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COMPUTER ANALYSIS OF SPECTRA

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ABSTRACT

Computers have contributed greatly to automation in the analysis of multichannel spectra and, more importantly, to the accuracies which can be achieved. The fundamental part of most spectral analysis methods—peak-shape analysis—is reviewed with emphasis on the present and potential level of accuracy in the determination of energies and intensities. The methods are illustrated with analyses of Ge(Li) gamma-ray spectra, although the techniques are quite general for high-resolution, multichannel spectra. It is found that gamma-ray energies can be determined to a few eV if suitable standards are available. Measurement of intensities to better than the present best error level of 1-2% seems possible. The resolution of closely-spaced multiplets can be done far more accurately than by graphical techniques.

Less basic problems pertaining to specific applications, such as automatic peak identification and grouping of peaks for fitting, are discussed less critically; some examples of programs in current use are given as illustrations.

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I. INTRODUCTION

The use of high-resolution, high-rate multichannel spectrometers has spurred the development of computer techniques for analyzing large amounts of spectral data. The quantitative comparisons shown in Fig. 1 illustrate the magnitude of the present data-analysis problem. If one appreciates that careful hand analysis of a single complex gamma spectrum, which may contain hundreds of lines, can require months of work, it is obvious that the use of a computer is mandatory for experiments or programs that produce several orders of magnitude more data.

The past few years have seen rapid growth in the use of computers to analyze spectra, due entirely to such considerations. However, for most physicists, the quality of the results will be even more important than the degree of automation. Section II of this chapter reviews the fundamental part of most methods—peak-shape analysis—and assesses the potential levels of accuracy in the determination of energies and intensities. Section III describes some additional techniques useful in automated analysis and illustrates these with examples of programs currently in use.
II. FUNDAMENTALS OF SPECTRAL ANALYSIS

The fundamental problem is the determination of the energies and intensities of individual spectral components (transitions). I shall restrict the discussion to monoenergetic transitions (line spectra). The illustrations given are for Ge(Li) gamma spectra, although the methods are equally applicable to electron or heavy-particle spectra.

The spectrum of a single transition, measured in a particular spectrometer under specified conditions, is characterized by a complex response function, which can often be determined experimentally. A complex spectrum is simply a sum of such response functions; spectral analysis is the decomposition of a complex spectrum into its individual components. With high-resolution spectrometers, most of the useful information is contained in the narrow peaks (full-energy or escape). I will further confine my remarks to peak analysis, although more general stripping analysis has been found advantageous in special cases.1 With most methods the problem can be separated into two parts: the determination of peak positions and areas, and the application of calibrations to obtain energies and intensities.

Peak Shape Analysis

The simplest method for the determination of position and area is moment analysis. If the background under a peak is defined, the area (A), the average position or centroid (x), the average half-width (w), and the statistical uncertainties in these quantities can be calculated from simple formulae (see Table I). The centroid so defined corresponds to the peak center if the peak is symmetrical, and \( \bar{w} \) is equal to \( \sigma = \text{FWHM}/2.355 \) if the
peak is Gaussian. The value of \( w \) can give some indication whether a peak is complex, but there is no way within the method to resolve complex peaks.

This fundamental deficiency of moment analysis is the major reason for the use of more complicated fitting procedures. Fitting can also determine the positions and widths more accurately when statistics are poor, since the moment formulae contain no independent information about the peak shape.

The most direct approach to fitting is to define the peak shape by parabolic interpolation of the data points of a strong, single peak.\(^2\) This approach is useful only when the peak shape can be fixed; since the peak shape usually varies with energy, the more commonly used approach is to approximate the true peak shape with an analytic function which contains variable parameters. The shape parameters then provide an easy method to characterize the energy dependence of the shape.

Many different functions have been used to represent spectral peaks. The quality of any fitting results depends on how accurately these approximate the true peak shape. It is also desirable to use as simple a function as possible, for reasons to be discussed below. Figure 2 illustrates some shapes which have been used to represent Ge(Li) gamma-ray peaks. (For simplicity, all functional forms are given for peaks at the origin with the major component having unit height.) The simple Gaussian (Fig. 2(a)) has been widely used; it is a good first approximation, although it fails to account for the low-energy tailing which is particularly evident with higher energy gamma rays, poor detectors, or high count-rates.

Tailing may be represented by other functions which are added to or, alternatively, joined smoothly with a Gaussian. An example of the former type
is the sum of two Gaussians (Fig. 2(b)). Figure 2(c) shows a widely used example of the latter, a Gaussian with an exponential tail on the low-energy side. Although tailing on the high-energy side of most peaks is very slight, the use of a gain stabilizer tends to reflect the low-energy tail, making the inclusion of exponential tails on both sides of the peak advisable. Some spectrometers also yield high-energy tailing at high count-rates.

None of the shapes shown in Figs. 2(a)-(c) accounts for the low-energy "step" observed on a strong gamma-ray peak. When these shapes are used, the step must be represented by a "pseudo-background" which joins the data points on either side of the peak. The use of a pseudo-background can introduce errors in the analysis of complex peaks and in the comparison of the areas of strong peaks with weak ones on a high background. Figure 2(d) shows a simple two-parameter form which represents the peak as a (broadened) Gaussian and the step as a constant. A Gaussian plus linear tail could be represented by the function

$$y = a \left( 1 + \frac{J}{j^2 + \sigma^2} x \right) + \left( 1 - \frac{ao^2e^j^2/2\sigma^2}{j^2 + \sigma^2} \right) e^{-x^2/2\sigma^2}$$

$$= e^{-x^2/2\sigma^2}$$

(1)

In a further generalization, a linear tail can be added to any peak shape $f(x)$, where $f(x)$ may be a simple function, a sum of functions, or a piecewise joined function, with the resulting shape represented by

$$y = a \left( 1 + \frac{x}{J + f'(-J)/f'(-J)} \right) + \left( 1 - \frac{a}{Jf'(-J) + f(-J)} \right) f(x)$$

$$= f(x)$$

(2)
Generalizations of the shape (2(d)) represented by the functions (1) and (2) have not yet been used for spectral analysis. A Gaussian with exponential tail plus a linear tail (four shape parameters) would probably be an excellent approximation to a gamma-ray peak.

Figure 2(e) shows another shape which is similar to that used by Varnell and Trischuk to analyze Ge(Li) spectra; Fig. 2(f) shows a shape which has been used by Sanders and Holm.

Some results of the analysis of single peaks having various numbers of counts are given in Table II. Particularly noteworthy are the small standard deviations in the peak positions; these are as low as 0.1% of the peak width, corresponding to an uncertainty of less than 2 eV for this gamma ray, the 570 keV transition in the decay of $^{207}$Bi. As expected, peak positions obtained by fitting are generally more accurate than those obtained by moment analysis. (The reason for the exception to this in the last entries of columns 3-4 is discussed below under Least Squares Fitting.) Values of the weighted variance ($\chi^2$/degree of freedom) show at what level of statistics deviations of the true peak shape from the functional representation become evident (see the last two columns of Table II). The estimated standard deviations in the fitted areas have not been given; these will be similar to those calculated by moment analysis so long as the weighted variance is near unity.

Further tests of fitting results under controlled conditions can be done with synthetic spectra, made by displacing and adding real spectra. Figure 3(a) shows the results of fitting a shape of the form depicted in Fig. 2(c) to a single peak ($^{203}$Hg, $\epsilon_\gamma = 280$ keV) of varying intensity relative to an underlying continuum. The sizeable overestimation of the peak area for low peak-to-background ratios is due to the pseudo-background problem mentioned.
above. When a real background and the peak shape 2(e) is used, the errors are smaller and more often within the standard deviations, as indicated in Fig. 3(b).

Figure 4(a) shows the results of analysis of a synthetic doublet with shape 2(c). The higher-lying component has a fixed intensity of 1.6 times the Compton background, and the peaks are separated by 10 channels, or 1.186 times FWHM; the results cover a rather extreme range of relative intensities. The errors for low $P_1/P_2$ ratios are due primarily to the use of a pseudo-background. Figure 4(b) shows similar results when peak shape 3(e) is used with a real background. Some results for a more closely spaced doublet, separation 5 channels = 0.593 times FWHM, are shown in Figs. 5(a) and 5(b). It would be very difficult to obtain meaningful resolution of such a doublet by graphical techniques.

It is of course desirable to test fitting procedures out on real standard spectra rather than on synthetic spectra. Since most standards provide known energies and intensities rather than positions and areas, such tests involve calibration accuracy as well as fitting accuracy. Unfortunately, the accuracy of most standards and calibration procedures is much poorer than the potential accuracy of fitting procedures (as good as a few eV for positions, and 100%/$\sqrt{\text{total counts}}$ for areas). Position determinations do receive strong support from calibration experiments, as described below. The resolution of multiplets can often be verified by analysis of the same spectrum measured in a spectrometer with higher resolution; an example is given in Section III. Other good test cases for multiplets are the known relative intensities of closely-spaced x-ray components or subshell conversion lines.
Area determinations are most difficult to test. In practice, these have seldom been determined to better than 1-2%, probably because the results are strongly dependent on the use of very accurate shape functions and background representation. Varnell and Trischuk\(^5\) claim relative area determinations to better than 0.2% for strong single peaks. Some further consideration of areas is made under the topics least-squares fitting and efficiency calibrations.

**Least Squares Fitting**

Most peak fitting procedures require the use of an iterative, nonlinear least-squares method. While it is not within the scope of this chapter to discuss the mathematics of such methods, it is worthwhile to reference some methods and to give cautions regarding their use.

The method of Gauss\(^*\) is based on a first order Taylor's series expansion of the analytic linear solution in \(\Delta p_i\), the change in each of the variable parameters. A Fortran program based on this method has been developed by Moore and Zeigler at Los Alamos.\(^7\) Another method, variable metric minimization, has recently been devised and programmed by Davidon.\(^8\) Another Fortran program based on Davidon's method has been developed at Berkeley.\(^9\) Although good comparative studies of the two methods applied to spectral analysis problems have not been done, the variable metric method is thought to converge more rapidly and reliably. With either method the user must supply a subroutine to compute the fitting function and its gradient with respect to the variable

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\(^*\) Also referred to as the Gauss-Seidel, Seidel, Gauss-Newton, or Newton-Raphson method.
parameters, and the fitting program should be carefully tested before use. Another method, which does not require calculation of the gradient, has not yet been used for spectral analysis.

Failure to converge to meaningful values can be a problem with any such iterative method. The speed and reliability of convergence is dependent on the functional forms employed, the number of parameters, and the statistical quality of the data. In general, $\chi^2$ is very sensitive to the height, width, and positions of strong, well resolved peaks and to low-order terms in the background function; it is rather insensitive to the parameters of weak peaks and weak components of multiplets, small tailing corrections to the shape function, and higher order background terms. Convergence to meaningful values is best obtained by minimizing the number of variable parameters to which $\chi^2$ is insensitive, or by constraining their values.

Constraints of two types are commonly used in peak-shape fitting. Ranges of the fitting parameters are best confined by functional substitutions such as those suggested in Table III. These constraints help to force reasonable solutions with poor statistics and to avoid many convergence problems. Equality constraints may be used to fix peak separations or

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*With "minimization" routines the user must supply $\chi^2$ and $\nabla_{p_i}(\chi^2)$; "least squares" routines include a calculation of these from $f$ and $\nabla_{p_i}(f)$. More efficient computation can often be obtained by coding the computation of $\chi^2$ and its gradient for a particular function.
area ratios. This latter type of constraint is particularly useful in the analysis of subshell lines of conversion spectra, and for known gamma-ray multiplets which occur, for example, in x-ray spectra.

Standard deviations in the fitting parameters found by least squares are given by the expression

$$\delta p_i = \sqrt{C_{ii} \times V'}$$

where $C_{ii}$ is the diagonal element of the covariance matrix and $V'$ is the larger of the weighted variance $V$ or unity.

One problem in the interpretation of this error estimate is that the mathematical parameters do not precisely represent the physical quantities sought. For instance, the peak position parameter $x_0$ is actually the x-position of the fitting function rather than that of the true peak; this distinction removes the apparent paradox in the fact that $\delta x_0$ can increase with better statistics due to an increase in $V'$, whereas physical intuition dictates that better statistics should always determine the peak position more accurately (see Table II, Col. 4). Although there is no rigorous way to handle this problem, it is probably safe to use the uncertainty in the centroid, $\delta \bar{x}$, (see Table I) for the peak position uncertainty when this quantity is smaller than $\delta x_0$.

Errors in the peak area are subject to additional subtleties. It is common to use a parameter representing peak height and to assign an error to the peak area

$$\delta A = \sqrt{C_{hh} V} \cdot R_h$$

where $R_h$ is the ratio of peak area to peak height.
This estimate does not account for the influence of errors in the background and peak shape parameters on the errors in the peak area. For the most precise area determinations, it will be necessary to consider these additional sources of error in detail.

Ciampi et al.\textsuperscript{12} have suggested a method of maximum probability as an alternative to least squares.

\textbf{Calibrations}

We have already seen evidence that peak positions can be determined to within 0.1\% of the peak width, or a few eV for gamma-ray spectra. Whether such accuracy can be utilized depends on how well it is possible to calibrate the energy scale. Calibration accuracy is limited by the non-linearities of the spectrometer system, (or the accuracy with which these are known), and the accuracy with which the energies of standard peaks are known in the vicinity of the unknown peak. A technique frequently used is to fit a low-order polynomial to the standard energies as a function of peak position.\textsuperscript{3,13,14} Such a function is not necessarily a good approximation to the spectrometer non-linearities (primarily those of the ADC), and Fig. 6 shows that a poor ADC is not well calibrated with any order polynomial. Nevertheless, with the high linearity obtainable from good ADC's, a polynomial fit can provide adequate correction. Table IV shows cubic polynomial calibrations for two of the most accurate low-energy standard sources, $^{192}$Ir and $^{182}$Ta. The spectra were measured with a Goulding-Robinson successive approximation type ADC.\textsuperscript{15} In the first case the fitting errors are smaller than the assigned errors in the standard energies.\textsuperscript{16} One concludes from the fit that the
assigned errors are conservative, and that they provide only an upper limit on the accuracy of the calibration. In the case of $^{182}$Ta, the assigned errors in the standard energies\textsuperscript{17} are of the same order as the calculated uncertainties of the peak positions. Even at these high levels of precision there is no evidence that the calibration procedure is inadequate, nor that the calculated uncertainties are too optimistic.

The ease with which such measurements can be made has important implications in the field of gamma-ray standard measurements. The determination of peak positions is only slightly less accurate at higher energies, so that one might hope to obtain standard energies up to about 1 MeV with an order of magnitude improvement over the present level of accuracy. This will require some primary standards of very high accuracy; hopefully these might be obtained with iron-free spectrometers. Some Ge(Li) measurements using the crossover-cascade sum relationship may also be helpful. Above 1 MeV, most primary standard energies will probably be obtained by the "bootstrap" method\textsuperscript{13,19,20} applied to full energy and escape peaks. Corrections for shifts due to the electric field in the detector\textsuperscript{13} are presently the limiting source of error in the use of escape-peak energies.

Detector efficiency calibrations are commonly done with absolute standards whose gamma-ray emission rates are known to 1-2%. With the potential for determining peak areas to greater accuracy, it is desirable to make more accurate efficiency calibrations. Since there are no measured standards with intensities determined experimentally to better than about 1%, the best hope would appear to be the relative intensities of lines from "pure cascade" sources, such as $^{60}$Co, $^{180m}$Hf, $^{46}$Sc, $^{108m}$Ag, $^{111}$In, $^{52}$Mn, $^{138}$Pr, $^{178}$Ta, etc.
Detectors calibrated with such standards could then be used to measure more convenient sources such as $^{110m}_{\text{Ag}}$, $^{166m}_{\text{Ho}}$, $^{182}_{\text{Ta}}$, $^{192}_{\text{Ir}}$, $^{226}_{\text{Ra}}$, and $^{56}_{\text{Co}}$. These and other convenient, long-lived standards with many gamma rays could provide rapid calibrations of detectors when used with careful analysis techniques. When efficiency calibrations are done to higher accuracy, the fitting of efficiency curves to the data will provide a test of peak area determinations in the same manner as the energy calibration fits test position determinations.

Efficiency calibrations can easily be applied to measured peak areas by fitting the efficiency curve with analytic functions,\textsuperscript{3,21,22} or by suitable interpolation from a small table of values.\textsuperscript{3}

It should be emphasized that the above discussion concerns potential levels of accuracy. Much additional study of calibration procedures is necessary, and considerable care is obviously required in any high-precision measurement. The determination of intensities within error limits approaching the statistical standard deviations is especially subject to systematic errors, both in the measurements and in the data analysis.
III. PROGRAMS FOR ANALYSIS OF SPECTRA

In the preceding section the fitting of individual peaks and multiplets was described in general terms. Any program for spectral analysis must also include means for identifying the peaks, grouping them for fitting and making initial guesses for the fitting parameters, and determining background.

Before describing some computer codes in current use, a brief discussion of these operations is in order.

Peak Identification

The positions of peaks may be specified simply by supplying the approximate channel positions as input data. For experiments which produce reasonably small quantities of data this procedure is entirely adequate. When large amounts of data are to be processed, automatic search routines may be used.

A simple approach is to examine the local curvature at each point in the spectrum. The method of generalized second differences, a more elegant approach proposed by Mariscotti and modified by Routti and Prussin, is based on a comparison of the curvature in the spectrum over a number of channels comparable to the total peak width with the curvature expected for a peak. The result of this comparison is characterized by a single quantity \( ss_i \) representing the statistical significance of a possible peak at channel \( i \):

\[
ss_i = \left( \frac{\sum_{j=-k}^{k} c_j n_{i+j}}{\left[ \sum_{j=-k}^{k} c_j^2 n_{i+j} \right]^{1/2}} \right)
\]
where \( n_{i+j} \) is the number of counts in channel \( i+j \),

the \( c_j \)'s are coefficients characterizing the curvature expected
for a peak,

and the summation includes \( 2k+1 \) channels centered on channel \( i \).

Optimum values for the coefficients \( c_j \) depend on the peak shape, the ratio of
peak height to background, and the separation of components in a multiplet.

However, good sensitivity is often obtained using a single set of coefficients
for an entire spectrum. Mariscotti has obtained optimal values for the \( c_j \)'s
by an averaging process; \(^{23}\) Routti and Prussin derive similar values as the
second derivative of a Gaussian. \(^3\) The peak search consists of establishing
coefficients from the shape of a strong peak or peaks and then testing each
point of the spectrum with the above expression for \( s_{i1} \). Points for which
\( s_{i1} \) is greater than some threshold value define the neighborhood of a
potential peak, the approximate position of which is given by the channel
with the maximum value of \( s_{i1} \). Further tests on the shape of the potential
peak can then be made. \(^3,^{23}\)

The second difference method is capable of detecting most weak
singlets without introducing spurious peaks. It is less successful at detecting
components of multiplets, and these are generally not found unless they are
sufficiently well resolved that there is a change in sign of the curvature
between them. Inouye et al. \(^{24}\) have recently developed a method involving
Fourier transforms which is capable of detecting very close doublets. The
principle of this method is easily visualized if one imagines a spectrum as a
plot of amplitude versus time rather than intensity versus channel number.
The Fourier transform of a spectrum then corresponds to a plot of amplitude versus frequency. Different frequencies on this plot correspond to characteristic oscillations in the original spectrum: \( \geq 1 \text{ ch}^{-1} \) for statistical oscillations, \( \approx 1/(\text{peak width}) \) for peaks, and very low frequencies for slow variations in the background. Figure 7 shows the Fourier transform of a spectrum.

The basis for the method is the application of "filter" functions which select desired "frequency" ranges during the inverse transform, thus enhancing the desired "signal" relative to the "noise". Figures 8(a)-(c) show how these are used; the initial spectrum (8(a)) is transformed and then retransformed with a filter function which excludes the high-frequency statistical variations to yield the smoothed spectrum (8(b)). The smoothed spectrum is then subjected to a second pair of transforms with a narrow filter characteristic of the width of a single peak. The original broad peak is cleanly resolved into a doublet (Fig. 8(c)). As is also evident, the transformations tend to introduce small oscillations which were not present in the original spectrum; care must be taken not to interpret these as additional peaks.

**Grouping of Peaks and Background Determination**

The grouping of peaks for fitting will depend on the nature of the data and the complexity of the fitting function. A general principle, based on the objective of maximizing the probability of obtaining good fits and minimizing the computation time, is to minimize the number of variable parameters in a single fit. Based on this principle, the following procedures are suggested:
1) First, fit the strong single peaks with variable shape parameters and fixed background. The appropriate shape parameters for other peaks can then be derived by fitting or interpolating the parameters found as a function of channel number. Next, divide the spectrum into intervals surrounding each peak or group of peaks in a multiplet, and fit each interval with the appropriate number of peaks of fixed shape. The background may be included in these fits as a simple function (e.g., linear or quadratic), or it can be fitted first to the data on either side of the peak(s) and subtracted before fitting. The latter method is necessarily of the "pseudo-background" type, but it is less likely to produce meaningless or non-convergent results in difficult cases.

2) The first procedure is not possible when there are few strong singlets or none at all. It may also be undesirable if one wants to fix some of the separations or relative areas of widely separated peaks. One must then group more peaks and larger regions together and fit multiple peaks with variable shapes. In this case, the number of free shape parameters should be reduced by setting them equal for all peaks, or by reparametrizing them as a simple function of channel number.

3) In difficult cases, the number of free parameters can be reduced if some prior information about the peaks is available. The positions or areas of some peaks, or the separations or area ratios can be fixed if any of these are known.

Many computer codes have been or are being developed to analyze spectra. Some of these are described in Refs. 2-6, 10, 14, 22, and 24-27. Brief descriptions of three programs in current use at Berkeley are given below.
This program is used routinely by a number of groups at the Lawrence Radiation Laboratory at Berkeley for the analysis of gamma and conversion-electron spectra from radioactive decay and nuclear reactions. The procedure employed is similar to that suggested in 1) above. As a minimum input, the user need only supply the fitting intervals for peaks to be used as shape standards and data for energy and efficiency calibrations, if these are desired. Peak searching may be done automatically by the second difference method already described. Fitting is done by the variable metric method, using Gaussians with exponential tails on both high- and low-energy sides of the peak. Figure 9 shows the set of shape parameters obtained from a spectrum of $^{177m}$Lu. The width and low-energy tail are well defined, and the high-energy tail is negligible except at the highest energies, so that the large fluctuations in the calculated joining point have almost no effect on the peak shape. After obtaining shape parameters and finding peaks, the program fits each peak or multiplet with fixed peak shapes and a quadratic or linear background. The present version of the program fits multiplets with up to 6 components.

In addition to the numerical results, the output includes printer plots of the fits and, if desired, Calcomp plots of the total spectrum. Any peaks not found by the search routine can easily be detected from the graphical output and included in a second run. A large variety of input control features, including on-line control with CRT display of the fits, is written into the program. When the program is used on-line, peaks missed by the search routine can be detected and added immediately, and difficult multiplets can be reanalyzed with operator control of the fitting intervals.
The program has been tested extensively on a CDC-6600 computer. Typical central processor times * are about 1 second per thousand channels for the search routine and about 1 second per photopeak for fitting a spectrum containing a mixture of singlets and multiplets. As an example of the results, in the spectrum of $^{177m}$Lu, all but one weak gamma ray and the weaker members of six closely-spaced doublets were found automatically. The energies and intensities computed agree well with a very careful graphical analysis of the same spectrum, except for the relative intensities in the 291.4-292.5 keV doublet. Figure 10(a) shows the computer fit to a quartet of lines including this doublet, where one component of the doublet has been missed by the search routine, as is obvious from the CRT graph; this line was then added and the analysis redone (Fig. 10(b)). The fit now appears to be good, but the doublet has an intensity ratio 1.00/0.80, in disagreement with the hand-done graphical result 1/1. The computer result is strongly supported by Fig. 10(c), which shows the analysis of these lines in a spectrum measured several years later with higher resolution.

SPECT

This program was designed by the author principally to handle timed spectra, angular distributions, and coincidence spectra from in-beam gamma-ray measurements. Since the quantities of data are very large, the major objective is to shorten the amount of time required to analyze the output.

* Corresponding computation time on an IBM-7094 is approximately five times longer.
The program is run on-line at a CDC-6600 computer. Each peak is indicated by the operator, who marks the left and right boundaries with a light pen on a CRT screen (see Fig. 11(a)). These markers define the fitting intervals and the intervals to be excluded from the background calculation. A multiplet is indicated by leaving zero or one data point between the second marker of one peak and the first marker of the next peak. (These inner markers are ignored during the fitting process.) Multiplets can contain up to 20 peaks. Sets of position markers can be stored and recalled for subsequent spectra with the same peaks.

After peaks have been marked, the computer fits a background to the entire spectrum as a piecewise cubic polynomial (Fig. 11(b)), the boundaries between regions occurring where neighboring peaks are separated by more than a specified number of channels (normally 15). The background routine tries to extend each region on either side up to a specified maximum number of channels, or until the fit gets worse or another peak boundary is encountered. In rare cases where the background is poor, the operator may redraw part of it with a light pen, (Fig. 11(c)). This method of drawing and inspecting background, together with the method of specifying peaks, results in good fits with a high degree of reliability. (Gunnink et al. 22 have devised a method of peak selection and background determination which can possibly retain this reliability while permitting almost totally automatic peak selection.)

Remaining operations are entirely automatic. The background-subtracted data are fit with Gaussians with low-energy tails. 9 Strong singlets distributed throughout the spectrum are used to establish width and tail parameters which are then fit to a linear function of energy. Alternatively, shape parameters
established from another spectrum can be used. Each peak or multiplet of the spectrum is then fit with a fixed shape peak or peaks.

Energy calibrations are established by designating desired spectra as calibrations and assigning energies from a table to peaks with the light pen. The resulting polynomial calibration may be applied to any other spectrum. Efficiency calibrations employ a functional representation whose variable parameters are read in on cards.

Only two lines of output are given for each transition: the first includes the position, area, energy, intensity, shape parameters, standard deviations, and the weighted variance; the second gives values calculated from moment analysis. Output can also be written on magnetic tape for subsequent analysis of angular distributions, decay curves, etc.

The program requires about 1 second of central processor time per 4000 channels for the automatic background routine, and an average of about 0.1 second per peak for the fitting process. Total on-line time for an experienced operator analyzing a long run ($\approx 3 \times 10^5$ channels of data and $10^4$ peaks; angular distributions) is about four hours, most of which is spent in peak selection. (The amount of central processor time used during this operation is negligible.) Typical on-line time for analysis of a single complex gamma-ray spectrum is 2-15 minutes.

FELSPAR

This program was written for detailed analysis of complex spectra with a high degree of correlation in the positions and areas of the lines, such as x-ray spectra of mixed fission products and photoelectron (ESCA)
spectra from an iron-free spectrometer. Gaussians or Lorentzians with constant or exponential tail on the low-energy side are fit by the method of Gauss. 7

The user supplies as card input the fitting interval and guesses for peak positions and shape parameters. He may also specify area ratios or peak separations to be fixed. Shape parameters may be set equal for all peaks or for all peaks within specified subsets, or may be free. In addition, each of the parameters, including those which define the shape, area, and position of each peak and the linear background, can be fixed at the initial estimate or left free. The program performs one fit with up to 42 parameters (including those which are fixed or dependent) for each set of input specifications. A companion program, AIRLIFT, fits large numbers of peaks with fixed shape parameters.

An example of such a fit28 is shown in Fig. 12. The program has been run routinely on a CDC-6600 computer with typical central processor times of 1-10 seconds per fit.
REFERENCES

FIGURE CAPTIONS

Fig. 1. Number of peaks and channels of data produced in some typical experiments with gamma-ray detectors:

1) NaI(Tl) gamma singles spectrum
2) Ge(Li) gamma singles spectrum
3) Ge(Li)-Ge(Li) gamma-gamma coincidence spectra, sorted from incremental tape
4) In-beam Ge(Li) gamma spectrum, 2-dimensional (energy vs. time after beam burst); ≤2 day experiment
5) In-beam Ge(Li) gamma-ray angular distributions; ≤2 day experiment.

Fig. 2. Some analytic functions which have been used to represent gamma-ray peaks. For simplicity the shapes are plotted at the origin with the major component of unit height. Fits to actual gamma rays are displaced upward in Figs. 2(a)-(e). Figure 2(f) is from Ref. 6.

Fig. 3. Results of fitting a single peak of varying height with respect to the underlying continuum

a) with peak shape 2(c) and a cubic pseudo-background
b) with peak shape 2(e) and a linear background.

Fig. 4. Results of fitting a doublet, separation 10 channels = 1.186 FWHM,

a) with peak shape 2(c) and a cubic pseudo-background
b) with peak shape 2(e) and a linear background.

Fig. 5. Results of fitting a doublet, separation 5 channels = 0.593 FWHM,

a) with peak shape 2(c) and a cubic pseudo-background
b) with peak shape 2(e) and a linear background.
Fig. 6. Polynomial fits to an energy calibration: poor ADC linearity.

Fig. 7. Fourier transform of a Ge(Li) gamma spectrum; from Ref. 24.

Fig. 8. Effect of successive pairs of Fourier transforms on a portion of a spectrum; from Ref. 24.
   a) a portion of the initial spectrum before transformation
   b) after smoothing transforms
   c) after "resolution improvement" transforms.

Fig. 9. Shape parameters derived from a gamma spectrum of $^{177m}_{\text{Lu}}$; from Ref. 3.

Fig. 10. Program SAMPO: Fits to a quartet of lines in the gamma spectrum of $^{177m}_{\text{Lu}}$ (Ref. 3).
   a) without one component of the 291.4-292.5 keV doublet missed by the automatic search routine
   b) after adding the missing component
   c) the same spectrum measured at higher resolution.

Fig. 11. Program SPECT: Display of the spectrum at the console (semilog plot)
   a) after marking some peaks with the light pen. These are indicated by left and right boundary markers (vertical dashed lines) and a marker at the top of the peak supplied by the computer
   b) after automatic background has been drawn
   c) correction of the background with the light pen.

Fig. 12. Program FELSPAR: Fit to a fission-product K-x-ray spectrum.

The K-x-ray components for each element are represented by four lines with fixed separations and relative areas. Fitting curves are shown for four elements.
Table I. Formulas for numerical analysis of peaks.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Area ((A))</td>
<td>(\Sigma (C_x - B_x)) (\sqrt{\Sigma (C_x + B_x)})^2 (\Sigma )</td>
</tr>
<tr>
<td>(\delta A)</td>
<td>(\Sigma (C_x - B_x) x) (\Sigma (C_x + B_x)) (\Sigma )</td>
</tr>
<tr>
<td>Centroid ((\bar{x}))</td>
<td>(\frac{\Sigma (C_x - B_x) x}{A}) (\frac{\Sigma (C_x + B_x) (x-\bar{x})}{A})</td>
</tr>
<tr>
<td>(\delta x)</td>
<td>(\frac{\sqrt{\Sigma (C_x - B_x) (x-\bar{x})^2}}{A}) (\frac{\sqrt{\Sigma (C_x + B_x) (x-\bar{x})^2}}{A})</td>
</tr>
<tr>
<td>Half-width ((\bar{w}))</td>
<td>(\frac{1}{2WA} \sqrt{(x-\bar{x})^2 \left(1 - 2 \frac{C_x - B_x}{A}\right) - \bar{w}^2} \left[C_x + B_x\right] )</td>
</tr>
</tbody>
</table>

where \(C_x\) = counts in channel \(x\)

\(B_x\) = background in channel \(x\)

* Error formulae based on the conservative assumption that \(\delta B_x = \sqrt{B_x}\).
Table II. Results of numerical analysis and fitting for a single peak
($^{207}$Bi, $E_x$ 570 keV, FWHM 10 channels = 1.8 keV).

<table>
<thead>
<tr>
<th>Area, counts</th>
<th>Standard deviation of area, %*</th>
<th>Standard deviation of position, channels</th>
<th>Weighted variance ($\nu$) of fit</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>numerical</td>
<td>fitting†</td>
<td>Gaussian</td>
</tr>
<tr>
<td>2.5x10$^2$</td>
<td>6.5</td>
<td>0.38</td>
<td>0.85</td>
</tr>
<tr>
<td>5.1x10$^2$</td>
<td>4.5</td>
<td>0.26</td>
<td>1.94</td>
</tr>
<tr>
<td>2.6x10$^3$</td>
<td>2.0</td>
<td>0.12</td>
<td>0.79</td>
</tr>
<tr>
<td>1.3x10$^4$</td>
<td>0.93</td>
<td>0.055</td>
<td>1.40</td>
</tr>
<tr>
<td>5.1x10$^4$</td>
<td>0.46</td>
<td>0.027</td>
<td>3.4</td>
</tr>
<tr>
<td>2.5x10$^5$</td>
<td>0.21</td>
<td>0.013</td>
<td>8.9</td>
</tr>
<tr>
<td>1.3x10$^6$</td>
<td>0.09</td>
<td>0.010</td>
<td>4.7</td>
</tr>
</tbody>
</table>

*Statistical value; fitting values are similar if $\nu$ is near unity.
†Fitting with Gaussians with low energy exponential tails.
Table III. Examples of parameter constraints by functional substitutions.

<table>
<thead>
<tr>
<th>Constraint</th>
<th>Functional substitution</th>
<th>Typical peak parameters to which constraint is applied</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ p &gt; A ]</td>
<td>[ p = A + (p' - A) \sin (\frac{p}{2}) ]</td>
<td>peak height, peak width</td>
</tr>
<tr>
<td>[ A &lt; p &lt; B ]</td>
<td>[ p = A + \frac{B - A}{2} \sin^2 (p') ]</td>
<td>peak position, tail joining parameter</td>
</tr>
</tbody>
</table>

or

\[ p = A + (B - A) \sin^2 (p') \]
### Table IV. Polynomial fit energy calibrations.

<table>
<thead>
<tr>
<th>192Ir</th>
<th>Computed peak channel (x)</th>
<th>Computed standard deviation (δx)</th>
<th>Assigned energy (E\text{\text{\text{std}}})</th>
<th>Deviation E\text{\text{\text{std}}}-E\text{\text{\text{fit}}}</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Channels</td>
<td>eV</td>
<td>eV</td>
<td>eV</td>
</tr>
<tr>
<td>1115.610</td>
<td>0.010</td>
<td>1.8</td>
<td>205810(10)</td>
<td>0.5</td>
</tr>
<tr>
<td>1615.926</td>
<td>0.006</td>
<td>1.1</td>
<td>295938(9)</td>
<td>-3.3</td>
</tr>
<tr>
<td>1685.282</td>
<td>0.007</td>
<td>1.3</td>
<td>308435(10)</td>
<td>-2.0</td>
</tr>
<tr>
<td>1729.933</td>
<td>0.010</td>
<td>1.8</td>
<td>316488(10)</td>
<td>6.0</td>
</tr>
<tr>
<td>2570.644</td>
<td>0.019</td>
<td>3.3</td>
<td>468053(14)</td>
<td>-0.7</td>
</tr>
<tr>
<td>3237.783</td>
<td>0.024</td>
<td>4.3</td>
<td>588557(17)</td>
<td>-0.5</td>
</tr>
<tr>
<td>3325.297</td>
<td>0.021</td>
<td>3.8</td>
<td>604385(17)</td>
<td>-1.3</td>
</tr>
<tr>
<td>3369.775</td>
<td>0.017</td>
<td>3.1</td>
<td>612435(17)</td>
<td>1.8</td>
</tr>
</tbody>
</table>

Fitting function:
\[E\text{\text{\text{fit}}} = A + Bx + Cx^2 + Dx^3\]
\[A = 4.7039 \text{ keV}\]
\[B = 0.1804559 \text{ keV/channel}\]
\[C = -2.3950 \times 10^{-7} \text{ keV/ch}^2\]
\[D = 6.1501 \times 10^{-11} \text{ keV/ch}^3\]

<table>
<thead>
<tr>
<th>182Ta</th>
<th>Computed peak channel (x)</th>
<th>Computed standard deviation (δx)</th>
<th>Assigned energy (E\text{\text{\text{std}}})</th>
<th>Deviation E\text{\text{\text{std}}}-E\text{\text{\text{fit}}}</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Channels</td>
<td>eV</td>
<td>eV</td>
<td>eV</td>
</tr>
<tr>
<td>443.137 (k\text{\text{A}}_2)</td>
<td>0.046</td>
<td>5.6</td>
<td>57981(1)</td>
<td>6.7</td>
</tr>
<tr>
<td>454.052 (k\text{\text{A}}_1)</td>
<td>0.027</td>
<td>3.3</td>
<td>59318(1)</td>
<td>-4.1</td>
</tr>
<tr>
<td>659.325</td>
<td>0.021</td>
<td>2.6</td>
<td>84681(3)</td>
<td>6.2</td>
</tr>
<tr>
<td>784.271</td>
<td>0.006</td>
<td>0.7</td>
<td>100106(1)</td>
<td>-0.3</td>
</tr>
<tr>
<td>1207.963</td>
<td>0.009</td>
<td>1.1</td>
<td>152435(4)</td>
<td>-0.3</td>
</tr>
<tr>
<td>1240.045</td>
<td>0.017</td>
<td>2.1</td>
<td>156395(5)</td>
<td>-2.5</td>
</tr>
<tr>
<td>1579.844</td>
<td>0.032</td>
<td>3.9</td>
<td>198362(7)</td>
<td>4.1</td>
</tr>
<tr>
<td>1772.240</td>
<td>0.012</td>
<td>1.5</td>
<td>222110(3)</td>
<td>-0.4</td>
</tr>
<tr>
<td>1830.624</td>
<td>0.019</td>
<td>2.3</td>
<td>299322(8)</td>
<td>4.8</td>
</tr>
<tr>
<td>2112.263</td>
<td>0.023</td>
<td>2.8</td>
<td>264072(6)</td>
<td>-1.4</td>
</tr>
</tbody>
</table>

Fitting function:
\[E\text{\text{\text{fit}}} = A + Bx + Cx^2 + Dx^3\]
\[A = 3.2649 \text{ keV}\]
\[B = 0.1234328 \text{ keV/ch}\]
\[C = 8.3402 \times 10^{-8} \text{ keV/ch}^2\]
\[D = -3.0368 \times 10^{-11} \text{ keV/ch}^3\]
Fig. 1.
Fig. 2a.
Shape parameters:
$\sigma_1, (\sigma_2), \delta, h_2$

Fig. 2b.
\[ y = e^{-\frac{x^2}{2\sigma^2}} \]

Shape parameters:
\( \sigma, J_l, (J_h) \)

Fig. 2c.
Fig. 2d.
Shape parameters:
\( \sigma_1, J_1, \sigma_2, J_2, h_2, h_2 \)

\( y_1 + y_2 + \text{background} \)

\( y_1 : \text{Gaussian with exp. tail} \)

\( y_2 : \text{Gaussian with exponential tail} \)

Background

Fig. 2e.
$Y_1 + Y_2 + Y_3 + \text{Background}$

$Y_2 = h_2 e^{K_2 x (1 - e^{2\sigma_2^2})}$

$Y_3 = h_3 (1 - e^{2\sigma_2^2})$

Fig. 2f.
Fig. 3a.
Fig. 3b.
Fig. 4a.
Error in computed area ratio

Error in computed separation

Fig. 4b.
Fig. 5a.
Error in computed area ratio

Error in computed separation

True area ratio, Lower peak/Upper peak

Fig. 5b.
Fig. 6.
Fig. 7.
Fig. 8a.
Fig. 8b.
Fig. 8c.
Fig. 9.
Fig. 10a.
Fig. 10b.
Fig. 10c.
High Z fission fragment x-rays at 5.4 min. transit time

Channel

Counts

XBL688-3826
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