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This paper discusses the relocation of counts in multichannel spectra. A method that preserves both the Poisson statistical fluctuation and the shape of the spectra is proposed. Also, results of tests are shown.

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I Introduction

The relocation of a multichannel spectrum may be necessary when spectra obtained with different calibrations are compared. For example, in the analysis of double beta decay experiments [1,2] it has been a common practice to sum the individual spectra relocated to the same calibration.

The usual way to relocate spectra is to divide the counts from an old (non-relocated) channel and place them into new channels. The division is usually done by assigning to each new channel a weighting factor which corresponds to the superposition of the old channel on the new one. However, this simple procedure leads to changes in the statistical fluctuation and shape of the spectrum. As a result, such relocation introduces correlations that prevent the application of fitting procedures and statistical tests in the usual manner.

The difficulty in performing a relocation which preserves both the Poisson statistical fluctuation and the shape of the spectra is due to the fact that part of the information originally contained in the experimental data is lost after building a histogram: we do not know the exact position of each count within a channel. However, if the spectrum is smooth, it is possible to estimate how the counts observed in a channel are distributed within it. From such an estimate, a new histogram can be constructed where the data is statistically redistributed through the new channels.

II Statistical Procedure

Consider a multichannel spectrum whose data obey the density function f(x), where

$$a = \int_{x_1}^{x_2} f(x)\, dx \qquad (1)$$

is the expected number of events in channel (x_1,x_2). In the case of a narrow channel, the observed number of events, n, is distributed

as

$$P_a(n) = \frac{e^{-a}\, a^n}{n!} \quad . \qquad (2)$$

Now, consider that a new spectrum is to be constructed and (x_3,x_4) is a new channel within (x_1,x_2). Suppose that n_{obs} events were observed in channel (x_1,x_2) and a binomial random number n′ is drawn from n_{obs} with a probability parameter

$$p = \frac{\int_{x_3}^{x_4} f(x)\, dx}{\int_{x_1}^{x_2} f(x)\, dx} \quad . \qquad (3)$$

The unconditional distribution of n′ is

$$P(n') = \sum_{n_{obs}=n'}^{\infty} P(n'|n_{obs},p)\; P_a(n_{obs}) \quad , \qquad (4)$$

where $P_a(n_{obs})$ is given by eq. (2) and $P(n'|n_{obs},p)$ is the conditional (binomial) distribution of n′,

$$P(n'|n_{obs},p) = \frac{n_{obs}!}{(n_{obs}-n')!\; n'!}\, p^{n'}(1-p)^{n_{obs}-n'} \quad . \qquad (5)$$

Substituting equation (5) into equation (4) yields

$$P(n') = \frac{e^{-(ap)}\, (ap)^{n'}}{n'!} \quad . \qquad (6)$$

Equation (6) shows that P(n′) is a Poisson distribution with mean $a{\cdot}p$. Thus, if f(x) is known, it is possible to construct a new spectrum preserving both the statistical fluctuation of the number of events and the shape of the spectra.

Since f(x) is not known, it must be estimated from the original spectrum. If f(x) is approximated by an Mth degree polynomial function, which coincides in value with the counts in the M+1 neighbor channels of the original spectrum, then the systematic error δn′ of the mean value of n′ obtained by the procedure above can be estimated from the remainder in Lagrange interpolation formula [3],

$$\delta n' = \frac{\Pi(x)}{(M+1)!}\, f^{(M+1)}(\xi)\; \delta x \quad , \qquad (7)$$

where $f^{(M+1)}(\xi)$ is the (M+1)th derivative of f(x) for some ξ in the analyzed region, $\Pi(x) = (x-x_1)\cdot(x-x_2)\cdots(x-x_{M+1})$, with x_i denoting the central abscissa of each of the M+1 channels, and δx is the width of the new channel.

In order to obtain an error δn′ which is negligible when compared to the statistical fluctuation of n′, $\sqrt{n'}$, we must have

$$n' \ll \left(\frac{(M+1)!\; f_0}{\Pi(x)\; f^{(M+1)}(\xi)} \right)^2 = n_{cr}, \qquad (8)$$

where f_0 is the value of f(x) for some x in the analyzed region.

Equation (8) is an estimate of the upper critical value n_{cr} that must not be attained if the statistical fluctuation is to be

kept larger than errors which are introduced when approximating f(x) by a polynomial function.

III Gamma-Ray Spectra

As can be seen from equation (8), the most difficult regions to relocate in a spectrum are those with larger $f^{(M+1)}/f_0$. When dealing with gamma-ray spectra, those regions occur near the peaks, and it is valid to assume, in the case of Gaussian peaks,

$$\frac{f^{(M+1)}}{f_0} \cong \frac{1}{\sigma^{M+1}} \quad , \qquad (9)$$

where σ=FWHM/2.35 and FWHM is the full width at half maximum. Using this approximation and also $\Pi(x)\cong(M/4)^{M+1}$ we can simplify eq. (8) to

$$n_{cr} \cong \left((M+1)! \left(\frac{4\sigma}{M}\right)^{M+1} \right)^2 . \qquad (10)$$

Table (1) shows n_{cr} estimated from equation (10) for some values of σ and M. For a very narrow peak ($\sigma \cong 0.5$), a relocation can be done only in the case of a very small number of events; otherwise, systematic errors will be larger than statistical fluctuations. Nevertheless, for wide peaks, σ>3, the relocation procedure can be applied for very intense peaks without introducing systematical errors.

Figure 1 shows the effect of relocating the doublet 1086 keV and 1090 keV from ^{152}Eu decay. The relocations were done using a 4th order polynomial fitted over 5 channels. The spectrum was analyzed using a parabolic background plus a Gaussian peak with a tail at the left side and a step under the peak [4]. Fig 1a shows the results of the original spectrum. The bad reduced χ^2 value, 3.4, is due to the distortion of the peak with respect to the fitted shape. Fig. 1b shows the results after a relocation given by x'=x-0.5, where x and x' denote the abscissa in the original and in the relocated spectra, respectively. Fig. 1c shows the results after the relocation given by x'=x/1.05. No significant change can be seen in these relocated spectra.

Fig. 1d shows the results of the fit after a relocation given by

$$x' = 1.5x - 0.15. \qquad (11)$$

No significant changes were observed in the peak positions and areas in this case as well. Concerning the peak width, we notice that the fitted FWHM is wider than the real $FWHM_0$,

$$FWHM = \sqrt{FWHM_0^2 + \frac{\lambda^2}{12}} \quad , \qquad (12)$$

where $\lambda = 2\sqrt{2\ln 2}$. After this correction, the width of the peaks in fig. 1d agrees with the width of the peaks in the original spectrum. The decrease in the reduced chi-square in fig. 1d is due to the fact that systematic errors in the peak shape are proportional to the number of counts per channel (which were reduced as a consequence of the calibration change), while the standard deviation is equal to the square root of the number of counts.

From these and other tests, we can conclude that for peaks with $\sigma \geq 2$ channels (FWHM≥4.7 channels) the change in calibration preserves the statistical fluctuation, and neither inhibits statistical tests nor alters peak shapes.

IV Example of Application

A relocation procedure has been used in the study of the gamma-ray spectra of ^{152}Eu. A large number of measurements have been made using two different HPGe detectors, two different ADCs and two different amplifiers, each one used with two different gains. The goal of the use of a large number of independent measurements is to randomize systematic errors[5]. The spectra resulting from these measurements were relocated to the same calibration. The initial

different calibration functions x'(x) were obtained by fitting parabolic curves to the centroids of the most intense gamma-ray transitions from ^{152}Eu. After relocation the spectra were summed up. Background measurements were also done and their energy spectra were relocated and subtracted from the total ^{152}Eu spectrum. Finally, the resultant spectrum was then analyzed.

The relocation procedure was also used in the analysis of the 121 keV gamma-ray from ^{152}Eu and the 123 keV gamma-ray from ^{154}Eu (present in the ^{152}Eu source as contamination). In order to eliminate the presence of the 123 keV transition in the spectrum, the spectrum was first divided by the activity ratio between the ^{152}Eu and the ^{154}Eu (experimentally determined as 265±17), then, shifted by an amount of channels corresponding to (1.36±0.04keV), the energy difference of the two transitions[8], and finally subtracted from the original spectrum. Table 2 shows the fitted position of the 121 keV after the subtraction of the shifted spectra. From table 2 it is clear that the effect of the uncertainties in ΔE (energy difference between the 123 keV and 121 keV transitions) and R (^{152}Eu-^{154}Eu activity ratio) on the uncertainty in the centroid of the 121 keV gamma-ray is negligible. Table 3 shows the obtained results for all gamma-ray transitions whose combined standard deviation

$$\sigma_E = \sqrt{\sigma_0^2 + g^2.\sigma_c^2 + \sigma_r^2} \qquad (13)$$

was less than 10 eV. In equation (13) σ_0 is the standard deviation of the adopted energy[6-8], σ_c is the standard deviation of the fitted peak position, g is the gain in keV/channel, and σ_r is the uncertainty due to the relocation, which is estimated from the fit x'(x).

Table 3 shows also the result of the fit of a fourth degree polynomial E=E(C), where E denotes the gamma-ray energy and C denotes the correspondent channel. The reduced chi-squared of this fit was 6.9. This bad value is mainly caused by the 271 keV, 324 keV and 416 keV transitions, as can be seen from the squared residues in table 3. However, those three gamma-ray transitions are not usually quoted as energy standards for calibration [7,9]. Squared residues of gamma-rays quoted as calibration standards are acceptable.

V Conclusion

The relocation of multichannel spectra can be done preserving both the shape and the statistical fluctuation of the number of events in each channel.

In this proposed procedure, the number of events in a channel of the relocated spectra is drawn from a binomial distribution with parameters n_{obs} (the observed number of events in the old channel) and p (the probability given by equation (3)). If the spectrum to be relocated is not very irregular, its shape can be estimated in a certain location through a polynomial fitted over some neighboring channels.

This procedure has been used in the analysis of gamma-ray spectra. No problems have been detected when the relocations are done within the limitations discussed in the text.

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TABLE CAPTIONS

Table 1 - Critical values n_{cr} from equation (10) for some values of M and σ. If $n \ll n_{cr}$, errors due to relocation are negligible compared to statistical fluctuations.

Table 2 - Fitted position of the 121 keV gamma-ray (in channel units) after the subtraction of the 123 keV transition component. R is the ratio of the ^{152}Eu and ^{154}Eu activities and ΔC is the shift described in the text.

Table 3 - Result of the analysis of the ^{152}Eu spectra. σ' is the uncertainty of the fitted energy E'.

FIGURE CAPTION

Results of the analysis of the 1086 keV and 1090 keV doublet from ^{152}Eu decay. (a) Original spectrum; (b) relocation given by $x'=x-0.5$, where x' and x correspond, respectively, to the abscissa of the relocated and the original spectra; (c) relocation given by $x'=x/1.05$; (d) relocation given by $x'=1.5x-0.15$. Standard deviations between parentheses are given in units of the last figure.

Table 1

σ	M				
	1	2	3	4	5
0.5	64	36	22	14	9
1.0	$1.0 \cdot 10^3$	$2.3 \cdot 10^3$	$5.8 \cdot 10^3$	$14 \cdot 10^3$	$36 \cdot 10^3$
1.5	$5.2 \cdot 10^3$	$26 \cdot 10^3$	$1.5 \cdot 10^5$	$8.3 \cdot 10^5$	$4.6 \cdot 10^6$
2.0	$1.6 \cdot 10^4$	$1.5 \cdot 10^5$	$1.5 \cdot 10^6$	$1.5 \cdot 10^7$	$1.5 \cdot 10^8$
3.0	$8.3 \cdot 10^4$	$1.7 \cdot 10^6$	$3.8 \cdot 10^7$	$8.5 \cdot 10^8$	$1.9 \cdot 10^{10}$

Table 2

ΔC(channel) ΔE(keV)	R		
	250	265	280
5.322 1.302	428.6028(2)	428.6027(2)	428.6026(2)
5.342 1.358	428.6028(2)	428.6027(2)	428.6026(2)
5.362 1.363	428.6029(2)	428.6028(2)	428.6027(2)

Table 3

Channel	E(keV)	σ(eV)	E′ (Fitted energy(keV))	σ′(eV)	$\frac{(E-E')^2}{\sigma^2}$
428.6027	121.7824*	0.4	121.7824	0.4	0.0
911.557	244.699	1.	244.6986	0.9	0.0
1015.17	271.135	9.	271.072	5.	34.
1112.76	295.939	8.	295.936	2.	0.1
1226.25	324.789	9.	324.841	8.	36.
1302.564	344.281	2.	344.283	1.	0.5
1394.860	367.789	5.	367.796	2.	2.3
1564.911	411.115	5.	411.124	2.	3.1
1584.10	416.052	8.	416.013	5.	23.
1693.809	443.976**	5.	443.970	2.	1.1
1927.29	503.487**	7.	503.475	5.	2.9
2164.78	564.021	8.	564.010	3.	1.5
2252.26	586.294	7.	586.312	3.	6.8
2598.85	674.678**	6.	674.680	6.	0.1
2614.293	678.623**	5.	678.617	6.	1.2
2653.74	688.678	6.	688.676	3.	0.0
2774.03	719.353	8.	719.354	6.	0.0
3007.52	778.903	6.	778.908	3.	0.4
3131.21	810.459	9.	810.461	6.	0.0
3354.34	867.388	8.	867.394	3.	0.6
3558.05	919.401	8.	919.389	7.	2.3
3733.306	964.131	9.	964.136	7.	0.3

Energy data and uncertainties from [6], except (*) from [7] and (**) from [8].