINT 55	A	170
	PRINT 39, (WT(I),I=1,NE)	A	171

38	PRINT 45	A	172
	PRINT 39, (EVEC(I), I=1, NC)	A	173
	GO TO 1	A	174
C		A	175
39	FORMAT (1P10E13.5)	A	176
40	FORMAT (12I6)	A	177
41	FORMAT (9E8.2)	A	178
42	FORMAT (/ * DATA *)	A	179
43	FORMAT (6E12.4)	A	180
44	FORMAT (/ * SIGMA *)	A	181
45	FORMAT (/ * REFOLDED DATA *)	A	182
46	FORMAT (/ * SPECTRUM *)	A	183
47	FORMAT (*1SOLUT IDV*)	A	184
48	FORMAT (* CHISQ =*, 1PE13.4, 10X*LAM =*, 1PE13.4)	A	185
49	FORMAT (/ * ENERGIES *)	A	186
50	FORMAT (10F13.4)	A	187
51	FORMAT (/ * UNCERTAINTIES *)	A	188
52	FORMAT (8A10)	A	189
53	FORMAT (*1*8A10)	A	190
54	FORMAT (12E6.0)	A	191
55	FORMAT (/ * SMOOTHING WEIGHT FACTORS *)	A	192
56	FORMAT (/ * TRIAL SOLUTION *)	A	193
57	FORMAT (/ * CHI SQUARED LARGER THAN NC *)	A	194
58	FORMAT (//// * SMOOTHING WEIGHTS CHANGED TO 1./S(J)*3H**2//)	A	195
	END	A	196