Improved FWHM fitting model in Genie 4.0

Introduction

In gamma spectroscopy, the energy resolution of a detector is measured by the width of a peak at a given energy. This is known as the Full Width at Half Maximum (FWHM). The FWHM at a specific energy is critical to many spectroscopy calculations, including those used in the Genie software applications. Algorithms that use the FWHM as input includes minimum detectable activity (MDA), fitted peak area, and peak locate algorithms. The typical way to determine FWHM at any energy is to create a least-squares fit function from measured FWHM values to establish a relationship of FWHM as a function of energy. This is often called the shape calibration or FWHM calibration.

In Genie 4.0, a new fit function has been included that better represents the FWHM behavior for High Purity Germanium (HPGe) and other semi-conductor detectors. This application note discusses the choice of fit function, shows the performance for several detectors, and the implications to analysis results.

Theory

The resolution of a semi-conductor detector can be described by three mayor components [1]:

- Electronic noise, $FWHM_E$: The electronics that the detector is connected to introduces electronic noise to the signal.
- Statistics of charge carriers, $FWHM_S$: The contribution to the detector resolution resulting from the statistical fluctuations of the number of electron-hole pairs created in the semiconductor when a photon of a fixed energy interacts with the detector.
- Variations in charge collection efficiency, $FWHM_C$: Ideally all charge created in the detector from a radiation event will be collected. However, for large detectors and detectors with low electric fields it is possible that not all charge will be collected for all radiation events. This factor represents the variations in the number of charges that will be collected from different interactions in the detector.

The FWHM can mathematically be represented by

$$FWHM^2 = FWHM_E^2 + FWHM_S^2 + FWHM_C^2$$

For the first component, the electronic noise contribution of the FWHM is typically independent of the photon energy. For the second component, the charge carrier statistics can be represented as the square root of the number of charge carrier which is proportional to the energy deposited in the detector. This means that the square of the charge carrier contribution is usually a linear function of the deposited energy. For the third component, the variation in charge collection efficiency varies linearly with energy and the square varies with the square of the energy. Using this information, we can arrive at a parameterization of the detector FWHM as a function of energy as follows:

$$FWHM = \sqrt{\mathrm{a} + \mathrm{b}E + \mathrm{c}E^2}$$

Where a represents the electronic noise, b the statistics of charge carriers and c the variations in charge collection efficiency. The values of the parameters a, b, and c for a particular detector are determined during the energy and shape calibration process. The detector resolution is measured at several energies spanning the energy range of interest for the analysis, and a least-squares fit algorithm is executed to determine the optimum value of the three parameters given the measured data points. Genie spectroscopy software applications refer to this fit function as the “Square Root of Polynomial” function.

Performance for different detector types

To determine the performance of the Square Root of Polynomial function, the new FWHM function is evaluated against measured FWHM values for a range of detector types. The legacy fit function $FWHM = a + b\sqrt{E}$ is also evaluated to provide a comparison of the two functions. In Figure 1 the two fits are compared for a 40% relative efficiency P-type HPGe detector for a typical energy calibration source standard spanning the energy range 59 to 1836 keV. To provide information at higher energies, these fits are also compared against the sum peak from Co-60 at 2505 keV and the Tl-208 background peak at 2614 keV.

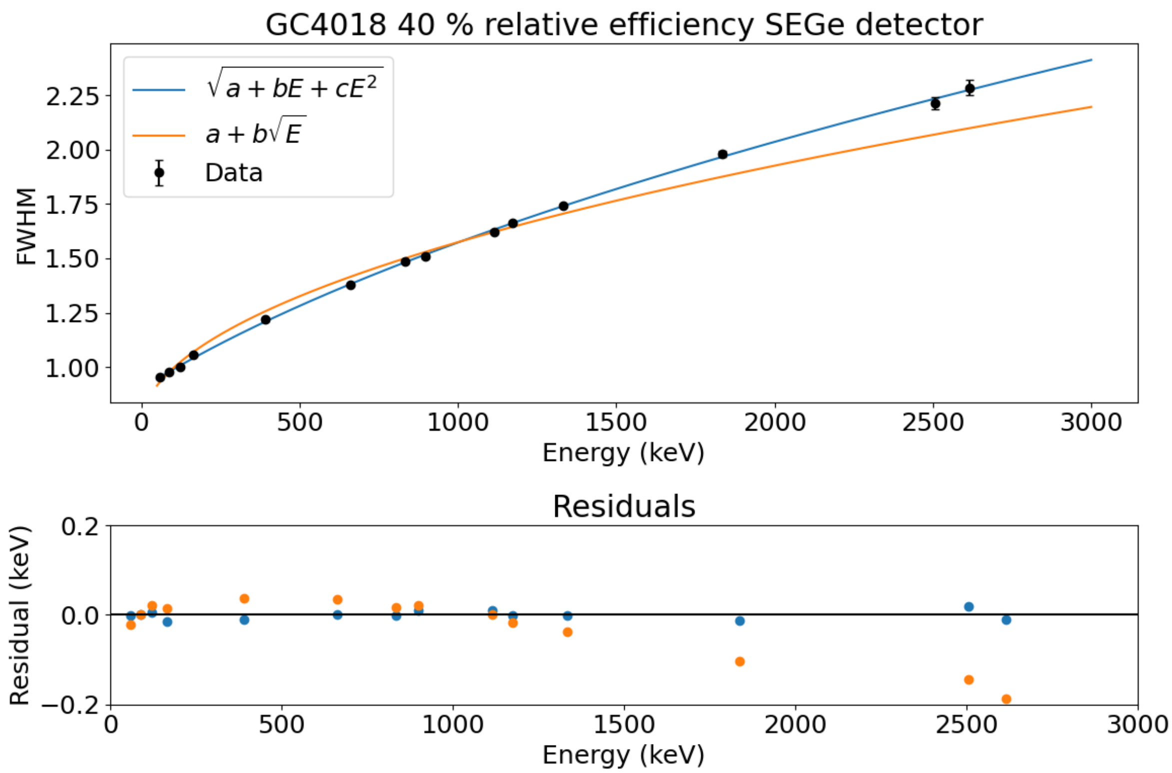

***Figure 1** The performance of the new fit function compared to the legacy fit function for a P-type 40 % relative efficiency HPGe (GC4018) detector. The top figure shows the two fits as a function of energy together with the measured FWHM values. The bottom figure shows the residuals between the fits and the measured FWHM values.*

It is clear from the figure that the Square Root of Polynomial function reproduces the measured FWHM values very well. This is evidenced by the residuals < 0.02 keV. The performance is better than the legacy fit function for all energies, but the improvements are most significant for higher energies where the variance in charge collection efficiency has the largest contribution.

Figure 2 and **Figure 3** show the performance for the Square Root of Polynomial function and the legacy fit function for several HPGe detectors of coaxial and planar types for the energy range 59 – 1836 keV. The new fit function reproduces the measured FWHM values better than the legacy fit function for all energies for all detectors. The largest differences are observed for high energies for large detectors.

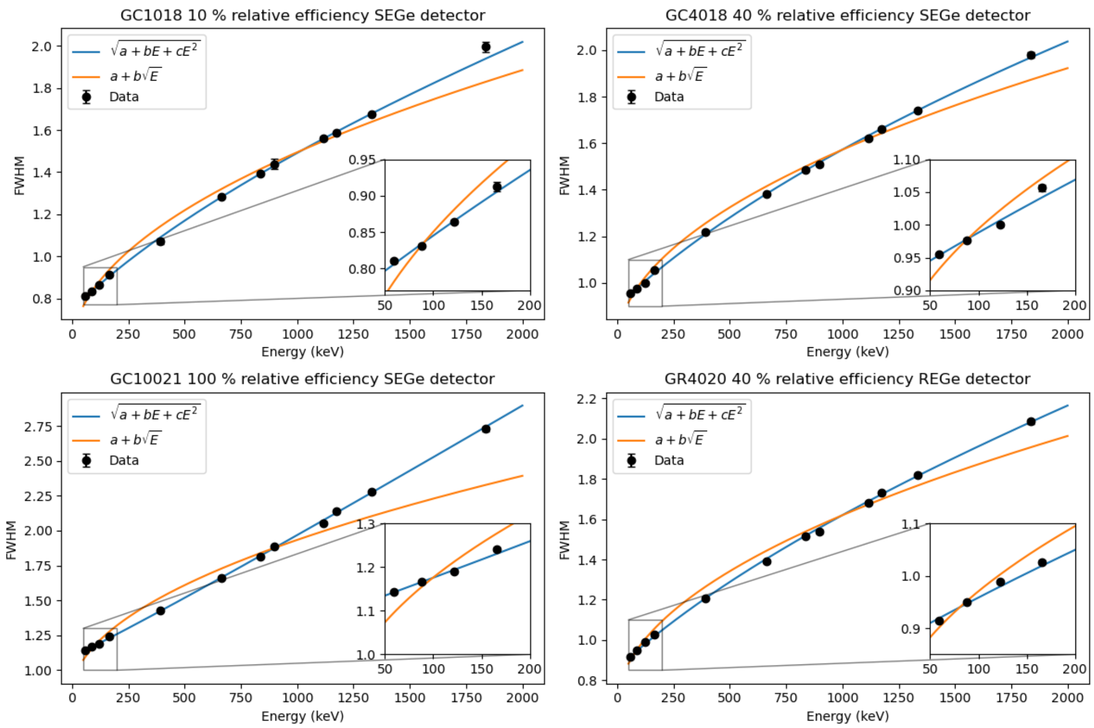

***Figure 2** The performance of the new Square Root of Polynomial function and legacy fit function compared to measured FWHM values for SEGe and REGe-type detectors of different relative efficiencies.*

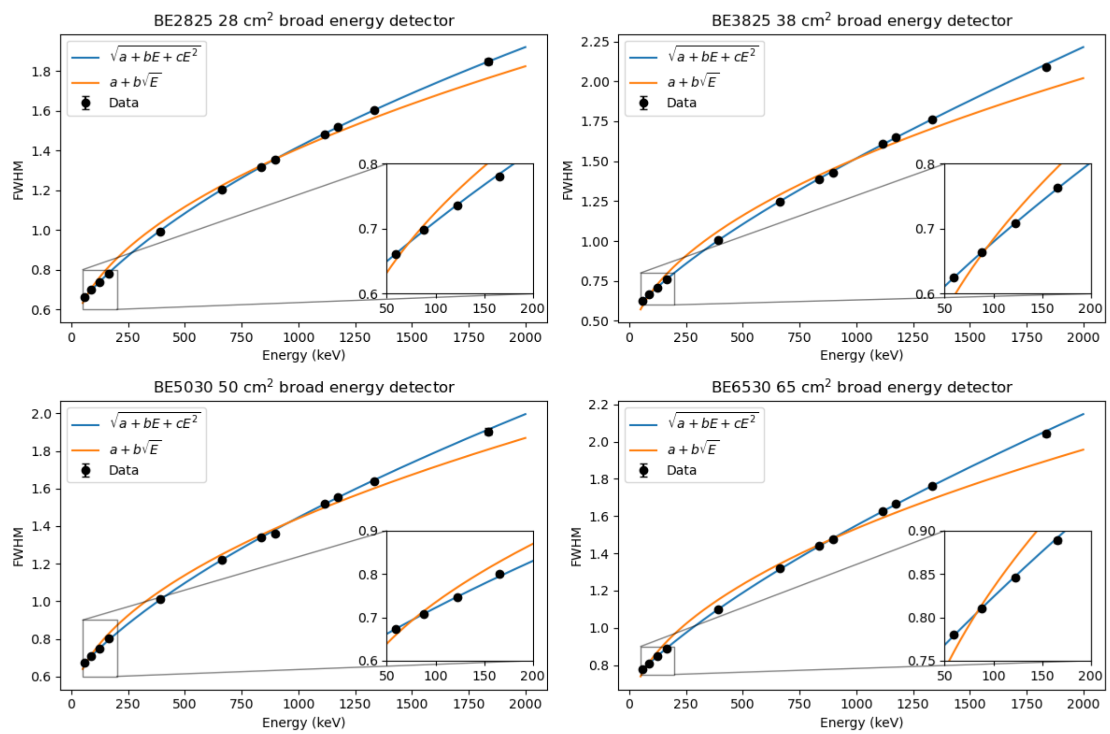

***Figure 3** The performance of the new Square Root of Polynomial function and the legacy fit function compared to measured FWHMs and the legacy fit function for different size point contact planar detectors.*

To determine the performance for non-HPGe detectors, additional comparisons against scintillators as well as a cadmium zinc telluride (CZT) detector are reviewed. The new square root of polynomial function produces almost identical results as the legacy fit function for scintillators, see Figure **4**. This is because the statistics of the charge carriers is the dominating contribution to the FWHM for scintillators. CZT is a semi-conductor, like HPGe detectors and the new fit function reproduces the measured data points much better than the legacy fit function for all energies.

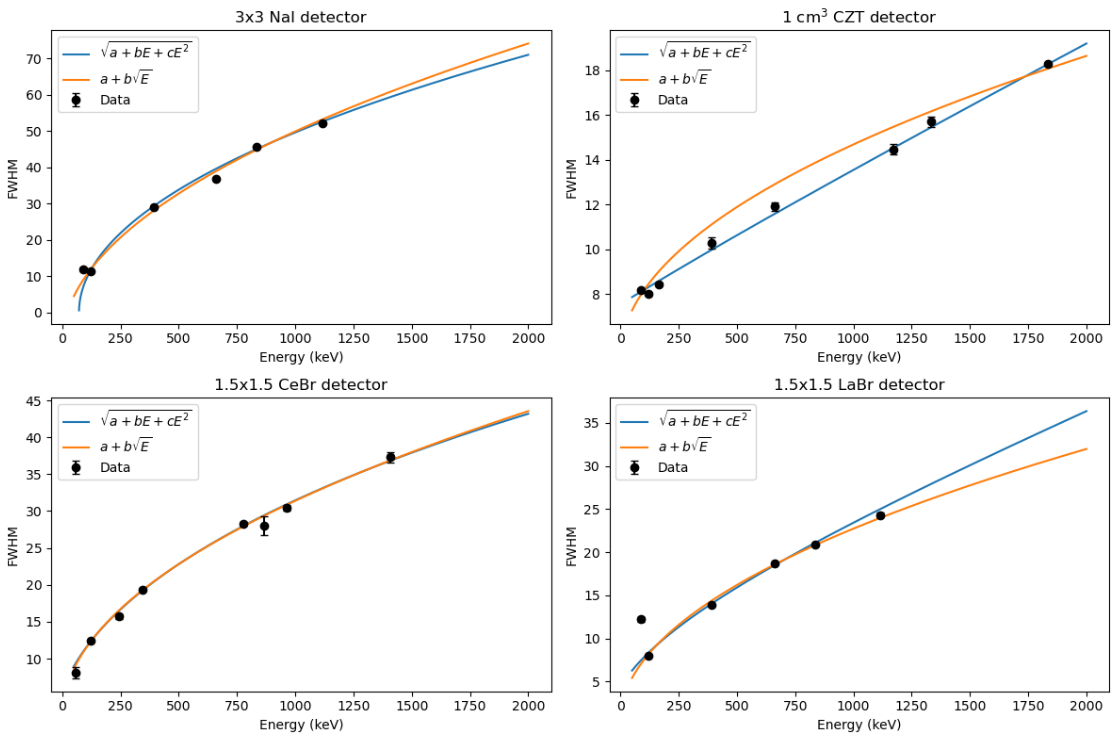

***Figure 4** The performance of the new Square Root of Polynomial function and the legacy fit function compared to measured FWHM values for three types of scintillator detectors and a cadmium zinc telluride (CZT) detector.*

Impact on analysis results

One of the quantities used for calculating critical level (CL) and minimum detectable activity (MDA) in Genie is the number of counts in a region of interest (ROI) around the energy of the peak of interest. The size of the ROI is dependent on the FWHM calculated from the FWHM calibration and therefore may be impacted by choice of the FWHM calibration model. It is important to recall that while ROI may be calculated in energy, the Genie software must use channel data to determine counts in a given ROI. Therefore, there will only be an impact to the CL and MDA if the choice of FWHM model changes the ROI sufficiently for the number of channels in the ROI to be different.

The ROI is most likely to be impacted by choice of FWHM model at high energies or when the spectrum consists of many channels (as a counterpoint, for a spectrum with a many channels, any change in channel count for a given ROI will have a smaller impact on change in peak counts). For peaks at low energy or if the spectrum has few channels, the likelihood that a change in the FWHM will change the number of channels in the ROI is low. That said, if the number of channels in the ROI is impacted, this will have a more significant impact on the number of counts in the ROI. Figure 5 illustrates this by showing the energy limits for an ROI centered around 2392.11 keV for different number of channels in the spectrum. For 32k channels the likelihood that the change in FWHM changes the number of channels is large but the number of counts in the channel added is small compared to the total number of counts in the original ROI. When only 4k channels are used and channel is added the number of counts in the added channel is larger compared to the total number of counts in the ROI.

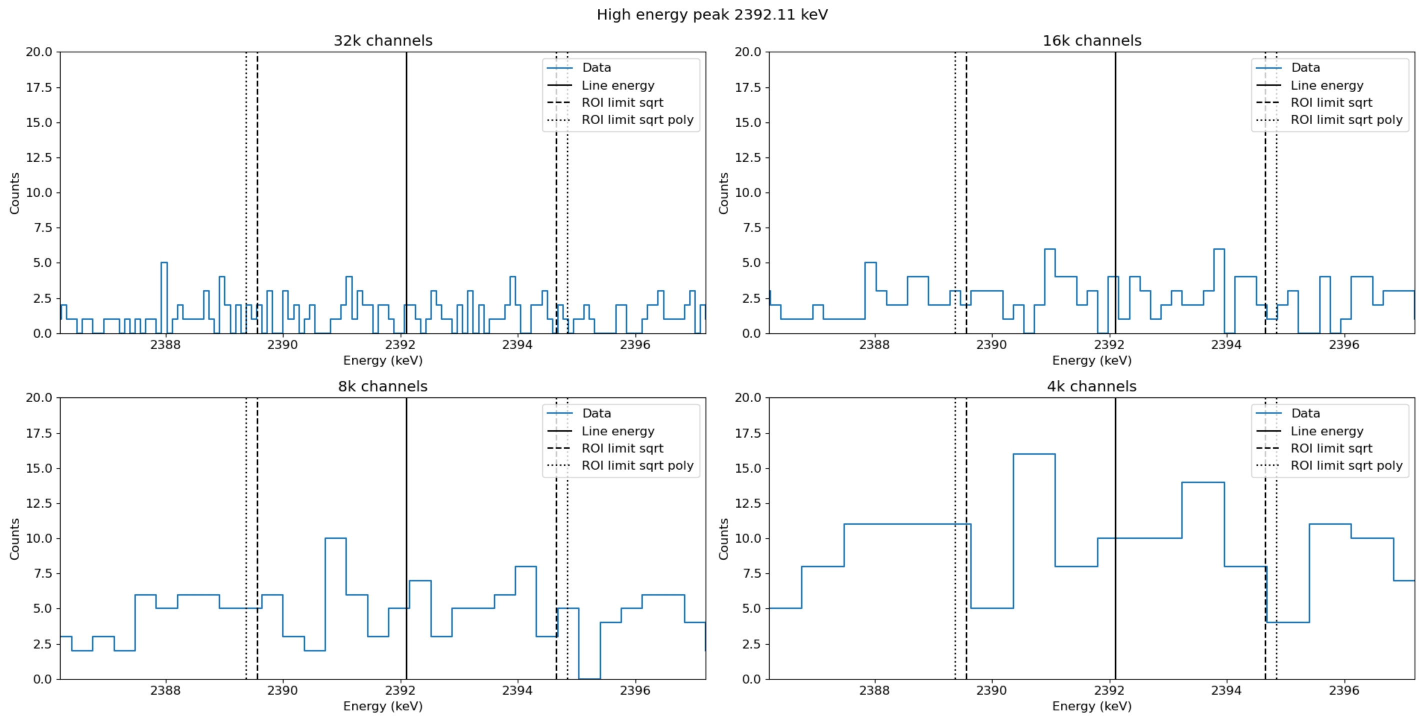

***Figure 5** Examples of the background ROI used to calculate MDA for a high energy emission line for various number of channels in the spectrum.*

Table 1 shows an example of the number of counts at the critical level for one low, medium, and high energy emission line. For the low and medium energy emission lines where the difference between the square root of polynomial and legacy fit functions are small and the number of channels in the ROI is small, there is no impact to the ROI. Therefore, no difference is observed in number of counts at the critical level. For the high energy emission line, where the size of ROI is larger and the typical difference between the square root of polynomial and legacy fit functions are also larger, there is a small impact to the number of counts at the critical level.

	95 % Critical Level in Counts							
Energy (keV)	**sqrt 4k ch**	**sqrt poly 4k ch**	**sqrt 8k ch**	**sqrt poly 8k ch**	**sqrt 16k ch**	**sqrt poly 16k ch**	**sqrt 32k ch**	**sqrt poly 32k ch**
59.5	224	224	224	224	209	209	206	206
661.7	70.6	70.6	64.7	64.7	64.7	64.7	64.7	64.7
2392.1	21.4	22.4	20.7	21.1	20.4	20.9	20.1	20.9

***Table 1** The 95 % critical level calculated for a low, medium, and high energy emission line for different number of channels in the spectrum.*

For peak area algorithms, the FWHM calibration is used for two calculations: determination of the ROI used for the peak area calculation and input to the least-squares optimization for fitted peaks. Using the square root of polynomial FWHM function for the inputs instead of the legacy FWHM function can impact the peak areas produced by the algorithm. Figure 6 shows the ratio of the peak areas calculated with the legacy fit function and the new fit function for four different options of the peak area calculation algorithm, and the error bars indicate the statistical uncertainty of the peak area ratio. The changes to the peak areas using the two fit functions as input is all within the expectation from statistical uncertainties. Therefore, it is not expected that the choice of the new square root of polynomial fit function versus the legacy fit function will significantly impact peak area results.

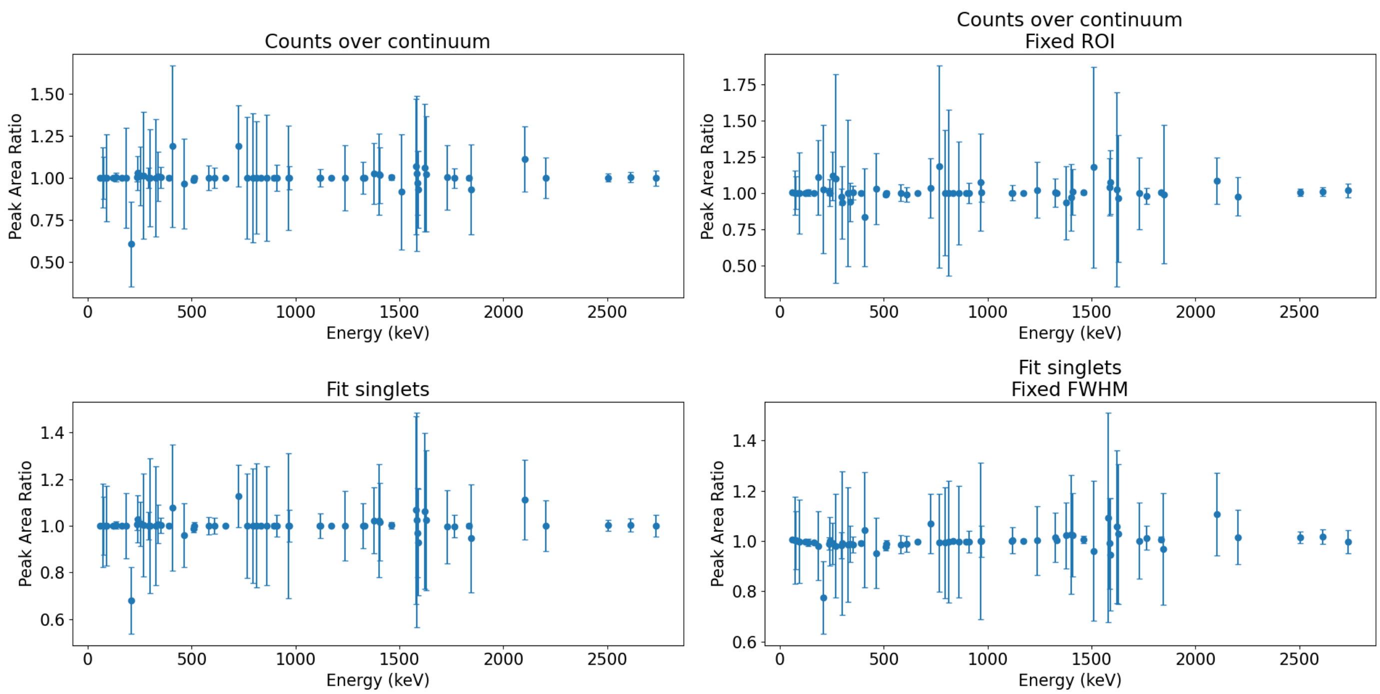

***Figure 6** The ratio of the peak area calculated using the legacy FWHM fit function and the square root of polynomial FWHM fit function for a range of peak area calculation settings. The top left figure shows the ratio for non-fitted singlets and non-fixed ROI limits. The top right figure shows non-fitted singlets and fixed ROI limits. The bottom left figure shows the ratio for fitted singlets where the FWHM are allowed to be optimized by the fitting algorithm. The bottom right figure shows the ratio for fitted singlets where the FWHM is fixed such that the fitting algorithm performs no optimization.*

Applying the new fit function in Genie

The new square root of polynomial fit function can be applied in Genie by performing a standard Energy and Shape calibration. First, measure an energy calibration source standard that emits gamma rays with known energies and that are well separated in energy. Count the calibration standard such that all peaks have sufficient statistics for the FWHM to be reliably determined. A typical recommendation is 10,000 to 50,000 counts in the calibration peaks. Use one of the Genie calibration methods to create energy, FWHM, and FWHM uncertainty triplets and open the Energy Calibration Dialog, shown in Figure 7. The square root of polynomial fit function can be selected in the dialog, and it is highlighted in red in Figure 7. Selection of the FWHM fit model during the Energy and Shape calibration process determines the FWHM fit model used throughout the analysis.

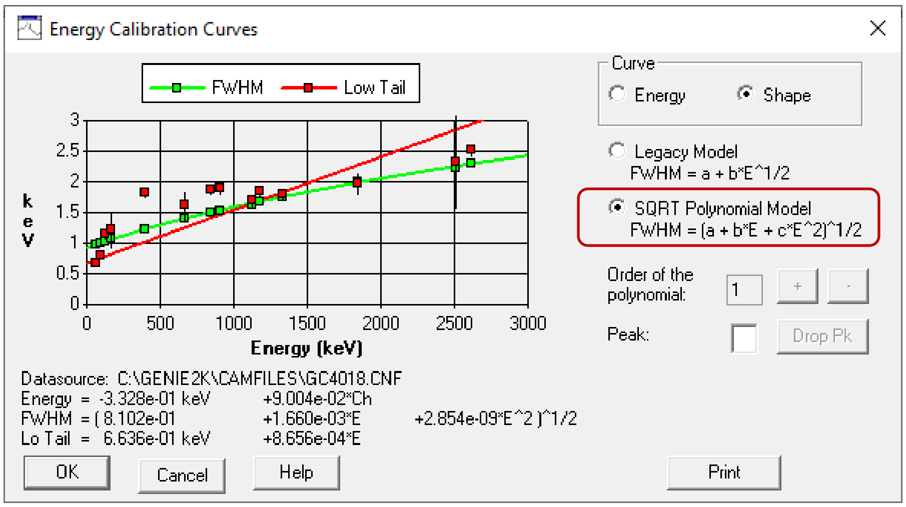

Figure 7 *The Energy calibration dialog in Genie. The square root polynomial model selection is highlighted in red.*

Comparing analysis results between the two fit functions

Mirion has created a python script that can be used to compare the analysis results produced using the legacy and new square root of polynomial fit function [4]. The python script can be run from Genie Spectroscopy Suite Post-NID processing analysis step on the spectrum of interest. It will produce two set of results using an ASF and store them in a .csv file. The results are expected to be close and within statistics for most analyses, but occasionally more significant changes are observed. An example is the calculated MDA, when the ROI of the peak of interest is close to an existing ROI from a peak that was found in the spectrum, and the ROI limits change significantly to account for the adjacent peak.

Conclusions

A new fit function for FWHM has been included in Genie 4.0 based on known physics of the behavior of FWHM for semi-conductor detectors. This function is of the form $FWHM = \sqrt{\mathrm{a} + \mathrm{b}E + \mathrm{c}E^2}$ and is referred to as the Square Root of Polynomial fit function in Genie applications. The new fit function reproduces measured FWHM better compared to the legacy fit function for all energies and HPGe detectors. For scintillating detectors, there is very small difference observed between the new and legacy fit function. The impact of using the new fit function during the analysis of a HPGe spectrum has been investigated and the impact on the results produced is typically small and within uncertainties. The greatest impact is observed in critical level and MDA calculations for high energy emission lines, although this impact is also minor. For HPGe and other semi-conductor detectors, it is recommended to use the new Genie 4.0 square root of polynomial fit function for better fidelity to detector resolution.

References and Additional Resources

1. Knoll G. **Radiation Detection and Measurement**, 4th edition, John Wiley & Sons, ISBN: 978-0-470-13148-0
   This excellent textbook includes discussion on detector physics principles and theory.

2. **Genie Operations User Manual**, Mirion Technologies (Canberra), Inc. 9233652K
   The Genie User Manual provides instruction on how to implement a FWHM calibration in Genie 4.0

3. **Genie Customization Tools Manual**, Mirion Technologies (Canberra), Inc. 9233653K
   The Genie Customization Tools Manual contains information on the algorithms implemented in Genie applications.

4. Genie FWHM Comparison Script at https://www.mirion.com/genie4/python
   This python script is available to be downloaded and used with Genie 4.0 applications that have the Python SDK for Genie installed. It will automatically compare peak area and MDA values for the square root of polynomial and legacy FWHM calibration fits for a particular spectrum and analysis sequence file.