A method for interpolating asymmetric peak shapes in multiplet γ-ray spectra[*]

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Abstract   The peak shapes of γ-rays at various energies must be known before unfolding the multiplet spectra obtained by using semiconductor or scintillation detectors. Traditional methods describe isolated peaks with multi-parameter fitting functions, and assume that most of these parameters do not vary with energy because it is rare to find a spectrum with enough isolated peaks to constrain their dependence. We present an algorithm for interpolating the γ-ray profile at any intermediate energy given a pair of isolated γ-ray peaks from the spectrum under consideration. The algorithm is tested on experimental data and leads to a good agreement between the interpolated profile and the fitting function. This method is more accurate than the traditional approach, since all aspects of the peak shape are allowed to vary with energy. New definitions of Left-Half Width at Half Maximum, and Right-Half Width at Half Maximum for peak shape description are introduced in this paper.

Key words   peak shape, peak asymmetry, γ spectrum, unfolding spectrum

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1   Introduction

When a γ-ray spectrum contains an isolated peak, its area can be assessed in two ways: by fitting an appropriate analytical function to the distribution and then integrating, or by summing counts in the peak region and then subtracting the background inferred from the neighboring bins.

In the case of several overlapping peaks, the source γ-ray spectrum can only be extracted by fitting the data with a response function. This function describes the spectrum created by γ-rays of constant energy. In semiconductor detectors such as high purity germanium (HPGe) and scintillation detectors such as NaI(Tl), a single high-energy photon will produce counts in nearby channels as well as in its own. The resulting peak has an asymmetric tail, for the following reason.

When a γ-ray deposits its energy inside an active area (for example, a HPGe crystal), many electron-hole pairs are created. The charge carriers then move towards the anode and cathode under the influence of a strong external electric field. However, some of the charge carriers will be "trapped" by impurities or defects, decreasing the height of the pulse and the output of the analog-to-digital converter (ADC) will show an asymmetry in the transfer spectrum.

Several fitting functions have been developed in the past decades to model peak areas[1—7]. One common choice is to model the peak as a Gaussian, while using separate functions to represent the two tails.

To unfold a multiplet spectrum, the peak shape functions must be known beforehand. Their parameters may be chosen by the researcher or determined

from the profiles of isolated peaks in other regions of the spectrum, if such exist. The latter method is generally more reliable, since the peak shape can also be influenced by experimental conditions such as dead time, incident energy, and the stability of electronics in the spectrometer system.

After obtaining the response function for an isolated peak, the question arises of how to deduce the appropriate peak shapes for other γ-rays in the multiplet. Because the asymmetry depends on several parameters, it is seldom possible to find a simple relationship between the peak shape and the energy. (In most cases there are simply not enough isolated peaks available to constrain all the variables.) For this reason, traditional methods[8] usually neglect the energy dependence of these parameters.

To take into account the energy dependence of peak shapes, this paper presents a new method: interpolating between two or more isolated peaks in the spectrum. This technique is more accurate than assuming a constant peak shape, yet requires fewer reference peaks and no assumptions regarding the energy dependence of additional parameters are necessary. In this way we can achieve more precise results when unfolding a multiplet spectrum.

2   Method

As the first step, all isolated peaks are fitted by the same response function.

2.1   Single peak profile

The fitting function is a Gaussian with two tails:

$$f(x) = G(x) + T_1(x) + T_2(x) , \quad (1)$$

where $G(x)$ is written as

$$G(x) = \exp\left[-\frac{(x-x_0)^2}{\sigma^2}\right]. \quad (2)$$

In this application, x_0 is set to the centroid of the peak. The tail function $T_1(x)$ is defined as

$$T_1(x) = \frac{1}{2}T\exp\left[\frac{x-x_0}{B\sigma}\right]\mathrm{erfc}\left[\frac{x-x_0}{\sigma}+\frac{1}{2B}\right], \quad (3)$$

where T is the relative amplitude and B is the slope. The complementary error function "erfc" is defined as follows:

$$\mathrm{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty \exp(-t^2)\mathrm{d}t . \quad (4)$$

The function $T_2(x)$ is defined as

$$T_2(x) = \frac{1}{2}S\mathrm{erfc}\left[\frac{x-x_0}{\sigma}\right], \quad (5)$$

where S is the relative amplitude.

The maximum likelihood method is used to obtain the fits[9].

2.2   Interpolating a peak profile

The model just described can describe isolated peaks more accurately than a pure Gaussian function, but will encounter difficulties when confronted with more complex spectra. For the Gaussian component (Eq. (1)), the variation with energy can be described by calibrating the resolution of the detector system. The relationship between σ and the peak energy is generally known for a given detector. However, in general the energy dependence of the tail function parameters cannot be determined, since not enough isolated peaks are available.

To accurately describe the variation of peak shapes with energy, we introduce two new concepts: Left-Half Width at Half Maximum (LHWHM), and Right-Half Width at Half Maximum (RHWHM). As an example, consider the 59.536 keV γ-ray peak shown in Fig. 1. This peak was generated by ^{241}Am radiation, and measured using a HPGe detector. Background events have been subtracted using a smoothed-step Compton function; for more details on this process, refer to page 124 of the book by Reilly, Ensslin and Smith[1].
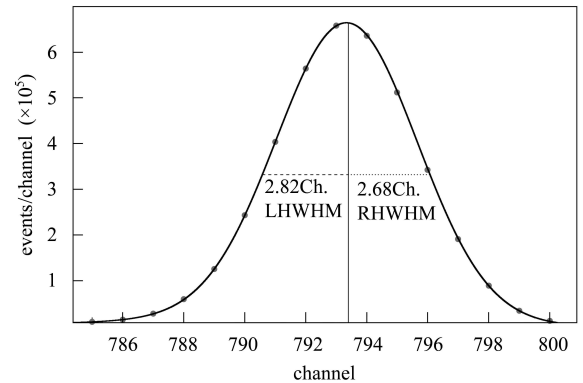

Fig. 1.   An isolated peak fitted with the function shown in Eq. (1). The left and right half widths at half maximum are labeled on the plot. Their values are calculated numerically from the fitting function, as described in the text.

After fitting Eq. (1) to an isolated peak, the LHWHM can be calculated numerically as follows:

(1) Calculate the peak amplitude $y_0 = f(x_0)$ using Eq. (1) and the fitted parameters.

(2) Evaluate $f(x)$ to the left of x_0, scanning outward at a fixed step length while monitoring the difference $\Delta h = f(x) - 0.5y_0$.

(3) When Δh drops below 0, decrease the step length and scan to the right until the value becomes positive. Then decrease the step length and scan to the left until the sign of Δh changes again, and so on.

(4) Repeat Step 3 until Δh is small enough. The distance between x_0 and x_1 at this point is the LHWHM.

The RHWHM can be calculated using a similar method.

Studies have shown[10, 11] that the shape of the low-energy tail may depend not just on the detector but also on its associated electronics. The peak shapes for γ-rays of different energies may also be different.

In this paper, we describe the relationship between LHWHM (or RHWHM) and energy as a simple function $f_{\mathrm{LHWHM}}(E)$ $(f_{\mathrm{RHWHM}}(E))$. The peak shape of a γ-ray with energy E_0 can be obtained by interpolation, as described below.

The shape of any other peak is described using a series of interpolated points. To calculate the height h_l^{E0} of an interpolated peak with energy E_0 at any point on the curve, we first express the distance l from its centroid x_0 in terms of the LHWHM or RHWHM as appropriate. Denote this value as l_1. If there are n $(n \geqslant 2)$ isolated γ-ray peaks in the spectrum, each one can be fitted with Eq. (1) independently. In this case each fitted function is normalized such that its height at x_0 is 1 and our interpolation contains only shape information. If we have n pairs of fitted peaks, then a linear function can be used between each pair to determine the relationship between h_{l1} and E for any other peak. It is then a simple matter to rescale the height h_l^{E0}. Through a series of such calculations, an accurate peak shape at any energy E_j can be obtained.

3 Test

The proposed method was tested on experimental data. A solid source containing Pu and Am was measured using a planar HPGe detector. The 129.294 keV γ-rays (of ^{239}Pu) form an isolated peak whose fitting function will be taken as a reference. The shape of the 129.294 keV γ-ray peak can also be obtained by interpolation between the isolated peaks at 59.536 keV (of ^{241}Am) and 208.000 keV (of ^{241}Am). To compare the fitted and interpolated peak shapes, all four functions are plotted together in Fig. 2 showing details of their low-energy tails. All of the peak shapes have been renormalized to an amplitude of 1, and their centroids have been shifted to the origin.

The x-axis is expressed in units of LHWHM for $x < 0$ and RHWHM for $x > 0$. B_{59}^{L}, B_{129}^{LI}, B_{129}^{L} and B_{208}^{L} are given for the left boundaries of the shapes.
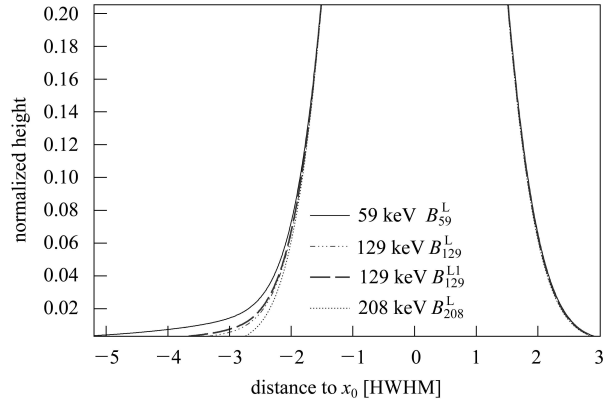

Fig. 2. An example of interpolation of a peak shape (labeled by "129 keV Inter.") with two measured shapes (labeled by 59 keV and 129 keV). A measured peak shape at the 129.294 keV (labeled by "129 keV Inter.") has also been presented as reference. See text for more detail.

The interpolation shape is calculated according to the method outlined above in the region where the 59 keV and 208 keV peaks both have counts. In the region where the 208 keV peak has zero counts $(x < B_{208}^{\mathrm{L}})$, the output of the algorithm is offset so that the interpolated counts decrease to zero at the correct position, B_{129}^{LI}. This position is calculated as follows.

The distance between B_{208}^{L} and B_{129}^{LI} is denoted as $d_{129\mathrm{I}}^{208}$, and distance between B_{208}^{L} and B_{59}^{L} is denoted as d_{59}^{208}. We require that the left-hand boundary of the interpolated peak meets the following condition:

$$\frac{d_{129\mathrm{I}}^{208}}{d_{59}^{208}} = \frac{208.000 - 129.294}{208.000 - 59.536} . \tag{6}$$

The numbers on the right-hand side of the equation are the energies of the γ rays. Since the left-hand boundaries of the two isolated peaks are known, B_{129}^{LI} can be determined.

An interpolated value $H_{129\mathrm{I}}$ at position x between B_{208}^{L} and B_{129}^{LI} can be calculated using the method outlined above even though the 208 keV peak has zero counts in this region. However, the value of $H_{129\mathrm{I}}$ is modified by the following offset:

$$O(x) = \left(\frac{x - B_{129}^{\mathrm{LI}}}{B_{208}^{\mathrm{L}} - B_{129}^{\mathrm{LI}}} - 1 \right) H_{129\mathrm{I}} . \tag{7}$$

This offset makes the interpolated function continuous across B_{208}^{L}, where $O(x) = 0$. The height at B_{129}^{LI} is always zero, as there the offset is equal to

$-H_{129\mathrm{I}}^{\mathrm{L}}$. The interpolated counts are forced to zero for $x < B_{129}^{\mathrm{LI}}$, outside the peak boundary.

Figure 2 shows that the four peak shapes are very similar in the $x \geqslant -2\mathrm{LHWHM}$ range. Slight differences are evident in the low-energy tail below this point. The interpolated 129 keV peak shape is in good agreement with the actual peak shape for energies down to the left boundary of the 208 keV peak. In the region $B_{129}^{\mathrm{LI}} \leqslant x \leqslant B_{208}^{\mathrm{L}}$, some difference between the two 129 keV shapes is observable.

4   Conclusion

Traditional methods for modeling complicated spectra assume that the complicated function used for fitting an isolated peak can be applied at all energies. This approach will introduce systematic errors, however, as the shape of the asymmetric low-energy tail is energy-dependent and may also vary with other experimental parameters. This paper has described an interpolation method capable of obtaining more accurate peak shapes at any given energy between two isolated peaks. The method takes into account the energy dependence of peak shapes, and can be used to unfold complex spectra for more accurate results.

We tested the method on three isolated peaks in a real radioactive spectrum. The 59 keV and 208 keV peaks were used for interpolation, while the 129 keV peak between them was used to verify the result. According to Fig. 2, the peak shape obtained by the interpolation is a good approximation to the 129 keV fitting function. (There are of course some slight differences.)

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