

SURVEY OF THE NONLINEARITIES STRUCTURES IN GAMMA RAY ENERGY CALIBRATION USING HPG_e DETECTORS.

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ABSTRACT

The present work aims to survey the typical fine energy calibration structure in gamma-ray spectroscopy systems which use successive approximation ADC and shows that the knowledge of this fine structure, about 5 eV per 10² channels, allows achieving correct statistic energy calibrations without the usually *ad hoc* introduction of uncertainties associated with the differential non-linearity inherent to those systems. Differently of previous works, the One Step Self-Calibration Procedure implementation allows the proper use of all covariances between the experimental data. At the end of the interactive scheme proposed in this work, it was achieved a reduced chi-square of 1.11 without the *ad hoc* introduction of uncertainties related to the differential nonlinearities.

INTRODUCTION

The uncertainties associated with gamma spectroscopy with High Purity Germanium (HPGe) detectors have achieved values of the order of a fraction of the electron-volt (eV) [1]. Such measurements use primary calibration standards, i.e. ¹⁹⁸Au and ¹⁹⁸Ir, whose respective uncertainties are around 0.15-0.78 eV, and methodologies which try to reduce systematic errors such as those produced by counting rate changing, fixed source-detector distance, and the use of just one type of calibration source [2].

After the correction of the most important systematic errors, the main energy calibration problem in the field of gamma-ray spectroscopy with semi-conductors is the non-linearity of the associated electronic systems. This non-linearity depends on the data acquisition system – fig. 1, for instance, different types of ADC (Analog-to-Digital Converter) systems produce completely dissimilar error structures.

A successive approximation ADC system shows oscillations which are due to the lack of homogeneity in comparison levels of its MCA (Multi Channel Analyzer). So, this work aims to survey the typical structure showed by gamma spectroscopy systems that use successive approximations ADC and show that the determination of such structure allows achieving energy calibrations statistically correct without introducing *ad hoc* uncertainties related to

those nonlinearities. The determination of this structure will allow future investigations of mathematical models used to describe such systems. Finally, the present survey uses the One Step Self-Calibration Procedure [4] adjusted to the methodology presented in [3], which in turn let to consider the proper covariances between the gamma-ray energies values involved in the calibration.

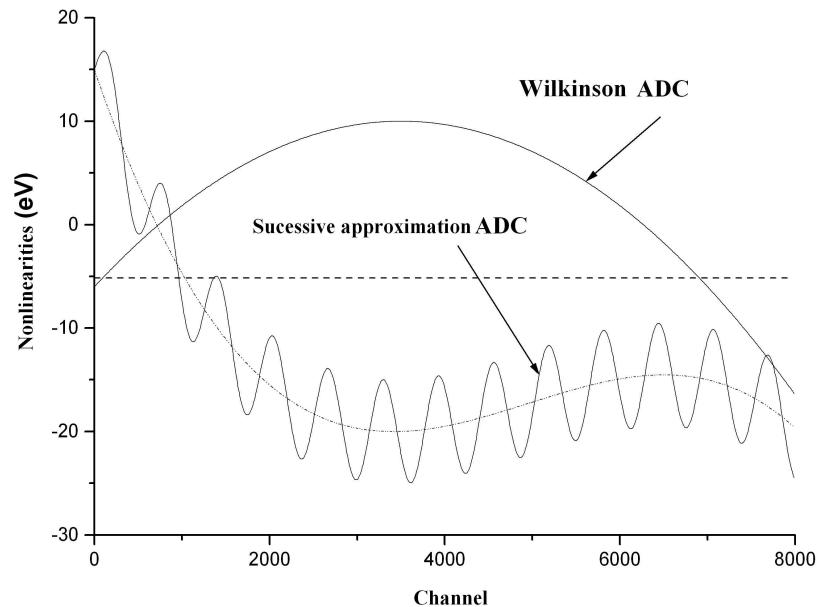


Figure 1 - Different types of nonlinearities associated to different types of ADC converters used in gamma-ray spectroscopy data acquisition systems. When the uncertainties are small enough, a polynomial fitting procedure is not sufficient. The nonlinearity is the subtraction between the true value of a gamma-ray energy and the respective linear term of the polynomial fitting function.

ENERGY CALIBRATION AND ITS FINE STRUCTURE

In the simple energy calibration procedures that are usually carried out, it is associated a polynomial function of the full-energy peak position to the respective gamma-ray energy. Then, the calibration procedure yields an estimation of the polynomial coefficients and its correlations through the Least Square Method (LSM) in its matrix approach.

The uncertainties related to the full-energy peak position in an usual experimental set up could be as small as hundredths of a bin channel. Such uncertainties when combined with those from primary or secondary gamma radiation sources yield a polynomial fitting whose goodness-of-fit test, such as chi-square (χ^2), is not satisfactory (i.e., the fitting chi-square is much bigger than the available degrees of freedom), fig. 2 (a).

Indeed, a polynomial function is not capable of yielding proper statistical results if a complicated fine energy structure starts to become important when it is confronted against the data uncertainties. For instance, in a typical experimental set up for precise measurement of gamma-ray energies, 10-50 eV/channel, the combined uncertainties from calibration source energies and full-energy peak positions ($\cong 10\text{-}50 \text{ eV/channel} \cdot 0.01\text{channel}$) do not allow a proper statistical analysis, because a typical fine energy 'amplitude' could be bigger than those combined uncertainties, probably yielding a poor goodness-of-fit.

The solution to this problem has been the introduction of an *ad hoc* uncertainty in the measurement of the full-energy peak position which is related to the fine energy structure, fig. 2 (b). In reference [2], which uses a Wilkinson ADC, the variance of the full-energy peak position, σ_{peak}^2 , is the combination of its value and another empirical one ($\sigma_{\text{final}}^2 \rightarrow \sigma_{\text{peak}}^2 + 0.0033^2$). This procedure is relayed on the hypotheses that the final effect of the energy fine structure is an increased full-energy absorption peak position variance.

On the other hand, besides the systematic nature of such errors components (which are of course undesirable), the resultant uncertainties from energies measurements of unknown gamma transitions after this calibration procedure became unnecessary large, hence underrating the modern gamma-ray spectroscopy systems capacity.

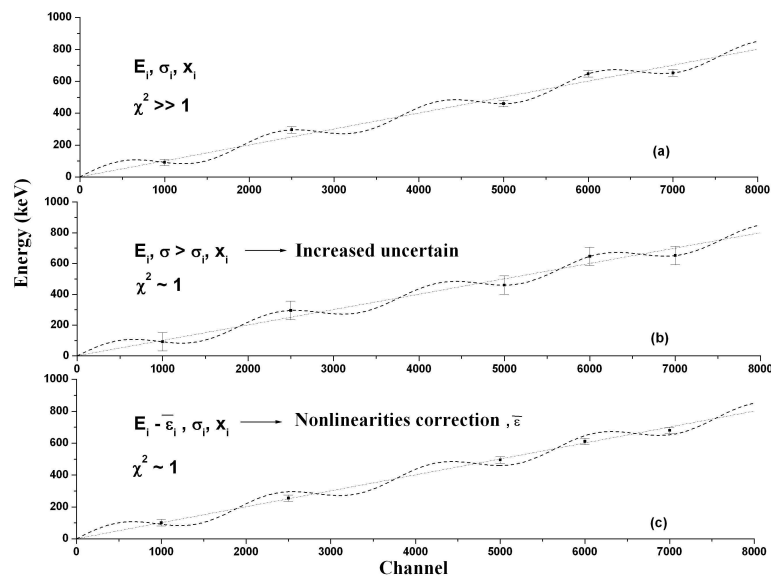


Figure 2 – Systematic error handling by means of the correction of the differential nonlinearities. (a) usual procedure which not uses the *ad hoc* introduction of additional uncertainties related to the full-peak position; in this case, the reduced chi-square of the fitting procedure is much bigger than one ($\chi_{\text{red}}^2 \gg 1$) (b) usual procedure with *ad hoc* increased uncertainties which produces $\chi_{\text{red}}^2 \approx 1$ (c) calibration procedure with nonlinearities correction which yields a fitting with a proper goodness-of-fit without the introduction of *ad hoc* uncertainties.

The resolution of this problem demands an increased number of gamma-ray transition lines, that is, unfolding the energy fine structure demands close transitions lines. In this sense, the propose of this work is to establish an experimental methodology similar to [5] which discloses the energy nonlinearities fine structure. However, the mathematical procedure used in reference [5] do not permit the full handling of all covariances between the calibration sources gamma-ray energies. Following this reasoning, the One Step Self-Calibration Procedure [4] was implemented to allow the proper blend between the experimental information (full-energy peak position) and those previously known experimental data (calibration source gamma-ray energies), allowing the proper use of covariances between all the fitting parameters involved.

ENERGY CALIBRATION AND ITS FINE STRUCTURE

The task of increasing the number of transition lines is achieved by an usual gamma ray spectroscopy system endowed of: an ORTEC 572 amplifier with a shaping time of 10 μ s and pile up rejection, an ADC ORTEC 114, a biased amplifier ORTEC 444 and an ORTEC HM413 (Histogram Module), fig. 3. Such set up is not a typical one and for this reason it was used a low counting rate of \approx 1700 cps, avoiding peak distortion due to pile up. In this work, the pulses amplitudes were changed only by modifying the bias level and keeping the ADC ORTEC 444 gain constant.

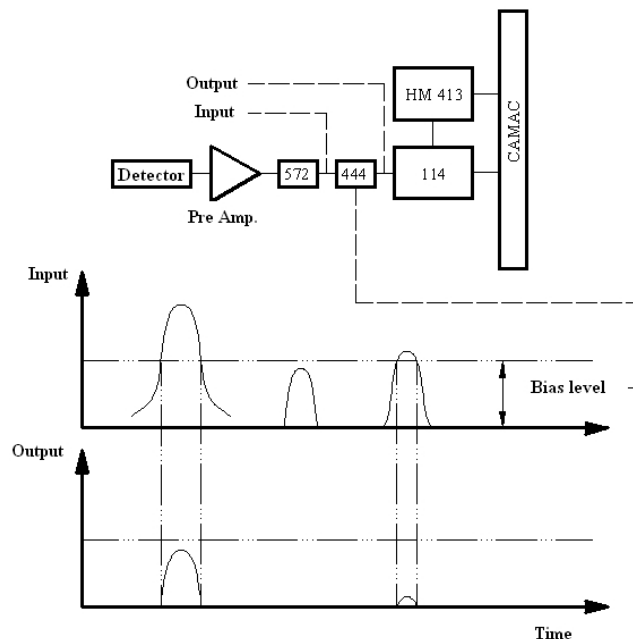


Figure 3 – Pulse amplitude variation through bias level changing. Pulses above the bias level are ‘cut’ at the bias level. The bias amplifier saves only what is above the bias level. When the signal is lower than the bias level nothing happens.

The bias amplifier can change gain and pulse amplitude. Pulses from the ORTEC 572 are eliminated if they are lower than the bias level. On the other hand, if the gain is unitary and pulses are bigger than the bias level output pulses amplitudes will be the inputted ones subtracted from the bias level, fig. 3. Consequently, bias level could be used to ‘move’ the full-energy peak position through the whole gamma spectrum, creating ‘new’ gamma transitions lines.

Using a ^{133}Ba gamma-ray source, an ORTEC HPGe detector (162 cm^3 , whose relative efficiency relative to a 3’x3’ NaI(Tl) crystal is 33%) and the described electronics it was obtained a set of 16 000 channels gamma-ray spectra in which each spectrum is ‘moved’ approximately 70-80 channels to its neighbors by means of bias level variation.

The full-energy peaks were fitted by a Gaussian function, a low energy exponential tail and a linear background through the program IDF [6]. In the fig. 5 it is shown a full-energy peak fitting of one of the 356.0134(6) keV gamma-rays used from the ^{133}Ba calibration source.

METHODOLOGY

Once one has acquired all ‘moved’ spectra (N: number of acquisition), is possible to relate to each acquired spectrum a third grade polynomial function, which includes all information related to experimental set up for all observed gamma-rays, according to the following matrix equation:

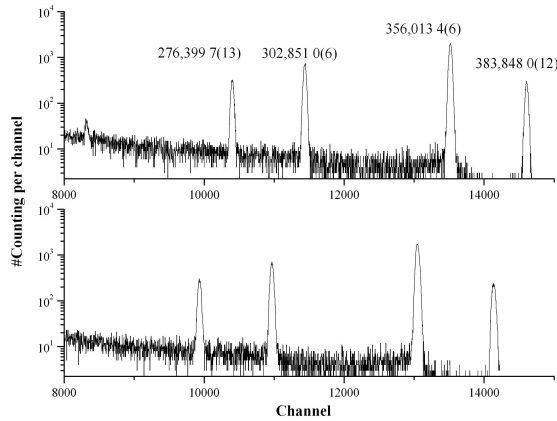


Figure 4 – Examples of two ^{133}Ba gamma-ray spectra ‘moved’ by the change in the bias level of the biased amplifier ORTEC 444. In the figure, the ^{133}Ba gamma-ray energy values and its respective uncertainties are indicated in keV.

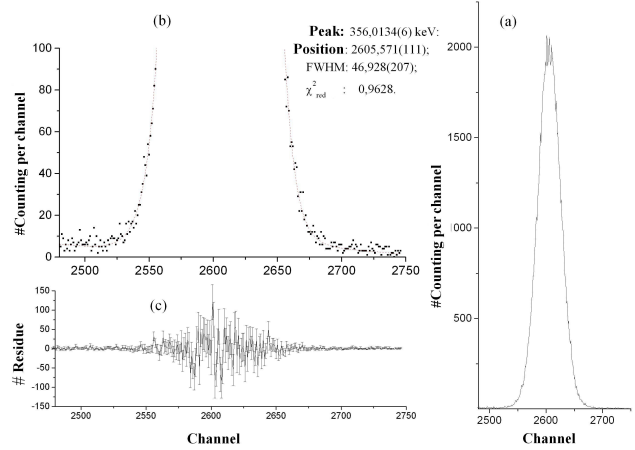


Figure 5 – Full-energy peak fitting of one a 356.0134(6) keV gamma-rays from the ^{133}Ba calibration source. (a) full-energy peak; (b) Gaussian and exponential tail fitting detail; (c) fitting residues.

$$\begin{aligned} \vec{0} &= -\vec{E}^0 + \mathbf{X}_P \vec{A}_P^0 + \vec{\epsilon}_P \\ 0 &= -E_{ij}^0 - a^j + bx_{ij} + cx_{ij}^2 + dx_{ij}^3 \end{aligned} \quad (1)$$

where, $\mathbf{0}$ is a null vector whose dimension is equal to the numbers of acquisitions, \mathbf{A}_P^0 represents the true value of the calibration coefficients, \mathbf{E}^0 the true value of the gamma-ray energy transitions, $\mathbf{\epsilon}_P$ the errors related to the measurement of the full-energy peak position. According to this scheme, one gets the following planning matrix \mathbf{X}_P ,

$$\begin{pmatrix} 1 & 0 & \cdots & 0 & x_{11} & x_{11}^2 & x_{11}^3 \\ 1 & 0 & \cdots & 0 & x_{12} & x_{12}^2 & x_{12}^3 \\ 1 & 0 & \cdots & 0 & x_{13} & x_{13}^2 & x_{13}^3 \\ 1 & 0 & \cdots & 0 & x_{14} & x_{14}^2 & x_{14}^3 \\ 0 & 1 & \cdots & 0 & x_{21} & x_{21}^2 & x_{21}^3 \\ 0 & 1 & \cdots & 0 & x_{22} & x_{22}^2 & x_{22}^3 \\ 0 & 1 & \cdots & 0 & x_{23} & x_{23}^2 & x_{23}^3 \\ \vdots & \ddots & \ddots & \ddots & \vdots & \vdots & \vdots \end{pmatrix}$$

where x_{ij} is the position of the full-energy peak and $i = 1, \dots, N$ is an index for spectrum and $j = 1, \dots, 4$ for the used ^{133}Ba gamma-ray energies. The previous knowledge of the ^{133}Ba gamma-ray energies values are gathered to the present experiment by means of

$$\vec{R} = \vec{E}^0 + \vec{\epsilon}_E \quad (2)$$

where \mathbf{R} represents the four ^{133}Ba gamma-ray energies used and $\boldsymbol{\epsilon}_E$ the errors related to their measurements. Gathering equations 1 and 2 one gets the mathematical statement of the problem according to the One Step Self-Calibration Procedure, eq. 3.

$$\begin{aligned} \begin{pmatrix} \vec{0} \\ \vec{R} \end{pmatrix} &= \begin{pmatrix} -\mathbf{I} & \mathbf{X}_P \\ \mathbf{I} & \mathbf{0}_M \end{pmatrix} \begin{pmatrix} \vec{E}^0 \\ \vec{A}_P^0 \end{pmatrix} + \begin{pmatrix} \vec{\epsilon}_P \\ \vec{\epsilon}_E \end{pmatrix} \\ \begin{pmatrix} -\mathbf{I} & \mathbf{X}_P \\ \mathbf{I} & \mathbf{0}_M \end{pmatrix} &= \mathbf{X}; \quad \begin{pmatrix} \vec{E}^0 \\ \vec{A}_P^0 \end{pmatrix} = \vec{A}^0 \\ &\quad \begin{pmatrix} \vec{0} \\ \vec{R} \end{pmatrix} = \vec{Y} \end{aligned} \quad (3)$$

The covariance matrix of \mathbf{Y} , \mathbf{V}_Y , is given by

$$\mathbf{V}_Y = \begin{pmatrix} \mathbf{V}_P & \mathbf{0}_M \\ \mathbf{0}_M & \mathbf{V}_E \end{pmatrix}$$

where \mathbf{V}_p and \mathbf{V}_E are the covariance matrix of the full-energy peaks and the ^{133}Ba gamma-ray energies, respectively. The presence of $\mathbf{0}_M$ indicates the independence between both experimental informations. Initially, the LQM solution to this problem is given:

$$\vec{A} = (\mathbf{X}^T \cdot (\mathbf{V}_Y)^{-1} \mathbf{X})^{-1} \cdot \mathbf{X} \cdot (\mathbf{V}_Y)^{-1} \cdot \vec{Y} \quad (4)$$

The calculation scheme aims to eliminate systematic errors by separating them from random ones. If it is supposed that the fine energy structure varies slowly with channel position it is possible to define a modified error vector, $\boldsymbol{\epsilon}_M = \mathbf{M}\boldsymbol{\epsilon}_p$, which is the averaged between neighborhood peaks, so that:

$$\epsilon_{Mi} \equiv \sum_{m=i-n}^{m=i+n} \epsilon_{P,m} / (2n+1) \quad (5)$$

where $2n+1$ is the number of peaks used in averaging process (in this work it was assumed $n=2$) and let $\boldsymbol{\epsilon}_M \equiv \boldsymbol{\epsilon}_s$ because it is supposed that:

$$\sum_{m=i-n}^{m=i+n} \epsilon_{a,m} \cong 0 \quad (6)$$

that is, random errors are supposed to have a null mean value ($\langle \boldsymbol{\epsilon}_a \rangle = 0$) and hence it is possible to associate the error mean value to the systematic one ($\langle \boldsymbol{\epsilon} \rangle = \boldsymbol{\epsilon}_s$). So, once one has calculated $\boldsymbol{\epsilon}_M$ it is possible to undertake the following interactive scheme (step $k \rightarrow k+1$),

$$\begin{aligned} \epsilon_{Mk} &= \mathbf{M} \vec{\epsilon}_{P,k} \\ \vec{Y}_{k+1} &= \vec{Y}_k - \begin{pmatrix} \epsilon_M \\ \vec{0} \end{pmatrix} \\ \vec{A}_{k+1} &= (\mathbf{X}^T \cdot (\mathbf{V}_Y)^{-1} \mathbf{X})^{-1} \cdot \mathbf{X} \cdot (\mathbf{V}_Y)^{-1} \cdot \vec{Y}_{k+1} \\ \mathbf{V}_{Y,k+1} &\rightarrow A_{P,k+1}(N+1) \\ \chi_{k+1}^2 &= (\vec{Y}_{k+1} - \mathbf{X}\vec{A})^T (\mathbf{V}_Y)^{-1} (\vec{Y}_{k+1} - \mathbf{X}\vec{A}) \end{aligned} \quad (7)$$

During the procedure, $\mathbf{V}_{Y,k+1}$ update follows from uncertainties propagation of the previous knowledge of gamma-ray energies uncertainties, σ_E , and full-energy peak positions uncertainties, σ_p , so that $\sigma^2 = \sigma_E^2 + b_k^2 \sigma_p^2$ ($b_k = A_{P,k}(N+1)$). The procedure is over when the fitting chi-square is approximately constant ($\chi_{k+1}^2 \cong \chi_k^2$).

ANALYSIS

After applying this procedure to forty ^{133}Ba spectra we got approximately 150 transitions lines in the range between channels 8000-14000. In the fig. 6 it is presented the results. At the end of the interactive scheme, it was achieved a reduced chi-square of 1.11 without the *ad hoc* introduction of uncertainties related to the differential nonlinearities.

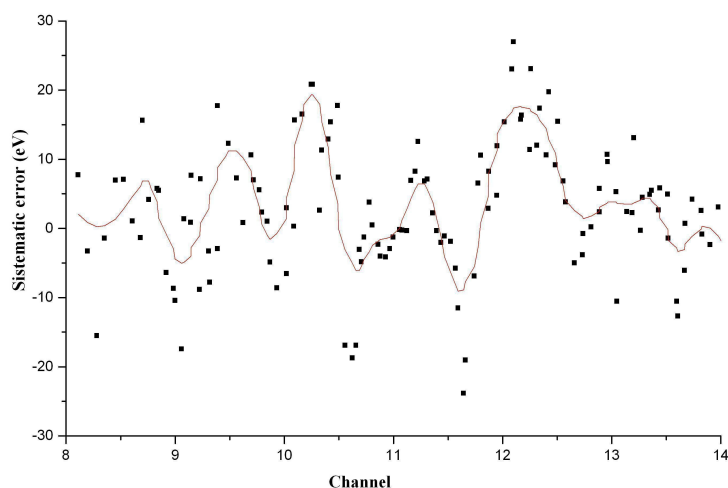


Figure 6 – Resultant fine energy structure between channels 8000-14000 from the application of the presented procedure. It was used forty spectrums ‘moved’ 70-80 channel per spectrum to each other.

Differently of [3] the implementation of One Step Self-Calibration Procedure adequately agrees to the methodology of [2]. Indeed, all the covariances between gamma-ray energies were properly used. The displacement between spectra accomplished by bias level changing was enough to unravel the fine energy structure by means of a Fast Fourier Transformation (FFT - using 5 close points), fig. 6. Yet, if the same procedure is applied to the fitting residues it will not shown any significantly structure, fig. 7.

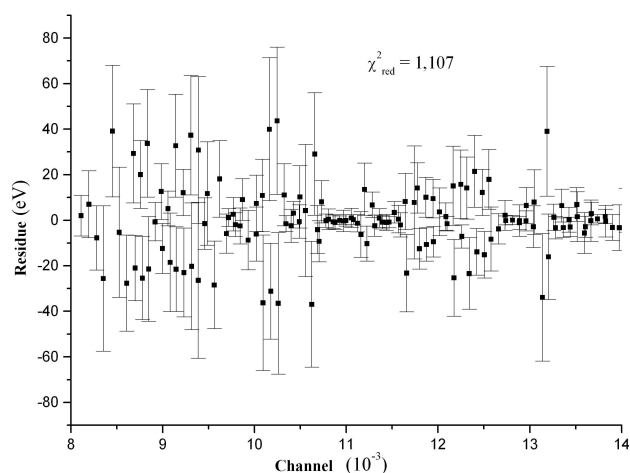


Figure 7 – Fitting residues.

3. CONCLUSIONS

In the present work, it was shown that the fine energy structure survey turns the energy calibration procedure of a semi-conductor gamma-ray detector (which uses a successive approximation ADC) into an adequate statistical one without the *ad hoc* introduction of uncertainties related to differential nonlinearities of the full-energy peaks positions. Differently of previous works, the One Step Self-Calibration Procedure implementation allows the proper use of all covariances between the experimental data. However, the procedure is time-consuming and future works aiming the fine structure modeling will demand as many transitions lines as possible. For this reason it is intended to improve the experimental set up, making it as more automate as possible to allow its day-basis use and to investigate different mathematical models for successive approximation ADC acquisition systems.

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