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LIVERMORE

A COMPUTER METHOD OF PEAK AREA DETERMINATIONS
FROM Ge-Li GAMMA SPECTRA

H. Robert Ralston, Bio-Medical Division

George E. Wilcox, Computation Division

August 30, 1968

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A COMPUTER METHOD OF PEAK AREA DETERMINATIONS
FROM Ge-Li GAMMA SPECTRA^{*}

H. Robert Ralston, Bio-Medical Division

George E. Wilcox, Computation Division

Lawrence Radiation Laboratory

University of California

Livermore, California

INTRODUCTION

The development of Ge-Li gamma detectors has made high resolution gamma spectrometry a readily usable laboratory tool. The resolutions which are routinely achieved have brought about a simplification in the problems of peak identification and at the same time posed problems of peak area integration.

Since the resolution is of the order of 3 keV fwhm, the number of points representing a peak on an analyzer with even 4096 channels is quite small for a spectrometer set to 2 or more MeV full scale. The peak area is determined by adding the counts in each channel within the peak and subtracting that portion which is contributed by the Compton contribution

* This work was performed under the auspices of the U.S. Atomic Energy Commission.

of higher energy peaks. This calculation requires that the limits of the peak be defined and that the amplitude of the Compton continuum at the location of the peak be known.

This task of determining an appropriate base line (Compton level) from which to begin and end the integration of a peak area appears easy when calculations are being done by hand and subjective judgment is exercised on each peak. When computer methods are used, the problem becomes one of translating a subjective evaluation into a computer program which will give consistent and accurate results.

A program which defines the base line and limits of integration is shown in the flow chart (Fig. 1). The computational method is as follows: A spectrum is generated by replacing the counts in any given channel of original data by the average of the original point plus $n/2$ points on each side. This generated spectrum is now compared to the original data point by point. If the original data exceeds the averaged data by more than k standard deviations, the original data is replaced by the averaged data at that point. The alternating process of averaging and replacing is continued with ever decreasing values of k down to .2. Each step of this process reduces the contribution of peaks whose significance is defined by the then current k .

This repetitive process reduces the significance of all peaks until the data at previous peak locations has no more significance than the

random scatter of the Compton continuum data points. Thus the final averaging represents the average of the Compton continuum with no superimposed photo peaks.

The alternating process is repeated ten times. The resulting spectrum is the base.

The base is now used in conjunction with the original raw data as a basis for defining and integrating significant peaks. The portions of spectra which can cause problems are the ends and regions of sharp changes in slope. The selection of n (the number of points in the averaging process) is dependent on the number of points in the spectrum, the resolution of the system, and the conversion gain. For 2048 channels at 1.0 keV per channel, values of 27 for n give satisfactory results for a 3 keV (fwhm 1332 keV) detector. The value of k is generally set at 9.2 and reduced by 1.0 for each pass until the value is 0.2.

EXPERIMENTAL

A quantitative evaluation of the program was obtained by the use of a pulser. The pulse was injected into the preamplifier at the point where the Ge-Li diode signal appears. The resolution was about 0.5 keV better than measured with diode pulses.

A series of pulses was placed at regular intervals along the energy axis of a Co^{60} spectrum. The pulser was timed so that the same number

of pulses was injected into the preamplifier for each position. The spectrum was then processed and the areas from each pulser peak integrated. Figure 2 shows the results of this test. The Co^{60} spectrum was counted for 10 minutes, and in a second run, for 100 minutes.

The pulses were paired in some portions of the spectrum so that it would be possible to determine the effects of peak separations. The separation of the peaks was varied.

A second series of pulser runs were done in which successive peaks were decreased in amplitude relative to the preceding peak. In this way, it was possible to determine a lower limit of peak height upon which the program will operate to distinguish the peak. It was also possible to determine how well the peak was integrated. Table 1 shows the results of these checks. The Co^{60} spectrum was run for 10 and 150 minutes. Figure 3 shows a portion of the spectrum with pulser peaks superimposed.

RESULTS AND DISCUSSION

The pulser tests, the results of which are shown in Table 1 and Figs. 2 and 3 show that the peaks can be located and quantitated to levels approaching 2 standard deviations from the averaged Compton background (base line). The determinations of peak areas is consistent in most cases with the calculated standard deviations and the uncertainties of gating the pulser on and off.

The program functions satisfactorily for most spectra with well defined peaks. It fails to quantitate two peaks which are not separated by having a low point between them less than $k\sigma$ above the base line. This is an inherent limitation on a generalized single pass program. "Double" peaks are identified. Although such peaks are not quantitated all pertinent parameters are saved. A later sub-routine will be required to resolve these "doubles."

Peaks which are on a Compton edge are readily identified and quantitated down to levels approaching twice the background under the peak.

Figure 4 is a portion of a mixed gamma spectrum. The peaks at the 520 keV region were identified by the program as separate peaks and satisfactorily quantitated. The peak at 720 keV was identified as a single peak. The peaks at 750 to 760 keV were identified as a triple peak. The program identified the step on the leading edge of the 750 keV peak as a maximum with a subsequent minimum greater than the 2σ level. Similarly, the minimum between the two major peaks was above the 2σ level. The peak area reported was for all three peaks combined. The peaks at 810 keV and 865 keV were identified and quantitated.

The triple peak can be resolved into its separate components by raising the $k\sigma$ level above $k = 2$ so that the minima are below the $k\sigma$ line.

Appendix 1 is the Fortran 400 listing of the program.

Table 1

Location (channel number)	Pulser peaks only (no Compton)	FSD	Peaks + 10 min Co ⁶⁰ spect.	FSD calc by computer program	Actual deviation from original value	Peaks + 150 min Co ⁶⁰ spect.	FSD calc by computer program	Actual deviation from original value
300	3581	.017	3540	.018	.012	3516	.025	.018
310	1802	.024	1756	.026	.026	1902	.038	.053
320	1068	.031	1060	.035	.007	1031	.063	.034
330	718	.038	701	.043	.024	795	.078	.032
340	368	.053	357	.066	.030	262.3	.158	.287
350	191	.074	146	.108	.236	—	—	—
360	154	.082	128	.118	.169	168.1	.254	.092
370	126.5	.091	96.4	.144	.238	—	—	—
380	84.2	.111	90.9	.165	.080	—	—	—
390	57.4	.136	49.0	.236	.146	—	—	—
800	3601	.017	3589	.017	.003	3528	.025	.020
810	1794	.024	1760	.026	.019	1750	.039	.025
820	1082	.031	1050	.035	.030	975	.058	.099
830	737	.037	700	.044	.050	662	.083	.102
840	369	.053	354	.068	.040	333	.159	.098
850	202	.072	182.3	.105	.098	182	.239	.099
860	162	.079	185.6	.112	.146	—	—	—
870	124.9	.090	93.6	.158	.250	—	—	—
880	90.6	.107	—	—	—	145	.316	.600
890	67.3	.123	53.7	.265	.200	—	—	—
950	3587	.017	3585	.018	.0006	4100	.026	.143
960	1792	.024	1781	.026	.006	1932	.045	.078
970	1085	.031	1043	.035	.039	926	.067	.147
980	721	.038	680	.045	.057	727	.090	.008
990	367	.053	335.5	.068	.086	279	.161	.240
1000	190	.074	189.2	.111	.004	258.3	.209	.360
1010	148.3	.084	120	.131	.190	141.3	.311	.047
1020	106.7	.099	86.7	.169	.187	—	—	—
1030	100.6	.101	64.5	.214	.360	—	—	—
1040	57.4	.133	—	—	—	—	—	—

LIST OF TABLES

Table 1. Integrated peak areas for pulser generated peaks.

Column 2 shows the calculated peak areas without any Compton continuum. Column 4 shows the peak areas as calculated after a Co^{60} source was counted for 10 minutes to give a relatively low Compton continuum. Column 7 shows the peak areas as calculated after a Co^{60} source was counted for 150 minutes. The fractional standard deviations were calculated by the computer program. Actual deviations from the original peak areas are shown for comparison.

LIST OF FIGURES

- Figure 1. Flow chart of basic program.
- Figure 2. Scatter of peak areas of equal area pulser generated peaks superimposed on a Co^{60} spectrum.
- Figure 3. Pulser produced peaks superimposed on the Compton edge of a Co^{60} spectrum. The lower line is the generated base and the upper line is the 2σ level.
- Figure 4. Portion of mixed gamma spectrum showing the generated base line and the 2σ line.

PRESET BASE = DAT

FIGURE 1

APPENDIX 1

```

C
C      PRESET BASE(J) = SPECTROMETER DATA(DAT)
C
C      SUBROUTINE REPSUM
COMMON BASE(2048),DAT(2048),NCHAN
DIMENSION SUMSPC(2048)
C
C      NCHAN = NUMBER OF CHANNELS
C
C      ICH=NCHAN-27
C
C      MAIN AVERAGING AND REPLACEMENT LOOP
C
DO 100 L=10,1,-1
  TL=L
  TL=TL-0.8
  K = 1
C
C      AVERAGING LOOP
C
DO 300 I = 1, ICH
  SUMSPC(I) = 0.0
  KUP=K+26
  DO 200 J = K , KUP
    SUMSPC(I) = BASE(J) + SUMSPC(I)
  200 CONTINUE
  SUMSPC(I)=SUMSPC(I)/27
  K = K+1
  300 CONTINUE
C
C      END AVERAGING LOOP
C
C      REESTABLISH CHANNEL POSITIONS OF AVERAGED POINTS
C
  ICH=NCHAN-13
  DO 400 J=ICH,1,-1
  400 SUMSPC(J+13)=SUMSPC(J)
C
C      END REESTABLISHING LOOP
C
C      BEGIN TESTING AND REPLACEMENT OF BASE POINTS
C
DO 500 J=1,NCHAN
  TEST=SUMSPC(J)+TL*SQRTF(SUMSPC(J))
  IF( DAT(J).GT.TEST),500
  BASE(J)=SUMSPC(J)
  500 CONTINUE
C
C      END TESTING
C

```



```

100 CONTINUE
C
C           END MAIN LOOP
C
    K = 1
    ICH = NCHAN - 13
C
C           SMOOTH FINAL BASE WITH RUNNING AVERAGE
C
    DO 700 I=1, ICH
        SUMSPC(I) = 0.0
        KUP = K + 12
        DO 600 J=K, KUP
            SUMSPC(I) = BASE(J) + SUMSPC(I)
600    CONTINUE
        SUMSPC(I) = SUMSPC(I)/13
        K = K+1
700    CONTINUE
C
C           END SMOOTH LOOP
C
    ICH=NCHAN-6
C
C           REESTABLISH CHANNEL POSITIONS OF SMOOTHED POINTS
C
    DO 800 J=ICH, 1, -1
800    BASE(J+6)=SUMSPC(J)
C
C           END REESTABLISHING LOOP
C
    RETURN
    END

```

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