A COMPUTER ANALYSIS OF COMPLEX
GAMMA-RAY SPECTRA

APPROVED:

Bruce P. Forster
Major Professor

John F. Malat
Minor Professor

Director of the Department of Physics

Robert B. Toro-loz
Dean of the Graduate School
A COMPUTER ANALYSIS OF COMPLEX GAMMA-RAY SPECTRA

THESIS

Presented to the Graduate Council of the North Texas State University in Partial Fulfillment of the Requirements

For the Degree of

MASTER OF SCIENCE

By

William K. Cunningham
Denton, Texas
August, 1965
# TABLE OF CONTENTS

List of Illustrations ........................................ iv

Chapter

<table>
<thead>
<tr>
<th>Chapter</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>I. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>II. PROBLEM STATEMENT</td>
<td>6</td>
</tr>
<tr>
<td>III. MATHEMATICAL DISCUSSION</td>
<td>9</td>
</tr>
<tr>
<td>IV. COMPUTER PROGRAMS</td>
<td>16</td>
</tr>
</tbody>
</table>

Appendix .................................................. 55

Bibliography ............................................... 58
# LIST OF ILLUSTRATIONS

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Decay Scheme of Ba$^{137}$</td>
<td>3</td>
</tr>
<tr>
<td>2.</td>
<td>Plot of Equation 1-1</td>
<td>4</td>
</tr>
<tr>
<td>3.</td>
<td>Altered Na$^{22}$ Spectrum</td>
<td>23</td>
</tr>
<tr>
<td>4.</td>
<td>Artificially Produced Co$^{60}$ Spectrum</td>
<td>24</td>
</tr>
<tr>
<td>5.</td>
<td>Co$^{60}$ Spectrum</td>
<td>47</td>
</tr>
<tr>
<td>6.</td>
<td>Cs$^{137}$ Spectrum</td>
<td>48</td>
</tr>
<tr>
<td>7.</td>
<td>Mn$^{54}$ Spectrum</td>
<td>49</td>
</tr>
<tr>
<td>8.</td>
<td>Na$^{22}$ Spectrum</td>
<td>50</td>
</tr>
<tr>
<td>9.</td>
<td>Complex Spectrum</td>
<td>51</td>
</tr>
<tr>
<td>10.</td>
<td>Complex Spectrum</td>
<td>52</td>
</tr>
<tr>
<td>11.</td>
<td>Plot of Each Term of Equation 3-3</td>
<td>53</td>
</tr>
<tr>
<td>12.</td>
<td>Plot of Residuals in Mn$^{54}$ Peak Region</td>
<td>54</td>
</tr>
</tbody>
</table>
CHAPTER I

INTRODUCTION

In recent years there has been much progress in developing theoretical and mathematical descriptions of the atomic nucleus. The innovations brought about by quantum mechanics have been used in conjunction with various nuclear models in an attempt to construct a mathematical formulation which will encompass all available information about the atomic nucleus.

The true test of any physical theory is that it predict the nature of physical phenomena under given conditions, as well as account for all existing data. In the search for a workable theory, it is necessary to know exactly in what area and under what conditions a mathematical formulation is valid and where it fails. To this end, large amounts of nuclear data and information must be collected.

One of the principal methods of determining properties of a particular nucleus is that of gamma-ray spectroscopy. As is dictated by quantum mechanics, every atomic nucleus exists in various discrete energy levels. The levels above the ground state are unstable, and a nucleus may lose all, or part, of its excess energy in the form of electromagnetic radiation. The analysis of this radiation is used principally to determine such properties of a particular nuclear
level, or isomer, as its parity, energy, total angular momentum, and orbital angular momentum; as well as probabilities of transition between two levels.

The transition probabilities are dependent upon the other properties, and therefore their determination can be very important is assigning various quantum number values to a particular level. Also, these probabilities are in themselves of considerable interest.

The probability of transition, or de-excitation, of a nuclear level is directly related to the mean life and half life of the level; and any one of these values may be determined to fix the values of the others.

The following is an example of the use of the mean life of a level to determine the relative, and even absolute, angular momentum, $I$, of the level. The diagram shown on the next page represents the ground state and an excited state of Ba$^{137}$. The excited level, with 0.6616 MeV more energy than the ground state, emits this energy in the form of a gamma ray and becomes the stable isomer of Ba$^{137}$. From various experiments, it has been determined that the mean life of the excited state is 2.6 minutes and that the ground state has an angular momentum of $3/2$.

Suppose that the gamma ray emitted is electric multipole radiation of order $2^L$; then Weisskopf has shown that the mean life of an excited level can be accurately represented by the relation
where $\bar{\tau}$ is the mean life, $L$ is the exponent in the radiation order, $S$ is a statistical factor involving $L$, $A$ is the mass number of the nucleus, $W$ is the energy of the emitted gamma ray in Mev, and $R_0$ is the characteristic nuclear radius.\(^1\)

Equation 1-1 is plotted for various values of $L$, $A$, $\bar{\tau}$, and $W$ in Figure 2. From this graph, it is seen that a mean life of 2.6 minutes and a gamma energy of 0.6616 Mev dictate that the emitted radiation be of multipole order 2\(^4\).

![Figure 1—Decay scheme of Ba\(^{137}\)](image)

The change in angular momentum in an isomeric transition, $\Delta I$, is almost always equal to the value of $L$ of the emitted radiation.\(^2\) In the case of Ba\(^{137}\), $\Delta I$ must be 4 and the angular momentum of the excited state is therefore $3/2$. In confirming angular momentum assignments and determining other


Figure 2—Plot of Equation 1-1
properties of the level, various other types of experimental measurements may be used.

Often, the mean life of a level is not easily determined. However, the relative transition probabilities of two separate transitions can be determined by observing the relative intensity of the two gamma radiation modes. This method will be enlarged upon in the next section.
CHAPTER II

PROBLEM STATEMENT

If a material is naturally radioactive, those levels that are involved in the radiation can be studied quite easily. If, however, nuclear levels other than those found excited naturally are of interest, they must be excited by some artificial means. One such method is that of bombarding the material with neutrons. The number of levels thus produced is dependent upon the energy of the incident neutrons and, if the energy is sufficient, several excited levels may be produced.

In detecting and analyzing gamma radiation, a multichannel analyzer is usually used. The output of the analyzer is the energy spectrum of the events caused in the detecting crystal by the gamma rays. The spectrum of a single type of gamma ray is shown in Figure 6. This shape is typical for gamma rays having energies between .5 and 1.5 Mev. If there are two gamma rays being simultaneously detected by the crystal, the result is a spectrum as shown in Figure 5. The energy at which the sharp peaks fall is the energy possessed by the gamma ray. In Figure 6, the height of the peak and the number of events counted represent the intensity of the transition. These sharp peaks are caused by the photoelectric
effect in the detecting crystal. The broad peak that falls about channel 130 is caused by compton scattering within the detecting crystal. If two such spectra of different gamma rays are observed over the same time period, using the same detecting apparatus, the relative heights of the peaks represent the relative intensities of the two gamma rays. However, in a spectrum such as in Figure 5, the number of counts in the channels at which the lower energy peak falls includes counts due also to the higher energy gamma ray. Due to this fact, the relative heights of these two peaks do not represent the relative intensities of the two transitions. To determine the relative intensities, other means must be used.

If more than one isotope is present in the material being bombarded by neutrons, and if several levels of the material are excited, then the spectrum becomes increasingly complex. The purpose of this investigation was to provide a method for determining the relative intensities of all gamma rays in a particular spectrum, and thereby determine the relative transition probabilities.

For this purpose, it may be noted that the spectrum of Figure 5 can be regarded as simply the sum of two spectra such as shown in Figure 6. Such a condition is true in general for all complex spectra. It is also true that the shape of a gamma-ray spectrum due to a single type of transition is constant for a given energy, providing the detecting apparatus and apparatus geometry is not changed in any way.
Therefore, if the shape of a gamma-ray spectrum of any energy can be determined, the shape of any of the "component" spectra may be artificially produced immediately. This statement is based upon the assumption that one knows the energies of the gamma rays present. All of these curves may be fitted to the complex curve by a least-squares process, yielding the height of the peaks of each component spectrum. The relative transition probabilities may then be obtained from the relative intensities of the component spectra.

It is desired, then, to facilitate this process by the use of a computer. The spectrum composed of several gamma rays and the component spectra may be used as the computer input so that one may fit the component spectra to the complex spectrum by a least-squares process, using a computer program, and obtain the relative amounts of each component spectrum present in the complex spectrum. Other computer programs can be used to perform most of the associated processes.
CHAPTER III

MATHEMATICAL DISCUSSION

In obtaining component spectra, the intensity of the spectrum may be arbitrarily assigned. Coefficients may then be determined, which, when multiplied by the number of counts in each channel, yield the actual number of counts in the complex spectrum due to a particular gamma ray.

Consider four arbitrary curves. It is desired to determine coefficients for three of the curves so that their sum closely approximates the fourth curve, called the complex curve.

Designate these coefficients $a_1$, $a_2$, $a_3$. Designate the number of counts assumed for each channel of each curve as $x(I,J)$, and as $y(J)$, or

$$x(I,J) = \text{no. of counts in } I^{th} \text{ channel of } I^{th} \text{ component curve}$$

$$y(J) = \text{no. of counts in } J^{th} \text{ channel of complex curve}$$

Then the residual in the $J^{th}$ channel is

$$R_J = a_1 x(I,J) + a_2 x(2,J) + a_3 x(3,J) - y(J) \quad ; \quad 3-1$$

or, for $k$ curves,

$$R_J = \frac{\sum_{I=1}^{k} a_I x(I,J) - y(J)}{k} \quad ; \quad 3-2$$
In order to determine coefficients, \(a_1, a_2, \ldots, a_k\), such that the sum of the squares of the residuals, divided by their statistical weights, is a minimum, consider the function,

\[
 f(a_1, a_2, a_3) = \frac{R_1^2}{Y(1)} + \frac{R_2^2}{Y(2)} + \cdots + \frac{R_n^2}{Y(N)} \tag{3-3}
\]

for \(n\) channels. It will be noted that the square of each residual has been divided by a weighting factor, the number of counts in the complex curve. Suppose that in one channel of the complex spectrum there are 10,000 counts and 100 in another. These numbers are subject to a statistical error on the order of the square root of the number of counts. Therefore, the counts in the two channels are actually 10,000 \pm 100 and 100 \pm 10. This means that a residual of 100 counts in the first channel is no worse than a residual of 10 counts in the second, and the two residuals should be weighted equally in the process of minimizing. It can be easily seen that Equation 3-3 accomplishes this requirement.

For this discussion, the statistical error in the component spectra will be ignored, since one may reduce this error considerably by using a very long counting time when the component spectra are obtained. For the function in Equation 3-3 to have a minimum value, the following set of equations must be satisfied.

\[
 \frac{\partial f}{\partial a_1} = 2 \left[ \frac{R_1}{Y(1)} \frac{\partial R_1}{\partial a_1} + \frac{R_2}{Y(2)} \frac{\partial R_2}{\partial a_1} + \cdots + \frac{R_n}{Y(N)} \frac{\partial R_n}{\partial a_1} \right] = 0
\]
\[
\frac{\partial F}{\partial a_2} = 2 \left[ \frac{R_1}{Y(1)} \frac{\partial R_1}{\partial a_2} + \frac{R_2}{Y(2)} \frac{\partial R_2}{\partial a_2} + \ldots + \frac{R_n}{Y(N)} \frac{\partial R_n}{\partial a_2} \right] = 0
\]
\[
\frac{\partial F}{\partial a_3} = 2 \left[ \frac{R_1}{Y(1)} \frac{\partial R_1}{\partial a_3} + \frac{R_2}{Y(2)} \frac{\partial R_2}{\partial a_3} + \ldots + \frac{R_n}{Y(N)} \frac{\partial R_n}{\partial a_3} \right] = 0
\]  
\[3-4\]

For three curves and \( n \) channels, these equations are

\[
\frac{\partial F}{\partial a_L} = \sum_{j=1}^{N} \frac{R_j}{Y(j)} \frac{\partial R_j}{\partial a_L} = 0 \quad \text{with} \quad L = 1, 2, 3
\]  
\[3-5\]

Therefore, to satisfy the conditions for a minimum, the equations are

\[
\sum_{j=1}^{N} \frac{R_j}{Y(j)} \frac{\partial R_j}{\partial a_L} = 0 \quad \text{with} \quad L = 1, 2, 3
\]  
\[3-6\]

From Equation 3-2, for \( k \) curves, we have

\[
\frac{\partial R_j}{\partial a_L} = \frac{\partial}{\partial a_L} \left[ \sum_{i=1}^{k} a_i X(I,J) - Y(J) \right], \quad \text{with} \quad L = 1, 2, \ldots, k
\]  
\[3-7\]

or

\[
\frac{\partial R_j}{\partial a_L} = X(L,J), \quad \text{with} \quad L = 1, 2, \ldots, k
\]  
\[3-8\]

so that the conditions become

\[
\sum_{j=1}^{N} \frac{R_j}{Y(j)} X(L,J) = 0 \quad \text{with} \quad L = 1, 2, \ldots, k
\]  
\[3-9\]

From Equation 3-2, this may be written as

\[
\sum_{j=1}^{N} \frac{X(L,J)}{Y(J)} \left[ \sum_{i=1}^{k} a_i X(I,J) - Y(J) \right] = 0 \quad \text{with} \quad L = 1, 2, \ldots, k
\]  
\[3-10\]

yielding, for three curves,

\[
\sum_{j=1}^{N} \frac{a_1 X(1,J) X(1,J)}{Y(J)} + \sum_{j=1}^{N} \frac{a_2 X(1,J) X(2,J)}{Y(J)}
\]

\[
+ \sum_{j=1}^{N} \frac{a_3 X(1,J) X(3,J)}{Y(J)} = \sum_{j=1}^{N} X(1,J)
\]  
\[3-11\]
\[
\sum_{J=1}^{N} \frac{a_1 x(2,J) x(4,J)}{Y(J)} + \sum_{J=1}^{N} \frac{a_2 x(2,J) x(2,J)}{Y(J)} \\
+ \sum_{J=1}^{N} \frac{a_3 x(2,J) x(3,J)}{Y(J)} = \frac{N}{j=1} x(2,J)
\]

\[
\sum_{J=1}^{N} \frac{a_1 x(3,J) x(4,J)}{Y(J)} + \sum_{J=1}^{N} \frac{a_2 x(3,J) x(2,J)}{Y(J)} \\
+ \sum_{J=1}^{N} \frac{a_3 x(3,J) x(3,J)}{Y(J)} = \frac{N}{j=1} x(3,J)
\]

For the general case, with \( k \) curves, we have

\[
a_1 \sum_{J=1}^{N} \frac{x(2,J) x(4,J)}{Y(J)} + a_2 \sum_{J=1}^{N} \frac{x(2,J) x(2,J)}{Y(J)} + \ldots \\
+ a_k \sum_{J=1}^{N} \frac{x(2,k) x(k,J)}{Y(J)} = \frac{N}{j=1} x(2,J)
\]

\[
a_1 \sum_{J=1}^{N} \frac{x(3,J) x(4,J)}{Y(J)} + a_2 \sum_{J=1}^{N} \frac{x(3,J) x(2,J)}{Y(J)} + \ldots \\
+ a_k \sum_{J=1}^{N} \frac{x(3,k) x(k,J)}{Y(J)} = \frac{N}{j=1} x(3,J)
\]

\[
\vdots
\]

\[
\vdots
\]

\[
a_1 \sum_{J=1}^{N} \frac{x(k,J) x(4,J)}{Y(J)} + a_2 \sum_{J=1}^{N} \frac{x(k,J) x(2,J)}{Y(J)} + \ldots \\
+ a_k \sum_{J=1}^{N} \frac{x(k,k) x(k,J)}{Y(J)} = \frac{N}{j=1} x(k,J)
\]

Thus the general element of the coefficient matrix of this system of equations, \( A(I,M) \), is

\[
A(I,M) = \sum_{J=1}^{N} \frac{X(I,J) X(M,J)}{Y(J)}
\]

and the element of the constant column of the augmented matrix is

\[
Z(I) = \sum_{J=1}^{N} X(I,J)
\]
The solution to the set of linear equations, 3-11, will yield the proper values of the coefficients to ensure a good fit.

The calculation of the elements of the augmented matrix is very lengthy, particularly if as many as 256 or 512 channels and ten component spectra are used. Clearly, such a process would be practically impossible to perform without the aid of a computer. Also, the solution of ten simultaneous equations dictates the use of a computer.

Perhaps the method of solving a set of linear equations most amenable to a computer solution is the one developed by Prescott D. Crout. The method is explained in the following paragraphs.

Denote the augmented matrix derived from the set of linear equations, 3-11, by \[ G(I,J) \]. An auxiliary matrix, \[ A(I,J) \], is computed from this given matrix by the following relations:

\[
A(I,J) = G(I,J) - \sum_{K=1}^{J-1} A(I,K) A(K,J) \quad I \geq J
\]

\[
A(I,J) = \left[G(I,J) - \sum_{K=1}^{J-1} A(I,K) A(K,J)\right] \frac{1}{A(I,I)} \quad I < J
\]

where the A's in the right-hand side of the equations are elements of the auxiliary matrix which have already been calculated. The solution matrix, \[ F(I) \], a column matrix, is

---

obtained from the auxiliary matrix by

$$F(I) = A(I, N+1) - \sum_{K=I+1}^{N} A(I, K) F(K)$$  \hspace{1cm} 3-16

where \( N \) is the number of equations and \( F(K) \) is a solution already obtained. It is understood that any sum whose lower limit exceeds its upper is zero. The proof of the validity of the solution is a straightforward inductive proof and is summarized in the appendix.

The solutions obtained from Equation 3-16 are exact, but in practice considerable error can result from the loss of significant figures. The magnitude of this error depends upon the number of significant figures carried by the calculating machine or computer. Indeed, for the purposes for which this analysis is designed, the elements of the augmented matrix may be of the order of \( 10^7 \). Also, the solutions will be more nearly exact if the diagonal elements of the matrix are not small in relation to the other elements. Therefore, the linear equations should be ordered with this fact in view.

The accuracy of the solutions, Equation 3-16, can be improved considerably in nearly all cases, usually to arbitrary accuracy. These solutions may be substituted into the original set of equations, Equations 3-11, and differences obtained between the left hand side and the constant on the right hand side of each equation. If this difference column then replaces the constant column in the augmented matrix,
the solutions to this set of equations will yield the corrections to the original solutions. This process may be repeated any desired number of times, yielding accurate coefficients for each component spectrum.
CHAPTER IV

COMPUTER PROGRAMS

Program I—Preparation of Standard Component Spectra

As was stated earlier, the component spectra are constructed by noting the detecting apparatus response to a gamma ray of a particular energy. Suppose that one wished to produce a synthetic spectrum typical of a 1.31 Mev gamma ray. The most obvious method would be to obtain a substance that emitted a single 1.31 Mev gamma ray and to use the data from this sample. However, only rarely could one obtain a nuclide which emits a single gamma ray of the desired energy. An alternative method would be to use the shape of a spectrum from a single gamma ray at some fairly close energy.

Consider a 1.26 Mev gamma ray whose peak lies in channel 180. The peak of a 1.31 Mev gamma ray should therefore lie in channel 186. It is desired that the 1.26 Mev spectrum be altered so that the peak is moved to channel 186, so that the linearity of the spectrum is preserved, and so that the total number of counts is approximately preserved.

Designate the 1.26 Mev spectrum as curve A and the 1.31 Mev spectrum as curve B. The following mapping then applies.

channel Y of B → channel Y(180/186) of A
For example,

channel 186 of B ——> channel 180 of A
channel 50 of B ——> channel 48.4 of A.

However, the curves are not continuous, and the mapping of channel 50 onto channel 48.4 is impossible. So, the counts in channel 50 of curve B must be composed of .6 of the counts in channel 48 of A and .4 of the counts in channel 49 of A. Also, the counts in every channel of curve must be multiplied by 180/186 in order to preserve total counts.

This process may be expressed generally as follows:

Define

\[ Q = \text{channel no. of peak in original spectrum} \]
\[ P = \text{channel no. of peak in new spectrum} \]
\[ X(J) = \text{no. of counts in } J^{th} \text{ channel of original spectrum} \]
\[ Z(J) = \text{no. of counts in } J^{th} \text{ channel of new spectrum} \]

Let

\[ R = J \frac{Q}{P} = M \cdot RA \quad . \]

R will in general be a decimal fraction. M is the number to the left of the decimal point and RA is the number to the right. We then have,

\[ Z(J) = \left( \frac{Q}{P} \right) \left[ (1-RA)X(M) + (RA)X(M+1) \right] \quad . \]

This expression yields the proper shape of the new spectrum.

It will be noted that if the peak is moved down in channel number, that more than 256 channels from the original spectrum will be required to compute 256 channels for the
new spectrum. This difficulty can be overcome if less than 256 channels of the new spectrum are calculated. For example, if a peak is moved down six channels, the new spectrum may be calculated through channel 240, assigning small values for the remaining 16 channels.

If a peak is moved more than a very few channels, the fact that the photoelectric cross section in the detecting crystal changes must be taken into account. According to theory, the cross section varies approximately inversely as the cube of the photon energy. Due to competing events in the crystal, the effective cross section varies closely as the square of the photon energy in the region of one Mev, for the equipment used.
Program I--Movement of Gamma-ray Peak

**Input**

Q = channel no. of original peak
P = channel no. of new peak
K = no. of new channels to be calculated

1. Read Q, P, K.
2. Read original spectrum, any no. of channels per card.
3. No switches are used.

**Output**

1. New spectrum is typed out, starting with channel 1, eight channels per line.
2. New spectrum is punched out, starting with channel 1, ten channels per card.
Program I—Flow Diagram

Read 
Q,P,K

Type
Q,P

Read original 
spectrum, X(J)

Compute 
M,RA

Compute new spectrum
\[ Z(J) = \frac{Q}{P} \left[ (1-RA)X(M)+(RA)X(M+1) \right] \]

Type
Z(J)

Punch 
Z(J)
C

PROGRAM 1

DIMENSION X(256),Z(256)

50 FORMAT(/8F9.0)
60 FORMAT(10F7.0)
70 FORMAT (/F10.0,7HCHANNEL,2X,F6.0)
80 FORMAT (16HM0VED TO CHANNEL,2X,F6.0)

1 READ,Q,P,K
   TYPE 70,Q
   TYPE 80,P
   DO 2 J=1,K
2 READ,X(J)
   DO 5 J=2,K
   S=J
   R=S*(Q/P)
   M=R
   AR=M
   RA=R-AR
   L=M-1
5 Z(J)=(Q/P)*((1.-RA)*X(M).*RA*X(L))
   DO 6 J=2,K,8
6 TYPE 50,Z(J),Z(J+1),Z(J+2),Z(J+3),Z(J+4),Z(J+5),Z(J+6),Z(J+7)
   DO 7 J=2,K,10
   A=Z(J)
   B=Z(J+1)
   C=Z(J+2)
   D=Z(J+3)
   E=Z(J+4)
   F=Z(J+5)
   G=Z(J+6)
   H=Z(J+7)
   T=Z(J+8)
   U=Z(J+9)
7 PUNCH 60,A,B,C,D,E,F,G,H,T,U
   GO TO 1
END
Test Problem for Program I

The spectrum of Co$^{60}$ is composed of two gamma-ray transitions and is shown in Figure 5. The two peaks fall at 1.17 Mev and 1.33 Mev. An altered Na$^{22}$ spectrum is shown in Figure 3 whose peak falls at 1.28 Mev. The annihilation peak has been subtracted from the original Na$^{22}$ peak. If the 1.28 Mev spectrum could be altered so that the peak fell at 1.17 Mev and again so that it fell at 1.33 Mev, the sum of the two spectra thus obtained should be identical to a Co$^{60}$ spectrum.

Assuming that the photoelectric efficiency of the detecting crystal varies inversely as the square of the photon energy, the spectrum constructed from Na$^{22}$ is shown in Figure 4. This spectrum should be compared with Figure 5. The ratio of the peak heights in the Co$^{60}$ spectrum is 1.44 while the ratio in the synthetic spectrum is 1.47. This appears, then, to be an acceptable method of obtaining component spectra.
Program II—Adjustment of Data for Least-Squares Fit

The calculation of the matrix elements from Equations 3-12 involves every component spectrum used. If ten component spectra are used, each consisting of 256 channels, this involves 2,560 numbers and 25,600 computer core locations. Due to the size of the computer available, it is impossible to store such a large amount of data. Therefore, a method must be devised to calculate Equations 3-12 without storing all the data.

This method may be developed by noting that each matrix element, $A(I,M)$, in Equation 3-13 involves only two component spectra. If the data are altered so that on each card of the input there is one channel from each spectrum, part of each matrix element may be calculated by computing all possible products, by pairs, of the numbers on one card. This process may be repeated 256 times, using all 256 channels, and the results of each product added to the previous corresponding product.

In effect, sums over $I$ and $M$ in Equation 3-12 are performed, leaving the sum over $J$ last. It is necessary, then, to alter the data so that the first input card contains the first channel from each spectrum, the second card the second channel from each spectrum, etc.
Program II—Adjustment of Data

Input

$M$ = number of component spectra
$N$ = number of component spectra channels per card
$KA$ = number of channels in total spectrum

1. From each deck of the $M$ component spectra, construct a single deck so that the first $M$ cards are the first cards from each of the decks, the second $M$ cards are the second cards from each deck, etc. The order of the spectra in each group of $M$ should be constant.

2. Read $M, N, KA$.

3. If the background is to be subtracted from the spectra, turn switch 2 on and read the background, $B(I)$.

4. With the exception of the last $M$ cards in the single deck, it is necessary that all cards contain the same number of channels.

5. If the data are to be typed out, turn switch 1 on.

Output

1. Adjusted data are punched out, $M$ channels per card, grouped according to channel number, in increasing order.

2. If switch 1 is on, data are typed out, $M$ channels per line, grouped according to channel number, in increasing order.

3. If switch 2 is on, all channels are less background.
Program II—Flow Diagram

Read
\(K, N, KA\)

Set
\(B(I) = 0\)

switch
2

on

off

Read background
\(B(I)\)

Type
heading.
Read component spectra, \( AX(I,J) \)

Compute \( X(I,J) \)
\[
X(I,J) = AX(I,J) - B(J)
\]

Punch altered data

switch
\[
\begin{align*}
\text{on} & \quad \text{Type altered data} \\
\text{off} & \\
\end{align*}
\]
Program II--Listing

C PROGRAM 2
DIMENSION AX(10,10),X(10,10),BA(256)
50 FORMAT(10F7.0)
70 FORMAT(7,10F7.0)
60 FORMAT(7,15X,6G6) GROUPING BY CHANNEL NUMBER IN INCREASING ORDER
1 READ,M,N,KA
DO 27 I=1,KA
27 BA(!)=0
IF(SENSE SWITCH 2)30,28
28 DO 29 I=1,KA
29 READ,BA(I)
30 TYPE 60
L=-N
2 L=L+N
DO 3 I=1,M
DO 3 J=1,N
3 READ,AX(I,J)
DO 26 I=1,M
DO 26 J=1,N
K=L+J
26 X(I,J)=AX(I,J)-BA(K)
DO 24 J=1,N
1=1
A=X(I,J)
B=X(I+1,J)
C=X(I+2,J)
D=X(I+3,J)
E=X(I+4,J)
F=X(I+5,J)
G=X(I+6,J)
H=X(I+7,J)
S=X(I+8,J)
T=X(I+9,J)
GO TO(1,4,5,6,7,8,9,10,11,12),M
4 PUNCH 50,A,B
GO TO 13
5 PUNCH 50,A,B,C
GO TO 13
6 PUNCH 50,A,B,C,D
GO TO 13
7 PUNCH 50,A,B,C,D,E
GO TO 13
8 PUNCH 50,A,B,C,D,E,F
GO TO 13
9 PUNCH 50,A,B,C,D,E,F,G
GO TO 13
10 PUNCH 50,A,B,C,D,E,F,G,H
GO TO 13
11 PUNCH 50,A,B,C,D,E,F,G,H,S
   GO TO 13
12 PUNCH 50,A,B,C,D,E,F,G,H,S,T
13 IF (SENSE SWITCH 1)14,24
14 GO TO (1,15,16,17,18,19,20,21,22,23),M
15 TYPE 70,A,B
   GO TO 24
16 TYPE 70,A,B,C
   GO TO 24
17 TYPE 70,A,B,C,D
   GO TO 24
18 TYPE 70,A,B,C,D,E
   GO TO 24
19 TYPE 70,A,B,C,D,E,F
   GO TO 24
20 TYPE 70,A,B,C,D,E,F,G
   GO TO 24
21 TYPE 70,A,B,C,D,E,F,G,H
   GO TO 24
22 TYPE 70,A,B,C,D,E,F,G,H,S
   GO TO 24
23 TYPE 70,A,B,C,D,E,F,G,H,S,T
24 CONTINUE
25 GO TO 2
END
Program III—Calculation of Augmented Matrix

M = number of component spectra
N = M + 1
K = number of channels fitted
Y(I) = number of counts in I\textsuperscript{th} channel of complex spectrum
B(I) = number of counts in I\textsuperscript{th} channel of background of complex spectrum
X(I) = number of counts in I\textsuperscript{th} channel of component spectra (output of Program II)
A(I,J) = matrix elements, Equation 3-13

**Input**

1. Read $M, N, K$.
2. Read $Y(I)$.
3. To subtract background, turn switch 1 on and read $B(I)$.
4. Read $X(I)$, output of Program II.

**Output**

1. Elements of augmented matrix, $A(I,J)$, are typed out, starting with first row.
Program III--Flow Diagram

1. Read M, N, K
2. Read complex spectrum, Y(I)
3. Switch
   - Off
   - On
4. Read background B(I)
5. Subtract background
   \[ Y(I) = Y(I) - B(I) \]
6. Read adjusted data
   X(I) (output of II)
7. Compute matrix elements, A(I,J)
8. Type A(I,J)
Program III—Listing

C                         PROGRAM 3
  DIMENSION A(10,11),X(10),Y(256),B(256)
  60 FORMAT(3F25.0,5X)
  50 FORMAT(/E18.8)
  1 READ,M,N,K
     DO 2 I=1,M
     DO 2 J=1,N
  2 A(I,J)=0
     DO 3 I=1,K
  3 READ,Y(I)
       IF(SENSE SWITCH 1)4,7
  4 DO 5 I=1,K
  5 READ,B(I)
     DO 6 I=1,K
  6 Y(I)=Y(I)-B(I)
  7 DO 10 L=1,K
     DO 8 I=1,M
  8 READ 60,X(I)
     DO 9 I=1,M
     DO 9 J=1,M
  9 A(I,J)=(X(I)*X(J))/Y(L)+A(I,J)
     DO 10 I=1,M
 10 A(I,N)=X(I)+A(I,N)
     DO 11 I=1,M
     DO 11 J=1,N
 11 TYPE 50,A(I,J)
     GO TO 1
END
Program IV--Final Solution

M = number of component spectra
N = number of columns in augmented matrix
K = number of channels fitted
Z = number of solution improvements desired

B(I) = coefficients of component spectra
DB(I) = corrections to coefficients, B(I)
A(I,J) = elements of augmented matrix (output of Program III)

X(I,J) = derived matrix as defined in Equation 3-15

Input

1. Read M, N, K, Z.
2. Read A(I,J) in order they are typed out by Program III.

Output

1. Coefficients, B(I), are typed out (B(1), B(2), ..., B(M)).
2. Corrections to B(I) are typed out (DB(1), DB(2), ..., DB(M)).
3. Corrected coefficients are typed out.
4. To type out X(I,J), turn switch 1 on.
Program IV—Flow Diagram

1. Read
   \( M, N, K, Z \)

2. Read
   Augmented matrix
   \( A(I,J) \)

3. \( AX(I) = A(I,N) \)

4. Compute derived matrix
   \( X(I,J) \)

5. Switch
   - off
   - on

6. Type derived matrix
Compute solution matrix $B(I)$

Type $B(I)$

Compute corrections to $B(I)$ $DB(I)$

Type $DB(I)$

Compute corrected solutions $B(I) = B(I) + DB(I)$

repeat $Z$ times

Type $B(I)$

after $Z^\text{th}$ loop
Program IV—Listing

C

PROGRAM k

DIMENSION A(10,11), X(10,11), B(10), R(10), D(10), DB(10), AX(10)

FORMAT('F18.8')

FORMAT(2X, F18.8)

FORMAT(//', 15X, 32H IMPROVED COEFFICIENTS OF SPECTRA)

FORMAT(//', 15X, 32H UNIMPROVED COEFFICIENTS OF SPECTRA)

FORMAT(//', 20X, 27H CORRECTIONS TO COEFFICIENTS)

FORMAT(//', 20X, 2HB(, I3, 2H) = )

READ, M, N, K, Z

DO 1 I = 1, M

DO 2 J = 1, M

2 READ, A(I, J)

Y = 0

DO 5 I = 1, M

5 AX(I) = A(I, N)

DO 6 J = 1, N

6 X(I, J) = A(I, J)

DO 7 J = 2, N

7 X(I, J) = X(I, J) / X(I, 1)

DO 13 J = 2, N

13 F = 0

DO 10 K = 1, N

10 F = X(I, K) * X(K, J) + F

X(I, J) = X(I, J) - F

GO TO 13

IF (SENSE SWITCH 1) 14, 16

14 DO 15 I = 1, M

15 TYPE k, I, M

16 Y = Y + 1.

17 B(M) = X(M, N)

DO 19 J = 2, M

19 I = M + 1 - J

E = 0

11 H = I + 1

DO 18 K = H, M

18 E = X(I, K) * B(K) * E
19 B(1)=X(1,M)-E
   TYPE 60
   DO 20 I=1,M
   TYPE 70,1
20 TYPE 50,S(1)
   GO TO 27
21 DB(N)=X(M,N)
   DO 23 J=2,M
   I=M+1-J
   E=0
   I=I+1
   DO 22 K=1,M
   E=X(I,K)*DB(K)+E
22 END
23 DB(1)=X(1,N)-E
   TYPE 65
   DO 24 I=1,M
   TYPE 75,1
24 TYPE 50,DB(1)
   DO 25 I=1,M
   B(I)=B(I)+DB(I)
   TYPE 55
   DO 26 I=1,M
   TYPE 70,1
26 TYPE 50,B(I)
   IF(Y-Z)27,27,1
27 DO 28 I=1,M
   R(I)=C
   DO 28 J=1,M
   R(I)=B(J)*A(I,J)+R(I)
28 END
29 D(I)=AX(I)-R(I)
   DO 30 I=1,M
30 A(I,N)=D(I)
   GO TO 6
END
Program V—Analysis of Fit

K = number of channels fitted
BA-BD = coefficients of component spectra
Y(I) = complex spectrum
A - D = output of program II
R(I) = residuals
X(I) = terms of Equation 3-3
T = function of Equation 3-3 / K

Input
1. Read K, BA, BB, BC, BD.
2. Read Y(I).
3. Read output of program II.

Output
1. Residuals, R(I), are typed out, six numbers per line
2. If switch 1 is on, X(I) are typed out.
3. T is typed out.
Program V—Flow Diagram

1. Read $K, BA, BB, BC, BD$

2. Read complex spectrum $Y(I)$

3. Read output of program II

4. Compute residuals $R(I)$

5. Compute each term of Eq. 3-3, $X(I)$

6. Compute Eq. 3-3, $T$
Type R(I)

switch

Type X(I)

Compute T

Type T
C
PROGRAM 5
DIMENSION Y(256), R(256), X(256)
50 FORMAT (/6F9.0)
60 FORMAT (/F18.8)
70 FORMAT (3F25.0, 5X)
80 FORMAT (/6F10.3)
1 READ, K, BA, BB, BC, BD
2 Q=K
DO 2 I=1, K
2 READ, Y(I)
3 READ 70, A, B, C, D
4 E=A*BA
5 F=B*BB
6 G=C*BC
7 H=D*BD
8 R(I)=E+F+G+H-Y(I)
9 DO 5 I=1, K
10 X(I)=(R(I)*R(I))/Y(I)
11 XA=0
12 DO 5 I=1, K
13 XA=X(I)+XA
14 DO 5 I=1, K
15 TYPE 50, R(I), R(I+1), R(I+2), R(I+3), R(I+4), R(I+5)
16 IF(SENSE SWITCH 1)7, 9
17 DO 8 I=1, K
18 TYPE 80, X(I), X(I+1), X(I+2), X(I+3), X(I+4), X(I+5)
19 T=XA/Q
20 TYPE 60, T
21 GO TO 1
22 END
Test Problem for Programs II, III, IV, and V

In order to test the validity and reliability of the whole method, a complex spectrum was obtained, composed of radiation from Na$^{22}$, Cs$^{137}$, Co$^{60}$, and Mn$^{54}$ sources. This spectrum is shown in Figures 9 and 10. These sources were placed very near the detecting crystal and their exact positions relative to the crystal carefully noted. The counts were recorded in 256 channels. It was desired to determine the relative intensities of the four gamma spectra making up the complex spectrum.

In order to accomplish this determination, each of the sources was returned to its position relative to the detector and four individual spectra obtained. The counting time was the same as for the complex spectrum and care was taken to ensure the same relation of energy to channel number in the multi-channel analyzer. These spectra are shown in Figures 5 through 8. If these spectra were used as the component spectra and fitted to the complex spectrum, one should find the coefficient of each component spectrum to be 1.0, since the complex spectrum should be simply the sum of the four spectra. In actual fact, the complex spectrum thus obtained was not simply the sum of the four spectra experimentally obtained, but differed from this sum in some channels by as much as 1,000 counts.

The four spectra and the complex spectrum were used in Programs II, III, and IV, fitting the first 240 channels.
Designating Co\textsuperscript{60} as spectrum 1, Cs\textsuperscript{137} as spectrum 2, Mn\textsuperscript{54} as spectrum 3, and Na\textsuperscript{22} as spectrum 4, the coefficients thus obtained were

\begin{align*}
B(1) &= .98330860 \\
B(2) &= 1.02004030 \\
B(3) &= .91542570 \\
B(4) &= .99823175
\end{align*}

The curve produced by multiplying each spectrum by its proper coefficient was produced using Program V. However, the result is too similar to Figures 9 and 10 to display on the same graph.

Each term of the minimized function, Equation 3-3, has been plotted, using Program V, in Figure 11 as a function of channel number. Only those terms larger than 5.0 have been plotted. It can be seen that the largest deviations are in the vicinity of peaks in the complex spectrum. The most marked deviation is in the region of the Mn\textsuperscript{54} peak. On each side of the peak channel there are sharp spikes in Figure 11. This fact would seem to indicate that there has been a shift in the energy calibration at some point in obtaining the data. In the region of the other peaks, there is little pattern in the scattering of points, indicating that perhaps the shift is not so large in these areas.

The nature of this shift can be determined by observing Figure 12, in which the residuals in the Mn\textsuperscript{54} region have been plotted as a function of channel number. In the lower
channels, the residuals are positive, and in the upper channels they are negative; indicating that the number of counts to the left of the center of the peak in the complex spectrum is smaller than in the fitted curve, and that the counts to the right are larger. This fact is undoubtedly due to the fact that the Mn\textsuperscript{54} peak in the complex spectrum is shifted to a higher channel, relative to the component spectrum. A shift on the order of three-fourths of a channel to one channel would account for this deviation.

It may also be noted that the coefficient for the Mn\textsuperscript{54} component spectrum is the one that differs most from the expected value of 1.0. Thus the major source of error seems to be in the calibration of the Mn\textsuperscript{54} component spectrum. The use of extremely stable power supplies in the detecting apparatus will help minimize shifts such as these.

It is clear, nevertheless, that Program V is very helpful in determining the nature and magnitude of errors involved in a particular analysis. If a random scatter of points were obtained for the terms of Equation 3-3, it would tend to indicate that the calibration and component spectra shape were approximately correct. If, however, there are peaks in the plot, as in this case, the accuracy of the data should be questioned. If a plot of the residuals, as in Figure 12, shows the residuals to have the same sign on either side of a questionable peak, the indication would be that there has been a resolution change in the analyzing apparatus.
In any case, the method seems to work satisfactorily, even for somewhat inexact data. A close scrutiny of the output of Program V will aid in determining the validity of the results, and indicate the nature of the necessary adjustments.
Figure 6—Cs137 spectrum

Counts (Thousands)

Channel number

Counts

150
100
50
0

199 keV
Figure 10—Complex spectrum
Figure 11--Plot of each term of Equation 3-3
Figure 12—Plot of residuals in Mn$^{54}$ peak region
APPENDIX

Proof of Crout's Method

Denoting the given matrix, the auxiliary matrix, and the final matrix by \( G_{i;j} \), \( A_{i;j} \), and \( F_{i;j} \), respectively, the method is contained in the following equations:

\[
A_{i;j} = G_{i;j} - \sum_{K=1}^{i-1} A_{i;K} A_{K;j} \quad i \geq j
\]

\[
A_{i;j} = \left[ G_{i;j} - \sum_{K=1}^{i-1} A_{i;K} A_{K;j} \right] \frac{1}{A_{i;i}} \quad i < j
\]  \hspace{1cm} (1)

\[
F_{i;j} = A_{i,n+1} - \sum_{K=i+1}^{n} A_{i;K} F_{K;j}
\]  \hspace{1cm} (2)

where any sum whose lower limit exceeds its upper vanishes.

Consider the usual case where the diagonal elements are not zero, in which case the final matrix has but one column.

We wish to prove that if the elements of the principal diagonal of the auxiliary matrix be replaced by 1's, and the elements below this diagonal be replaced by 0's, the resulting matrix is the augmented matrix of a set of equations entirely equivalent to the given set. More explicitly, the set of equations having the augmented matrix

\[
\begin{vmatrix}
G_{11} & G_{12} & \cdots & G_{1,n-1} \\
G_{21} & G_{22} & \cdots & G_{2,n-1} \\
\vdots & \vdots & \ddots & \vdots \\
G_{n1} & G_{n2} & \cdots & G_{n,n-1}
\end{vmatrix}
\]  \hspace{1cm} (3)

55
and that having the augmented matrix

\[
\begin{vmatrix}
1 & A_{12} & A_{13} & A_{14} & \cdots & A_{1n} & A_{1,n+1} \\
0 & 1 & A_{23} & A_{24} & \cdots & A_{2n} & A_{2,n+1} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 1 & A_{n,n+1}
\end{vmatrix}
\]

have the same solution. Since the solution of the equations corresponding to an augmented matrix is not altered if the rows are multiplied by any numbers, or if to any row there is added a linear combination of the other rows; the above statement will be proved by induction if we note that the first row of (4) is \(1/A_{11}\) times the first row of (3), and if we can show that the \([i\text{th row of (3)}] = 1/A_{11}\{[1\text{th row of (3)}] - A_{11}[1\text{st row of (4)}] - A_{12}[2\text{nd row of (4)}] - \cdots - A_{1,i-1}[\text{\((i-1)\text{th row of (4)}\)]\},\) or more explicitly,

\[
1 = \left[ G_{i,i} - \sum_{k=1}^{i-1} A_{ik} A_{k,i} \right] \frac{1}{A_{i,i}}
\]

\[
O = \left[ G_{i,j} - \sum_{k=1}^{j-1} A_{ik} A_{k,j} - A_{ij} \right] \frac{1}{A_{i,i}} \quad j = 1, 2, \ldots, i-1
\]

\[
A_{i,j} = \left[ G_{i,j} - \sum_{k=1}^{j-1} A_{ik} A_{k,j} \right] \frac{1}{A_{i,i}} \quad j = i+1, i+2, \ldots, n+1.
\]

But these equations follow directly from (1); hence the above statement is proved.

In a similar manner we can show that the equations corresponding to the final matrix, whose augmented matrix is
are equivalent to those of (4), for the \( n \)th rows of (4) and (6) are identical \((F_{nl} = A_{n,n+1})\), and the \([i]th row of (6)\) \[= \text{[i]th row of (4)} - A_{1,i+1} \text{[(i+1)th row of (6)]} - A_{1,i+2} \text{[(i+2)th row of (6)]} - \ldots - A_{1n} \text{[nth row of (6)]}, \] as is expressed by Equation (2). The equations corresponding to (6), which constitute the result given by the final matrix, are thus equivalent to (4) and hence (3); and therefore express the required solution.\(^1\)

\(^1\)Crout, op. cit.
BIBLIOGRAPHY

Books


Articles
