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Spline and polynomial models of the efficiency function for Ge gamma-ray detectors in a wide energy range

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In one of our recent papers, the applicability of linear parameter functions for fitting the full-energy peak efficiency of n-type Ge gamma-ray detectors has been examined over a wide energy range of 50–8500 keV. In that paper we compared six different analytical functions and showed that higher-order polynomial functions on a log-log scale gave the best performance. However, there is a drawback to using the log-log scale when an additive function of efficiency at different energies or of the inverse efficiency has to be used in a fitting procedure. In the present study, the applicability of higher-order polynomial and spline functions to linear and inverse efficiency, but logarithmic energy scales, is examined.

Introduction

In gamma-ray spectroscopy, one of the most important tasks is to determine the full-energy gamma-ray peak efficiency ε. The simplest procedure for its determination is the counting of multi-gamma-ray sources placed at the sample position, with full spectrum analysis.[1,2] The full-energy efficiency of the detector can be determined from Eq. (1) (neglecting coincidence summing) at the energies of the peaks provided by the sources:

$$\varepsilon(E_\gamma) = \frac{A}{NP_\gamma} K \qquad (1)$$

where N is the number of disintegrations during the measurement, A is the integrated peak area in counts, P_γ is the emission probability of the peak located at an energy of E_γ and K is a correction factor for losses.[3] If the energy range of interest is densely covered with calibration peaks, they will define an efficiency curve that is a smooth, continuous function of the energy (except at X-ray absorption edges) which lends itself for fitting with a smooth curve. The main characteristics of the efficiency curve are a maximum at about 100 keV and then an exponential decrease towards higher energies. Thus, it is a quite general practice to fit the logarithm of the efficiency instead of the efficiency itself.[4] Linear parameter functions, which were suggested to fit the efficiency, have generally failed to describe it over a wide energy range.[3,4] In the recent paper of KIS et al., the only linear parameter function,[4] which was able to describe the whole energy range had the following form:

$$\log(\varepsilon) = \sum_{i=0}^{n-1} a_i (\log(E_\gamma))^i \qquad (2)$$

where $1 \le n \le 9$ and a_i are the fitting parameters. This function is defined on a log-log scale. However, there is a drawback to this functional form. Namely, if one needs to use a linear combination of efficiency values (ε) or its inverse values ($1/\varepsilon$) at different energies, and tries to fit the parameters, then using Eq. (2) leads to a very nonlinear problem. This situation may occur when the efficiency is to be fit using intensity balances. Unfortunately, fitting polynomials with logarithmic energy scale to a linear or inverse efficiency scale was not studied,[4] nor were fits with cubic splines, which are also suitable for interpolation.

Splines have already been used in fitting Ge gamma-ray detector efficiency curves.[5] JANSSEN used cubic and quintic B-splines in fitting the efficiency of various detectors on a log-log scale in the 2 keV–3 MeV energy regions with a p-type Ge(Li), an n-type HPGe and a Si(Li) detectors. Here, we will study how a special, easy-to-use form of cubic splines performs in a wider energy range from 50 keV–10.8 MeV with an n-type Ge detector. Furthermore, we will compare its capability of fitting the efficiency on the log-log, log-linear and log-inverse scales to that of the polynomial fitting function.

Experimental

To study the linear-parameter efficiency-fitting functions we have chosen recent experimental data that was measured as part of our regular efficiency determination procedure at the prompt gamma activation analysis (PGAA) facilities of the Budapest Research Reactor.[6–8] The PGAA detector is an n-type, Compton-suppressed high-purity Ge (HPGe) detector of 25% efficiency and 1.8 keV energy resolution at the 1332 keV ^{60}Co line.[8] The detector to source distance was 23 cm. The true coincidence summing at this detector to source distance is negligible, therefore, no effort was made to perform a correction for it. In the series we include data accumulated with ^{60}Co, ^{133}Ba, ^{152}Eu, ^{207}Bi and ^{226}Ra standard sources purchased from

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Table 1. Full-energy-peak absolute efficiency of the PGAA system at the Budapest Research Reactor

Source	Energy, keV	Efficiency	Relative uncertainty, %	*Z*-score
^{24}Na[12]	1368.7	2.3787E-04	0.5	–0.2
	2754.2	1.3318E-04	0.7	0.3
^{60}Co[12]	1173.2	2.6584E-04	0.1	0.3
	1332.5	2.4248E-04	0.2	–0.5
^{110m}Ag[12]	446.7	5.3668E-04	0.9	0.0
	620.2	4.1548E-04	0.9	–0.7
	677.4	3.9903E-04	0.9	2.1
	686.8	3.9285E-04	0.7	1.9
	744.1	3.6720E-04	0.9	0.3
	763.7	3.5745E-04	0.4	–1.2
	817.8	3.4131E-04	0.6	–0.4
	937.2	3.1005E-04	0.4	–0.8
	1384.1	2.3713E-04	0.4	1.1
	1475.6	2.2529E-04	0.9	0.0
	1504.9	2.2146E-04	0.4	–0.6
	1562.2	2.1490E-04	1.3	–0.4
^{133}Ba[12]	53.3	9.5603E-04	1.9	–0.1
	79.8	1.0802E-03	3.2	1.0
	276.4	7.7490E-04	0.5	1.1
	302.8	7.2194E-04	0.4	0.1
	355.9	6.3874E-04	0.2	–0.5
	383.8	6.0316E-04	0.4	–0.2
^{152}Eu[12]	121.8	1.0898E-03	0.9	–0.2
	244.7	8.3962E-04	0.9	0.5
	344.2	6.5535E-04	0.8	–0.1
	411.0	5.7345E-04	0.9	0.2
	443.9	5.4100E-04	1.0	0.3
	778.7	3.5381E-04	0.9	–0.2
	867.2	3.2587E-04	1.0	–0.7
	963.9	3.0290E-04	0.8	–0.8
	1085.7	2.8055E-04	0.9	0.0
	1089.6	2.8442E-04	1.1	1.5
	1111.9	2.7814E-04	0.9	0.9
	1212.8	2.5952E-04	1.2	0.0
	1299.1	2.4799E-04	1.1	0.3
	1408.0	2.3260E-04	0.9	–0.3
	1457.6	2.2239E-04	1.6	–1.4
^{207}Bi[12]	569.7	4.4537E-04	0.1	–0.2
	1063.5	2.8498E-04	0.3	0.4
	1770.2	1.9679E-04	0.7	0.6
^{226}Ra[12]	242.2	8.1981E-04	1.3	–1.9
	295.4	7.3700E-04	1.6	0.2
	352.1	6.4404E-04	1.4	–0.1
	609.5	4.3010E-04	1.1	1.4
	768.5	3.6174E-04	1.5	0.8
	934.2	3.1905E-04	1.7	1.4
	1120.4	2.7631E-04	1.4	0.5
	1155.4	2.6814E-04	2.5	–0.1
	1238.3	2.5234E-04	1.4	–1.0
	1281.1	2.4871E-04	2.2	–0.2
	1377.8	2.4069E-04	2.1	0.8
	1509.4	2.2165E-04	2.0	0.0
	1729.8	1.9495E-04	2.2	–1.1
	1764.7	1.9560E-04	1.3	–0.3
	1847.7	1.8544E-04	2.1	–1.0
	2118.9	1.6985E-04	2.8	0.2
	2204.5	1.6229E-04	1.9	–0.3
	2448.2	1.5172E-04	2.8	0.7
$^{14}N(n,\gamma)^{13}$	1678.2	2.0677E-04	1.1	1.0
	1681.1	2.0445E-04	2.4	0.1
	1884.8	1.8614E-04	1.1	–0.1
	1999.6	1.7515E-04	1.3	–1.0
	2520.4	1.4265E-04	1.6	–0.9
	2830.8	1.2905E-04	2.3	–0.1
	3532.0	1.0429E-04	1.3	1.1
	3677.7	9.8640E-05	1.2	0.2
	4508.7	7.7640E-05	1.1	–0.1
	5269.1	6.3815E-05	1.0	–0.1
	5297.8	6.3286E-05	1.2	–0.2
	5533.4	5.9863E-05	1.2	–0.1
	5562.0	5.9626E-05	1.3	0.2
	6322.5	4.9731E-05	1.3	–0.1
	7299.0	3.9847E-05	1.4	–0.3
	8310.0	3.1948E-05	2.3	–0.1
	9149.0	2.8506E-05	4.6	1.5
	10829.1	1.7554E-05	4.4	–0.4

metrological laboratories, plus home-made ^{24}Na and ^{110m}Ag sources. High energy gamma rays from the $^{14}N(n,\gamma)^{15}N$ reaction were also included. Since the data were taken separately we normalized them together with the efficiency routine of the HYPERMET-PC program.[9,10] The reduced chi-square of the 8th order polynomial fit was 0.82 on the log-log scale. The resulting data set is listed in Table 1, together with reference to the literature of the source gamma-ray intensities, as well as the fitted efficiency from HYPERMET-PC.

The data set in Table 1 was used to test the performance of the polynomial and spline model functions for linear, logarithmic and inverse scales of the efficiency axis mentioned above.

The efficiency functions and discussion

The mathematical form of the efficiency-fitting spline function is defined as:

$$g(\varepsilon) = \sum_{i=1}^{n} a_i C_i(\log(E_\gamma)) \qquad (3)$$

where C_i are the so called cardinal spline functions[11] and function g can be a logarithmic, linear or inverse function. Each cardinal spline C_i has the form of a cubic spline function:

$$S(x) = \alpha_0 + \alpha_1 x + \sum_{s=1}^{n-1} \gamma_s (x - x_s)_+^3 \qquad (4)$$

where n is the number of nodes and x_s are the nodes, which are predetermined. The α_0, α_1 and γ_s are

parameters to be fixed. The '+' index has the following meaning:

$$z_+ = \begin{cases} 0 & \text{if} \quad z < 0 \\ z & \text{if} \quad z \geq 0 \end{cases} \tag{5}$$

The definition of the cardinal spline function C_i is:

$$C_i(x_k) = \delta_{i,k} \tag{6}$$

where $\delta_{i,k}$ is the Kronecker-delta and the set of node points x_k are conveniently spaced. The cardinal spline C differs from spline S only in this orthogonality requirement expressed in Eq. (6).

The remaining free parameter in Eq. (4) may be fixed with the following boundary condition:

$$S''(x)|_{x=x_n} = 0 \tag{7}$$

With linear combinations of n cardinal splines C_i [Eq. (3)] the solution of a set of complicated nonlinear equations may be reduced to simple algebraic equations.[11] Although, this is not the task in our case, the flexibility of cardinal splines may be superior to other functions. Since cardinal splines C_i are determined completely by their node points through Eqs (4)–(7), they can be used in least square fitting like any other functions such as polynomials. In the case of a polynomial fitting function, the C_i in Eq. (3) is defined as:

$$C_i(x) \mapsto x^{i-1} \tag{8}$$

The least square expression for a set of efficiency-points ε_j at energies E_j is:

$$Q^2 = \sum_{j=1}^{m} \frac{\left[\mathrm{g}(\varepsilon_j) - \sum_{i=1}^{n} a_i C_i(\log(E_j)) \right]^2}{\sigma_j^2} \tag{9}$$

where σ_j are the uncertainties of $\mathrm{g}(\varepsilon_j)$. The index j runs up to the number of data points m, while n is the number of nodes or number of free parameters in case of the polynomial. The number of free parameters in Eq. (9) is $2n$ for cardinal splines, however, for a fixed set of node points it is only n. This is a crucial point, since there is also the question of which placement of nodes gives the minimum for Eq. (9). The simplest choice for the placement of the node points is an equidistant distribution between and including the boundary values, which are chosen to be 5% smaller and 5% larger than the minimum and maximum of the logarithm of the measured energies. The 5% refers to 5% of the distance between maximum and minimum. We must note that in all cases the energies used were in MeV and when using $\log_{10}(E)$, this transforms the energies roughly to in the interval (–1, 1). This helps to increase the numerical stability, especially in the case of the high order polynomials. If the boundaries differ considerably from the boundaries of the (–1, 1) interval, then it may be advisable to transform the energy values to the (–1, 1) interval before doing the least square fit.

Table 2 summarizes the resulting reduced chi values $\chi = \sqrt{Q^2/f}$ obtained from fits with different number of free parameters, where equation $f = m - n$ defines the number of degree of freedom.

From Table 2 one may note that the fitting performance of cardinal splines in the linear ε case is slightly better than the polynomial with the same number of free parameters. However, the polynomial model performs similarly or better at larger n order in the case of logarithmic and inverse efficiency scale. To make this overview easier, a plot of Table 2 is presented in Fig. 1.

From Fig. 1 it is easy to recognize that from 7 parameters onwards the reduced chi values stabilize and the improvement slows down considerably. It is also interesting that on the log-log scale the stabilization happens earlier than in the other two cases. To show what the fits look like, we present the nine-parameter fit to the inverse (shown on a log scale for clarity) in Fig 2. The results show that the major difference happens at the low and high energy ends. Since the cubic spline does not go to infinity as fast as a high-order polynomial with increasing argument values, their behaviors differ significantly at the boundaries. In general the spline seems to be more appropriate for extrapolation at the low energy end, since from more detailed experiments with our n-type HPGe detector we know that at low energy the efficiency does not have such a large curvature as the polynomial fit would indicate (Fig. 2). Although in this particular case, the polynomial seems to give a better description at the high energy end, we suggest caution in taking it seriously since the uncertainties in the extrapolation grow very rapidly just beyond the last fitted point. At the high energy end the requirement in Eq. (7) may not let the spline approach the last point closely enough.

Table 2. Comparison of χ values by changing the number of free parameters n, for polynomial function and cardinal splines

n	Spline linear ε	Polynom linear ε	Spline log ε	Polynom log ε	Spline inverse ε	Polynom inverse ε
	χ	χ	χ	χ	χ	χ
3	5.86	8.47	6.97	6.19	5.20	13.36
4	6.05	6.61	6.53	6.20	10.09	10.28
5	5.47	6.20	1.47	1.93	3.93	5.76
6	0.84	3.27	1.16	1.82	2.12	1.97
7	1.49	1.79	1.11	1.24	1.46	1.16
8	0.86	1.46	0.88	0.82	1.19	1.07
9	0.79	0.86	0.84	0.80	1.02	0.90

The value of m is 76 in all cases.

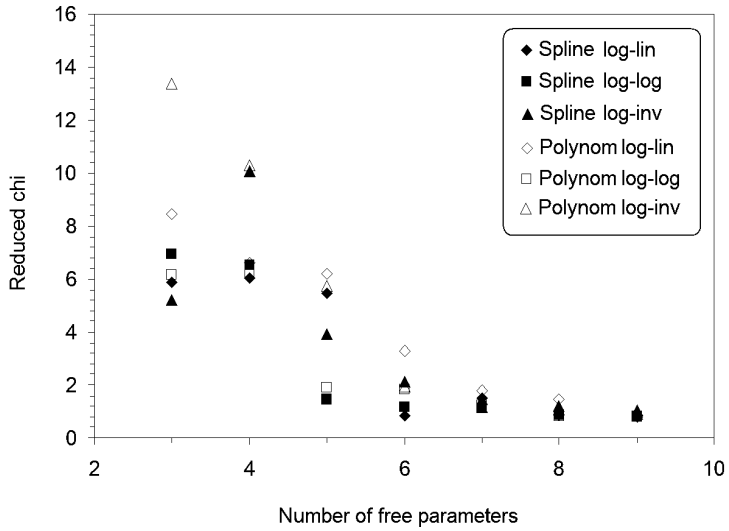

Fig. 1. Reduced chi-values of spline and polynomial fits of detector efficiency on linear, logarithmic and inverse efficiency scales as a function of number of parameters

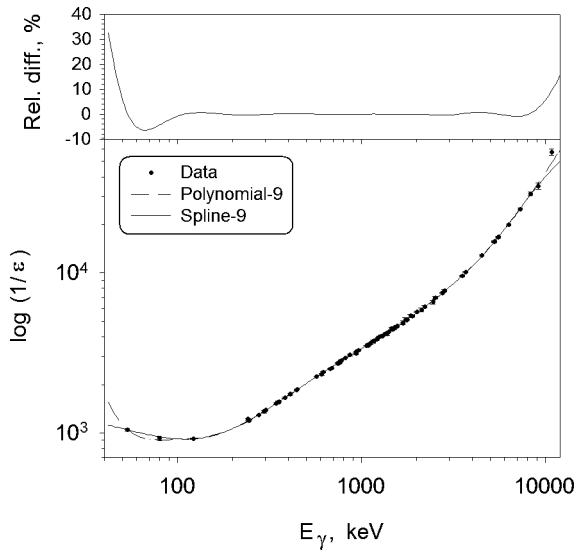

Fig. 2. Comparison of the performance of polynomial and spline models on log-inverse scale with 9 parameters. The lower panel shows the experimental data with our n-type HPGe detector and the fitting functions. The upper panel presents the relative difference of the fitted polynomial and spline functions in percentage

In general, we can summarize that both the polynomial and the spline model provide good fits to the data, but at the ends of the data set, the reliability of the fit decreases rapidly. This latter is reflected also by the uncertainties of the fitted curves, which are not shown here for the sake of clarity.

In the remaining part of this article we will concentrate on the spline model itself, and study the question of what distribution of the node points gives a minimum reduced chi-square $\chi^2 = Q^2/f$ for a fixed number of node-points n. Since this leads to a strongly nonlinear problem we cannot give a definite answer. Instead we will study the distribution of node points as a function of reduced chi-square χ^2. By randomly selecting node points between the lowest and the highest boundaries we can obtain such a distribution. Here we present only the case where the number of node points is 9. This leads to a study of points in a parameter space of 7 dimensions. With a random number generator 5000 sets of node points have been generated and for each set of node points the fit has been repeated.

Figure 3 shows results for about fifty of random node point sets out of the total number of 5000 as a function of the reduced chi-square. Lines guiding the eyes connect the node points with the same serial number from the sets. The rest of the remaining nearly 5000 sets have reduced chi-square values are larger than 0.85, and were left out of the figure. It is interesting that even around the minimum chi-square, the locations of the node points are changing rather rapidly, while for higher reduced chi-square values (above 0.85) the changes are extremely rapid. As a result there seems to be a rather complicated rule for determining the set of node points that gives the lowest reduced chi-square value for the fit, which we cannot determine.

Due to this chaotic behavior the equidistant distribution of nodes points (which yielded a reduced chi-square of 1.04, see Table 2) is almost as good as many others. Other general observations are, and this can also be seen in Fig. 3, that a lower reduced chi-square could be achieved when one of the node points is close to the last (highest energy) data point and when the

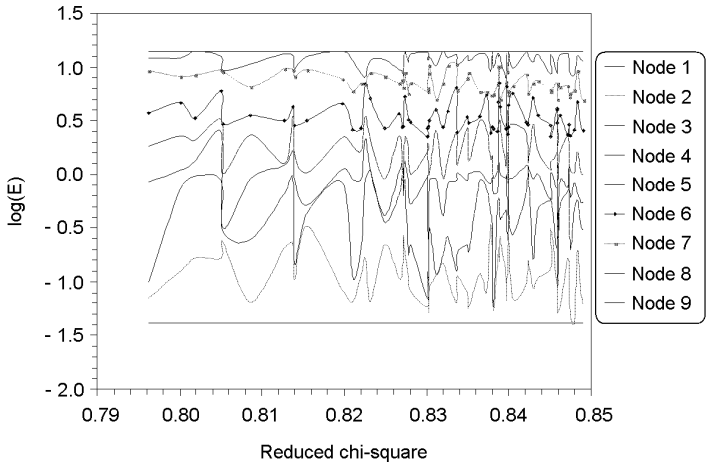

Fig. 3. Common logarithm of the energy of the randomly selected node points as a function of reduced chi-square (χ^2). The dots show the energy positions of the node points in each set (only shown for nodes 6 and 7)

node points are more dense where more of the accurate data points are. One way of handling this situation is to take the simple average of node point values from Fig. 3. Doing so and performing a calculation with this set of node points, the reduced chi-square of the fit was 0.806, which is fairly close to the minimum value. This also yields two node points at higher energy than the last experimental point and manages to fit the last point by avoiding the end condition of Eq. (6). Finally we think that these features of the cubic spline should be studied in more detail by mathematicians.

Conclusions

In summary, we can state that although the setting up to fit with the cubic splines is somewhat more complicated than with simple polynomials, there are applications where they can be used more efficiently than simple polynomials, especially for extrapolation. However, care must be taken with the endpoint behavior. One such application is the fit of a Ge detector full-energy-peak efficiency on a linear scale. For this case, the cubic splines provide better reduced chi-squares with the same number of free parameters than the polynomials. Spline and polynomial models perform similarly on the logarithmic and inverse efficiency case.

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