Behavior of Several Germanium Detector Full-Energy-Peak Efficiency Curve-Fitting Functions

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This article presents in qualitative terms some of the behaviors of three frequently used germanium detector full-energy-peak efficiency curve-fitting functions. It is written from the viewpoint of doing routine gamma-ray counting at the accuracy of several percent using commercially available software and standards with only 8 to 11 major gamma rays. Some of the limitations of this calibration procedure are discussed.

The germanium detector full-energy-peak efficiency curve-fitting functions investigated are: the polynomial function in log-log coordinates, the exponential (or four factor) function, and the spline. Most commercial gamma-ray-spectroscopy software packages provide for the utilization of one or more of these curve-fitting functions without providing any discussion of their behavior in the documentation. The effects of variations in the data points on interpolated and extrapolated efficiencies (in the energy range 60-2000 keV) using these curve fits are compared.

An excellent discussion of the physical basis for a number of germanium detector full-energy-peak, efficiency fitting functions as well as a general discussion of the mathematics of curve fitting can be found in the book by Debertin and Helmer.[1] While using some of those efficiency curve-fitting procedures in the analysis of the efficiency data from the coincidence-free, Marinelli-beaker standard presented previously,[2] several questions arose. The first question was why did one particular set of data from the coincidence-free, Marinelli-beaker standard result in interpolated efficiencies differing by as much as 6% when using different curve-fitting functions in the 700-keV to 900-keV region? Second, since the coincidence-free standard only covered the energy range of 59.5 keV to 1115.5 keV, how much uncertainty would be introduced by extrapolating the curve fits to higher energy where there were no experimental points? Third, what effect would one inaccurate data point have on an efficiency curve? Fourth, if it is suspected that a particular point is less accurate than the others in a data set, is it better to use it or delete it? Since most commercial software packages do not allow weighted fits, weighted fits will not be considered here.

The coincidence-free, Marinelli-beaker standard in reference 2 emitted gamma rays at 59.5, 88, 122, 165.9, 279.2, 391.7, 661.6, 810, 834.8, 1099.3, and 1115.5 keV. Using a least-squares procedure, the efficiency data from one count was fitted to a fifth-order polynomial of the form:

$$\ln(\varepsilon) = C0 + C1\ln(E) + C2\,(\ln(E))^2 + C3\,(\ln(E))^3 + C4\,(\ln(E))^4 + C5\,(\ln(E))^5$$

where

ε = counting efficiency
E = energy.

The uncertainty due to counting statistics was ±1% (1 σ) for all measured points. The maximum difference between the measured efficiency and calculated

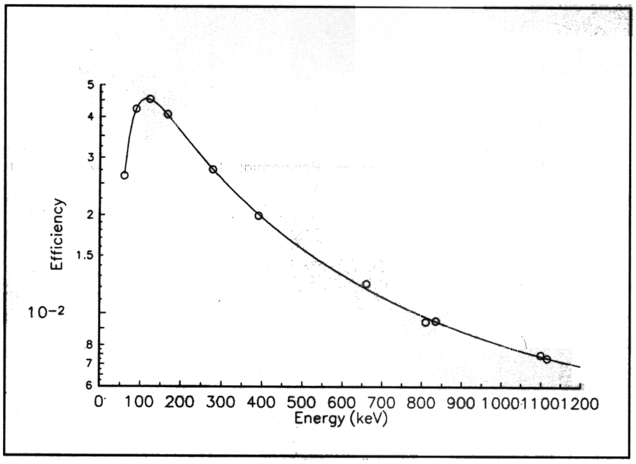

Figure 1 Efficiency data and polynomial fit.

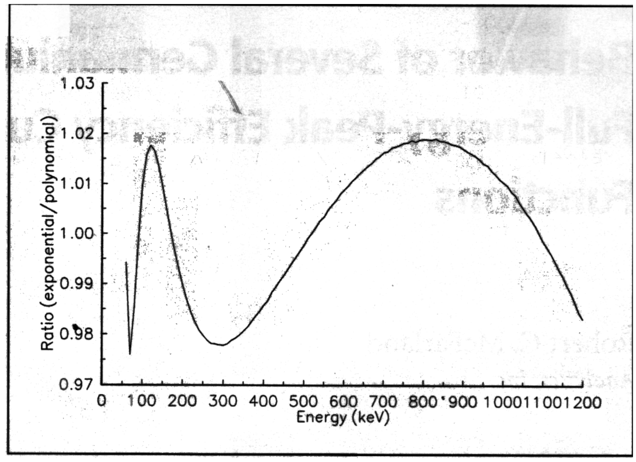

Figure 2 Comparison of polynomial and exponential curve fits.

efficiency was +3.39% at the 661.6-keV point. The 810-keV point fell below the curve 3.21%. Figure 1 shows the experimental points and the polynomial curve fit.

After noticing that these differences were higher than generally encountered in this energy region, two additional fitting procedures (the exponential or four-factor fit and a spline fit) were used in an attempt to improve the agreement between calculated and measured efficiencies. The exponential or four-factor function has the form:

$$\varepsilon = 1 / (C1 * E^{C2} + C3 * E^{C4}).$$

The simple spline fit without smoothing, as described by Debertin and Helmer,[1] uses a set of cubic polynomials joined at and passing through each experimental point.

Figure 2 shows the ratio of calculated efficiencies from the polynomial function to the exponential function in the energy region bounded by the experimental points. The maximum difference between the two functions is 2.5%. Use of the fifth-order polynomial allows the polynomial curve to oscillate as shown in the graph. The ratio of the polynomial to the spline fit is shown in Figure 3. Use of the cubic spline and the fifth-order polynomial allows more oscillation in the difference function. The maximum difference is approximately 4.4%. Figure 4 compares the spline and the exponential function showing a maximum difference of approximately 6%. The graphs are presented to facilitate a qualitative discussion of efficiency curve fits. Although no quantitative significance should be attached to this data, as it applies only to one detector, one standard and one counting run, it is useful in demonstrating some of the problems with efficiency curve fitting.

Inspection of Figure 1 leads to the hypothesis that the differences are caused by a 5% low-efficiency point at 810 keV. The polynomial fit was recalculated omitting the 810-keV point and compared to the original polynomial fit. Figure 5 compares the original polynomial function to the function obtained by omitting the 810-keV point. Notice that omitting the 810-keV point made only about 2% difference in the energy region bounded by the experimental points, but the two functions diverged rapidly as the energy increased beyond 1200 keV. Since there were three higher energy points in the data set, it was not expected that the polynomial fit would be that sensitive to the 810-keV point even when extrapolating beyond the data points. Next, the exponential fitting procedure was repeated omitting the 810-keV point and compared to the original fit (the dashed line in Figure 5). The exponential fit is not as sensitive as the polynomial fit to the 810-keV point as the maximum difference is only about 1% even at 2000 keV. This is not really surprising since the exponential function does not allow as many degrees of freedom as the fifth-order polynomial. In all cases the fifth-order-polynomial functions gave better fits to the data than did the exponential fits as measured

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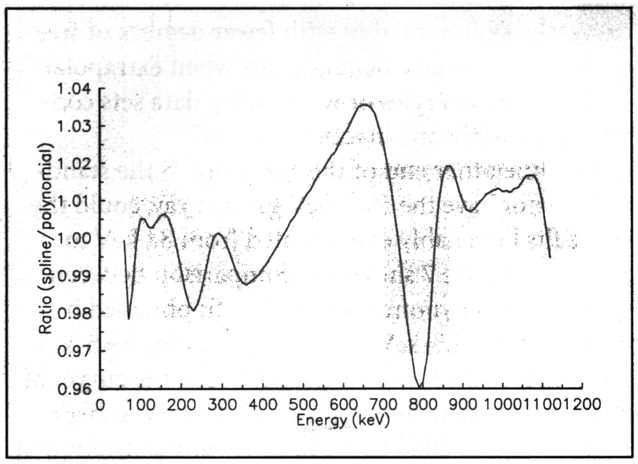

Figure 3 Comparison of spline and polynomial curve fits.

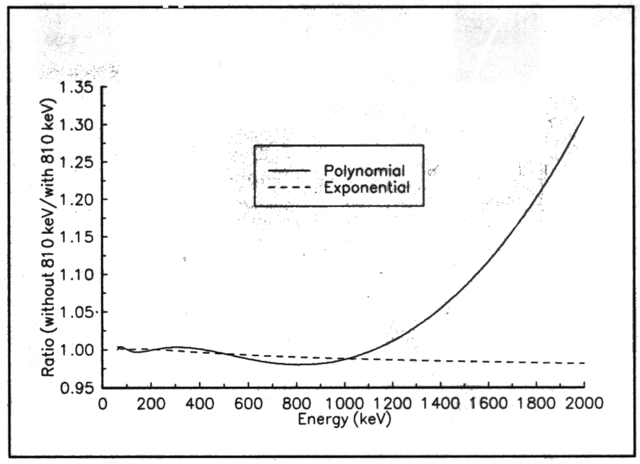

Figure 5 Effect of deleting the 810-keV point.

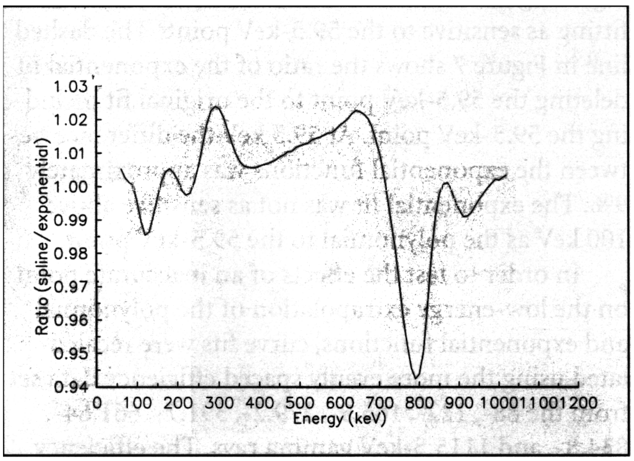

Figure 4 Comparison of spline and exponential curve fits.

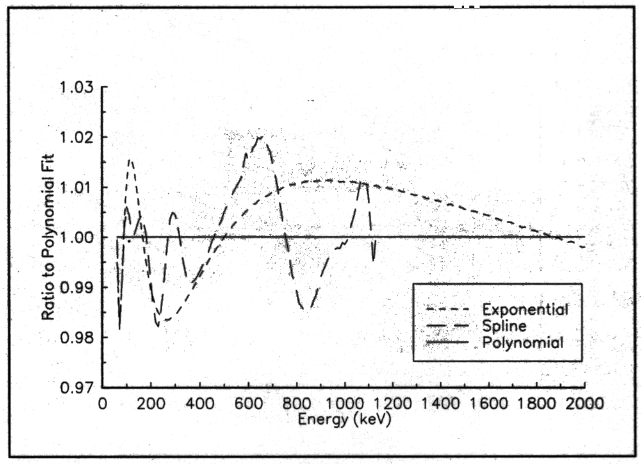

Figure 6 Exponential, spline, and polynomial fits omitting the 810-keV point.

by the sum of the absolute magnitudes of the percent differences. The extra degree of freedom of the polynomial function allowed it to fit the experimental data more closely. However, when extrapolating beyond the region of the data points that degree of freedom may allow too much variation in some cases.

Figure 6 shows a comparison of the three fitting functions after omitting the 810-keV point. The exponential and spline functions were divided by the polynomial function only for ease in graphing. By definition, the spline fit does not exist outside the energy region of the experimental points, therefore, no comparison was possible past 1120 keV for the spline. Omission of the 810-keV point brought all three fits into better agreement. As shown in Figure 6, the maximum difference was approximately 2%. The calculated efficiencies at 1836 keV from the polynomial and exponential fits (omitting the 810-keV point) were surprisingly close to the measured value for this particular data.

The data in Figure 5 indicates that extrapolation of an efficiency curve to higher energies could introduce a large uncertainty in high-energy measurements. The data in Figure 6 shows that an extrapolation might be performed if there is no other choice and if the data points give a very close fit. As long as there are an adequate number of points to define the

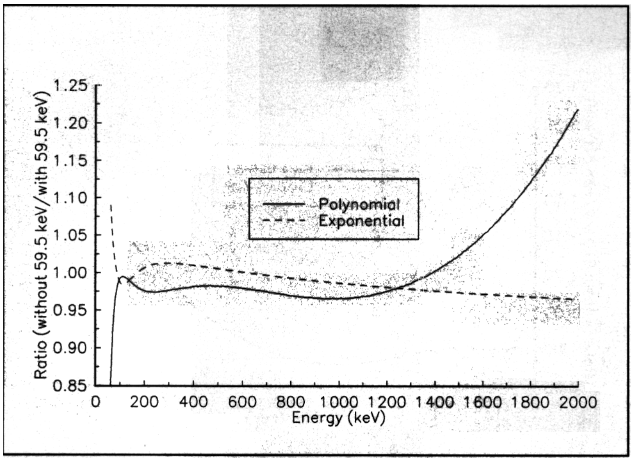

Figure 7 Effect of omitting the 59.5-keV point.

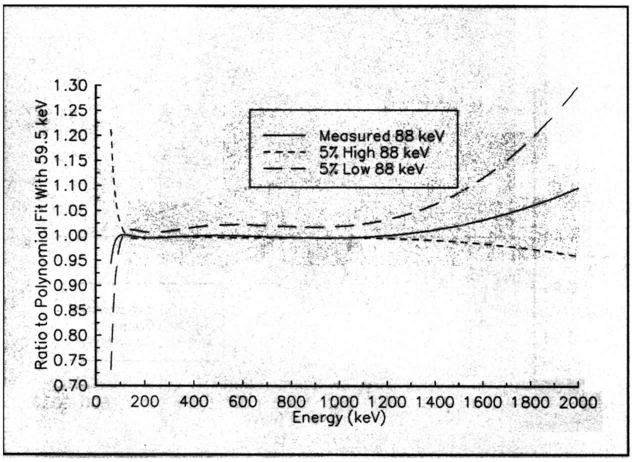

Figure 8 Effect of variation in the 88-keV point using polynomial fit.

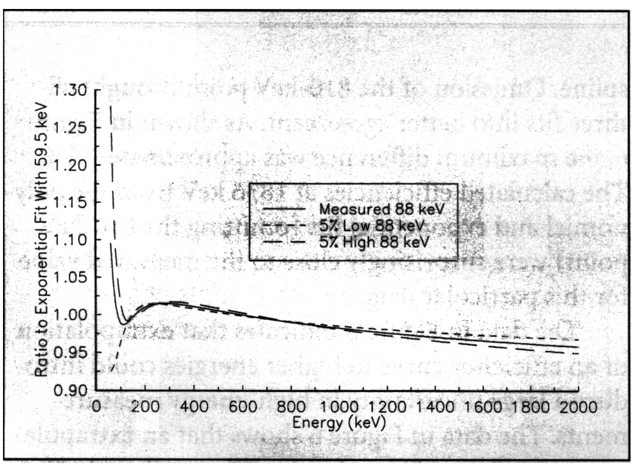

Figure 9 Effect of variation in the 88-keV point using exponential fit.

curve, the exponential fit with fewer degrees of freedom appears to give better results when extrapolating to higher energies or when using data sets containing possibly one inaccurate point.

On the other end of the spectrum, if the standard did not have the 59.5-keV gamma ray, could the curve fits be reliably extrapolated from 88 keV to 59.5 keV? Figure 7 shows the comparison between the original polynomial fit and the fit obtained by omitting the 59.5-keV point. Omitting the 59.5-keV point caused a 15% difference between the curves at 59.5 keV. More surprising is the difference at high energy: 20% at 2000 keV due solely to the deletion of a point at 59.5 keV. Also, the deletion of the 59.5-keV point caused some differences of about 3% in the energy range 88 keV to 1115.5 keV. Is the exponential fitting as sensitive to the 59.5-keV point? The dashed line in Figure 7 shows the ratio of the exponential fit deleting the 59.5-keV point to the original fit including the 59.5-keV point. At 59.5 keV the difference between the exponential functions was approximately 9%. The exponential fit was not as sensitive above 100 keV as the polynomial to the 59.5-keV point.

In order to test the effects of an inaccurate point on the low-energy extrapolation of the polynomial and exponential functions, curve fits were recalculated using the more evenly spaced efficiency data set from the 88-, 122-, 165.9-, 279.2-, 391.7-, 661.64-, 834.8-, and 1115.5-keV gamma rays. The efficiency at 88 keV was varied from 0.95 to 1.05 times the measured value and the curves extrapolated to 60 keV. For comparison, the values at each energy were divided by the values obtained from the curve fit which included the 59.5-keV point. The results for the polynomial curves are shown in Figure 8 and the exponential curves in Figure 9. Variations in the 88-keV efficiency caused great differences in the extrapolated 60-keV efficiency with both functions. Large differences were also observed at the high-energy end of the polynomial function due solely to variations in the 88-keV efficiency.

To investigate the effect of variations in an interior point, curve fits were recalculated with the 834.8-keV efficiency varied between 0.95 and 1.05 times the measured value. Figure 10 shows the results of the polynomial fits and Figure 11 the exponential fits. Inside the energy region bounded by the

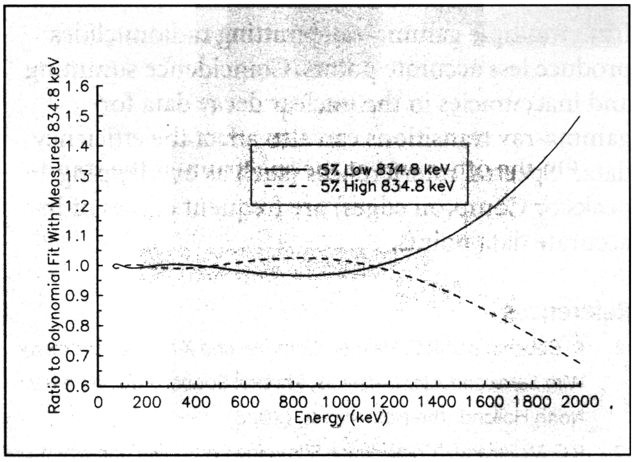

Figure 10 Effect of variation in the 834.8-keV point using polynomial fit.

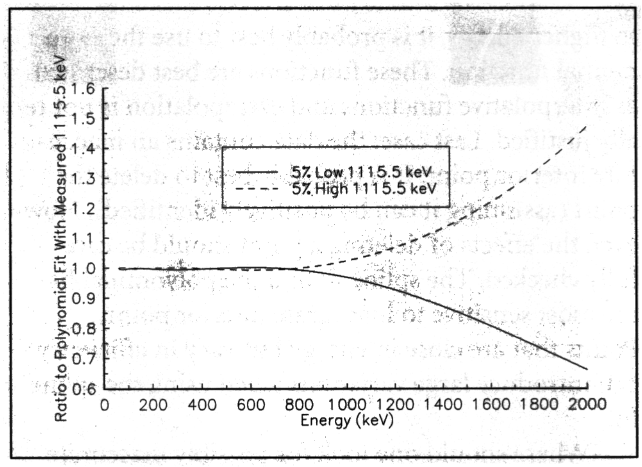

Figure 12 Effect of variation in the 1115.5-keV point using polynomial fit.

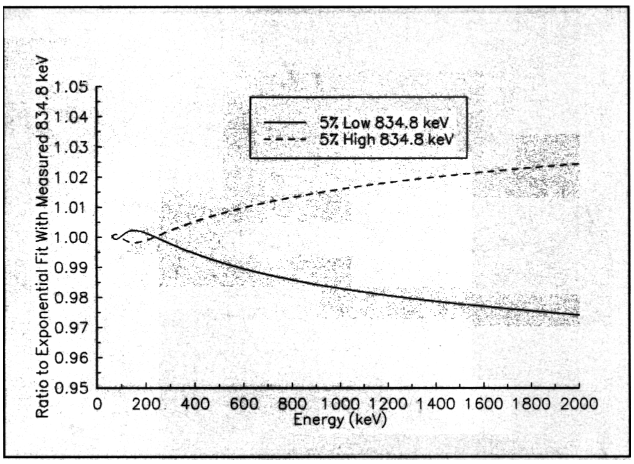

Figure 11 Effect of variation in the 834.8-keV point using exponential fit.

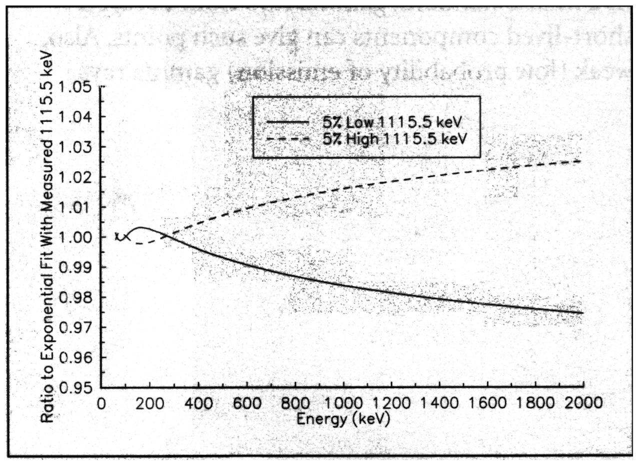

Figure 13 Effect of variation in the 1115.5-keV point using exponential fit.

experimental points, both functions exhibited some resistance to the variation: that is, deviations were less than the 5% introduced into the 834.8-keV point. The exponential fit was slightly less sensitive to the variation in the data than the polynomial fit. At higher energies the variation at 834.8 keV caused large differences with the polynomial function.

For completeness, the effect of variation in the highest energy point (1115.5 keV) was investigated. The efficiency at 1115.5 keV was varied between 0.95 and 1.05 times the measured value. The results for the polynomial functions are shown in Figure 12 and the exponential functions in Figure 13. The curves are very similar to the curves obtained by varying the 834.8-keV point especially for the exponential functions.

Besides computer operator exhaustion, what has been derived from these 23 tedious curve fits? First, consider the case: the efficiency data set to be fit contains an inaccurate boundary point. Apparently, less uncertainty is introduced by using the point in the curve fit rather than reducing the energy range covered by measured points. If the polynomial function is used to fit the data, extrapolation outside the bounds of the measured points will probably not be very accurate. Low-energy extrapolation with either function is very sensitive to inaccuracies in the lowest energy point. If absolutely forced to extrapolate to higher energy, it is probably best to use the exponential function. These functions are best described as interpolative functions and extrapolation is not really justified. Last case: the data contains an inaccurate interior point. It is probably best to delete the point (assuming it can be positively identified). However, the effects of deleting a point should be carefully checked. The spline fit and the polynomial fit are most sensitive to inaccurate interior points. Points that are close in energy but vary in efficiency can introduce large variations when using the spline fit.

Where should one look for possibly inaccurate efficiency data points? Data points with the lowest signal-to-background ratio should be investigated. In a mixed standard, gamma rays from decayed short-lived components can give such points. Also, weak (low probability of emission) gamma rays from multiple gamma-ray-emitting radionuclides produce less accurate points. Coincidence summing and inaccuracies in the nuclear decay data for gamma-ray transitions can also affect the efficiency data.[2] Spectral interferences (such as overlapping peaks or Compton edges) are frequent causes of inaccurate data points.

References

1. K. Debertin and R.G. Helmer; *Gamma- and X-Ray Spectrometry With Semiconductor Detectors*, Physical Science Publishers B.V.; North Holland: The Netherlands, (1988).
2. R.C. McFarland, "Coincidence Summing Considerations When Using Marinelli-Beaker Geometries in Germanium Gamma-Ray Spectroscopy," *Radioact. Radiochem.*, 2 (3), 4-7, (1991).

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