ImplicitFWHMcalibration for gamma-ray spectra (Postprint)

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Abstract

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Full Text

Preamble

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Implicit FWHM Calibration for Gamma-Ray Spectra

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Abstract: FWHM calibration is one of the essential procedures in gamma-ray spectral analysis. Traditional methods are time-consuming and lack flexibility because they require additional measurements with calibration sources. This paper introduces an implicit calibration method based on symmetric zero-area conversion. Single peaks can be differentiated from doublets, while the extracted FWHM values can be applied in the fitting process. Various forms of calibration equations are introduced and compared with practical spectral data using this method.

Key words: Gamma-ray spectrum, FWHM, Implicit calibration, Symmetric zero-area conversion

Introduction

The full width at half maximum (FWHM) of peaks in gamma-ray spectrometry serves as a key measure of the gamma spectroscopy system's resolution. The FWHM expressed in keV has a well-defined relationship with the energy of incident gamma rays. Knowledge of the FWHM as a function of energy is crucial when analyzing gamma spectra, particularly for peak searching and fitting []. Therefore, accurate FWHM calibration must be performed as a fundamental step in spectrum processing.

2 Physical Essence of FWHM

A gamma-ray spectrum represents the energy response of the detection system to gamma rays of particular energies. Peaks in the spectrum are spread over several channels and can be characterized by a Gaussian distribution, whose standard deviation can be predicted by []:

$$\sigma^2 = \sigma_I^2 + \sigma_P^2 + \sigma_C^2 + \sigma_E^2$$

where σ is the overall uncertainty of the peak in energy units. σ_I is the intrinsic width of nuclear energy levels, which is extremely small compared to σ and can be ignored []. σ_P represents the statistical fluctuation in the production of electron-hole pairs (n) in the detector. The number of electron-hole pairs created by a gamma ray of energy (E) follows a Fano distribution (F) []. Defining W as the average energy required to create an electron-hole pair, the expected uncertainty in n is $\sigma_n = (F \times n)^{0.5} = [(F \times E)/W]^{0.5}$. σ_C is the uncertainty in charge collection by the detector caused by trapping effects. Due to the complexity of this effect, there is no simple way to express this uncertainty as an energy function []. However, a linear relationship $\sigma_C = cE$ appears satisfactory, though without theoretical justification []. σ_E, the contribution from electronic noise in the pulse processing system, is treated as constant for gamma rays of any energy.

3 FWHM Calibration Equations []

Three independent effects mainly influence the resolution of gamma-ray spectra. Using the energy form ΔE to express the FWHM of a Gaussian-shaped peak in the spectrum, we can write:

$$\Delta E \approx 2.355\sigma$$

where p, c, and e are constants related to fluctuation, collection, and electronic noise, respectively. Taking the square root of both sides of Eq.(2) yields the form found in commercial programs such as Genie 2000 []. Debertin and Helmer [] introduced Eq.(4) by ignoring the factor of incomplete charge collection:

$$\Delta E = a_0 + a_1\sqrt{E} + a_{2E}$$

In addition, Eq.(5) with a simpler expression can be used. Gilmore conducted a series of experiments to compare FWHM calibrations using different formulae [] (Table 1). The best fit comes from the square root quadratic function, followed by a simple quadratic fit. The Genie 2000 fitting performs worse than the linear equation.

Results of fitting FWHM data to different functions []

Fitting type	Formulae	RMS differences
Linear	$a_0 + a_{1E}$	
Quadratic	$a_0 + a_{1E} + a_{2E}^2$	
Genie 2000	$a_0 + a_{1E}^{0.5}$	
Debertin and Helmer	$(a_0 + a_{1E} + a_{2E}^2)^{0.5}$	
Square root quadratic		

4 Traditional FWHM Calibration

Similar to energy calibration, traditional FWHM calibration is accomplished by measuring gamma rays of precisely known energy and establishing the relationship between peak width and energy []. Three approaches can provide appropriate gamma-ray emission sources: (1) selecting and mixing several nuclides with single or discrete energies; (2) choosing one specific nuclide that emits a variety of energies covering the entire spectrum range, such as ^{152}Eu; or (3) using known nuclides present in the test sample for calibration.

Explicit methods can be used for fine calibration, but their calibration sources require additional time-consuming measurements. Particularly when experimental conditions change, the spectroscopy system must be recalibrated through new measurements, except when using nuclides that are always present. This paper develops an implicit FWHM calibration method that utilizes self-information gained from the target spectrum itself.

5 Implicit FWHM Calibration Method

5.1 Method Introduction

Ge(Li) detectors provide high energy resolution, producing numerous gamma peaks with sufficient separation to easily distinguish single peaks. The implicit method involves two calibration procedures: first, single peaks are examined and extracted from the spectrum; second, the width of each singlet is calculated.

Together with the peak position, the calibration curve is obtained by fitting these data.

Among various peak searching algorithms, the implicit FWHM symmetric zero-area conversion method (SZA) offers advantages in low noise sensitivity, fine multi-peak resolution, and weak peak identification capabilities [].

5.2 Method Description

The spectrum data are convolved using the SZA method with a zero-area window. The linear baseline tends to zero after convolution, while maximum values appear at the positions of gamma peaks. The conversion process is described by Eq.(6):

$$y_i' = \sum_{j=-m}^{m} C_j y_{i+j}$$

where y_i and y_i' are the spectrum data before and after conversion, and C_j is the window coefficient.

Among various window functions, the Gaussian second derivative has the best properties [], with coefficients expressed as Eq.(7):

$$C_j = \frac{1}{\sqrt{2\pi}\sigma_w^3}\left(\frac{j^2}{\sigma_w^2} - 1\right)\exp\left(-\frac{j^2}{2\sigma_w^2}\right)$$

where σ_w is the standard deviation from the original Gaussian distribution $G_w(j)$.

[Figure 1: see original paper] shows a Gaussian second derivative formed SZA window function with $\sigma_w = 4$.

Gamma peaks in the spectrum can be approximated as Gaussian shapes:

$$G_\gamma(i) = H\exp\left(-\frac{(i-p)^2}{2\sigma_\gamma^2}\right)$$

where H, p, and σ_γ are the amplitude, position, and standard deviation, respectively.

Due to the convolution property [], a Gaussian peak convolved with the window function maintains the second derivative form, as shown in Fig.2. The σ_γ of the gamma peak is deduced from intercept D and σ_w, and subsequently the peak FWHM is expressed by Eq.(11):

$$\text{FWHM} = 2.355\sigma_\gamma = 2.355\frac{D}{2\sqrt{2}}$$

Eq.(11) is only valid for single peaks, and the calculated FWHM is constant for every pair of D and σ_w. For multi-peaks, the intercept D relates to the intervals and ratios between component peaks, making the FWHM obtained from Eq.(11) meaningless.

Consequently, the same spectrum can be converted using several windows with different σ_w values. When the FWHM value becomes invariant, the corresponding peak is considered a singlet, thus distinguishing multi-peaks through their invalid FWHM values. Additionally, the FWHM of each single peak can be obtained, implementing the FWHM calibration process.

5.3 Method Modification

To apply this to practical spectra, a simulation dataset is established to test the calibration method. Eight window functions with σ_w values from 1 to 8 are convolved with four individual Gaussian peaks having σ_γ values of 1, 2, 4, and 8. The calculated and theoretical FWHM values are compared (Table 2, Fig.3).

The convolution of a gamma peak with the window function is:

$$R(i) = G_\gamma(i) \times W(j) = G_\gamma(i) \times G_w(j) = G_{\text{conv}}(i)$$

where $G_{\text{conv}}(i)$ is the convolution of the gamma peak and the original Gaussian distribution of the window, which has a Gaussian form with $\sigma_{\text{conv}} = (\sigma_\gamma^2 + \sigma_w^2)^{0.5}$.

The distance between two zero-crossing points beside the conversion maximum can be obtained from the Gaussian second derivative:

$$D = 2\sigma_{\text{conv}} = 2(\sigma_\gamma^2 + \sigma_w^2)^{0.5}$$

[Figure 3: see original paper] shows the error between calculated and theoretical FWHM values under different windows.

Difference between calculated FWHM and theoretical value

Theoretical σ_γ	Error between calculated and theoretical FWHM values
1	-1.71e-4
2	
4	
8	

To reduce the difference in Eq.(11), a modification factor is introduced in Eq.(12):

$$\text{FWHM} = 2.355 \cdot a \cdot \frac{D}{2\sqrt{2}}$$

The resultant reliability depends on the uncertainty of peak height and background level. The constant a is determined by applying an iterative method to optimize the average error under every window function for each Gaussian peak.

[Figure 4: see original paper] shows the result using Eq.(12). Under every window with different σ_w, the mean of residual errors approaches zero, and the fluctuation is suppressed to some extent.

In practical application, appropriate σ_w values should be selected. The SZA method can separate multi-peaks with small σ_w but is sensitive to noise. Conversely, large σ_w windows are reliable but inadequate for multi-peak processing. A σ_w value approximating σ_γ suggests optimal results. Therefore, σ_w can be determined within a rough range related to FWHM variation in the spectrum.

This method is also compared with a direct calculation process. The average background level above and below the peak is subtracted from the estimated peak height to obtain the expected count. The two positions of half-height on the peak are obtained by linear interpolation, and the distance equals the FWHM. Quadratic background and noise with constant SNR are added to a Gaussian peak with $\sigma_\gamma = 4$ to simulate an actual gamma peak. One hundred sets of simulation data with random background and noise are processed by both methods (Table 3).

Eq.(12) approximates the theoretical value well. For the direct approach, the result is relatively fluctuant due to noise. When a smoothing process is first applied to reduce the standard deviation, it impacts the FWHM value to a certain extent.

Comparison of direct process and method in this paper

Method	Theoretical FWHM	Error of 100 experiments
Direct-without smoothing		
Direct-with smoothing		
This paper		

6 Method Verification

A gamma-ray spectrum from a sand sample measured by an HPGe detector is used to test the implicit FWHM calibration method (Fig.5). Three windows with σ_w values of 2, 3, and 4 are employed to convert the spectrum and calculate the FWHM for each peak. The three sets of FWHM deviations are used to identify single peaks, and their mean value is used in the fitting procedure.

HYPERMET, a mature gamma spectrum analysis code, and the Genie 2000 program are employed for validation (Table 4). HYPERMET uses a region fitting method to obtain accurate peak position and FWHM, which can be used as the standard value, while Genie 2000 applies a direct process to calculate FWHM. Together with FWHM values, the relative errors compared to HYPERMET are calculated for the other two processes, as shown in Table 5. The relative errors within $±$3% are obviously better than Genie 2000, except for one point. Additionally, both HYPERMET and Genie programs require a rough FWHM calibration as input to obtain proper results, while the novel method is fully automatic.

Calculated FWHM and position of each single peak

Peak position	Calculated FWHM

The FWHM calculated by different methods

Peak position	HYPERMET	Genie	This paper
		Relative error / %	Relative error / %

Table 6 and Fig.6 show the position-FWHM data from Table 4 fitted to the five equations in Section 3. The square root quadratic function provides the best fit, and the linear fit performs better than the Genie 2000 function, consistent with the conclusion in Section 3.

Comparison of different equations fitting FWHM data

Calibration equation	RMS differences
Square root quadratic	
Quadratic	
Linear	
Debertin and Helmer	
Genie 2000	

[Figure 6: see original paper] Fitting curves of the 5 calibration equations.

The performance of the three typical equations is shown in Fig.7 using simulation data first. Ultimately, this method is applied to a practical gamma-ray spectrum, and the calibration result proves to be satisfactory.

[Figure 7: see original paper] Error between fitted functions and FWHM data.

7 Conclusions

This paper introduces an implicit FWHM calibration algorithm as a complement to traditional methods. The new algorithm is developed based on the symmetric zero-area conversion method and utilizes self-information from the target spectrum. The method is tested, modified, and compared with a direct calculation process. First using simulation data, the method is ultimately applied to a practical gamma-ray spectrum, and the calibration result proves to be effective.

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Note: Figure translations are in progress. See original paper for figures.