AUTOMATED ANALYSIS OF GAMMA RAY SPECTRA

AUTOMATED ANALYSIS OF GAMMA RAY SPECTRA

BY

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SCOPE AND CONTENTS: Contemporary approaches to data analysis suffer from being both time-consuming and subjective; however, the application of numerical techniques to the automated (non-interactive) analysis of gamma ray spectra often leads to considerably improved performance. The foundations and limitations of such techniques lie in the applicability of certain mathematical operations such as deconvolution, and the careful study of stochastic models. The use of digital filters as a method of enhancing detector response has been applied to a triple-coincidence counting arrangement, after modelling undesired physical effects. An objective background estimation method has been described based on the statistical nature of nuclear measurements. Finally, the application of such techniques is demonstrated with a package of FORTRAN programs designed to be used in a variety of situations with minimal modifications.

ACKNOWLEDGMENTS

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I thank all the members of our group, past and present, who daily contributed their own time and skills to making my sojourn both pleasant and profitable.

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Finally, I thank my parents, in recognizing that their efforts contribute to whatever I happen to be doing.

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CHAPTER I

INTRODUCTION

The analysis of gamma ray spectra from multichannel analyzers is an integral part of much work in the field of nuclear physics. Historically, the use of sodium iodide [NaI] detectors, posessing inherently poor resolution, led to the development of many diverse methods of extracting energy and amplitude information from measured spectra. In the last two decades, however, two important developments have served to revolutionize nuclear measurements. First, the introduction of high-speed digital computers heralded the possibility of automating analytical methods, more promising still in the light of major developments such as the discovery of the fast Fourier transform [FFT] algorithm. Secondly, the appearance of solid state germanium [Ge] and lithium-drifted germanium [Ge(Li)] detectors allowed the collection of gamma ray spectra with unheard of resolution. Combined, these developments served to provide major impetus for much of today's work in experimental nuclear physics, simplifying data analysis while providing a richer store of precise nuclear data. However, the burden of analysis work often is left to the experimenter, despite the availability of more sophisticated methods. This situation may prove

unmanageable in the presence of large data records, or where closely-spaced components make resolution impossible.

As practical limits of resolution are approached, the development of improved computer codes becomes as important as the amelioration of existing experimental apparatus, since any technical improvement is ultimately reflected in the precision of a given measurement. By linking the techniques of numerical analysis to the domain of instrument design, the inherent physical limitations of a given experimental setup may be surmounted. In keeping with this philosophy, the wise use of computer methods serves to satiate a physicist's natural desire to make objective judgements.

Any approach to numerical analysis demands that the methods employed be consistent with the mathematical nature of the collected data, and more fundamentally to the nature of the physical phenomenon being measured. While methods which mimic human 'intuitivity' are attractive, the more secure footing of a mathematical argument lends itself not only to the goal of unbiased, reproducible results, but also to the actual construction of computer codes. Therefore, a careful study of the mathematical origins of nuclear data and the appropriateness of certain operations must be performed before any such applications are made. Only then may techniques such as digital filtering be confidently

introduced as a step in the analysis stream, while techniques to estimate background continuum in complex spectra may rely solely on the mathematical justification to be accepted. Of course, any methods are ultimately subject to careful scrutiny through use in the laboratory and comparison with results obtained in other ways.

In the end, such analysis programs must be combined in a convenient manner to facilitate their use and study. They must be combined with other, more mundane, programs which simply read data from magnetic tape, or produce numerical listings of results. Such a package of programs is far more powerful than either isolated routines or one all-purpose program. Only with such an efficient method of access and use will these methods be accepted in the laboratory and used to their fullest.

In summary, the application of numerical methods to a given measurement should be viewed as an extension of the measurement process rather than a completely separate procedure to be performed at a later time. Ideally, an instrument faithfully reports a measurement under all conditions; such performance is approachable with the enhancement produced by automated analysis.

CHAPTER II

ANALYSIS OF GAMMA RAY SPECTRA

Spectral analysis encompasses all the procedures through which an experimenter determines the energy and relative intensities of gamma rays incident on a detector. In more practical terms, it is an effort to determine the presence of, the centroid position of, and the area under, peaks which have been somewhat broadened, [and often distorted] by the measurement process. Of course, if one could immediately determine these parameters, spectral analysis would be a fait-accompli. Unfortunately for the nuclear physicist, no detection system exists which would provide perfect resolution with accurate energy information. In short, the purpose of spectral analysis is to approach the response of an ideal system after the measurement has already been made. Automated analysis is the [computerized] application of such procedures in a manner which requires little or no human intervention to reach this end.

Mathematical Basis of the Automated Approach

Even the nature of nuclear measurement precludes such a perfect arrangement. Counting experiments follow Poisson statistics and, by definition, an error is introduced into

each measurement.(BR65) While such effects may be minimized by long acquisition times, the presence of background [both instrumental and environmental contributions] and the finite time allotted for any experiment, may combine to make this recourse impractical. Fortunately, many experiments involve the measurement of events which are far more dominant than background contributions, and the percentage-error introduced through counting statistics becomes manageable at large counts. [Where such error varies as the square-root of the count.]

Every measurement made with any instrument involves a certain 'colouration' of the desired result with an effect characteristic of that particular instrument. The effect a given instrument or acquisition system has on a measurement is called the response-function of the device. This effect is not necessarily due to poor design or mis-use; it may be physically impossible to construct a device to perform the desired measurement to the necessary precision. Secondly, all electronic devices are 'noisy'; that is, an amount of random signal is introduced at every stage of the measurement chain. The latter effect is unavoidable; thermal noise and shot noise are inevitably present in any solid state devices. (DI72) Careful design of instruments and careful use of detectors may serve to minimize these effects; solid state detectors, for example, are usually

operated at liquid-nitrogen temperatures [as is the pre-amplifier stage] to minimize noise contributions. The mathematical implications of such effects, when combined in series, leads to the use of convolution theory and with it, the theory of Fourier transforms. Statistical theory, and the treatment of stochastic processes will also play a role in spectral analysis.

The use of multichannel analyzers implies that energy information must be quantized. While it is not a serious problem in determining gamma ray energies [given that the system has been wisely assembled], this condition implies that analysis of spectral data will be performed on discrete, rather than continuous data. This, of course, will be true for both energy and intensity information; raw data is positive-integral in both the abcissa and ordinate dimensions. Ultimately, these facts dictate the mathematical methods which will be applicable to spectral analysis.

Finally, it may be impossible to isolate a desired phenomenon from other, similar events; in this instance the measurement may include undesired information which is left to be separated at a later stage. This problem, of course, is not unique to nuclear measurements; rather, it is fundamental to experimental physics. In light of the objectives of automated analysis, the obvious implication is that all events must be detected and classified even if they

are not directly related to the process involved.

Physical Basis of the Automated Approach

To appreciate the approaches specific to the problem of gamma ray measurements, the interaction of gamma rays within a detector and the physical construction of such detectors must be considered. Three principal processes characterize a gamma ray's interaction in a material; photoelectric effect, Compton scattering, and pair-production events. [A fourth possibility is that no interaction results; an effect nonetheless crucial to experimental and instrumental design.] Of course, an interaction must occur if the gamma ray is to be detected and its energy established. Since the relative probability of each type of interaction varies as the atomic number of the target, different detector configurations are often used at different gamma ray energies. Since the cross-section for each process also varies as the gamma ray energy, different effects may dominate within the same measured spectrum. Ultimately, whichever interaction occurs within a detector must be translated into an electrical impulse which is distinguished only by the energy of the gamma ray that caused it. Because the energy of the incident gamma ray is to be determined, it is of paramount importance that the type of interaction be known, and that all consequences of a given interaction be

considered. The ability of a given detector to distinguish between gamma rays of nearly-equal energies is referred to as the resolution.

Although many types of detection systems are in use, scintillation counters and solid state detectors are most commonly encountered in gamma ray experimentation. The superior quality of solid state detectors lends itself more readily to automated spectral analysis.(EW64)

Sodium iodide [NaI] detectors are 'scintillation-counters'. An energetic electron produced by the gamma ray causes a small flash of light in the crystal of sodium iodide. This light is translated into a measurable electrical impulse through a photomultiplier tube in contact with the crystal. The resolution of such a detector is poor; generally five or ten percent of the incident energy.

Solid state detectors provide superior resolution to that of NaI detectors, principally because the incident gamma ray energy is more efficiently translated into the production of charge carriers. This detector is basically a reverse-biased PN-junction, and the gamma ray's energy serves to create a large number of electron-hole pairs which are swept away by a large reverse potential to appear as a pulse in the accompanying circuitry. While intrinsic germanium (Ge) is a preferred semiconductor, unavoidable impurities have been tolerated in the past with the addition

of small quantities of lithium, creating a lithium-drifted germanium, Ge(Li) detector.[KN79] Figure 2.1 compares the resolution of NaI and Ge(Li) detectors.

The physical interaction of an incident gamma ray on a detector provides the necessary secondary effects which make it possible to translate the gamma ray energy into a specific electrical impulse. However, as discussed above, more than one event may occur as a result of the interaction. Even worse, an interaction may have side effects which do nothing but add uncertainty to the measurement. While an experiment may be constructed to favour certain events through effective collimation or by virtue of the atomic weight of the detector substrate, these side effects may be unavoidable. An example of such an effect is a direct result of a pair-production interaction. Here, the incident gamma ray has the immediate effect of converting all its energy into an electron-positron pair, and many possible fates unfold from this point. If the full gamma ray energy is to be determined, the electron and positron must remain within the detector, where the positron will ultimately annihilate with a nearby electron, releasing two 511 KeV gamma rays which in turn must interact within the detector. It is the untimely escape from the detector crystal of one or both of the latter gamma rays which

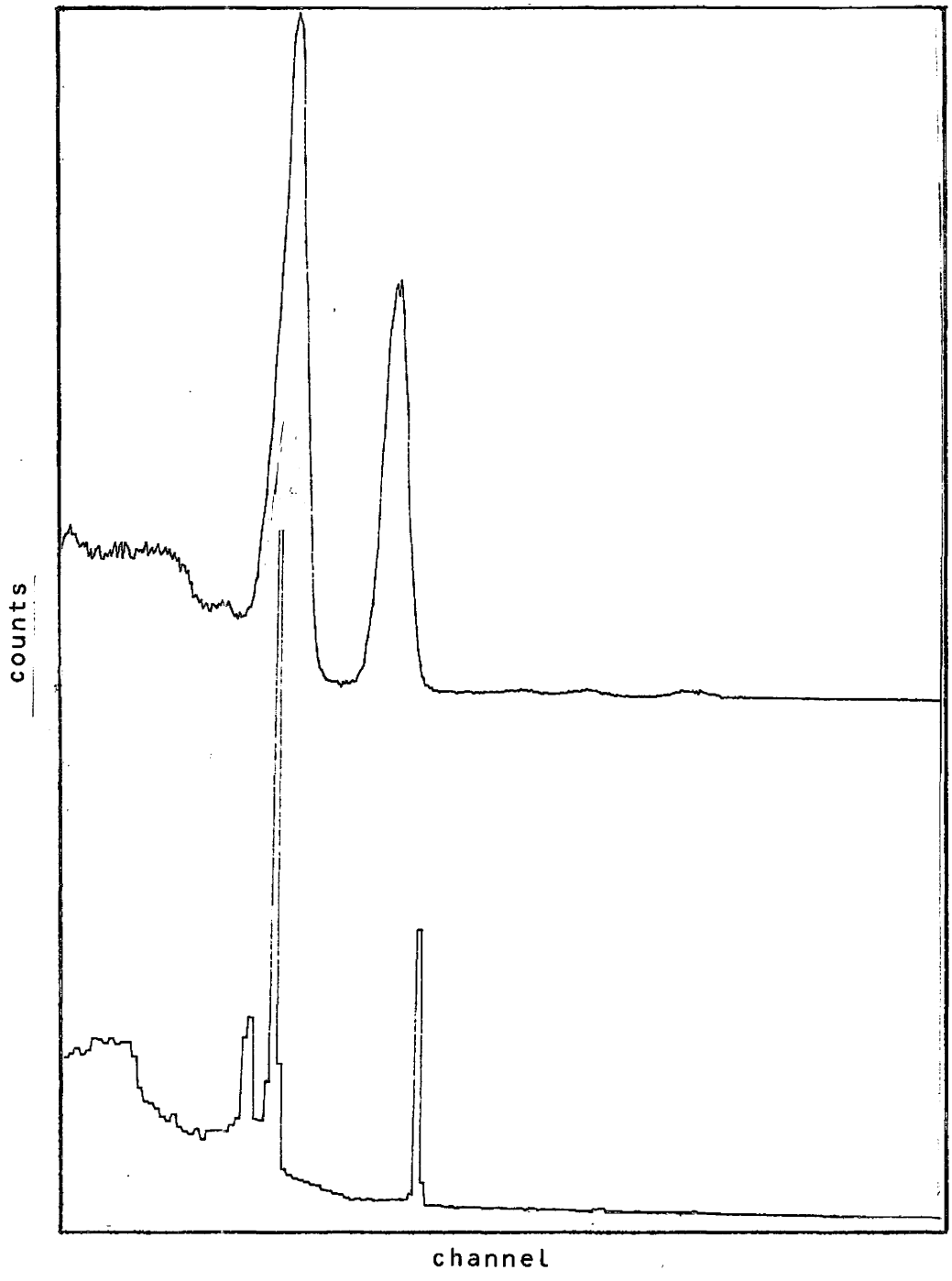

FIGURE 2.1 COMPARISON OF Ge(Li) AND NaI DETECTORS

Spectrum of ^{134}Cs illustrates the superior resolution of the solid state Ge(Li) detector [below]. Clearly defined peaks collected with the Ge(Li) detector are ideal candidates for automated methods, while a doublet [40 Kev separation] is completely masked when the NaI detector is used.

results in the "single-escape" and "double-escape" peaks familiar to spectroscopists. If a Compton interaction precedes the escape, some residual energy will remain in the detector, resulting in a different energy again. Finally, the original electron or positron itself may escape from the crystal, leaving behind only a fraction of the incident gamma ray energy. Clearly such physical effects are beyond the control of an experimenter, yet the success of an experimental technique often depends on dealing with such phenomena. It is these effects, and others, which determine the response-function of solid state detectors. The question of which output signal results from a given gamma ray energy and the feasibility of calculating that energy given only the resulting signal determines whether or not a detector is useful at all. Detector electronics, such as fast-coincidence circuits, or applied numerical techniques [based on the known interactions] can improve such results considerably.

Much work in numerical analysis is concerned with dealing with effects such as those described above. Each procedure may be viewed as a specific approach to a well-defined problem, just as a certain instrument may be used to selectively remove or enhance certain effects. The over-riding goal of such work is to approximate the ideal spectrum given actual experimental results.

CHAPTER III

DIGITAL FILTERING

If the response function of a detection system was known, it would seem reasonable that the original information could be extracted by an inverse mathematical operation performed on the measured data. Such a process is called unfolding, or deconvolution. Unfortunately, while it is a promising proposition, the procedure is not easily implemented in practice. The response function of an acquisition system [detector, amplifier, pulse-height analyzer etc.] is not always known per se; although it may be determined by the response at an isolated peak, [impulse input], or approximated by a Gaussian function, [central-limit theorem (BR65)] . However, it is the unavoidable presence of random noise in a measurement which ensures that a straightforward approach to deconvolution will result in an intolerable increase in background contribution.

Principle of Deconvolution

In the notation of Kennett et al.(KE78), a measured signal M(x), of a process T(x), by a system with linear response function R(x,x'), is expressed as

$$M(x') = \int R(x,x')T(x)\ dx + N(x')$$

which is clearly the convolution of the input data with the response function. N(x') is an [unknown] noise contribution.

By Fourier-transform theory, this convolution becomes a multiplication in the transform domain, giving

$$M(s) = R(s)\ T(s) + N(s)$$

It may be seen that only the presence of a noise term, N(s) prohibits the use of simple division to arrive at the desired result T(s), all other variables being known.

Various iterative approaches to this problem have been discussed, notably by Van Cittert, and by Kennett et al. (KE78). The latter group have outlined an approach based on probabilistic operations, the Bayesian deconvolution, which assures positivity of solution while maintaining noise growth at tolerable levels. This method, although demonstrated to be extremely effective, is too time-consuming to be performed as part of the routine analysis of large spectra, and it is best reserved for the cases of resolving poorly defined structure or closely spaced peaks. Of course, any deconvolution method demands a translationally invariant response function. [at least locally] (BR65)

There are cases where a considerable amount of improvement may be made to measured spectra without a complete deconvolution taking place. Such cases include those where definable linear contributions have been made to each peak. These effects may be readily reversed by modelling the undesirable response and constructing an inverse function to remove its contribution. (TE81)

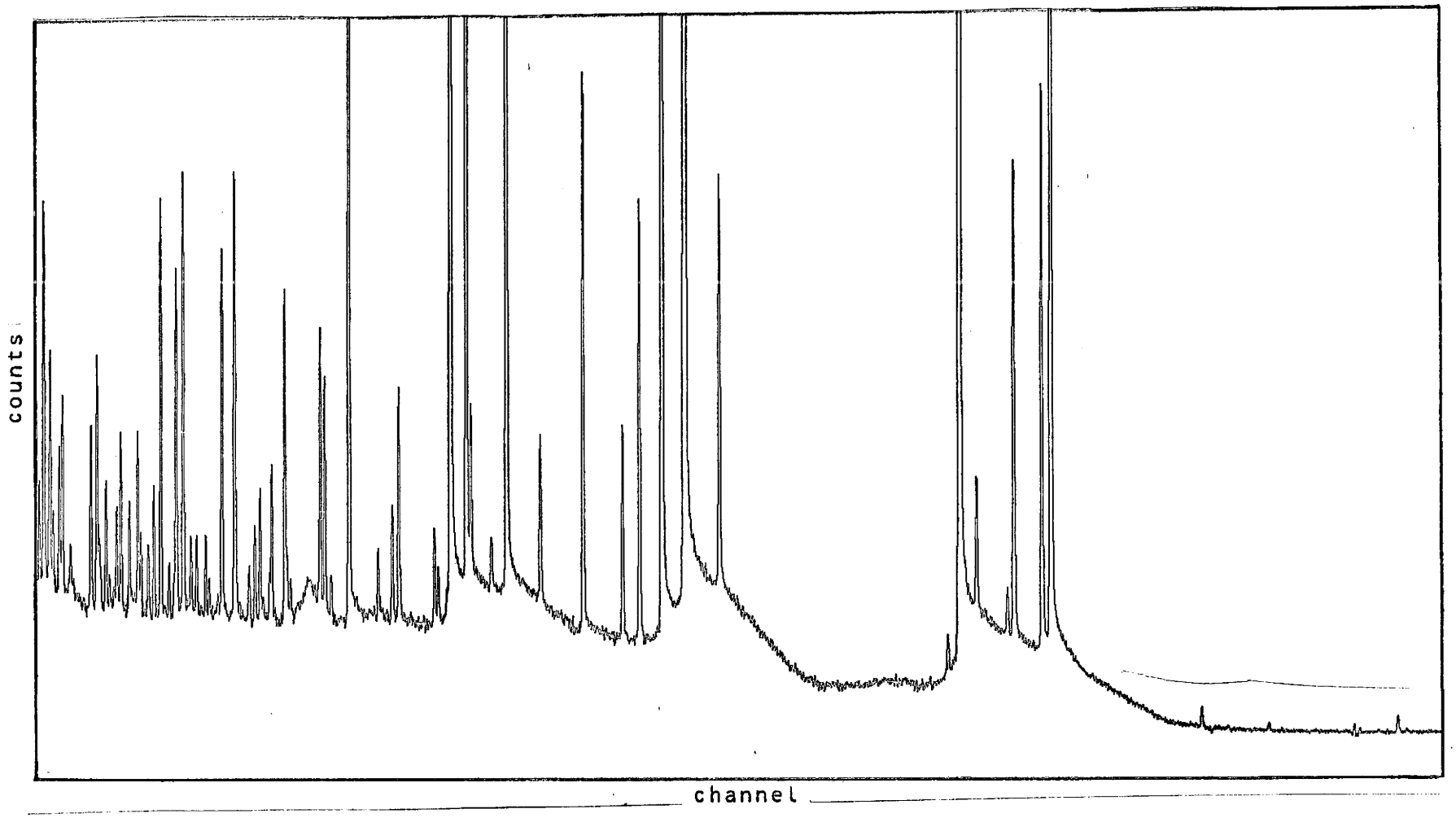

FIGURE 3.1 TYPICAL SPECTRUM BEFORE FILTERING

A high-energy "toe" has appeared on every peak in this spectrum, collected with the triple-coincidence spectrometer. Contributed by the detection system, such a definable, linear contribution is readily attacked with digital filtering techniques.

Defining a Filter

If the physical origins of such effects are known, the conditions of linearity and omni-presence may be easily verified, and a mathematical model constructed. An example of such an effect is shown in Fig 3.1 , where a distinctive high-energy toe has appeared on every peak of the $^{141}Pr(n,g)^{142}Pr$ spectrum. In this case, the offending toe has well defined origins in the triple-coincidence detector used (KN79). In this arrangement, only pair production events leading to double escape are selectively chosen by accepting only events accompanied by the emission of two 511 KeV gamma rays. [Of course, the measured energy will be exactly 1.022 MeV too low.] The toes are formed when one of the 511 KeV rays undergoes Compton scattering before escape, leaving a small amount of energy behind, but still satisfying coincidence conditions by being nearly 511 KeV. (OR67) The toes, caused by events independent of the incident gamma ray energy, are expected to be a linear contribution present in every peak. [Fig. 3.2]

This process may be represented as the convolution of the original signal T(x), by some unknown function ?(x), resulting in a measured spectrum with toes M(x).

$$T(x) * ?(x) = M(x)$$

where "*" represents convolution, following the notation of Bracewell (BR65). T(x) is considered, in this case, to be

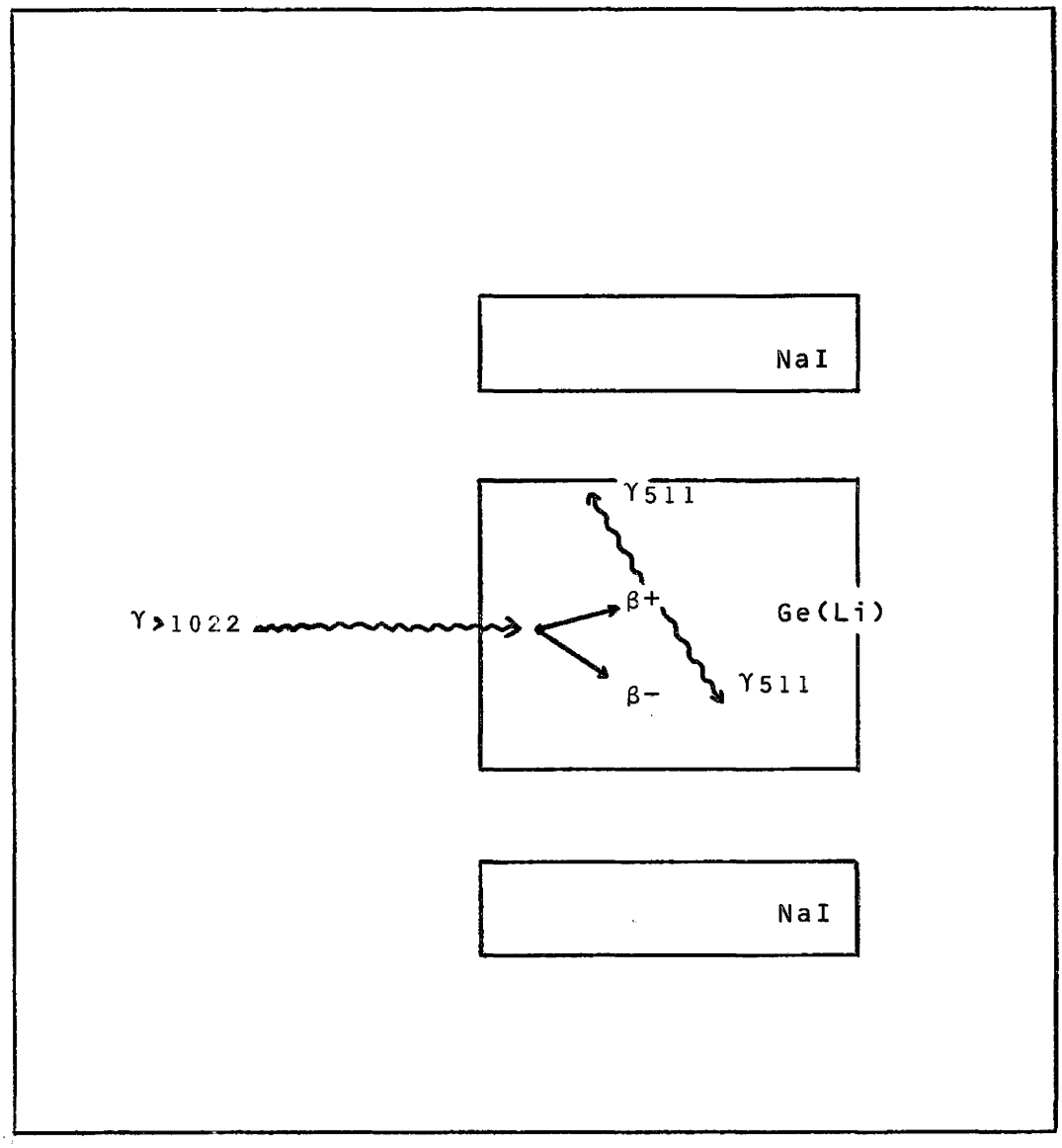

FIGURE 3.2 TRIPLE-COINCIDENCE DETECTOR

In this arrangement, pair-production events in the central [Ge(Li)] detector are selected by accepting only those accompanied by two 511 KeV annhilation gamma rays in the diametrically opposed NaI detectors.

A high-energy component appears on peaks when a Compton event precedes the escape from the central detector; while energy is left behind, the gamma ray is still nearly 511 KeV when a coincidence is recorded.

a spectrum which has already suffered the effects of measurement, the toe contribution being but the last of these effects. This notation is valid since convolution is a commutative operation. (BR65)

A function F(x) is desired which, when acting on M(x), will yield the desired T(x).

$$F(x) * M(x) = T(x)$$

This process may be modelled by convolving the function F(x), with a peak-and-toe model $P_t(x)$, leaving only a peak P(x), modelled as a Dirac delta function with amplitude **c**.

$$F(x) * P_t(x) = P(x)$$

The form of $P_t(x)$ is simply a Dirac delta function with a triangular base. [Both the length of the triangle and its area ratio to the peak may be adjusted] If the components of the modelled process are transformed, the filter may be obtained by a simple division,

$$F(s) = \frac{P(s)}{P_t(s)}$$

Observing that the Fourier transform of a delta function is a constant, the inverse filter is simply

$$F(s) = \frac{\mathbf{c}}{P_t(s)}$$

where **c** is simply the amplitude of the delta function, since $P(s)_{s=0}$ gives the integral of the function P(x). (BR65)

If this function, suitably transformed, acts on raw data such as that is Fig.3.1, the toe contribution will be

effectively suppressed, as Fig.3.3 shows. Furthermore, an inspection of the difference between the original and filtered spectrum reveals the remarkable smoothness of the subtracted data, despite the unavoidable presence of noise in the original spectrum. The result is a considerable improvement in background regularity, and an important step in approaching the response of an ideal system.

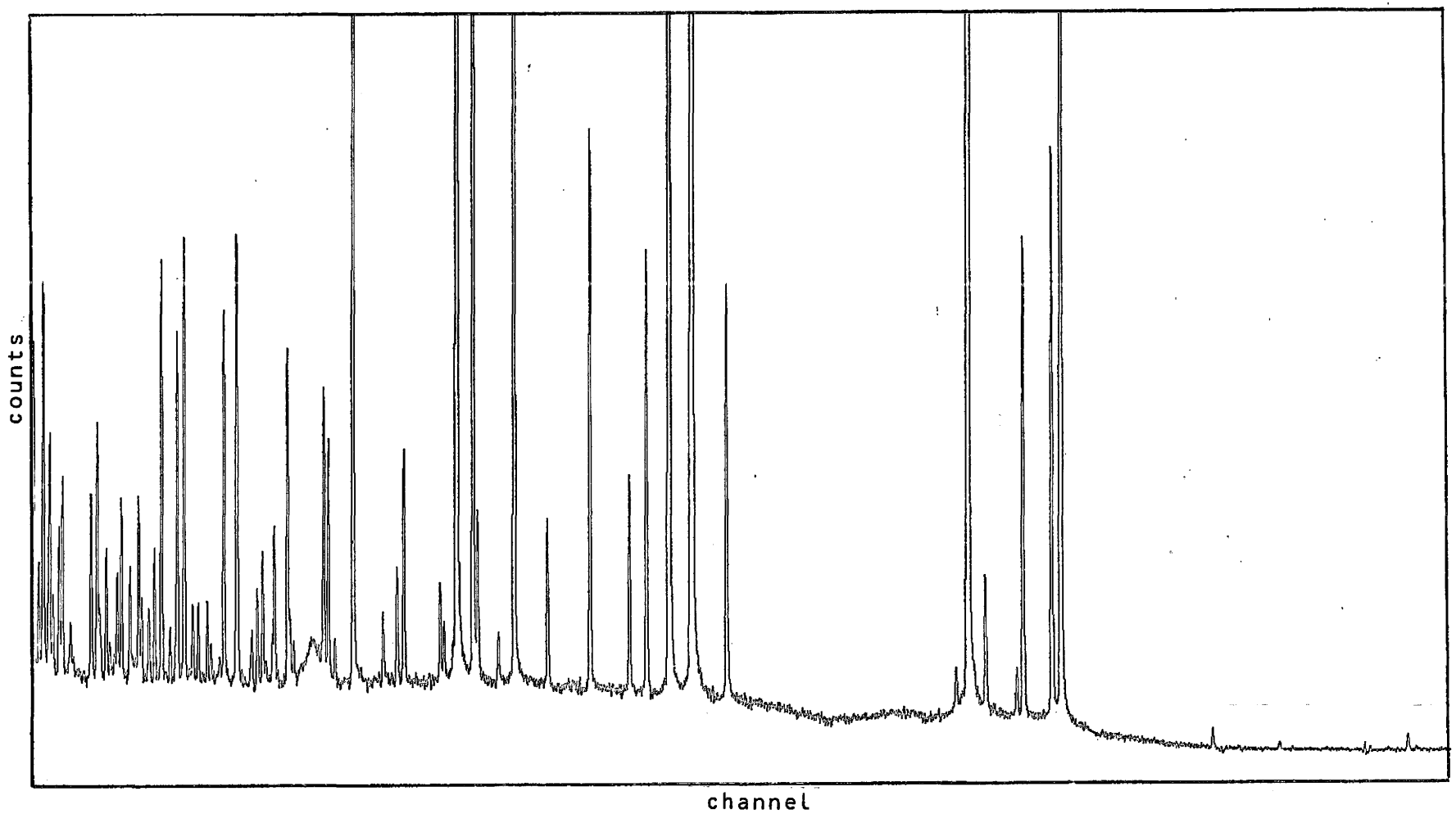

FIGURE 3.3 SPECTRUM AFTER FILTERING OPERATION

The spectrum of Fig 3.1 is shown after treatment with a digital filter. A considerable improvement in background regularity has been achieved with the use of the peak-and-toe model.

CHAPTER IV

BACKGROUND ESTIMATION

Ideally, gamma ray spectra could be collected without any information present but the desired peaks. Multi-channel analyzer data would appear as a vector containing zeroes where there were no peaks, and the peak amplitudes could be read directly from channels corresponding to their energy. The purpose of any background estimation procedure is to render results in this form given raw data having somewhat less than ideal characteristics.

An innumerable variety of effects combine to make measured spectra less than ideal. While some effects are common to all gamma ray spectra collected with Ge or Ge(Li) detectors, such as counting statistics, others appear only under certain experimental conditions, such as pileup [at high count rates], or the presence of Compton edges [at low energies]. Other effects may be specific to a certain detection system, as with the triple-coincidence arrangement of Chapter Two. Effects such as the latter must often be dealt with separately to permit any kind of reasonable background estimation.

Assuming the measured spectrum is relatively free from untoward distortions [such as overflows in certain channels]

and that the number of counts across the spectrum is high enough to permit a meaningful approach to the analysis, the problem of background estimation is one of removing a smoothly varying background continuum upon which peaks have been superimposed. Such a background continuum is made up of stray counts at other than the desired energies, created through some statistical or physical process which, by nature of its origins, cannot be treated directly. Obviously, random effects, or even non-linear contributions to background, cannot be dealt with through simple digital filters. Unfortunately, these conditions encompass almost all contributions to the background continuum.

One is not confined to procedures which would remove this continuum, leaving peaks on a zero background. Indeed, statistical methods are in use, based on the expected shape of peaks and the expected behaviour of the continuum, which allow peak detection and area estimation without any background treatment. Mariscotti (MA67) and, Robertson et al.(RO72) have outlined second-differencing methods which detect the [Gaussian] peak shape through its characteristic second-derivative. These methods rely on the background being locally linear to arrive at reliable results; they could be misled by sharp, peak-like Compton edges, or may fail to detect small peaks at all.

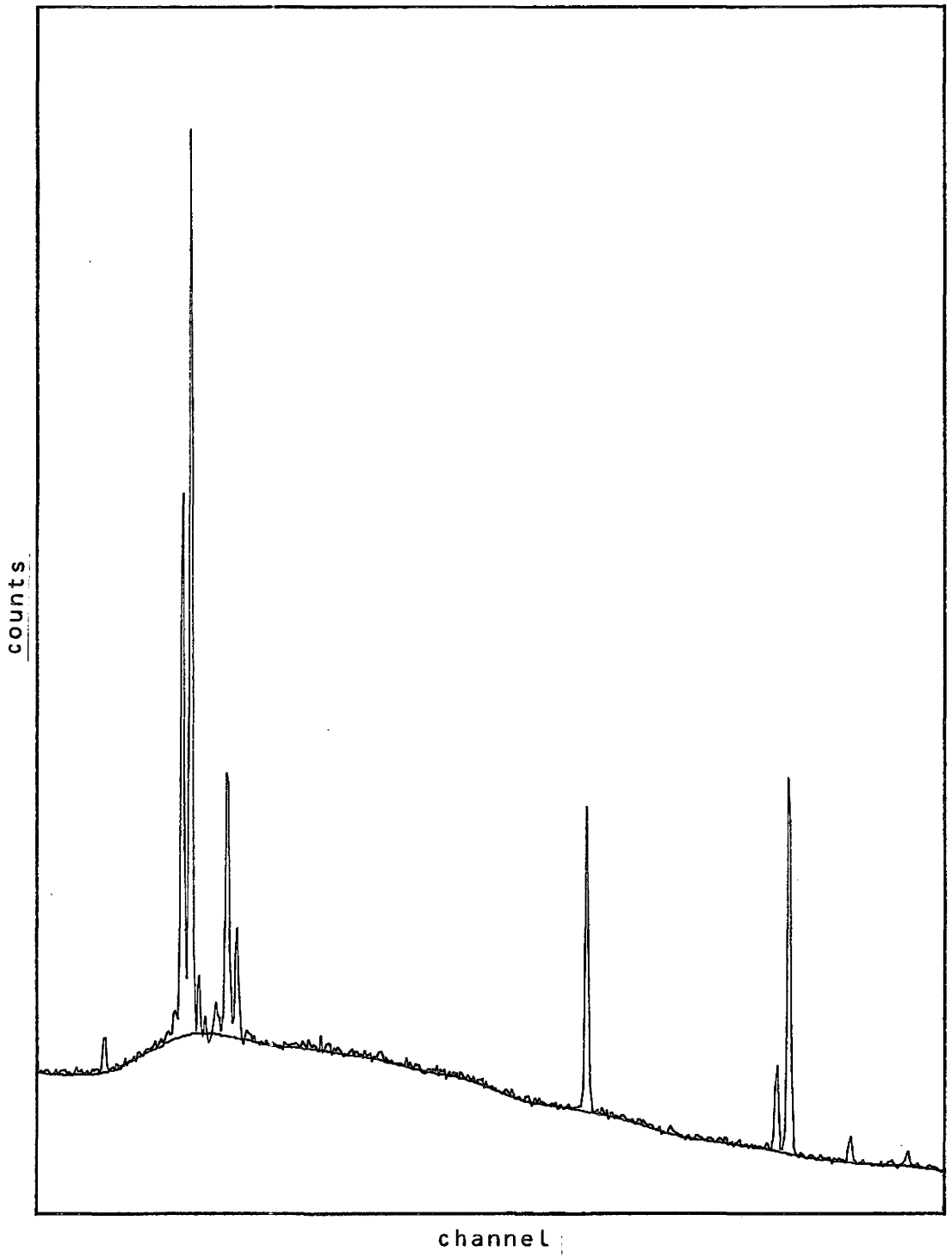

FIGURE 4.1 TYPICAL SPECTRUM WITH ESTIMATED BACKGROUND

This Radium spectrum illustrates the non-zero continuum which is to be removed through background estimation procedures. Also shown is the calculated background generated with the outlined method.

At some point however, a background must usually be estimated under a peak (even if only locally) in order to determine its area.(QU69) Conventional hand-analysis methods, of course, involve determining peak position by eye, and drawing a line across the base of the peak, perhaps by sampling nearby background points as being typical of the region.(KO73) (BA77) The computer-aided extension of this approach is to determine peak areas directly by fitting a Gaussian model to the peaks, often with a correction applied to the shape to compensate for particular detector response-functions. Much work has been done in this domain.(RO69),(KI71),(HI76),(HE67) This technique, although extremely popular, requires a degree of parameter-fitting around each peak and, like other procedures, special steps must be taken in the presence of doublets.(FA70) It is noteworthy that many of these methods were developed to analyze data from NaI detectors; where a characteristically wide response-function demands that poorly-resolved peaks be analyzed on an essentially undefinable background. Contemporary solid state detectors supply peaks which are in general much more sharply defined, and a more fundamental approach may be taken.

While the above methods are useful in situations where the detection system prohibits continuous background estimation, there exists a large class of situations where

it is desirable to first remove the background continuum. Simple spectra, of course, may be readily analyzed without the need for large investments in computer time if the background is first removed. More complex spectra may be better analyzed through Bayesian-deconvolution methods which allow the resolution of fine details in an unbiased and reproducible fashion. (KE78) Athough extremely effective, the latter methods work best when performed on data from which the background continuum has been removed.

The problem of automatically estimating a background continuum has been approached in the past. In general, most methods begin by assuming that background is a minima-event, that is to say that background channels contain lower counts than those containing peaks. By choosing minima along the spectrum, the shape of the continuum may be estimated, and subtracted. Such a method was proposed by Inouye (IN69), and by Weismeier(WE81). Kennett et al. (KE81) performed a systematic study of the background shape, concluding that, through choosing minima, the shape of a true background could be estimated through a statistical calculation. Given a sampled background, the smooth continuum could be modelled by interpolating between samples using a cubic-B spline calculation. These methods rely on choosing suitable intervals for background sampling, a parameter which could change with the nature of the data at hand. Unfortunately,

such a minima search to determine background behaviour presupposes that the background has zero slope within the region being examined, or sampled points will not accurately represent the background. Choosing smaller intervals will ultimately render a background estimation which is too readily seen to mistake peaks for fluctations in the background. Secondly, the use of minima within intervals as a criterion for choosing background overlooks the nature of Compton edges; these wide, rising, deviations from a smooth background are, by definition, maxima events in the background. Approaches which serve to correct the estimation around Compton edges quickly fall short of the justifications which allowed minima-sampling to take place, while other modifications which rely on the detection of upward deviations to signal the presence of Compton edges may lead to totally unacceptable results, such as the removal of entire peaks, mistaken for simple deviations from the background.

A Method for Calculating Background Continuum

In light of all these problems, a whole new approach to the problem must be considered. By definition, the background channels contain fewer counts than those harbouring peaks, and the concept of choosing channels with minimum counts is sound in this respect. However, in order to accurately follow the background, a different sampling

strategy is necessary, one which eliminates the bias of fixed interval lengths. This problem was anticipated by Weismeier (WE81), who attempted to eliminate it by taking the intersection of two sampling runs using different interval lengths. Of course, this approach makes it even less likely that Compton events will be included in the background estimation.

Instead of choosing a minimum point within an interval as a background sample, the entire spectrum may be examined point-by-point to determine background behaviour. A local minimum point is defined as any channel having counts less than both adjacent channels. This condition will be met for a large percentage of background points, where statistical fluctuations prevail. Peaks, on the other hand, predominantly span channels where at least one of the adjacent channels is much lower. Here, statistical fluctuations create fewer local minima, since the channel-to-channel changes through a peak are greater than fluctuations due to counting error. However, this is not the case on a Compton edge, where the background has strayed from monotonicity in a much slower fashion. Thus the channels corresponding to local minima may be considered to represent background, including both regular background and Compton events.

Following the work of Kennett et al.(KE81), the

observed background may be viewed as statistical fluctuations about a [still to be estimated] continuous line. Assuming the cumulative distribution function [CDF] across the line is f(x), [for every channel] then

$$Pr[\mathbf{x}<x] = f(x)$$

Since successive samplings may be considered independent events, then

$$Pr[\mathbf{x}<x \; ; \; x] = Pr[\mathbf{x}<x] \; Pr[\; x \;]$$

where Pr[x], the probability of choosing an x, is the density function for this distribution, evaluated at x. Defining Pr['local minimum'] as

$$Pr[\text{ two larger points } ; \; x \;]$$

the probability of a chosen x being a local minimum (M[x]) is given by

$$M[x] = Pr[x] \; [\; 1 - f(x) \;]^2$$

Obviously, the probability of a given point being a chosen mimimum varies inversely as its position with respect to the background. [A very small point is likely to be surrounded by two larger points.] Since counting statistics are the major contributor to the form of f(x), then Pr[x] may be considered Gaussian with mean m, and variance s. (BR79)

The integral of M(x) over all x gives the percentage of points in regular background expected to tagged as local minima. Since Pr[x] is by definition the derivative of the

cumulative distribution function, f(x), the integral reduces to

$$\int M(x)\ dx = \int f'(x)[\ 1 - f(x)\ ]^2\ dx$$

which gives, by inspection,

$$\int M(x)\ dx = (-1/3)\ [\ 1 - f(x)\ ]^3 = 1/3$$

or about one-third of all typical background points will be chosen as a sampling. [This may be compared to choosing one minimum in an interval perhaps 50 channels wide.] This result may be intuitively reached by considering the permutations of three equally-likely events; one-third of the events place the smallest choice in-between the other two.

The algorithm to accomplish this procedure stores in a vector the addresses of all the channels defined as local minima. This vector is filled in one pass with the addresses of every channel containing less counts than both of the adjacent channels. This procedure alone may select points [such as in doublets] which are not to be included as background, and such points may be ignored if they lie several standard devations above the previously defined minimum. On the other hand, when the background is interpolated from a sampling of these minima, the uncharacteristic position of such points may be weighted against them.

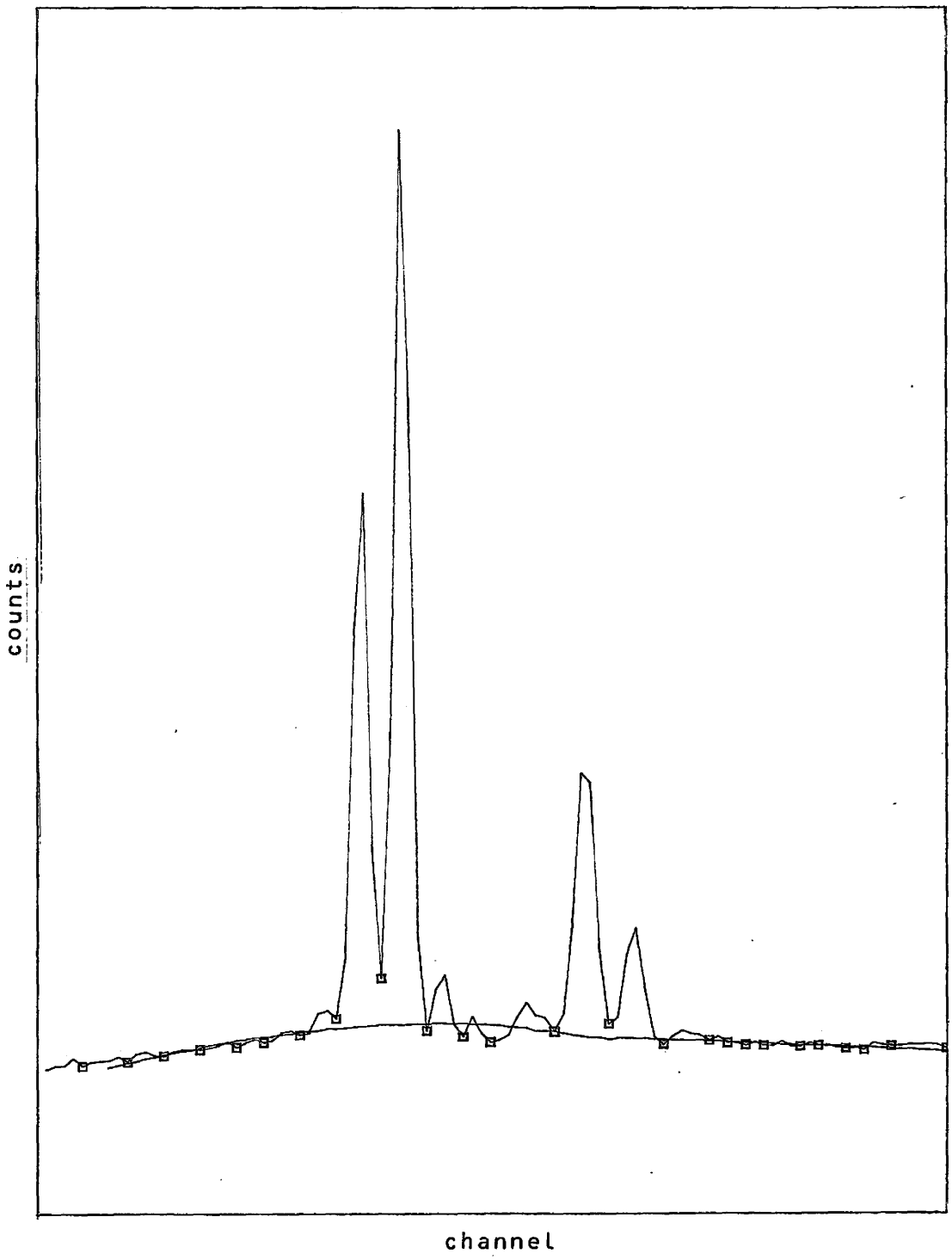

FIGURE 4.2 MAGNIFIED SPECTRUM SHOWING DEFINED MINIMA

The background is defined by selecting 'local-minima', points which are lower than both adjacent channels. A least-squares fit interpolates the background at every point using a number of these minima.

The local minima form a set of points which closely track background fluctuations. Therefore, the separation between points will be an indication of the peak density along the spectrum. Where there are many peaks, the background minima will be widely spaced, and vice versa. Since a sampling of the background is still desired for a curve fit, a fixed number of these chosen minima may be used to define an average value for the background. The fixed number will span differing channel numbers, meaning that wide intervals will be chosen under large peaks, and smaller intervals under event-free sections. Although a similar criterion was chosen by Kennett (KE81) for establishing sampling regions, the choice is now made dynamically and will adjust with the spectrum being analyzed. The average value chosen for background within this interval will be interpolated from a weighted fit of all the local minima in the interval.

To estimate the background at any point, the ten nearest local minima within a symmetric region are chosen using the vector defined above. These points will correspond to a range of somewhat more than thirty channels in regular background [from the preceding analysis], and more under peaks. Their values form a sampling of background behaviour in the region, and a linear [or quadratic] least-squares fit provides a reliable background point at each channel in the

spectrum. In this case, since several adjacent channels will share the same set of [ten] nearby minima, the interpolated value of the background will tend to change in steps as different samples are included. This effect may be lessened by weighting minima closest to the channel being calculated, or by smoothing the final answer. Such smoothing must be performed with due care, since the representation of true, sharp background events would be muddied by the same process.

The line constructed from the local minima passes under the data, grazing the background at each point along the spectrum. In order to subtract the background continuum, this line must be raised to lie at the mean of the background, rather than at the mean of the local minima. This is similar to an operation suggested by Kennett et al.,(KE81) in which a correction term was calculated as a function of the interval spacing. In this case, the local minima are sampled and distributed in such a manner that such a correction may now be made which depends only on the standard deviation of the background distribution. This term, of course, varies as the square root of the counts in each channel, and is expected to be relatively constant across an interval. Since the correction factor is to be applied in a continuous manner throughout the entire spectrum, it would normally be applied to each of the chosen

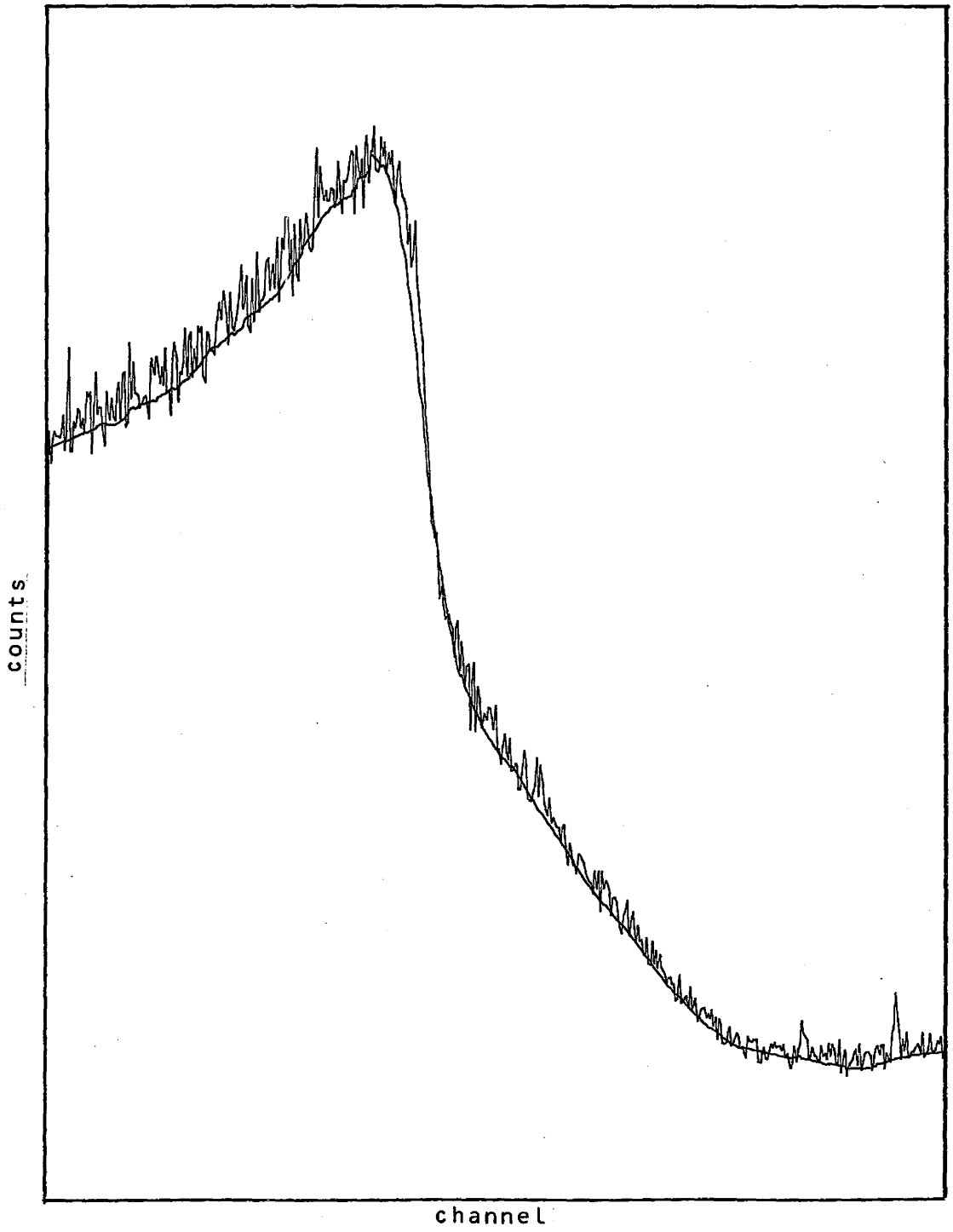

FIGURE 4.3 ILLUSTRATION OF BACKGROUND ON A COMPTON EDGE

The sharp, peak-like structure of a Compton edge makes it a classic troublespot for both peak-detection programs and background-estimation procedures. In this case, the illustrated background shows the ease with which the edge is removed without the need for special procedures.

points before the background curve was calculated.

The combinatorial nature of the problem prohibits a straightforward analytical result, but the correction value may be estimated numerically. Ten thousand trials of Gaussian-distributed random values on a zero-sloped background were performed with various means to determine a value for this parameter. For means of 100 and 1000, the correction was found to be .83 and .85 standard deviations respectively, while similar results were obtained in other trials. It should be noted that the background estimation of Figure 4.3 has not been corrected in this manner.

Finally, if the background is simply subtracted based on this [or any other] estimation procedure, a great deal of information is lost, principally the absolute magnitude of spectral features which is essential to determining Poisson statistics. Therefore, the interpolated background would normally be stored in a separate vector for later reference rather than being immediately subtracted.

In practice, the ability of a computer program to estimate a background continuum is not judicable solely by eye. Of course, it is easy to spot an entirely meaningless fit, but there are cases where the 'correctness' of a given line may be in question, or where no predictable background continuum may be drawn. In the latter case, merit is founded only on the accuracy of the final values [either peak

position or amplitude]. In many cases, where relative, rather than absolute figures are required, the reproducibility of results is paramount. Computers can excell in such a domain, provided that no hidden bias exists in the program.

An Assessment of the Background Estimation Procedure

To complete any discussion of background continuum estimation, some numerical results should be presented. While exhaustive testing under all conditions is clearly not a practical possibility, some fair test in light of the expected applications may be performed.

Background estimation techniques generally preceed peak-detection procedures in the analysis of [a priori] unknown spectra. Often, as in the example of neutron-activation analysis, the presence of statistically-significant peaks is used to determine chemical composition through a study of their position and intensity. Clearly, a background estimation procedure should preserve these quantities while removing any underlying continuum.

A test was devised to determine the effect of background removal on a typical spectrum. Two criteria were chosen which would normally be independent of detector efficiencies and therefore solely dependent on the method used to determine peak position and amplitude; the separation and the relative intensities of escape-peaks. As

described in Chapter II, escape peaks are spectral artifacts resulting from the escape of one or both 511 KeV gamma rays from a pair-production interaction. Their relative intensities are expected to be constant for a given detector configuration, and they must by definition be separated by 511 KeV from the incident gamma ray energy and from each other. The test would be to remove the background from a typical spectrum and to verify these values.

Typical (n,g) spectra were collected at the McMaster Nuclear Reactor with a solid-state detector, using three different samples containing nitrogen and another element. The background continuum was estimated and removed according to the outlined methods [with no operator intervention], and dominant nitrogen peaks were selected for close examination. Peaks with counts ranging from 20,000 to 300,000 were chosen to minimize the effects of statistical fluctuations. Six such peaks and their associated escape-peaks were to be used for each of the three samples; however, interferences prohibited the use of the double-escape peaks in two of the cases.

A comparison was made between the measured intensities of the escape peaks in all three samples. Any error introduced by the background estimation procedure would be expected to affect these ratios. Figure 4.4 illustrates the results, while averaging the values obtained for each of the

three samples gives [showing percentage error]

Sample 1.	0.2884 $\pm$ 0.0019	[0.6%]
Sample 2.	0.4457 $\pm$ 0.0074	[1.7%]
Sample 3.	0.2656 $\pm$ 0.0073	[2.7%]

Since some peaks used for comparison backgounds and possible interferences are different, actual error could be smaller. The average ratio of double/single escape peaks was for all cases 1.42 $\pm$ 0.05 [4.0%]

ENERGY [KeV]	SAMPLE NUMBER	FULL ENERGY	SINGLE ESCAPE	DOUBLE ESCAPE	single / double
10829	1	.289	.287	.286	1.36
	2	.458	.450	.448	1.36
	3	.253	.263	.266	1.38
6322	1	.286	.289	.289	*
	2	.457	.446	.447	see
	3	.256	.265	.263	text
5562	1	.291	.286	.292	1.40
	2	.449	.450	.437	1.41
	3	.260	.263	.271	1.33
5532	1	.287	.290	.290	*
	2	.449	.440	.445	
	3	.264	.271	.264	
5298	1	.289	.289	.289	1.44
	2	.447	.446	.437	1.41
	3	.263	.264	.274	1.50
5269	1	.287	.290	.286	1.44
	2	.451	.436	.429	1.44
	3	.262	.274	.285	1.52

FIGURE 4.4 ESCAPE-PEAK ANALYSIS ON TEST SPECTRA

Test spectra [1: N + Be, 2: N + C, 3: N_2 + Si] were treated with the background estimation procedure, and the escape-peak ratios calculated for some significant peaks. Results show that peak areas are preserved by the background estimation procedure.

CHAPTER V

CONCLUSIONS

The use of automated [non-interactive] methods in gamma ray spectroscopy is justified by a study of the physical and mathematical nature of nuclear measurements. Deviations from an ideal spectrum may be traced to the inherent statistical uncertainty in counting experiments, the unavoidable instrumental contributions called 'response-function', and the unwelcome 'random-noise' present in every measurement. While methods of minimizing such effects could be effected in the mechanical design of instruments, their nature precludes their complete elimination, and the numerical analysis of measured data seeks to reduce their contributions after the measurement has been made.

Digital filtering has been proposed as an effective method of eliminating some characteristic linear distortions, using the high-energy toes from a triple-coincidence instrument as an example.

An effective method of estimating background continuum in complex spectra has been outlined, one which proves particularly effective on Compton edges, a classic trouble-spot for automated procedures.

Finally, these methods have been implemented in FORTRAN IV in a package of analysis programs.

APPENDIX

Implementation of the numerical techniques required that a system of data handling be developed which would allow the efficient transfer of intermediate results from one step to the next. While many of the manipulations are well suited to implementation on a small computer, the desire to analyze raw spectra of up to 8192 channels led to the choice of the McMaster University CYBER 170 computer as primary computer. An assortment of peripherals; plotters, printers, tape drives etc., and a variety of pre-packaged programs available also made this choice desirable. On the other hand, some of the development and part of the final analysis would be more conveniently performed on a Data General NOVA II minicomputer within the laboratory, meaning that such a system should also allow the transfer of raw data and intermediate results between the two systems. Developed computer methods must, of course, be general enough to accommodate future changes to the available service.

No one multi-purpose program would fulfil the above requirements, so a package of modular programs was developed in which each step of the analysis procedure could be performed independently. Written in FORTRAN IV, the programs each form but one step in the analysis stream, a stream which could be constructed simply by placing the desired

procedures in a sequential set, just as one constructs a flow-chart. In this way, the analysis could be as limited or as varied as the user desired with an absolute minimum of reprogramming effort. The plot of an intermediate result, for example, could be obtained by simply placing program PLOT in the list of analysis programs. Specialized routines, such as for tape reading and writing, which depend heavily upon the demands of the computer in use, may, in this manner, be customised and tested independently of the analysis routines, at which point they appear to the user only as TAPEIN, or TAPEOUT--- the intricacies of a particular hardware configuration disappear.

By definition, this system allows for future changes or improvements to be made by writing a FORTRAN program to perform the desired manipulation [bearing in mind the formalities of the system as a whole] and incorporating the new program into a library of routines available to the user.

TERVLIB: A Spectrum Analysis Package

This package of programs was written in FORTRAN IV using a CDC CYBER 170 computer under the NOS operating system. An effort has been made to implement only standard FORTRAN functions and syntax, despite the fact that CDC FORTRAN features a number of additions to the language. Of course, if another system is used to run these programs, some modification may be necessary; particularly where library routines have been used [special routines were used from the IMSL collection of programs] and especially where tape reading and writing is performed. The latter case ensuing, input/output routines must be written which transfer data in blocks of 8192 channels to and from the computer, usually to be stored on disk until analysis is complete.

The package itself consists of a number of programs which may each be used as one step in the analysis stream. By sharing common features, each routine [although a complete program in itself] may accept and modify data produced by any of the others.

The operating system allows a certain amount of file manipulation such as storing and retrieving files from disk and renaming files to allow output data to be designated as input for the next step in analysis. This flexibility further extends the usefulness of the package.

Common Features :

1/ All programs work on 8192 channel integer data.

2/ All programs accept as input
the FORTRAN logical file TAPE3.

3/ All programs write output to TAPE4;
all leave TAPE3 [input] intact.
Certain programs may also use TAPE7 as output.

4/ All programs begin by rewinding the TAPE#s to be used

5/ Certain programs require additional information such as gain or zero-energy information. Such information is accepted as INPUT directly from the procedure file [TAPE10].

Figure 1 illustrates the way in which various programs interact through FORTRAN logical files. The programs shown were typical of those which would be included as an absolute minimum in such a package. More specifically, the programs FILTER, and BACKGR are implementations of the procedures described in chapters three and four. Each of these programs is to be described in some detail.

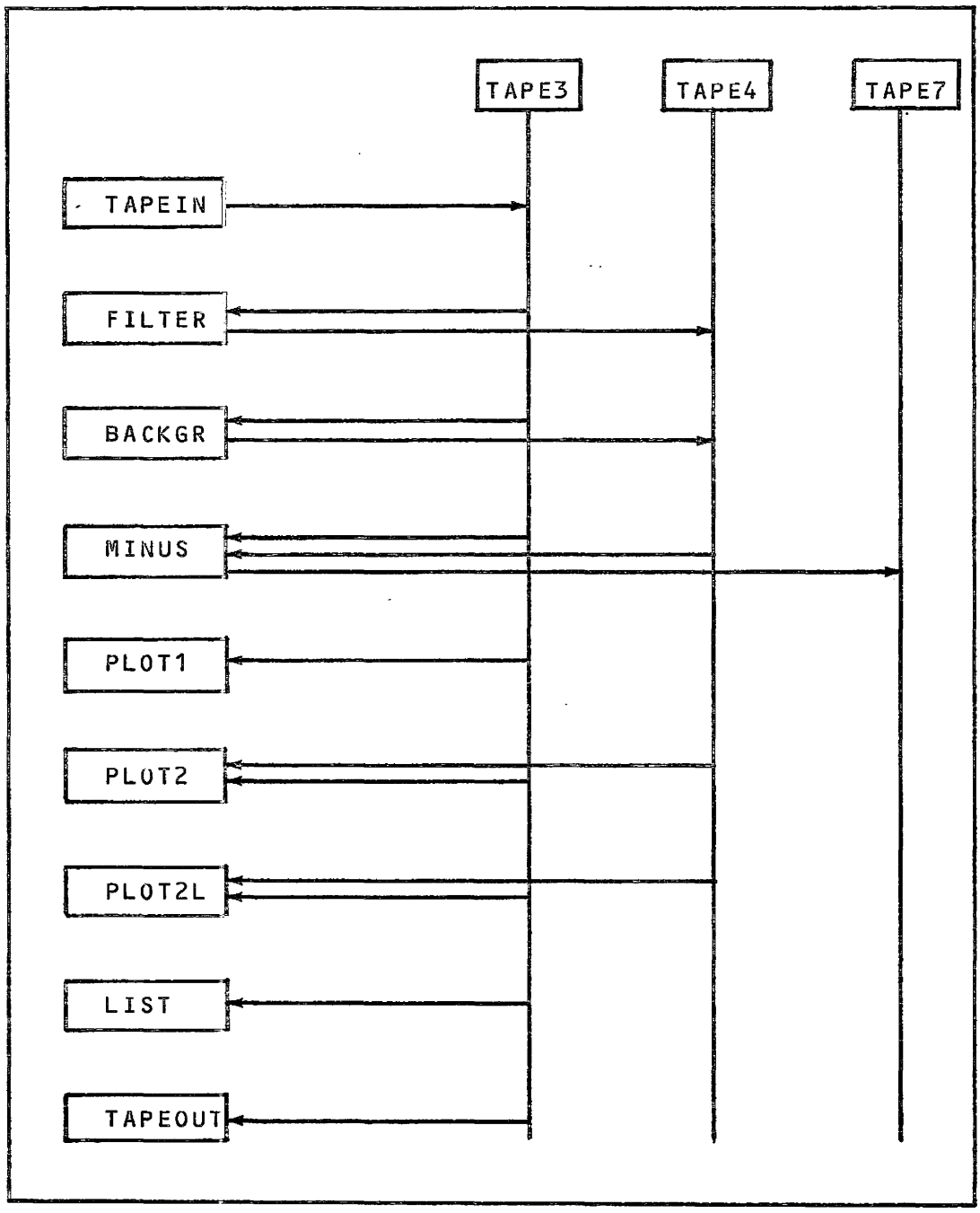

FIGURE 1. TERVLIB File Structure

The various programs in the package interact through FORTRAN logical file names. Combined with other common features, this allows the programs to be rearranged in various combinations depending on specific applications.

The Programs of TERVLIB

1.TAPEIN & TAPEOUT: These two programs combine to allow data to be passed in and out of the computer. They both contain assembly-language code to convert tape formats between computers. Since their use and structure is so machine-dependent, no effort is made to explain further.

TAPEIN allows files on magnetic tape to be read by file number [or for various files to be summed], creating an 8192 channel integer file called TAPE3. The file number to be read must be specified in a procedure file.

TAPEOUT writes an 8192 integer file [from TAPE3] onto magnetic tape, readable by another computer.

2. FILTER: This program is an implementation of the techniques in Chapter Three to remove a high-energy toe from collected data [in TAPE3]. The toe parameters being a constant for a given detector arrangement, only the system gain [energy per channel ($KeV \cdot channel^{-1}$)] need be specified in the procedure file. The filtered spectrum is written into TAPE4.

FILTER calls a system program to accomplish a complex Fourier transform of the 8192 channel data [and to perform the inverse operation]. If such a program was not available, then it would need to be included as a subroutine.

3. BACKGR: This program implements the background-generation technique described in Chapter Four, reading the original spectrum from TAPE3, and writing the generated background into TAPE4. No other information is necessary.

4. MINUS: This program simply subtracts two spectra, [from TAPE3 & TAPE4] channel-by-channel, and writes the result into TAPE7. It may be used, for example, in removing the background generated by BACKGD.

5. PLOT1, PLOT2, PLOT2L: These three programs call the plotter, producing respectively a plot of the data in TAPE3, a plot of the data in TAPE3 & TAPE4 on the same graph, and a log-scale plot of TAPE3 & TAPE4 on the same graph. The latter two programs are especially useful in checking the generated background of BACKGR.

6. LIST: Produces a numerical printout of the value of all 8192 values in TAPE3.

Useful Operating System Commands

The package relies on the presence of some system commands, interspersed between programs, to ensure data flow. Of course, these are specific to CDC computers.

1. GET(filename = TAPE3) : retrieves a file called "filename" from disk for analysis, giving it the name TAPE3.

2. RENAME(TAPE4=TAPE3) : assigns the name TAPE3 to a file called TAPE4, used to allow output data to be passed into the next program.

3. SAVE(filename = TAPE3) : saves on disk the contents on TAPE3 under the name "filename" [also use REPLACE]

Typical Data Analysis Procedure

The programs may be stored either as source listings, complied when needed, or stored in the compiled form for immediate use. The obvious trade-off is between the cost and time of compilation, and the cost of storing files on disk. Data too, may be stored on disk or read from tape whenever needed. In general, however, data would be read from tape, processed, and written out as one procedure. Such a procedure is outlined below.

Suppose that a file resides on magnetic tape which is to be filtered, the background removed and the result placed on disk as a file called RESULT, and a plot made of the filtered-only data. The programs to be run need only be listed [assumed compiled versions] as follows;

```
RESTAPE(MT=1)
LABEL(TAPE18,D=556,MT,F=L,LB=KU,VSN=7U1248,PO=W)
          [specifies tape parameters for CDC computer]

GRAB,PLOTVER.
LIBRARY,PLOTVER. [ specifies plot-package for computer]

GET, TAPEIN, FILTER, BACKGR, PLOT1, MINUS.

TAPEIN.    [reads data (100,200) and puts into TAPE3]

FILTER.    [reads data (0.75 = gain) and removes toes]

RENAME(TAPE3 = TAPE4).

PLOT1.     [plots intermediate result now named TAPE3]

BACKGR.    [generate background into TAPE4]

MINUS.     [subtract background, result in TAPE7]

SAVE(RESULT = TAPE7).

/EOR.      [these numbers are read as data]

100  200

/EOR.

0.75

EXIT.
```

```
      PROGRAM FILTRE(INPUT,OUTPUT,TAPE3,TAPE4,TAPE10=INPUT)
*
*    ...A NON-INTERACTIVE TOE-REMOVAL PROGRAM...  R.TERVO  JAN/81
*
*    THIS PROGRAM READS AN 8K SPECTRUM FROM .TAPE3.
*    AND  WRITES THE TOE-LESS SPECTRUM INTO .TAPE4.
* >>>> GAIN MUST BE PROVIDED IN PROCEDURE FILE <<<<
*
      COMPLEX PEAKFFT, SPECTRA(8192),TOE(8192),FILTER(8192)
      DIMENSION IWK(14)
      EQUIVALENCE (TOE,FILTER)
       DATA AREA/0./
*
      REWIND3
      REWIND4
*
      DO 1 J=1 , 8192
    1   TOE(J) = CMPLX(0.,0.)
*
*... THIS PART CREATES THE PEAK-WITH-TOE MODEL ...
*     ..............................
      READ(10,*) GAIN
      LENGTH=INT(230./GAIN)
      LHEIGHT=LENGTH
      TOEPERC=.35
*     ..............................
*
      DO 2 J=1 , LENGTH
       TOE(J) = (FLOAT(LHEIGHT-J))
    2  AREA   = AREA+ FLOAT(LHEIGHT-J)
*
      TOE(1)  = TOE(1)+((AREA*(1.-TOEPERC)/TOEPERC))
      PEAKFFT = TOE(1)
*
      CALL FFT2C(TOE,13,IWK)
*
* TRANSFORM THE TOE MODEL (STILL CALLED .TOE.)
* AND DIVIDE TO GIVE THE SOUGHT FUNCTION, CALLED FILTER(X).
*
      DO 3 J=1 , 8192
      FILTER(J) = PEAKFFT / TOE(J)
*
* THE FILTER COMPLETE, THE SPECTRA MAY NOW BE READ IN
*
       READ(3,*) ITEMP
    3  SPECTRA(J) = CMPLX(FLOAT(ITEMP),0.)
*
      CALL FFT2C(SPECTRA,13,IWK)
*
      DO 4 J=1 , 8192
       SPECTRA(J) = FILTER(J) * SPECTRA(J)
    4  SPECTRA(J) = CMPLX(REAL(SPECTRA(J)),-AIMAG(SPECTRA(J)))
*
* AFTER ANOTHER TRANSFORMATION, THE RESULT IS IN SPECTRA(X)
*
      CALL FFT2C(SPECTRA,13,IWK)
*
* SPECTRA(X) MUST BE DIVIDED BY .8192. TO NORMALIZE
* SEND FINISHED DATA OUT VIA  .TAPE4.
*
      DO 5 J=1 , 8192
    5 WRITE(4,*) MAX1( (REAL(SPECTRA(J)) / 8192.) , 0.)
*
      STOP
      END
```

```
      PROGRAM BACKGR(INPUT,OUTPUT,TAPE4,TAPE3)
      DIMENSION MINIMA(3000),NSPEC(8192)
      DATA NSPEC/8192(0)/,MINIMA/3000(0)/
*
* A BACKGROUND GENERATION PROGRAM        R.TERVO OCT/81
*
* READ SPECTRUM IN FROM  .TAPE3.
* WRITE BACKGROUND INTO  .TAPE4.
*
       SIGMA(X,NCHAN) = NSPEC(NCHAN) + X * SQRT(FLOAT(NSPEC(NCHAN)))
       REWIND 3
       REWIND 4
*
      DO 1 J= 1 , 8192
       READ(3,*) NSPEC(J)
    1  NSPEC(J) = MAX0( NSPEC(J) , 0 )
*
       MINTOTL = 0
       PREVIUS = 999999
*
* ADDRESSES OF DEFINED LOCAL MINIMA ARE STORED,
* IGNORING POINTS > 3*SIGMA ABOVE PREVIOUS MINIMUM
*
       DO 2 J=1 , 8192
       IF(NSPEC(J).GE.NSPEC(J-1).OR.NSPEC(J).GE.NSPEC(J+1)) GOTO 2
       IF(NSPEC(J).GT.PREVIUS) GOTO 2
       PREVIUS = SIGMA( +3.   , J )
       MINTOTL = MINTOTL + 1
       MINIMA(MINTOTL) = J
    2  CONTINUE
*
       ISTART = 1
       IWIDTH = 15
*
* A QUADRATIC LEAST-SQUARES FIT INTERPOLATES BACKGROUND
* AT EVERY POINT, USING THE .IWIDTH. NEAREST MINIMA
*
      DO 6 J=1 , 8192
       IF(J.EQ.1) GOTO 3
       IF(J-MINIMA(ISTART).LE.MINIMA(ISTART+IWIDTH)-J) GOTO 5
       IF(ISTART.GE.MINTOTL - IWIDTH) GOTO 5
       ISTART = ISTART + 1
*
    3  X1  = 0
       X2  = 0
       X3  = 0
       X4  = 0
       Y1  = 0
       YX  = 0
       YXX = 0
       N   = IWIDTH
*
      DO 4 K=1 , N
       Y   = NSPEC(MINIMA(ISTART+K))
       X   = MINIMA(ISTART + K) - MINIMA( ISTART)
*
       X1  = X1 + X
       X2  = X2 + X*X
       X3  = X3 + X*X*X
       X4  = X4 + X*X*X*X
       Y1  = Y1 + Y
       YX  = YX + Y*X
    4  YXX = YXX+ Y*X*X
*
      D= 1 / ( N*(X4*X2-X3*X3 ) -X1*(X4*X1-X2*X3 ) +X2*(X3*X1-X2*X2 ) )
      A= D * (Y1*(X4*X2-X3*X3 ) -X1*(X4*YX-X3*YXX) +X2*(X3*YX-X2*YXX) )
      B= D * ( N*(X4*YX-YXX*X3) -Y1*(X4*X1-X3*X2 ) +X2*(X1*YXX-X2*YX) )
      C= D * ( N*(YXX*X2-X3*YX) -X1*(YXX*X1-X2*YX) +Y1*(X3*X1-X2*X2 ) )
*
    5  X = J - MINIMA(ISTART)
*
    6  WRITE(4,*) MAX1( A + B*X + C*X*X   ,    0.0 )
*
       STOP
      END
```

```
      PROGRAM PLOT1(INPUT,OUTPUT,TAPE3)
*
* A PLOTTING PROGRAM        R.TERVO  FEV/81
*
* THIS PROGRAM PLOTS AN 8K INTEGER FILE FROM .TAPE3.
*
      REWIND3
*
      CALL PLTIN(400. , 0600. , 0.5 , 0.5 , 0.0 , 8193. , 0.0 , 65000.)
*     ----------XSCALE--YSCALE---X0----Y0---XMIN--XMAX----YMIN--YMAX---
*
      DO 1 J = 1,8192
       READ(3,*) ITEMP
       TEMP = AMAX0( ITEMP , 0 )
       CALL UNITTO( FLOAT(J)       ,  300.+ TEMP      , XP , YP )
        IF(YP.LT.0.) YP = 0.
        IF(YP.GT.10.) YP = 10.
       CALL PLOT ( XP , YP , 2 )
    1 CONTINUE
*
       CALL GRIDGS( 0.0 , 0.26 , 0.25 , 0.04, 10 , 0 , 81 , 0 )
*
       CALL NEWPEN(5)
*
      DO 2 J=1 , 8
       ENCODE(1,100,BCD) J
       XL=FLOAT(J) * 2.5
    2  CALL LETTER( 1 , .22 , 0. , XL , 0.02 , BCD )
  100  FORMAT(I1)
*
       CALL PLOT(0.01 , 0.01 , -3)
*
      STOP
      END
```

```
      PROGRAM PLOT2(INPUT,OUTPUT,TAPE3,TAPE4)
*
* A PLOTTING PROGRAM        R.TERVO  SEPT/81
*
* THIS PROGRAM READS AND PLOTS DATA FROM TWO FILES....
* .TAPE3. AND .TAPE4. , BOTH ON THE SAME GRAPH ,
* RIGHT ON TOP OF EACH OTHER.
*
* ADJACENT POINTS ARE SUMMED AND THE Y-SCALE IS HALVED
*
       REWIND 3
       REWIND 4
*
      CALL PLTIN(400. , 1200. , 0.5 , 0.5 , 0.0 , 8193. , 0.0 , 65000.)
*     -----------XSCALE--YSCALE---X0----Y0---XMIN--XMAX----YMIN--YMAX---
*
      DO 1 J =  1,8192,2
       READ(3,*) IFIRST
       READ(3,*) ISECOND
       POINT = AMAX0( 0 , IFIRST + ISECOND )
       CALL UNITTO( FLOAT(J) ,  1000.+ POINT  , XP , YP )
        IF(YP.GT.9.) YP = 9.
    1 CALL PLOT( XP , YP , 2 )
*
       CALL PLOT( 0.01 , 0.01 , 3 )
*
      DO 2 J = 1,8192,2
       READ(4,*) IFIRST
       READ(4,*) ISECOND
       POINT = AMAX0( 0 , IFIRST + ISECOND )
       CALL UNITTO( FLOAT(J) ,  1000.+ POINT     , XP , YP )
        IF( YP.GT.9. ) YP = 9.
    2 CALL PLOT( XP , YP , 2 )
*
       CALL GRIDGS( 0. , .26 , .25 , .04 , 10 , 0 , 81 , 0 )
       CALL NEWPEN(5)
*
      DO 3 J=1 , 8
       ENCODE( 1,200,BCD ) J
       XL = FLOAT(J) * 2.5
    3  CALL LETTER( 1 , .22 , 0. , XL , .02 , BCD )
  200  FORMAT (I1)
      CALL PLOT(.01 , .01 , -3 )
*
      STOP
      END
```

```
      PROGRAM PLOTL2(INPUT,OUTPUT,TAPE3,TAPE4)
*
* A LOGARITHMIC PLOTTING PROGRAM        R.TERVO  OCT/81
*
* THIS PROGRAM READS AND PLOTS DATA FROM TWO FILES....
* .TAPE3. AND .TAPE4. , BOTH ON THE SAME GRAPH ,
* RIGHT ON TOP OF EACH OTHER.
*
* ADJACENT POINTS ARE SUMMED AND THE Y-SCALE IS HALVED
*
       REWIND 3
       REWIND 4
*
      CALL PLTIN(400. ,  2.    , 0.5 , 0.5 , 0.0 , 8193. , 0.0 ,   12. )
*     ----------XSCALE--YSCALE---X0----Y0---XMIN--XMAX----YMIN--YMAX---
*
      DO 1 J =  1,8192,2
       READ(3,*) IFIRST
       READ(3,*) ISECOND
       POINT = AMAX0( 0 , IFIRST + ISECOND )
       CALL UNITTO( FLOAT(J) ,   1 + ALOG( 1. + POINT )  , XP , YP )
        IF(YP.GT.9.) YP = 9.
       CALL PLOT( XP , YP , 2 )
    1 CONTINUE
*
       CALL PLOT( 0.01 , 0.01 , 3 )
*
      DO 2 J = 1,8192,2
       READ(4,*) IFIRST
       READ(4,*) ISECOND
       POINT = AMAX0( 0 , IFIRST + ISECOND )
       CALL UNITTO( FLOAT(J) ,   1 + ALOG( 1. + POINT )  , XP , YP )
        IF( YP.GT.9. ) YP = 9.
       CALL PLOT( XP , YP , 2 )
    2 CONTINUE
*
       CALL GRIDGS( 0. , .26 , .25 , .04 , 10 , 0 , 81 , 0 )
       CALL NEWPEN(5)
*
       CALL LETTER( 8 , .22  , 0.  , .02 , .02 , "LOG PLOT" )
      DO 3 J=1 , 8
       ENCODE( 1,200,BCD ) J
       XL = FLOAT(J) * 2.5
    3  CALL LETTER( 1 , .22 , 0. , XL , .02 , BCD )
  200  FORMAT (I1)
      CALL PLOT(.01 , .01 , -3 )
*
      STOP
      END
```

```
      PROGRAM MINUS(INPUT,OUTPUT,TAPE3,TAPE4,TAPE7)
*
* A SUBTRACTION ROUTINE       R.TERVO MAR/81
*
*    .TAPE7.  =  .TAPE3. - .TAPE4.
*
*  NEGATIVE RESULTS ARE SET TO ZERO
*
      DIMENSION KTHREE(8192),KFOUR(8192)
*
      REWIND 3
      REWIND 4
      REWIND 7
*
       READ(3,*) (KTHREE(J),J=1 , 8192)
       READ(4,*) (KFOUR(J) ,J=1 , 8192)
*
       DO 1 J=1 , 8192
    1  KFOUR(J) = MAX0( KTHREE(J) - KFOUR(J) , 0 )
*
       WRITE(7,*) (KFOUR(J),J=1 , 8192)
*
      STOP
      END
```

```
      PROGRAM LIST( INPUT,OUTPUT,TAPE3 )
      DIMENSION IDATA(8193)
*
* A PRINTING OUT PROGRAM           R.TERVO MAI/81
*
      REWIND3
*
       DO 1 J= 1 , 8192
    1  READ(3,*) IDATA(J+1)
*
       DO 3 J= 1 , 8001 , 500
       PRINT200, (M-1,M=1,10)
       DO 2 K= 1 , 500 , 10
       IF(J+K .GE. 8192) STOP
       PRINT100,J+K-2, (IDATA(J+K+L-2),L=1,10)
    2  CONTINUE
    3  CONTINUE
*
  100  FORMAT(1H ,I10,3H ..,10I10)
  200  FORMAT(1H1,13H              ,10I10)
*
      STOP
      END
```

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