

VARIABLE VARIANCE MODEL FOR γ -SPECTRA ANALYSIS

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A spectral processing program "GAMMAPEAKS", approximating the peaks in the γ -spectra by simple Gaussian, Gaussian with variable variance and sectionally defined function, in which the peak center is described by the simple Gaussian, and the edges – in the form of an exponent, has been developed. For the approximation we used conjugate gradient method by which the sum of squared deviations of approximating function values and values in the range of channels belonging to the peak was minimized. The developed algorithm allows with sufficient precision to determine the area under the peak in the spectrum needed to determine the differential scattering cross section.

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1. INTRODUCTION

One of the main issues of γ -spectroscopy is the processing and analysis of γ -spectra obtained from experimental studies of nuclear reactions. Development and improvement of semiconductor detectors and analyzers for the measurement of the complex γ -spectra requires the use of modern computing tools to process experimental results.

Currently, firms producing equipment for detectors and spectrometric analysis, complement its production software analysis and processing of γ -spectra.

In the analyzing of γ -spectra with the help of programs such as GammaVision, BaltiSpectr, AnGamma et al., differences in the definition of areas under some peaks reach 25%, which affects the precision of the determination of intensities γ -lines of the corresponding peaks. This leads to large imprecisions in the calculations of various nuclear reactions parameters (scattering cross sections, radiation strength functions (RSF), and so on). The purpose of this paper is to analyze the peak processing in γ -spectra using as much as possible precision approximation of a single peak form (SPF). It achieves by using a Gaussian function with a variable variance.

The main tasks of processing γ -spectra measured by semiconductor and scintillation detectors are a precision description of the SPF and processing of overlapping peaks. The shape of the peak is determined by many physical processes associated with the interaction of the detected particles (γ -rays) with the detector material, as well as the quality of the detector and electronic equipment. Attempts to describe the SPF, taking into account these processes encounter substantial difficulties, because expressions used to describe the SPF are bulky and contain a large number of unknown parameters. Therefore, usually to approximate SPF try to use a variety of empirical and phenomenological expression.

2. PROBLEM DEFINITION

Most programs used for processing of γ -spectra used as processing models of standard Gaussian distribution with constant variance, described by the formula

$$f(x) = A \exp \left\{ -\frac{(x - B)^2}{2\Delta^2} \right\}, \quad (1)$$

where A represents the peak amplitude, B – the peak center position, Δ – the variance.

Since the peaks in the γ -spectra are often non-central, in the present paper to describe the SPF in addition to the above functions we used a Gaussian function with a variable variance, and sectionally defined function, in which the peak center is described by the usual Gaussian, and the edges – in the form of an exponent.

The Gauss function with variable variance [1] can be described by the expression

$$f(x) = A \exp \left\{ -\frac{(x - B)^2}{\Delta(x)} \right\}, \quad (2)$$

where $\Delta(x)$ is a parameter describing the peak width (variable variance). From the results of analysis of a large number of peaks, it was found that in most cases, this parameter has the shape of a hyperbola and can be represented as

$$\Delta(x) = |C| + |D| \sqrt{|E|(x - B - F)^2 + 1}, \quad (3)$$

where C and D describe the peak width, E and F – the peak widening and peak asymmetry respectively.

The sectionally defined function describing partially by the gaussian and the exponents [2], can be described by the following: when $x < B - C$, the function is

$$f(x) = A \exp \left\{ \frac{|C|(2(x - B) + |C|)}{2\Delta^2} \right\}, \quad (4)$$

where the parameter C is fixed at $2, 355\Delta$. If $x > B + D$, the function has the form

$$f(x) = A \exp \left\{ \frac{|D|(2(B - x) + |D|)}{2\Delta^2} \right\}, \quad (5)$$

where the parameter D is initially set equal to $\Delta/2$, and changes during the approximation, in the other cases, this function has the form of a usual Gaussian with constant variance. Parameters A and B in this function determines the height of the peak and its center position, respectively. Expressions for this function was taken from [3].

Coefficients C , D and E in the formula (3) and the coefficients C and D in the formula (4) and (5) are taken modulo, because $\Delta(x)$ in Gaussian function must be non-negative, and the calculations of the expressions for the exponents in the case of sectionally defined function at negative coefficients may lead to overflow.

3. APPROXIMATION METHOD

When approximating the peak of the various functions deviation of the experimental data obtained from the calculated using the approximate function is calculated by the method of least squares. It was necessary to minimize the sum of squared deviations of the experimental data obtained from mathematical given function that approximates the peak in spectrum. For this purpose one used an iterative method of finding the minimum function which is called *conjugate gradient method*. This method was used for the fitting of peaks approximating function parameters so that the sum of squared deviation between values calculated by this function and the experimentally obtained values was minimal, i. e. that the condition

$$F(a_1, \dots, a_n) = \sum_i (f_i(a_1, \dots, a_n) - y_i)^2 \rightarrow 0, \quad (6)$$

was satisfied. In this formula variables y_i represent experimental measured data for i specter channel, f_i – calculated values of theoretical peak approximating function, and a_1, \dots, a_n – approximating function parameters (peak amplitude, peak center position, variance, widening, asymmetry and other).

Phrase "conjugate gradient method" has no deep meaning, because in most cases the gradients are not conjugated, and conjugated directions have nothing mutual with gradients. Therefore, from a mathematical point of view, it would be correct to call this method "method of conjugate directions and gradients". Methods name "conjugate gradient method" reflects the fact that this approach combines the concepts of the gradient of the objective function and conjugate directions. In science, the name stuck and is used quite often.

To conjugate gradient method converges after a small number of iterations, the function $F(a_1, \dots, a_n)$ can be conveniently represented in the form of:

$$F(a_1, \dots, a_n) = \frac{1}{2}A\tilde{a}^2 - b\tilde{a}, \quad (7)$$

where \tilde{a} represents the function parameters vector (a_1, \dots, a_n) (unknown vector, to be determined

through optimization); A – some known, square, symmetric, positive definite matrix; b – some known vector. As is known, the function has an extreme at the point where its gradient (or antigradient) is zero. In the present case, it corresponds to

$$A\tilde{a} - b = b - A\tilde{a} = 0. \quad (8)$$

In the case of finding the minimum of a function in the calculations necessary to minimize its antigradient, i. e. is necessary to make sure that \tilde{a} defined by the condition

$$b - A\tilde{a} = 0. \quad (9)$$

During the calculation process one suppose that on the each iteration

$$r_k = b - A\tilde{a}_k, \quad (10)$$

where the k – iteration number, r_k – minimizing function antigradient value on the iteration number k . One also suppose that

$$\tilde{a}_{k+1} = \tilde{a}_k + \alpha_k d_k, \quad (11)$$

where d_k represents a direction associated with antigradient by a certain correlation, α_k – a corrective coefficient recounting on each iteration. Parameters d_k and r_k are bound by the correlation

$$d_{k+1} = r_{k+1} + \beta_k d_k, \quad (12)$$

in which β is the linking coefficient which value calculates on each iteration. Initially (before the calculation) d_0 considers to be equal to r_0 .

Let's now turn to the derivation of the expression for the coefficients α_k and β_k . First, we write the expression for r_k and r_{k+1} :

$$\begin{aligned} r_k &= b - A\tilde{a}_k, \\ r_{k+1} &= b - A\tilde{a}_{k+1}, \end{aligned} \quad (13)$$

and subtract the r_k form the r_{k+1} . One gets that:

$$\begin{aligned} r_{k+1} - r_k &= b - A\tilde{a}_{k+1} - b + A\tilde{a}_k = \\ &= -A(\tilde{a}_{k+1} - \tilde{a}_k), \end{aligned} \quad (14)$$

hence

$$r_{k+1} = r_k - A(\tilde{a}_{k+1} - \tilde{a}_k). \quad (15)$$

By definition $\tilde{a}_{k+1} = \tilde{a}_k + \alpha_k d_k$, so, $\tilde{a}_{k+1} - \tilde{a}_k = \alpha_k d_k$. Substituting this expression in the formula (15), one gets that:

$$r_{k+1} = r_k - \alpha_k A d_k. \quad (16)$$

Multiplying this equality by r_k on the left one finds that:

$$s(r_k, r_{k+1}) = (r_k, r_k) - \alpha_k (r_k, A d_k). \quad (17)$$

The value of r_{k+1} is chosen so that it is orthogonal to r_k . This means that $(r_k, r_{k+1}) = 0$. Hence one obtains:

$$(r_k, r_k) - \alpha_k (r_k, A d_k) = 0. \quad (18)$$

Thereby one receives the expression for α_k :

$$\alpha_k = \frac{(r_k, r_k)}{(r_k, Ad_k)}. \quad (19)$$

Replacing in expression (12) index $k+1$ to k , and $k -$ to $k - 1$, one gets: $d_k = r_k + \beta_{k-1}d_{k-1}$. Then $r_k = d_k - \beta_{k-1}d_{k-1}$. Substituting r_k in the denominator of expression (19) and taking into account the fact that d_k is orthogonal to d_{k-1} one gets that:

$$\alpha_k = \frac{(r_k, r_k)}{(d_k, Ad_k)}. \quad (20)$$

Let's now get the expression for β_k . By definition $d_{k+1} = r_{k+1} + \beta_k d_k$. Multiplying this expression by Ad_k , one finds:

$$(d_{k+1}, Ad_k) = (r_{k+1}, Ad_k) + \beta_k (d_k, Ad_k). \quad (21)$$

The expression on the left side of this formula which is equal to zero, because d_{k+1} is taken to be orthogonal to d_k . Hence one obtains:

$$\beta_k = -\frac{(r_{k+1}, Ad_k)}{(d_k, Ad_k)}. \quad (22)$$

From the expression (16) follows:

$$Ad_k = \frac{1}{\alpha_k} (r_k - r_{k+1}). \quad (23)$$

Thus, the numerator in the formula (22) can be written as

$$\begin{aligned} (r_{k+1}, Ad_k) &= \frac{1}{\alpha_k} (r_{k+1}, (r_k - r_{k+1})) = \\ &= -\frac{1}{\alpha_k} (r_{k+1}, r_{k+1}), \end{aligned} \quad (24)$$

because r_{k+1} is chose to be orthogonal to r_k . The denominator of expression (22) can be rewritten like this:

$$\begin{aligned} (d_k, Ad_k) &= ((r_k + \beta_{k-1}d_{k-1}), Ad_k) = \\ &= \frac{1}{\alpha_k} (r_k, (r_k - r_{k+1})) = \frac{1}{\alpha_k} (r_k, r_k). \end{aligned} \quad (25)$$

Therefore one can find the expression for β_k :

$$\beta_k = \frac{(r_{k+1}, r_{k+1})}{(r_k, r_k)}. \quad (26)$$

The resulting expression is called the formula of Fletcher-Reeves [4]. In some cases, using this formula, the method can not converge in a very large number of iterations. Therefore, in practice most often used Polak-Ribiere formula. This formula can be represented as follows [4]:

$$\beta_k = \frac{(r_{k+1}, (r_{k+1} - r_k))}{(r_k, r_k)}. \quad (27)$$

In this paper, the function $F(\tilde{a})$ is equal to $\sum_i (\tilde{F}_i(\tilde{a}))^2 = \sum_i (f_i(\tilde{a}) - y_i)^2$. The matrix element of gradient of this function is

$$r_j = 2 \sum_i \tilde{F}_i(\tilde{a}) \frac{\partial \tilde{F}_i(\tilde{a})}{\partial a_j}, \quad (28)$$

where a_j – vector \tilde{a} element number j .

To find the matrix A one needs to get the second derivative of the function $F(\tilde{a})$, or the first derivative of its gradient. From this we find the expression for the matrix element A_{jk} [5]:

$$A_{jk} = 2 \sum_i \left(\frac{\partial \tilde{F}_i(\tilde{a})}{\partial a_j} \frac{\partial \tilde{F}_i(\tilde{a})}{\partial a_k} + \tilde{F}_i(\tilde{a}) \frac{\partial^2 \tilde{F}_i(\tilde{a})}{\partial a_j \partial a_k} \right). \quad (29)$$

4. RESULTS AND DISCUSSION

To test the program processing spectra measured with detectors, model spectra were designed. They contained two partially overlapping peaks described ideal constant variance Gaussians. In mode which approximated resonances in the spectrum by the various theoretically determinable Gaussians was performed preliminary smoothing of the spectrum by six points, so smooth spectrum differed from the original. Consequently, the resonance in the model created spectra a little differed from the ideal Gaussian. When calculating the area under the peak was used per-channel summation of physical values described by approximating function, which is then compared with the sum of the per-channel measured or modeled physical values in smoothed spectrum.

Since the fitting results obtained by the conjugate gradient method, depends on the initial setting values, the ability to set these settings manually (with the keyboard) has been provided in the program. For this purpose, the window was made by the program, which was possible to set the text in the input fields of the initial values of the functions parameters that approximate resonance (Fig.1).

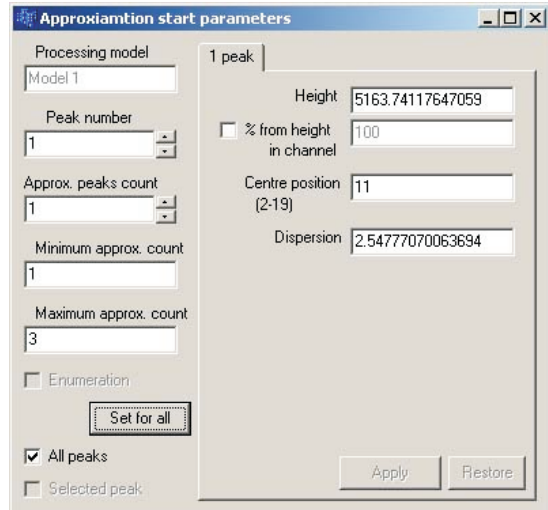


Fig.1. Start parameters setting window

After pressing the button "Count" in the main program window, the approximation of resonances in the spectrum of Gaussian functions started. If the result for any resonance had a rather large error, one was possible to change the initial settings, causing the

window shown in Fig.1, and set other initial values, and then recalculate the spectrum or the single peak.

The results of the approximation of the spectrum with two overlapping Gaussians model set shown in Fig.2. Before the approximation of the parameters set in accordance with Table. The error computing the area under the overlapping resonances in this range was equal to 4.81 % as a result of the fact that before the spectrum processing the spectrum smoothing was carried out and the resonances processed by program differs from the ideal Gaussians with a fixed variance.

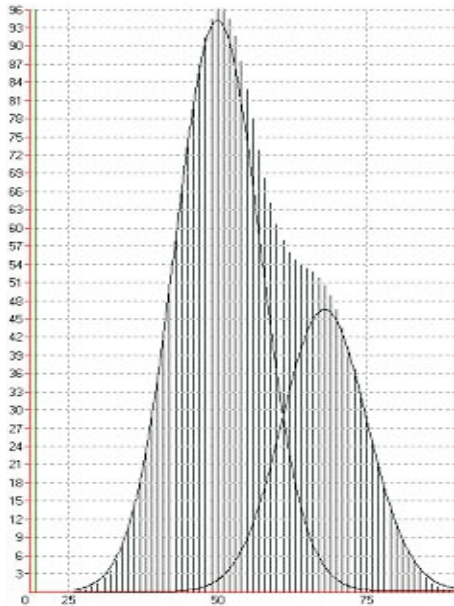


Fig.2. Overlapped peaks processing result

Start parameters values for overlapped peaks counting

N	Amplitude	Center	Variance
1	97.8	50	6
2	53.6	68	6

Also approximation was carried out by two types of two Gaussians model set of non-overlapping peaks. When approximating peaks by the usual Gaussian variance start value was set equal to 6, and in the case of approximation Gaussian with variable variance its start parameters were set as follows: for the first peak values of the parameters were as follows: $C = 95$; $D = 0.01$; $E = 10$; $F = 10$, and for the second - as follows: $C = 96$; $D = 0.01$; $E = 10$; $F = 10$. The results differ very little, and general appearance of the picture for them is shown in Fig. 3. In the approximation of these peaks by usual Gaussian errors are equal to 4.49 and 3.33 % for the first and second peaks, respectively. In the case of a Gaussian with variable variance approximation of the same peaks error are equal to 1.47 % for the first peak and 2.66% for the second one. In the case where these same

peaks were approximated by sectionally defined function, errors are equal to 5.63 % for the first peak and 3.98 % for the second one.

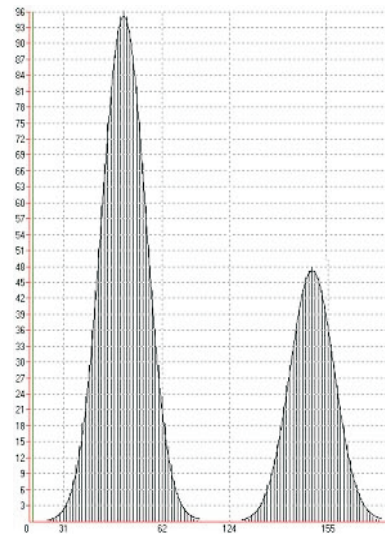


Fig.3. Single peaks processing result

5. CONCLUSIONS

The results of calculations carried out with the help of the developed program, show that the approximation of the Gaussian peaks with variable dispersion gives a more exact result than the approximation by the usual Gaussian. The result of sectionally defined function approximation to the peaks is less accurate than using conventional Gaussian.

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МОДЕЛЬ С ПЕРЕМЕННОЙ ДИСПЕРСИЕЙ ДЛЯ АНАЛИЗА γ -СПЕКТРОВ

А. Ю. Бережной, С. Н. Утенков

Разработана программа обработки спектров «GAMMAPEAKS», аппроксимирующая пики в γ -спектрах простым гауссианом, гауссианом с переменной дисперсией и кусочно-заданной функцией, в которой центр пика описывается обычным гауссианом, а края – в форме экспонент. Для аппроксимации использовался метод сопряжённых градиентов, с помощью которого минимизировалась сумма квадратов отклонений значений аппроксимирующей функции от значений в каналах спектра, принадлежащих пику. Разработанный алгоритм позволяет с достаточной точностью определить площадь под пиком в спектре, необходимую для определения дифференциального сечения рассеяния.

МОДЕЛЬ ІЗ ЗМІННОЮ ДИСПЕРСІЄЮ ДЛЯ АНАЛІЗУ γ -СПЕКТРІВ

А. Ю. Бережний, С. М. Утенков

Розроблено програму обробки спектрів «GAMMAPEAKS», що апроксимує піки в γ -спектрах за допомогою простого гауссіану, гауссіану із змінною дисперсією та кусочно-заданої функції, у якій центр піку описується звичайним гауссіаном, а боки – експонентами. Для апроксимації застосовувався метод спряжених градієнтів, на основі якого мінімізувалася сума квадратів відхилень значень апроксимуючої функції від величин у каналах спектра, що належать піку. Розроблений алгоритм дає змогу визначити з достатньою точністю площину під піком у спектрі, яка потрібна для визначення диференціального перерізу розсіяння.