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A revision of energy and resolution calibration method of Ge detectors

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Abstract

The energy and resolution calibration of germanium detectors being basic procedures in gamma-ray spectrometry have not been usually studied in depth. In this paper a new approach to these calibration methods based on the Orthogonal Distance Regression (ODR) algorithm is presented. This algorithm treats more adequately all uncertainties involved in the calibration process and produces better results than the usual Ordinary Least Squares (OLS) algorithm. Additionally a study of the functions involved in energy and resolution calibration of germanium detectors has been also carried out.

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Keywords: Gamma-spectrometry; Energy calibration; Resolution calibration

1. Introduction

Gamma-ray spectrometry with germanium detectors is a powerful and widely used technique. For many applications the final result of the measuring process consists of a pulse-height spectrum. The centroid and the area of the fitted peaks presented in the spectrum are turned, respectively, into gamma-ray energies and emission rates by using different calibration procedures of the germanium detector. Many efforts have been carried out on efficiency calibration of germanium detectors in order to obtain an accurate emission rate [1–5]. However, too little attention has been paid to energy and resolution calibration procedures of the germanium detectors.

The meaning to perform an energy calibration is to obtain a relationship between peak centroid in the spectrum and the corresponding gamma-ray energy. On the other hand the resolution calibration of the detector gives the width of a peak (by convention the full-width at half-maximum, FWHM) as a function of energy. These calibrations are accomplished by measuring the spectra of various sources emitting gamma-rays of precisely known energies at the working conditions. The final calibrations are carried out by fitting the experimental variables (energies and peak centroids, and peak widths and energies for energy and resolution calibration, respectively) to an appropriate function.

However, a main problem appears during the calibration procedure. The experimental variables have their respective uncertainties that are in general of the same order of magnitude. But the fitting algorithm usually used is based on Ordinary Least Squares (OLS) algorithm that ignores the uncertainties of the independent variable to simplify the fitting process [6]. The uncertainties associated to both dependent and independent variables have to be included in the fitting algorithm in order to perform correctly the calibration. For this purpose we have used in this work an Orthogonal Distance Regression (ODR) algorithm [7] that have in consideration both uncertainties for energy and resolution calibration of the germanium detectors. To test the validity of the ODR algorithm, a comparison between both algorithms has been carried out.

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On the other hand many functions have been proposed in the literature to fit the experimental energy and resolution data [6,8]. Therefore a comparison between the fits of the experimental energy and resolution data using those functions has been carried out.

2. Experimental data

In this work two different detector systems have been used. The first one consist of a Canberra type-n Ge detector (REGe) connected to a preamplifier (Canberra 2002), a linear amplifier (Canberra 2020) with quoted integral linearity of 0.05%, and an ADC (Canberra 8075) with 0.025% of linearity over total energy range. The second detector system is composed by a Canberra type-p Ge detector (XtRa), a preamplifier (Canberra 2002), a linear amplifier (Canberra 2022) with integral linearity of 0.05%, and an ADC (Canberra 8701) with an integral linearity equal or less than 0.025% of selected channel range. The output data from both ADC were collected by an Accuspec^{TM} card.

The energy and resolution calibration procedures were performed using ^{133}Ba and ^{152}Eu point sources supplied by DAMRI (France). Additionally two-point sources containing ^{201}Pb and ^{137}Cs were obtained by pipeting and drying a volume of standard solutions supplied by CIEMAT (Spain) over aluminium planchets in order to check the goodness of the calculated energy calibrations.

The sources were placed at 15 cm from the detectors. The pulse-height spectrums were collected separately and afterwards analysed with Genie2K^{TM} software obtaining the peak centroid, peak width, and its corresponding uncertainties for each energy emission (see Table 1). The uncertainties of energies were obtained from database [9] and the uncertainties corresponding to peak centroid channel were calculated using Generalized Second Difference method [10] implemented into Genie2K^{TM} software.

Table 1
Experimental data for energy and peak centroid channel, together with their uncertainties, using REGe and XtRa detectors

Source	Energy (keV)	Channel-REGe	Channel-XtRa
^{133}Ba	53.150(3)	232.07(5)	166.5(2)
^{133}Ba	80.997(1)	353.54(2)	250.25(6)
^{133}Ba	276.40(4)	1207.95(4)	838.61(8)
^{133}Ba	302.84(3)	1323.57(3)	918.35(6)
^{133}Ba	356.01(2)	1555.81(2)	1078.56(5)
^{133}Ba	383.85(4)	1676.98(4)	1162.46(7)
^{152}Eu	121.78(2)	532.15(2)	373.00(6)
^{152}Eu	344.28(2)	1504.55(3)	1043.23(6)
^{152}Eu	778.92(4)	3401.27(4)	2354.80(7)
^{152}Eu	964.05(7)	4208.70(7)	2913.88(7)
^{152}Eu	1112.08(4)	4852.74(4)	3360.93(7)
^{152}Eu	1408.02(3)	6140.14(4)	4254.92(6)

3. Energy calibration

The existence of non-linearity associated to the detector electronic chain affects the energy calibration, because the relationship between peak centroid and gamma-ray energy is represented ideally by a linear function. In order to overcome the non-linear response of the system, different functions (i.e., quadratic function) have been proposed in the literature [6].

In modern germanium detectors a linear fit of the experimental data is enough for energy calibration. The residuals obtained using a linear function for energy calibration of REGe and XtRa detector are displayed in Fig. 1. A deviation from linearity is clearly shown. The obtained residuals vary from −1 to 1 keV being large at the ends of the energy range of the ADC. We have used the OLS and ODR algorithm for each fit procedure. ODR algorithm overcomes OLS one taking into account both uncertainties of the peak centroid and energies. The statistical parameters (see Appendix A) show that the ODR algorithm (standard deviation: SD = 47.27; weighted sum of squares: WSS = 22300) is more suitable that usual OLS algorithm (SD = 197.9, WSS = 391000) for energy calibration of REGe detector. Also the ODR algorithm (SD = 11.04; WSS = 1219.7) overcome the OLS one (SD = 155.3, WSS = 241000) for energy calibration of XtRa detector.

In order to check the linear energy calibration we have also measured a ^{210}Pb and ^{137}Cs point sources. The resulting fitted energies using the linear relationship are shown in Table 2. The uncertainties of the fitted energies are subestimated if the OLS algorithm is used. We would use the ODR algorithm for precise determination of energy emission and its uncertainty together with error obtained from this method. However, the deviation between these fitted energies and the extracted from Ref. [9] denotes that if a precise calibration is required we would use a quadratic fit.

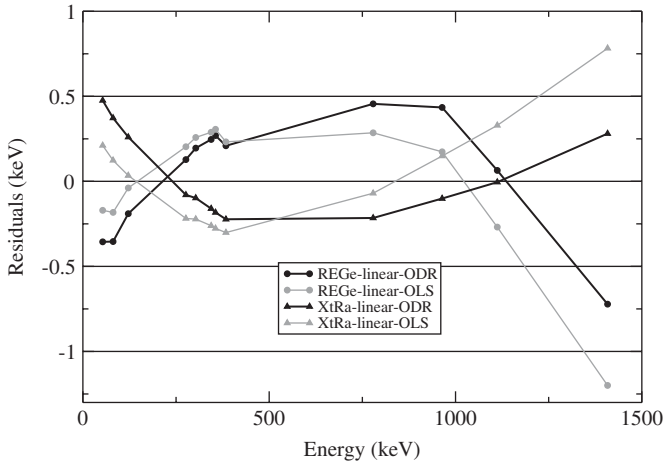

Fig. 1. Experimental residuals obtained with a linear fit for energy calibration of REGe and XtRa detector. Both OLS and ODR algorithms have been utilized.

Table 2
Fitted energies for measured ^{210}Pb and ^{137}Cs point sources using different functions, algorithms and detectors. The deviations D between fitted and reference values from Ref. [9] are also shown

Detector	Function	Algorithm	^{210}Pb	D (%)	^{137}Cs	D (%)
REGe	Linear	OLS	46.34(7)	0.43	662.13(21)	−0.07
REGe	Linear	ODR	46.20(14)	0.73	662.25(25)	−0.09
XtRa	Linear	OLS	48.41(6)	4.02	663.16(16)	−0.23
XtRa	Linear	ODR	48.42(11)	4.04	662.82(16)	−0.17
REGe	Quadratic	OLS	46.59(1)	−0.11	661.76(6)	−0.02
REGe	Quadratic	ODR	46.62(2)	−0.17	661.75(8)	−0.02
XtRa	Quadratic	OLS	46.60(2)	−0.13	661.79(14)	−0.02
XtRa	Quadratic	ODR	46.67(7)	−0.28	661.74(20)	−0.02
Reference data			46.539(1)		661.657(1)	

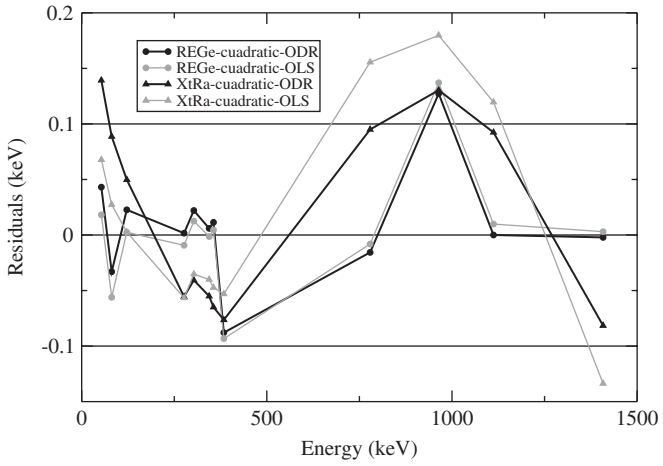

Fig. 2. Experimental residuals obtained with a quadratic fit for energy calibration of REGe and XtRa detector. Both OLS and ODR algorithms have been utilized.

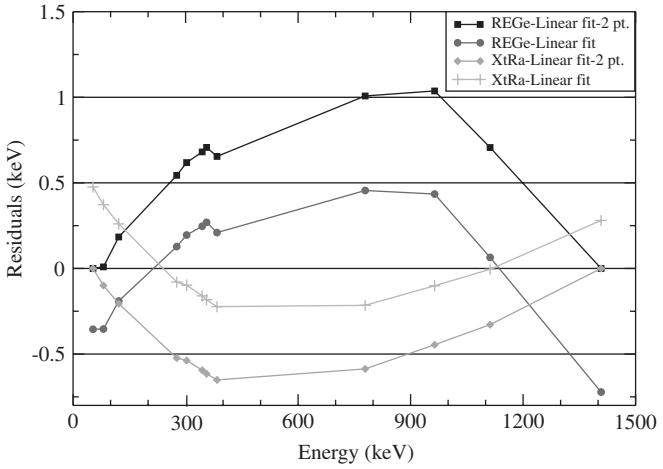

Fig. 3. Experimental residuals obtained with a two-point fit and a full data set linear fit for energy calibration of REGe and XtRa detector. The ODR algorithm has been utilized.

The obtained residuals using a quadratic fit are shown in Fig. 2. Their values drop ranging from −0.1 to 0.1 keV. A comparison between ODR (SD = 4.8, WSS = 211.5) and OLS (SD = 18.1, WSS = 2957.9) algorithm indicates that the proposed calibration method works well. As well as the ODR algorithm (SD = 4.03, WSS = 146.6) fit the energy calibration of XtRa detector better than OLS algorithm (SD = 41.65, WSS = 15400). The fitted energies for ^{210}Pb and ^{137}Cs point sources are shown in Table 2. The precision of energy calibration using a quadratic fit is better than 0.1% at the ends of the energy range and better than 0.02% at the middle of the energy range. Besides the uncertainties associated to the fitted energies are larger using ODR than OLS algorithm. On the other hand a upgrade to a cubic function does not improve the energy calibration.

Other functions have been suggested by Dryak [11] to handle the non-linearity of the system. The standard deviation SD obtained with these functions is around seven times higher than using a quadratic function. Alternatively a faster procedure based on a two-point fit has been proposed in the literature [6,8]. The residuals obtained with a two-point fit and a linear fit using the full experimental data set are shown in Fig. 3.

4. Resolution calibration

This resolution calibration plays a very important role in spectrum analysis software to extract the peak area of the gamma-ray emission.

On the other hand the resolution calibration of the detector gives the width of a peak (by convention, FWHM) as a function of energy. This resolution calibration plays a very important role in spectrum analysis software to extract the peak area of the gamma-ray emission. The peak width (FWHM) is given by the square sum of three factors [6,12]: the statistics of the charge-creation process ($\mathrm{FWHM_{stat}}$), the uncertainty in charge collection process ($\mathrm{FWHM_{elect}}$), and the electronic noise ($\mathrm{FWHM_{noise}}$). The first of these contributions is inherent to the detector material. This factor is given by the expression $\mathrm{FWHM^2_{stat}} = 2.35^2 F E \varepsilon$, where F is the Fano factor, ε the energy required to create a free electron–hole pair in Ge, and E the energy of the incident photon [6]. The second factor is proportional to the square of the energy $\mathrm{FWHM^2_{elect}} \propto E$ [8]. And finally the electronic noise is a

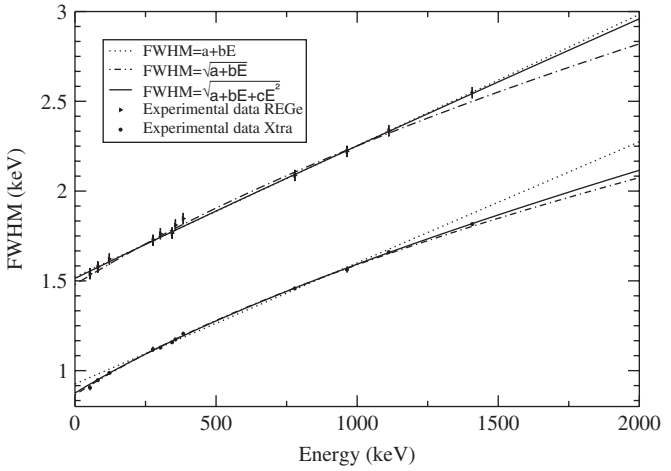

Fig. 4. Resolution calibration of the REGe and XtRa detector using three different functions.

constant uncertainty added to every pulse processed by the electronic chain $\mathrm{FWHM}^2_{\mathrm{noise}} = \text{constant}$ [8].

Three different functions presented in the literature have been involved in resolution calibration [6,8]: a linear function ($\mathrm{FWHM} = a_1 + a_2E$), a square root of a linear function ($\mathrm{FWHM} = \sqrt{a_1 + a_2E}$), and a square root of a quadratic function ($\mathrm{FWHM} = \sqrt{a_1 + a_2E + a_3E^2}$).

The resolution calibration is independent of the fit algorithm (ODR or OLS) used. This is because of the uncertainties associated to the experimental resolution data is much higher than the uncertainties related to the energy of the emission. The ODR algorithm have been selected for resolution calibration.

The fitted functions are shown in Fig. 4 for REGe and XtRa detector. The linear function gives a SD of 0.79 for REGe detector. On the other hand the uncertainties associated to the experimental resolution data for XtRa detector are much lower than for REGe detector. However, the same function provides a SD of 5.4 for XtRa detector. It seems that a linear function is not adequate to reproduce in general the resolution of the germanium detectors.

Both the square root of a linear function and the square root of a quadratic function reproduce quite well the experimental data for REGe and XtRa detector. The obtained values of the SD are similar for both functions. However, the WSS using the square root of a linear function is equal to 14.0 and 22.6 for REGe and XtRa detector, respectively. Whereas if the square root of a quadratic function is used the WSS takes a value of 6.1 and 8.3 for REGe and XtRa detector, respectively. Therefore we can deduce that the square root of a quadratic function reproduces accurately the experimental resolution data for germanium detectors.

5. Conclusions

We propose a new method for the energy calibration of germanium detectors. The method is based on the ODR algorithm that treats correctly all the involved experimental uncertainties fitting the experimental data better than the usual OLS algorithm. The comparison between different functions for energy calibration shows that a quadratic fit of a set of experimental data produces more accurate results than other functions. Finally, the resolution calibration performed using the functions presented in the literature indicates that the square root of a quadratic function reproduces perfectly the resolution of different germanium detectors.

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Appendix A. Orthogonal distance regression

ODRPACK is a collection of subroutines written in Fortran 77 and designed for solving the weighted orthogonal distance regression problem (ODR) when all the variables have significant uncertainties [7]. It can also solve the ordinary least squares problem (OLS) where the errors are assumed to occur in only one of the variables.

Let (x_i, y_i), $i = 1, \ldots, n$ be a set of experimental data where $x_i \in \Re^1$ and $y_i \in \Re^1$. Suppose that exists a function f with a set of unknown parameters $a \in \Re^p$ that defines the relationship between the variables, but that both the y_i and the x_i contain unknown errors $\varepsilon_i \in \Re^1$ and $\delta_i \in \Re^1$, respectively. Then the values of y_i satisfies for some unknown value $\mathbf{a}$:

$$y_i = f(x_i + \delta_i; \mathbf{a}) - \varepsilon_i. \tag{A.1}$$

The ODR problem is to find the $\mathbf{a}$ for which the sum of the squares of the n orthogonal distances from the curve $f(x; \mathbf{a})$ to the n experimental data points is minimized. This is carried out by the minimization problem:

$$\min_{\mathbf{a},\boldsymbol{\delta}} \sum_{i=1}^{n} w_i^2 \{[f(x_i + \delta_i; \mathbf{a}) - y_i]^2 + d_i^2 \delta_i^2\} \tag{A.2}$$

where σ_{ε_i} and σ_{δ_i} are the experimental uncertainties, and $w_i = 1/\sigma_{\varepsilon_i}$ and $d_i = \sigma_{\varepsilon_i}/\sigma_{\delta_i}$, therefore the equations looks like

$$\min_{\mathbf{a},\boldsymbol{\delta}} \sum_{i=1}^{n} \left\{ \left(\frac{f(x_i + \delta_i; \mathbf{a}) - y_i}{\sigma_{\varepsilon_i}} \right)^2 + \left(\frac{\delta_i}{\sigma_{\delta_i}} \right)^2 \right\}. \tag{A.3}$$

ODRPACK finds the solution iteratively using a trust region Levenberg–Marquardt method. If OLS method are used the weights included in the algorithm correspond to $w_i = 1/\sigma_{\varepsilon_i}$.

In order to check the goodness-of-fit the algorithm calculates the weighted sum of squares (WSS) and the

standard deviation (SD) using the following equations:

$$\mathrm{WSS} = \sum_{i=1}^{n} w_i^2 \{[f(x_i + \delta_i; \mathbf{a}) - y_i]^2 + d_i^2 \delta_i^2\} \quad \text{(A.4)}$$

and

$$SD = \sqrt{\mathrm{WSS}/(n-p)}. \quad \text{(A.5)}$$

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