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AEC Research and Development Report

GSSLRN - II
A LEAST-SQUARES COMPUTER CODE
FOR THE ANALYSIS OF PEAK SHAPES
WHICH CAN BE DEFINED ANALYTICALLY

G.D. Seybold

June 1971

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GSSLRN-IIA LEAST-SQUARES COMPUTER CODE FOR THE ANALYSIS OF
PEAK SHAPES WHICH CAN BE DEFINED ANALYTICALLYABSTRACT

A computer code, GSSLRN-II, is presented which is written in generalized form so as to allow analysis of any data containing peak shapes which can be adequately represented by an analytical function form.

GSSLRN-II utilizes a second order Newton-Raphson least-squares iterative scheme in its analysis of peak shapes. Effective use has been made of the measurement variance and the least-squares deviations to justify automatic recycling attempts of least-squares fits on groups of peaks.

The code will locate peaks, group them in appropriate sets, optimize the interval-of-fit, least-squares fit the set of peaks, recycle for another fit if necessary, and upon option will generate plots of the fitted results. Many other options are available which allow the user a high degree of versatility with respect to input and/or output options.

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GSSLRN-IIA LEAST-SQUARES COMPUTER CODE FOR THE ANALYSIS OF
PEAK SHAPES WHICH CAN BE DEFINED ANALYTICALLYI. Introduction

A computer code, GSSLRN-II, is presented which is written in generalized form so as to allow analysis of any data containing peak shapes which can be adequately represented by an analytical function form.

GSSLRN-II is a much more versatile code than GSSLRN-I⁽¹⁾ because it is not limited to the analyses of fission-product data using a fixed analytical function. In addition, GSSLRN-II contains a major improvement with respect to the use of measurement variance obtained from the least-squares fits for the purpose of justifying recycle (multiple fitting) attempts.

The code makes use of the least-squares package, LEARN,^(2,3) which utilizes a second order Taylors' expansion in its least-squares iterative scheme.

The code contains a wide variety of options which are designed to allow the analyst many override features with respect to the input and/or output options.

The net result is a code which is adaptable to many types of data with a minimal amount of necessary modification. Some examples of its possible applications are gamma scanning analysis, Mossbauer analysis, neutron activation analysis, radiochemical analysis, reactor fuel burnup, half-life determinations, volcanology studies, ecological studies, environmental

and pollutant applications, or any other analysis which requires the use of relative or absolute intensities of peak shapes in order to identify composite properties.

I. Highlights of the Code

Some of the features of GSSLRN-II which allow a wide variety of application are:

- Ability to rewrite the analytical function which describes a continuum under the peak shapes without destroying the integrity of the code
- Use of nonlinear least-squares techniques accompanied by a substantial regression analysis
- Judicious use of the measurement variance in order to quantify the performance of a fit
- An automatic recycling logic which enables the code to build in hidden or unaccounted for peaks
- Optional use of a peak searching routine⁽⁴⁾ to locate peaks from data spectra collected on large multichannel analyzers
- Optional input and/or output specifications including automatic on-line or off-line plotting features
- CALCOMP plotting options which display the measured spectrum, fitted curves and their root-mean-square deviation envelope, fitted parameters, curves of each peak as they are resolved from a multiplet, or a three-dimensional plot of multiple spectra
- No prior knowledge required to locate and successfully fit hidden or overlapping spectral components

- Useful results from the least-squares analyses which include:

1. Fitted parameters and statistical errors for each peak
2. Net peak intensities and their errors
3. Relative or absolute intensities including normalization
4. Corrected energies for the mean of each peak

III. Method of Fitting

In the least-squares analysis of GSSLRN-II it is assumed that data points in a portion of the experimental spectrum can be represented by an explicit scalar theory $Y=Y(x,\underline{a})$, where x and $\underline{a}$ represent the independent variable and a single vector set of parameters, respectively.

The code minimizes the mean square misfit Q , which is formulated as

$$Q = \sum_m W_m \left[Y_m - Y(X_m, \underline{a}) \right]^2 \quad (1)$$

where

W_m represents the weighting property of each data point,
 Y_m represents the measured data point,
 X_m represents the independent variable (channel number) for each Y_m ,
 Y represents the theoretical value of the analytic function,

The parameters $\underline{a}$ are computed at each successive iteration using the basic iterative algorithm⁽²⁾

$$\underline{a}_{new} = \underline{a} - (\partial Q / \partial \underline{a}) \cdot (\partial^2 Q / \partial \underline{a} \partial \underline{a})^{-1} \quad (2)$$

where $\frac{\partial Q}{\partial \underline{a}}$ represents the misfit gradient, defined by,

$$\frac{\partial Q}{\partial \underline{a}} = \sum_m 2W_m [Y_m - Y(X_m, \underline{a})] \left[-\partial Y(X_m, \underline{a}) / \partial \underline{a} \right] \quad (3)$$

and $\partial^2 Q / \partial \underline{a} \partial \underline{a}$ is the second misfit gradient (or matrix of second partial derivatives), defined by,

$$\begin{aligned} \frac{\partial^2 Q}{\partial \underline{a} \partial \underline{a}} = \sum_m 2W_m \left[\left\{ \partial Y(X_m, \underline{a}) / \partial \underline{a} \right\} \left\{ \partial Y(X_m, \underline{a}) / \partial \underline{a} \right\} \right. \\ \left. - \left\{ Y_m - Y(X_m, \underline{a}) \right\} \left\{ \partial^2 Y(X_m, \underline{a}) / \partial \underline{a} \partial \underline{a} \right\} \right]. \end{aligned} \quad (4)$$

The measurement variance, σ^2 , can now be defined as

$$\sigma^2 = Q / (M - J), \quad (5)$$

where M and J denote the number of measurements and parameters, respectively.

Using the measurement variance σ^2 , one may compute the parameter variances $V(\underline{a})$ as $V(\underline{a}) \equiv \langle (\delta \underline{a})(\delta \underline{a}) \rangle = 2\sigma^2 (\partial^2 Q / \partial \underline{a} \partial \underline{a})^{-1}$ and the parameter standard deviation doubt as $\delta a_i = \pm [V_i(a_i)]^{1/2}$.

One can describe the peak shapes by almost any nonlinear function represented by Y above.

The method described above⁽²⁾ uses the second derivatives of the analytical function, the quantity $\partial^2 Y / \partial \underline{a} \partial \underline{a}$ in Equation 4, and has been shown to be superior to the same least-squares technique using only the first derivative. The second derivative least-squares technique has proven itself invaluable in determining whether or not an assumed peak

is real or a result of a large amount of scatter in the data or from other anomalies.

IV. Code Description

GSSLRN-II has been coded with the use of an overlay structure which consists of a main segment and six overlay segments. Each of the overlay segments has a particular overall function which is almost entirely independent from the others. This permits the allocation of the code to minimize the storage requirements while maintaining an efficient mode of execution.

In addition to the overlay structure, there exists an element for the "Procedure Definition Processor" (PDP), which is used to define the dimensions of all the common storage in the code. It is written so as to allow the user the means by which he can recompile the entire code with redefined dimensions on all the parameters without making appropriate modifications to individual subroutines.

There are many options which are required in order to maintain a general coded package which is capable of performing the analyses needed for spectra of almost any type. However, the primary purpose of GSSLRN-II is to perform analyses requirements, using least-squares methods, for fission-product spectra obtained from a (Ge(Li)) detector system. Although GSSLRN-II was designed for this specific purpose, it is necessary to present some explanation of each of the above mentioned overlay segments in order to use the code in a more general way. Thus, the following descriptions are written in an order somewhat analogous to a flow diagram of the code.

A. Segments 0, 1, and 2 (Main Link)

These segments contain the main program, the systems routines, utility routines, and others which are or can be called at any time during execution of the code.

The input routine, LOAD, is also allocated to the main link. Its only function is that of reading all input from cards, magnetic tape, or data elements from fastrand drum files. Except for the data spectrum, the input cards defining the problem requirements (or options) are read by a utility input package, NAMELIST⁽⁵⁾.

B. Segment 3. (Peak Location Subroutines)

The function of this segment is to automatically locate peaks from a spectrum, put them in selected groups, and then set up the initial interval-of-fit for each group.

There are many methods from which to choose a peak searching algorithm. If the data spectra have good resolution (i.e. Full-width-at half-maximum, FWHM > 10 energy points), it is possible to locate most, if not all of the peaks by using methods which employ approximations of high order derivatives. However, in practice, most data collected from Germanium systems do not allow such resolution. In fact, most of the peaks found, using present day available detector systems, have from two to six energy points at FWHM. Therefore, a simple second difference function was adapted from Mariscotti⁽⁴⁾ which has been modified for GSSLRN-II to be the following:

$$S_i \triangleq 1/7 (2 N_{i-2} - N_{i-1} - 2N_i - N_{i+1} + 2N_{i+2})$$

where

S_i represents the difference function for channel i , and

N_i represents the count at channel i .

This modified difference function will not necessarily locate all of the peaks in a data spectrum, especially hidden peaks. However, with the proper choice of input parameters one can optimize the smoothing properties of the function such that all the prominent peaks are located. Problems in fitting data caused by the combination of insufficient detector resolution and the inadequate properties of the above difference function can be overcome by use of the least-squares recycling options in the code. These options check each fit for allowable deviations and an acceptable value of the measurement variance in order to discern if another fit with more or less peaks is justified.

C. Segment 5 (Input Parameters and Fitting Intervals)

Subroutine PUTIN functions as a starting point for each initial least-squares fit. This routine computes the initial fitting estimates and sets up many of the least-squares parameters which are specifically related to the iterative properties of the code.

In addition to the fitting estimates, this segment also contains the routines necessary to attempt to optimize the initial interval-of-fit.

D. Segment 6. (Fitting and Recycling Routines)

This segment constitutes the heart of the code. It contains all the subroutines necessary to perform the least-squares fits, saddle

point logic, theory-measurement correlations, regression analysis, variance-covariance matrices, and recycling logic.

Following the acceptance of the best fit from the recycling logic, this segment of the code also computes the net intensity and its uncertainty for each peak in the group. Assuming the analytic function has been described by Gaussian terms, the intensity is computed as

$$I_k = A_i/A_{i+1} * \sqrt{2\pi}$$

where A_i and A_{i+1} represent the Gaussian amplitude and inverse width parameter $1/\sigma_k$, respectively, for the k(th) peak.

The uncertainty of each intensity is computed as

$$\delta I_k = \left\{ \frac{2\pi}{A_{i+1}^2} \left[\overline{(\delta A_i)^2} - \frac{2A_i}{A_{i+1}} \cdot \overline{(\delta A_i \delta A_{i+1})} + \left(\frac{A_i}{A_{i+1}} \right)^2 \cdot \overline{(\delta A_{i+1})^2} \right] \right\}^{1/2}$$

where $\overline{(\delta A_i)^2}$ and $\overline{(\delta A_{i+1})^2}$ are the measurement variance uncertainties and $\overline{(\delta A_i \delta A_{i+1})}$ represents the cross-correlation term, all of which are obtained from the variance-covariance matrix.

E. Segment 7. (CALCOMP Plotting Routines)

The subroutines in this segment are called on option and allow the user to display various types of data for graphical purposes. Basically, there are three types of plotting demands satisfied by these routines:

1. Plots which are generated from each successful fit which contain the count per channel, its assumed error, the fitted curve, the root-mean-square deviation envelope, a plot of each resolved peak shape, and finally some

of the fitted results in numerical form.

2. Plots of the measured data spectrum.
3. Three-dimensional displays of multiple data spectra.

F. Segment 8. (On-Line Plotting Routines)

This segment contains the subroutines used to provide on-line printer plots of each fitted group. It is called on option and displays only the data measurements and their fitted values.

G. Segment 4. (Summary Routines)

This segment is called last. It provides a summary of output results for each successfully fitted group of peaks at the termination of all least-squares fits for any one case.

H. GSSLRN-II (Overlay of Program Segments)

The overlay structure, or groupings of subroutines, used to execute the various options of the code are defined relative to the segment names as:

SEG 0	LIKELY-PRESET-COMMON
SEG 1	SYSTEMS ROUTINES
SEG 2	PAGE-SPILL-INVERT-CHANCE-THEORY-ERF-RECOVR-WGT-ENGCON-BKG-WIDTH-CALCOM-LOAD
SEG 3	*ANALIZ-INTEGR-OUTPUT-PKCHK-OVRLOD-VALLEY-POLY
SEG 4	*TALLY-STRAIT-EFFICY
SEG 5	*PUTIN-LIMITS-SPLIT-SPLICE-LIST-REDUCE-FIXIT-FORCE-NORM
SEG 6	*MIX-MINMAX-DOUBT-SADDLE-PUTOUT-WORTH-WIT-WITTY-ADJI-ADJUST-DROP-INTSTY-MISFIT
SEG 7	*CONTRL-PLTTER-SCLE-SHUTLE-MAPS-PLOT-ARTIST-LOGAXS-THERY1
SEG 8	*SETUP-IMAGE-SORAS-CHAR-SORT

V. THEORY Subroutine

As mentioned in the introduction, the code can be easily modified or adapted to other functional representations for the data spectra. This versatility allows the analyst the capability of pursuing various functional forms without the necessity of major code revision. Modifications of this type are made by re-writing the THEORY subroutine along with some auxiliary routines. However, if one chooses to complete the modification to the extent of obtaining absolute intensities, there are available auxiliary subroutines for this purpose to which would require a minimum of coding.

Except for a few minor changes, the THEORY routine for GSSLRN-II requires the same basic coding properties as it would for the LEARN^(2,3) code. The structure used for coding the THEORY subroutine is presented in Section A. The specific THEORY subroutine used for the fission product analyses (see Section VII) currently in GSSLRN-II is presented in Section B.

A. Generalized Setup for THEORY

```

C     GENERALIZED SETUP FOR A 'THEORY' SUBROUTINE.
      SUBROUTINE THEORY
      DIMENSION Z(100)
      EQUIVALENCE (Z,DDY(1,178))
      L1=LOT(1,2)+1      'REFER TO INPUT INSTRUCTIONS FOR 'LOT' DEFINITION.
      L2=LOT(2,2)
      IF(JJ.LE.LOT(1,2)) GO TO 40      'NECESSARY FOR A STRAIGHT LINE FIT.
C     SET UP Z CONSTANTS FOR EXPONENTIALS USED WITH GAUSSIAN TERMS.
      40 COMPUTE 1ST DERIVATIVES 'DY' FOR THE BACKGROUND PARAMETERS.
      IF(JJ-LOT(1,2)) 30,50,60
      60 COMPUTE 1ST DERIVATIVES FOR GAUSSIAN TERMS.
      30 IF(MAX.LT.2) GO TO 50      'CHECK IF 2ND DERIVATIVES ARE NEEDED.
C     INITIALIZE ALL 2ND DERIVATIVES TO ZERO.
      IF(JJ-LOT(1,2)) 50,50,70
      70 COMPUTE ALL NON-ZERO 2ND ORDER PARTIALS 'DDY'.
      50 IF(JJ.LT.LOT(1,2)) A(3)=0.0
      IF(JJ.LE.LOT(1,2)) GO TO 101      'FOR STRAIGHT LINE FIT ONLY.
C     COMPUTE THE ANALYTIC FUNCTION USING GAUSSIAN TERMS.
      101 Y=FUNCTION      'RETURN 'Y' AS ANALYTIC FUNCTION.
      RETURN
      END

```

As described, the subroutine demands that the analytic function be expressed in two parts, one containing some continuum term (background), plus those terms required to express the peak shapes (Gaussian). The tests on JJ and LOT are included because of special optional requirements which are described in Section X.

B. PRESENT THEORY ROUTINE IN GSSLRN-II

```

      IT FR5 THEORY,THEORY
      SUBROUTINE THEORY
C  MULTIPLE PURPOSE ROUTINE---STRAIGHT LINE, PARABOLA, OR SUMS OF GAUSSIA03/18/70
C  SUBROUTINE FOR FITTING A POLYNOMIAL + AN UNDETERMINED
C  SUM OF SYMMETRIC GAUSSIAN FUNCTIONS.
C  DERIVATIVES FOR THE GAUSSIANS ARE RECURSIVE.
C  GD SEYBOLD AUGUST 1968      (LEARN-2)
      INCLUDE NAME0              03/25/70
      INCLUDE NAME1              03/25/70
      DIMENSION Z(100)
      EQUIVALENCE (Z(1),DDY(1,178))
      COMPUTE 1ST ORDER DERIVATIVES.
C  SET UP CONSTANTS
      J1=0
      L1=LOT(1,2)+1              03/18/70
      L2=LOT(2,2)                03/18/70
      IF(JJ.LE.LOT(1,2)) GO TO 40  03/18/70
      DO 10 J=L1,JJ,L2           03/18/70
      J1=J1+1
      J2=J1+50
      Z(J2)=A(J+1)*X(M,1)-A(J+2)
      10 Z(J1)=EXP(-Z(J2)*Z(J2)/2.)
      40 DY(1)=1.0                03/18/70
      DY(2)=X(M,1)-X(1,1)
      DY(3)=DY(2)*DY(2)
      IF(JJ-LOT(1,2)) 30,50,      03/18/70
      COMPUTE THE RECURSIVE FIRST ORDER DERIVATIVES.
      J1=0
      DO 15 J=L1,JJ,L2           03/18/70
      J1=J1+1
      J2=J1+50
      DY(J)=Z(J1)
      DY(J+2)=A(J)*Z(J2)*DY(J)
      15 DY(J+1)=-X(M,1)*DY(J+2)
      CHECK FOR FIRST AND/OR SECOND PARTIAL BRANCHING.
C  INITIALIZE ALL SECOND ORDER PARTIALS.
      30 IF(MAX.LT.2) GO TO 50    03/18/70
      DO 20 J1=1,JJ
      DO 20 J2=J1,JJ
      20 DDY(J1,J2)=0.
      IF(JJ-LOT(1,2)) 50,50,      03/18/70
      COMPUTE ALL NON-ZERO SECOND ORDER PARTIALS.
      COMPUTE ALL NON-ZERO SECOND ORDER RECURSIVE PARTIALS.
      J1=0

```

```

DO 25 J=L1,JJ,L2
J1=J1+1
J2=J1+50
J11=J+1
J22=J+2
DDY(J,J22)=Z(J2)*DY(J)
DDY(J,J11)=-X(M,1)*DDY(J,J22)
CSQ=Z(J2)*Z(J2)
DDY(J22,J22)=A(J)*DY(J)*(CSQ-1.)
DDY(J11,J11)=X(M,1)*X(M,1)*DDY(J22,J22)
25 DDY(J11,J22)=-X(M,1)*DDY(J22,J22)
50 IF(JJ.LT.LOT(1,2)) A(3)=0.
SUM=A(1)+A(2)*DY(2)+A(3)*DY(3)
IF(JJ.LE.LOT(1,2)) GO TO 101
DO 100 J=L1,JJ,L2
100 SUM=A(J)*DY(J)+SUM
101 Y=SUM
RETURN
END

```

03/18/70

03/18/70

03/18/70

03/18/70

03/18/70

VI. Auxiliary Subroutines

In addition to the THEORY routine, there are other routines available for modification, depending on user requirements.

- Subroutine FIXIT - This routine is necessary to supply the initial estimates for some of the fitting parameters. It requires change if THEORY is modified.
- Subroutine REDUCE - If peaks are discarded while executing recycle attempts, this routine is used to reorder the least-squares parameter set properly. It requires change if THEORY is modified.
- Subroutine PUTOUT - This is an output routine which is used to compute and store some of the errors needed in the summary output. It requires change if THEORY is modified.
- Function WIDTH - A function which can be used to simplify some of the properties of terms represented by the analytic expression. It is used only as a means of simplifying the least-squares width parameter. Non-functional if the THEORY is modified.
- Subroutine INTSTY - This routine computes the relative intensity of each peak. It requires change if THEORY is modified.
- Function WGT - This function provides the weighting properties necessary for the fit. Improper use of the weights will cause the criteria for recycling to be incorrect.
- Subroutine ENGCON - This routine converts the channel numbers to their proper energy. It can be modified by the user without causing any ill effects to the code.

- Subroutine BKG - This routine supplies the initial least-squares estimates for the fitting parameters used to express the background continuum. It requires change if the background terms in THEORY are modified.
- Subroutine STRAIT - This routine is used to supply the code with parameter estimates for fitting a straight line function before terminating a case. It requires change if some other function is desired to fit the resultant energy versus full-width-at-half-maximum values.
- Subroutine EFFICY - Presently this routine is a dummy, however it can be called by option in order to compute absolute intensities from the relative intensities by coding the desired functions which are used to make the efficiency corrections.
- Function PEST - This function simply provides a conversion term for the position and width parameters used for each peak. It requires change if THEORY is modified.

VII. Functional Representation of Peaks and Background Continua

The analytical function which is currently used in GSSLRN-II for analysis of fission-product spectra is one which establishes a compromise between accuracy, quality, and simplicity so as to ensure the user consistent results.

Two basic assumptions are made with respect to the current function in the code which is used for analyzing spectra obtained by gamma-scanning techniques.

1. The background continuum is expressed as a quadratic function. This is not unrealistic so long as the interval-

of-fit is consistently maintained so as to ensure that it does not rob any appreciable amount of intensity from the peak shape.

2. The peak shapes are represented as symmetrical Gaussian distributions. This form does not truly represent photopeaks but it does allow the data to be fit well under adverse conditions.

The analytical function used for the analysis of photopeaks is described by the following:

$$N(X) \cong A_1 + A_2 + A_3 X^2 + \sum_{\substack{JJ \leq 49 \\ i = 4,7,10,13,\dots}} A_i \exp [-1/2(A_{i+1}X - A_{i+2})^2]$$

where

A_1 , A_2 , and A_3 are the quadratic function coefficients (background),

A_i is the amplitude of each photopeak,

σ_i is a function of the width of each i th peak,

$A_{i+1} = 1/\sigma_i$ for each i th peak, and

$A_{i+2} = X_i/\sigma_i$ where X_i represents the mean position of the i th peak.

Another example for which GSSLRN-II has been applied is the analysis of Mössbauer spectra. In this problem the analytical function is expressed as a quadratic plus the sum of Lorentzian terms which is shown as

$$N(X) \equiv A_1 + A_2 X + A_3 X^2 + \sum_{\substack{JJ \leq 49 \\ i=4,7,10,13,\dots}} \frac{A_i}{1 + A_{i+1} (X - A_{i+2})^2}$$

where

A_1, A_2 , and A_3 are the quadratic function coefficients (background),
 A_i represents the amplitude of each Lorentzian peak,
 A_{i+1} is a function of the full-width-at-half-maximum, and
 A_{i+2} is the mean value of each Lorentzian peak.

GSSLRN-II has been used extensively with both of the above analytical forms. The recycling and fitting logic has performed well even when the FWHM parameters for the Lorentzian function were factors of as much as 500% different for peaks within the same interval-of-fit.

VIII. Least-Squares Recycling

Typically, least-squares fitting of multiple (overlapping) peaks has presented problems which at best have been only partially solved. Within the GSSLRN-II code, there are two subroutines, WIT and WITTY, which are used to attempt to determine if recycled least-squares attempts should be made. Their functions are as follows:

Subroutine WIT is executed after each least-squares fit. Its primary function is twofold:

- (a) It investigates the properties from each fit such as saddle points, goodness-of-fit, meaningful parameters, and spurious or unreal peaks.

- (b) If the conditions in (a) are conclusive enough, subroutine WIT will eliminate doubtful peaks from the interval of fit and cause a recycle attempt on the remaining peak(s) until all peaks are considered acceptable. If necessary the initial interval-of-fit will be modified to one which is more realistic for a fewer number of peaks if any have been eliminated.

Subroutine WITTY is called after the doubtful peaks have been eliminated in WIT. This routine contains the tests necessary to determine if the peak group might possibly contain hidden or unaccounted for peaks. The criteria for determining the existence of hidden peaks are under user control and can therefore be restrained or relaxed to any level which the user feels is appropriate.

There are two tests which must be satisfied in subroutine WITTY in order to allow a recycle attempt with additional peaks.

The first test is one which requires a search of the relative magnitudes of the deviations of each measurement from the least-squares fitted value. (i.e. $(Y - Y_m) * \sqrt{W_m}$, where Y and Y_m represent the fitted value and the measured value, respectively, and W_m represents the weighting function).

After the magnitudes of the deviations are computed, subroutine WITTY will then test the set of deviations to locate a minimum number of them (in sequence, and under user control) which are large enough to suggest the presence of a hidden peak. To test the deviation requirement criteria, the value T_m is computed which is

$$T_m = [((Y - Y_m) * \sqrt{W_m}) + \text{AMIN}(99) * \sqrt{Q}]$$

and

Q = goodness-of-fit (measurement variance) resulting from the least-squares fit, and

AMIN(99) = an input value used to determine a multiple of the measurement variance.

If $T_m \leq 0$, then the first test is satisfied and the particular data point, m, is flagged as one of a series of possible candidates for suggesting the presence of a hidden peak.

When the first test has been satisfied, then subroutine WITTY will demand a second test on the least-squares fit which must be satisfied before any peak(s) is allowed to be artificially built-in. This second test is used as justification of an attempt to improve the recycling decision analysis to a level which is statistically significant.

The code, GSSLRN-1⁽¹⁾, relies upon a test of the measurement variance, but suffers from lack of significant interpretation in order to discern if a recycling attempt is justified. Therefore, the following discussion is directed toward making use of the measurement variance (within GSSLRN-II), in a way which will allow the code to establish sufficient significance to the measurement variance in order to discern with added reliability whether or not the results are useful and/or meaningful.

Since the measurement variance is defined as $\sigma^2 = Q/(M-J)$ we can express its expected value as

$$\left\langle \frac{Q}{M-J} \right\rangle \doteq 1.0 \pm \sqrt{\frac{2}{M-J}} \quad (6)$$

From eq. (6), we have established a quantity which can be used as a limiting criteria for justifying a recycle attempt.

However, in practice eq. (6) is modified within GSSLRN-II to allow the user to intervene and dictate the potential worth of the test by the use of a multiple factor as input. The result becomes a test of the error implied in eq. (6) which has the following form:

YEXP = multiple factor mentioned above

If $\left[(\sigma^2 - 1)^2 > \left(\frac{2 * YEXP}{M - J} \right) \right]$, then the code will assume it has sufficient justification to postulate the success of a recycled least-squares fit with more peaks having been identified.

The two basic tests, discussed above, have been used very successfully in order to allow the code maximum resolution of multiplets. They are not intended as final judgement for any least-squares fit, but instead are used as an important step which allows the logic of the code to be fluid enough to process entire sets of spectra with minimal intervention by the user.

IX. GSSLRN-II FLOWCHART (MAIN PROGRAM LIKELY)

The following represents a brief flow chart of the main program, LIKELY. The intent is to give the user a brief idea of the general flow of the code.

X. Input Instructions

Although the code GSSLRN-I⁽¹⁾ has been updated, the input instructions which are used with GSSLRN-I can also be used in GSSLRN-II. Any and all additional input which results from the updated version GSSLRN-II is strictly optional. However, in order to eliminate any misunderstandings, the entire list of input instructions are listed.

<u>Code Limitations:</u>	<u>GSSLRN-I</u>	<u>GSSLRN-II</u>
Number of peaks/fit	10	15
Number of channels/fit	250	500
Total peaks/case	200	100
Total channels/case	2048	2048

The input variables used in GSSLRN-II are supplied with the use of an input utility package, NAMELIST⁽⁵⁾, which is available with most FORTRAN V compilers. Knowledge of NAMELIST and its use or replacement is assumed.

<u>NAME</u>	<u>DESCRIPTION</u>
IMIN	Defines the beginning channel number for the analysis of a case. ($1 \leq \text{IMIN} < 2048$)
IMAX	Defines the last channel number for the analysis of a case. ($\text{IMIN} < \text{IMAX} \leq 2048$ when NPAP $\neq$ -2 or -3) ($\text{IMIN} < \text{IMAX} \leq 4096$ when NPAP = -2 or -3)
NPAP	A control integer which is used to identify major options of execution. = -3; 3-dimensional perspective plots can be generated for a CALCOMP plotter. No axis labels or identification are supplied on the plots.

NAME

DESCRIPTION

- = -2; 2-dimensional perspective plots can be generated for a CALCOMP plotter. Complete titles and plot labeling must be supplied by the user.
- = -1; On-line printer plots are supplied with each interval-of-fit throughout the least-squares analysis. The measured data (*) and the fitted curves (-) are printed for each channel within the interval.
- = 0; A least-squares analysis is done, as in the NPAP = -1 option. However, no plotting is done as it is replaced with the theory-measurement correlation for each measurement.
- = 1; A least-squares analysis is done, complete with CALCOMP plots for each successfully fitted interval, which displays the measurements, measurement uncertainties, the best fit and its root-mean-square deviation envelope, each resolved peak shape excluding the background contributions, and fitted numerical quantities such as the mean, FWHM, net area, and energy or amplitude of each peak.
- = 2; Only least-squares output is obtained. No plotting of any kind is attempted.

LIP

A control feature used to designate the output results as they are defined with the NPAP options or to suppress the majority of output into a mini-edit form. This feature is useful when receiving output on a remote teletype terminal.

- = 0; All above NPAP options are available as described.
- = 1; All above NPAP options are available, but the printout is in a mini-edit suppressed form. LIP is preset to zero.

The following three variables INTEG, LENT, and FWHM are used to identify and optimize the peak search analysis if and when it is used. The peak search, when optimized, can be very effective in locating peaks from the data spectrum. It provides an attempt at recovering the mean-position, an approximated relative area, and an estimate of the starting and ending channels which are used to identify the initial interval-of-fit for each of the peaks it locates.

INTEG = $\pm n$, where n represents the number of times the measured data is to be smoothed for the peak search.

= $-n$; the user may execute successive cases for the same spectrum in order to optimize INTEG without supplying the spectrum more than once. No least-squares analysis is allowed as long as $\text{INTEG} = -n$.

= $+n$; then n smoothes will be applied to the data after which the least-squares analysis will begin.

Optimum values for INTEG are usually 4 or 5. INTEG is preset to 4.

LENT Defines the number of channels to be used for each smooth. LENT may be optimized by allowing INTEG to be negative.

Optimum value for LENT is usually $\pm 0.6 * \text{FWHM}$. LENT is preset to 3.

FWHM Except in runs where the peak search is overridden, FWHM is an estimate of the full-width-at half-maximum for all of the peaks.

In cases where the FWHM varies from peak to peak by large amounts, the widths are supplied by other means, as will be explained later.

FWHM is preset to 3.0.

Note: If $\text{INTEG} < 0$ and $\text{NPAP} = -2$ or -3 , then a peak search and a CALCOMP spectrum plot can be obtained.

Additional input variables are supplied which allow the user an override feature for the specified initial interval-of-fit, the sensitivity of locating hidden peaks (peaks not defined via input or the peak search), and use of a normalization quantity. They are as follows:

- AMIN(97) Defines the initial interval-of-fit for each peak. (i.e. $\bar{X}_i \pm \text{AMIN}(97) * \text{FWHM}$ in channels).
Preset AMIN (97) = 3.0
- AMIN(98) This quantity, combined with the test on AMIN(99), defines the minimum number of required deviations ($Y_{\text{calc.}} - Y_{\text{meas.}}$) which must occur sequentially, with the same algebraic sign in order to validate the location of hidden peaks.
Preset AMIN(98) = 2.0
- AMIN(99) Defines the minimum allowable rms deviation multiple in order to establish a limiting criteria for hidden peaks.
Preset AMIN(99) = 1.0
- YEXP Defines the minimum allowable multiple of the measurement variance which is used to allow a search for a hidden peak.
Preset YEXP = 50.0
- AMIN (100) If used, AMIN (100) defines the value about which all the resultant intensities are normalized. If not used, the largest intensity of the case is used for the normalization.
Preset AMIN (100) = $1. \times 10^6$

The following two variables, UGEN and UEXP, can be used to convert channel number to energy. At present this conversion assumes $E = \text{UGEN} * (\text{channel number}) + \text{UEXP}$.

<u>NAME</u>	<u>DESCRIPTION</u>
UGEN	Defines the slope coefficient. Preset UGEN = 1.0
UEXP	Defines the displacement coefficient. Preset UEXP = 0.0
C(1), C(2)	These quantities may be used to overload the use of FWHM so far as making estimates of the widths of peaks is concerned. They represent the slope and intercept, respectively, of the conversion necessary when calibrated peaks may have already been fitted. Preset C(1) = C(2) = 0.0
C(3)	A normalization constant which can be used to adjust the scale of the measurement spectrum. This is usually used when generating 3-dimensional plots (NPAP = -3). exp. $Y_m = Y_m * C(3)$ Preset C(3) = 1.0.
C(4)	Another constant which is used when NPAP = -3. It represents the angle of decline for the X-axis of the spectrum. The user must input C(4) as the tangent of the angle of declination. Preset C(4) = 0.0.
C(5)	This quantity is used to define the multiple of the FWHM that is used to help select peak groupings within the same interval-of-fit. (i.e. Peaks whose mean channels are within C(5) * FWHM channels are initially considered within the same fit. Preset C(5) = 3.5

<u>NAME</u>	<u>DESCRIPTION</u>
C(6)	Used within the same context as C(5), except that it defines the minimum relative percentage area allowed in order for a peak to be considered within the same interval-of-fit as its neighboring peaks. Used only with the peak search. Preset C(6) = 0.03 or 3% relative area.
C(7)	<p>If multiple peaks are defined within the same interval-of-fit, C(7) is used to help decide if the peaks should be fitted separately, where possible.</p> <p>(e.g. If $\left\{ \left \bar{X}_i - \bar{X}_{i+1} \right \geq C(7) * FWHM \right\}$, and if $\frac{Area_{i+1}}{Area_i} < C(6) * Area_i$, then the interval-of-fit is appropriately split. Preset C(7) = 1.75</p>
C(8), C(9), C(10)	<p>Define the estimates of the 3-term quadratic which describes the current background continuum. Necessary input when the value LOT(11,9) $\neq$ 0.</p> <p>Preset C(8) = C(9) = C(10) = 1.0</p>
<p>For generalization purposes, the values LOT(1,2) and LOT(2,2) are used to define the character of the analytic function.</p>	
LOT(1,2)	<p>Defines the number of fitting parameters present to describe the background continuum.</p> <p>Preset LOT(1,2) = 3.</p>
LOT(2,2)	<p>Defines the number of fitting parameters used to describe each peak shape.</p> <p>Preset LOT(2,2) = 3.</p>

The following list of input variables, LOT(1,9) - LOT(22,9), are all optional with the exception of LOT(1,9) through LOT(6,9). These LOT variables are particularly valuable when the user wishes to identify a specific set of data to be analyzed and which will not utilize the normal logic path of the code.

<u>NAME</u>	<u>DESCRIPTION</u>
LOT(1,9)	Identifies the first channel of data to be read from cards, tape, or drum. Preset LOT(1,9) = 1
LOT(2,9)	Identifies the last channel of each data block, card, or record. Preset LOT(2,9) = 10
LOT(3,9)	Identifies the total number of data blocks, cards, or records. Preset LOT(3,9) = 50
LOT(4,9)	Identifies an integer value which can be used to shift the fitted means of the peaks. This is done only on the summary of fitted results. Preset to zero, not required input.
LOT(5,9)	An integer used to identify the columnar output of the results. = 0; then a 72 column output format is used for teletype printout. (For use with mini-edit only). = 1; then the normal 132 column output for UNIVAC-1108 format is used. Preset LOT(5,9) = 1.

<u>NAME</u>	<u>DESCRIPTION</u>
LOT(6,9)	<p>Logical unit specification for inputting the spectrum measurements.</p> <p>= 5; cards are used for the input media.</p> <p>= 1, 4, 7, 9, 10, 11, 12, 13, or 15; magnetic tape is the input media.</p> <p>= 25, 26, 27, 28, or 29; DAT elements on cards or magnetic tape are stored as data elements on drum and then used as the input media.</p> <p>Preset LOT(6,9) = 5</p>
LOT(7,9)	<p>Used when NPAP = -2, or -3 only. Defines a factor which determines the length of the abscissa of a CALCOMP plot when the input value KK = -1 is used. Preset to 10. <u>exp.</u></p> <p>LOT(7,9) = 10 yields a plot of 2100 data points which is 21" along the abscissa.</p> <p>LOT(7,9) = 20 yields a plot of the same data, except it would be 42" along the abscissa.</p> <p>i.e., x-axis length (inches) = $(IMAX-IMIN+1) * LOT(7,9)/1000$.</p>
LOT(8,9)	<p>Control integer.</p> <p>= 0; no change in the program logic.</p> <p>= 1; then the input spectrum will be refreshed at the end of each case and can be used for subsequent cases. Preset to zero.</p>
LOT(9,9)	<p>Control integer.</p> <p>= 0; no change in the spectrum input logic.</p> <p>= 1; then an identification integer is required at the beginning of each set of spectrum measurements. Preset to zero.</p>

<u>NAME</u>	<u>DESCRIPTION</u>
LOT(10,9)	<p>Control integer.</p> <p>= 0; no change in the output logic.</p> <p>= 1; then punched card output is obtained which yields some of the quantities normally obtained in the summary of fitted results. Preset to zero.</p>
LOT(11,9)	<p>Control integer.</p> <p>= 0; no change.</p> <p>= n, ($0 < n \leq 15$); then n defines the number of peaks which are to be fit as a special case. In this case the user must input the values C(8), C(9), C(10), and C(50) through C(79). LOT(11,9) preset to zero.</p> <p>C(50) - C(64) - Represent estimates for the mean of each peak.</p> <p>C(65) - C(79) - Represent estimates for the width of each peak.</p> <p>The numbers for C(50) - C(79) override any previous estimates of FWHM.</p>
LOT(12,9)	<p>Control integer.</p> <p>= 0; no change.</p> <p>= n, ($0 < n$); then n represents the number (or pseudo count) that all the spectrum measurements are subtracted from. This feature allows the user to invert his spectrum such as is often the case when attempting to analyze Mössbauer Spectra. Preset to zero.</p>

NAME

DESCRIPTION

LOT(13,9)

Defines the CALCOMP plotting density of the measurements along the abscissa when NPAP = 1. LOT(13,9) preset to 200.

Example of use:

LOT(13,9) = 200 yields 5 points per inch.
 LOT(13,9) = 100 yields 10 points per inch.
 LOT(13,9) = 50 yields 20 points per inch.
 etc.

LOT(14,9)

Control integer.

= 0; no change.

= 1; then the user will initialize a call to subroutine EFFICY where he may compute and correct for the efficiency of his detector system and apply this correction to the fitted intensities. Currently, EFFICY is a dummy routine which needs to be supplied by the analyst. Preset to ZERO.

LOT(15,9)

Control integer.

= -1; no change, the code chooses the iteration limit.

≠ -1; then LOT(15,9) defines the iteration limit of the least-squares fits. LOT(15,9) preset to -1.

LOT(16,9)

Control integer.

= 0; no change in the printout.

≠ 0; then a fit of the resultant widths versus means is done using a straight line approximation. This fit is printed out the same as if NPAP = -1. LOT(16,9) is preset to zero.

LOT(17,9)

Control integer which is used for special "one fit" cases.

= 0; not inacted.

≠ 0; then it allows a preliminary fit to the background continuum. This obviously requires that enough measurements be present which are not influenced by any of the peaks. In addition, some further input is required.

Preset LOT(17,9) = 0.

The following represents the additional input; JJ = the number of parameters describing the background (JJ = LOT(1,2)).

LOT(3,2) = the number of pairs of channel numbers being specified to identify the background continuum.

LOT(4,2), (5,2) . . . = identify the first and last channel of each pair, all of which are included in the fit.

LOT(18,9)

Control integer to define piecemeal fitting.

= 0; not inacted.

≠ 0; then it allows the analyst to fit only those channels of data for which he specifies. No recycled attempts at least-squares are allowed. The following additional quantities are required:

Preset LOT(18,9) = 0

LOT(3,2) = identifies the number of pairs of sequential channels to be used in the least-squares fit.

LOT(4,2), (5,2) . . . identify the pairs by selecting the first and last channels denoted.

LOT(19,9)

Peak search overload option.

- = 0; then the peak search identified by INTEG and LENT is used.
- = $n(0 < n \leq 100)$; then n identifies how many peaks are being specified for the spectrum. Some additional input is as follows;
LOT(1,3) --- LOT(50,3) and LOT(1,4) --- LOT(50,4) are used to identify the approximate mean positions of each peak specified by LOT(19,9).
Preset LOT(19,9) = 0.

LOT(20,9)

Recycle control limit.

- = 0; no recycling of least-squares is allowed.
- = n ; then $n+1$ recycle attempts will be allowed depending upon whether or not the criteria for locating hidden peaks are met.
Preset LOT(20,9) = 1

LOT(21,9)

Defines the minimum measurement count level for establishing and accepting peaks located by the peak search.
LOT(21,9) preset to 10 counts per channel.

LOT(22,9)

CALCOMP control integer.

- = 0; energies are printed on the plots.
- ≠ 0; amplitudes of the peaks are printed on the plots. Used only when NPAP = 1.
Preset LOT(22,9) = 0.

• Optional Input

The following input variables are required when using any CALCOMP plotter options.

<u>NAME</u>	<u>DESCRIPTION</u>
MAP	<p>Due to the automated plotting specialties written for GSSLRN-II, the function of MAP has been limited from that which it was normally used in program LEARN⁽²⁾ to the following choices:</p> <ul style="list-style-type: none">= 0; No plotting will be attempted.= -1; and NPAP $\neq$ -2, plots for each successfully fitted peak will be generated.= -1; and NPAP = -2, plots of measured spectrums may be generated. <p>Preset MAP = 0.</p>
FCTR	<p>This is a special scaling feature which allows the user to magnify or reduce the total size of any desired graph.</p> <p>Preset FCTR = 1.0.</p>
NPLOT	<p>NPLOT specifies one of two scaling choices.</p> <ul style="list-style-type: none">= 1; Semi-logarithmic scales are generated.= 2; Linear scales are generated. <p>Preset NPLOT = 2.</p>
MARK	<p>This quantity specifies which CALCOMP symbol is to be used to symbolize the measured data.</p> <p>When NPAP $\neq$ -2, MARK must be positive in value.</p> <p>When NPAP = -2, refer to "Special Features".</p> <p>Preset MARK = 1.</p>
CYCLE	<p>This quantity specifies the maximum height, in inches of each plot.</p>

<u>NAME</u>	<u>DESCRIPTION</u>
	When NPAP $\neq$ -2; $2 \leq \text{CYCLE} \leq 29$ When NPAP = -2; refer to "Special Features" Preset CYCLE = 10.0.
KK	KK is a control integer used to specify automatic scale features. When NPAP $\neq$ -2, KK = 1. Not required input. When NPAP = -2, refer to "Special Features". Preset KK = 1
LINE	Control integer for NPAP = -2 option; refer to "Special Features." When NPAP $\neq$ -2, LINE = 2. Not required input. Preset LINE = 2.

- Special Features

The following list of input variables have special functions which are available when NPAP = -2.

<u>NAME</u>	<u>DESCRIPTION</u>
MAP	MAP = -1 is mandatory for each case.
MARK	This quantity specifies which CALCOMP symbol is to be used to symbolize the measured data. MARK may be positive or negatively valued. If MARK = + in a successive case execution, each case (or spectrum) will be plotted individually. If MARK = -, then each successive plot of a spectrum will be superimposed on the same graph up to and including the case where MARK = +.

<u>NAME</u>	<u>DESCRIPTION</u>
KK	<p>This is a control integer used to specify automatic scaling.</p> <ul style="list-style-type: none"> = 1, then no automatic scaling is attempted, and the variable ZDZSDS is required input data. = -1; then the program will automatically scale each plot and the variable ZDZSDS is not required.
LINE	<p>This is a control integer used to specify line or symbol plots.</p> <ul style="list-style-type: none"> = 2, yields a plot with lines drawn between each data point. = -2, yields a plot with only data symbols.
CYCLE	<p>Maximum height of plot, in inches.</p> <p>If KK = 1 and NPLOT = 1, then CYCLE defines the height in inches of each logarithmic cycle.</p> <p>If KK = 1 and NPLOT = 2, then CYCLE has no function.</p> <p>If KK = -1 and NPLOT = 2, then CYCLE defines the maximum height in inches of the total graph.</p>
TITL1(1) = 54H TITL2(1) = 54H TITL3(1) = 54H TITL4(1) = 54H	<p>These four input quantities are available so as to specify four lines of alpha-numeric information which identifies each spectrum plot. They are plotted in the lower left corner of each graph.</p>
ZDZSDS	<p>These quantities are used to specify plotting ranges.</p> <p>= ZDZSDS (L, K, M); L=1, 6; K=1, 2 ; M=1.</p> <p>If KK = -1, these quantities are not required input. Otherwise, they are used in the following manner:</p>

Example for a plot ranging from 1 to 1×10^6 on the Y-axis over a span of 24 inches and the X-axis ranging from 0 to 4096 channels over a span of 40.96 inches.

Y-axis definition when NPLOT = 1.

ZDZSDS(1,1,1) = 1., 0., 1. + 6, 0., 0., 24000.,

Y-axis definition when NPLOT = 2.

ZDZSDS(1,1,1) = 0., 0., 1. + 6, 0., 0., 24000.,

X-axis definition:

ZDZSDS(1,2,1) = 0., 0., 4096., 0., 0., 40960.,

The second and fifth values for each axis card are always zero.

The following list of input variables have special functions when NPAP = -3.

<u>NAME</u>	<u>DESCRIPTION</u>
MAP	= -1, mandatory.
MARK	No function.
KK	= 1, mandatory
LINE	Same use as when NPAP = -2
CYCLE	Same use as when NPAP = -2, except KK = +1 is required.
TITL1 TITL2 TITL3 TITL4	Non-functional
ZDZSDS	
FCTR	
NPLOT	

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XII. References.

1. G. D. Seybold, "GSSLRN-I, An Automated Least-Squares Computer Code For the Analysis of Photopeak Spectra", BNWL-1227, November 1969.
2. B. H. Duane, "Maximum Likelihood Nonlinear Correlated Fields (BNW Program LIKELY)", BNWL-390, September 1967.
3. G. D. Seybold, "Users Aid Programs LEARN and LIKELY", BNWL-1057, May, 1969.
4. M. Mariscotti, "A Method for Automatic Identification of Peaks in the Presence of Background and its Application to Spectrum Analysis", Nucl. Inst. Methods, 50(1967) 309-320.
5. NAMELIST, UNIVAC-1108 Programmer Reference Manual, Fortran V, UP-4060, Section 7, pg. 12-15.

XIII. Input Sample

The following example represents input for a sample problem for GSSLRN-II for the UNIVAC-1108 system. The sample problem is one which demonstrates the required input for analysis of a portion of a fission product gamma scan. The approximate means of the peaks of interest are specified and the options are exercised which will yield a CALCOMP plot of each least-squares fit.

```
'O RUN      8,CUBXXX,,180,5100      GD SEYBOLD (GSSLRN-II TEST CASE)
'X  ASG,R A=U0975
'  ASG,W H=(,NH,AT)      'NECESSARY FOR CALCOMP PLOTS.
'  MSG **CALCOMP PLOTTER INSTRUCTIONS, IF USED**
'  XQT CUR
IN A
TRI A
'  XQT GSSLRN
$LEARN
  IMIN=424,      IMAX=1130,      INTEG=4,      LENT=3,      FWHM=4.,
  AMIN(97)=3.,  2.,  1.,      NPAP=1,      YEXP=50.,
  MAP=-1,      NPLOT=2,      MARK=1,      CYCLE=10.,      KK=1,      LINE=2,
  LOT(1,9)=1,256,8,0,1,5,10,0,0,0,0,0,200,0,-1,1,0,0,24,2,10,0,
  LOT(1,3)= 455, 468, 552, 567, 580, 603, 634, 659, 689, 697, 724, 737,
           794, 804, 821, 852, 905, 912, 953,1024,1056,1064,1083,1092,
$
C  DATA SPECTRUM GOES HERE.
' FIN
```

Expected execution time will range from one to six seconds per peak, depending upon the frequency of hidden peaks and the amount of CALCOMP plotting required.

XIV. Appendix

Illustrations of Plotting Options

The following list of figures will refer to some of the different types of plotting features which are available within the code.

- Figure 1 These two plots, A and B, represent output from the least-squares fitting option (NPAP=1) where the measurements were fitted using Gaussian forms. It also demonstrates the relative additional power of doing second order least-squares fits.
- Figure 2 This plot is shown only as a demonstration of use for the option (NPAP = -3)
- Figure 3 This plot represents a set of synthetically computed measurements, with known parameters. The least-squares fitting process was allowed twenty-five iterations as an approach to verify that the iterative scheme of the code can result in the unique set of parameters. The analytical form is a composite of Lorentzian peak shapes.
- Figure 4 This plot represents a least-squares fit to a set of Mossbauer data using Lorentzian peak shapes. It is shown only to demonstrate the option (NPAP=1) while making use of a special case run.

FIGURE 1A

COMPARISON OF FIRST VERSUS SECOND ORDER FITTING

FIGURE 1B

FIGURE 2

FIGURE 3

FIGURE 4

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