MODIFICATION OF SEARCH SPECTRA AND METHODS OF DEFINITION OF PEAKS POSITION IN γ-SPECTRA USING THE STUDENT'S TEST

A.Yu. Berezhnoy, Yu.V. Lyashko
National Science Center "Kharkiv Institute of Physics and Technology", Kharkiv, Ukraine

In the program of processing of γ-spectra "GAMMAPEAKS" the algorithm of automatic search of peaks in γ-spectra based on use of convolution of sites of a spectrum from a negative smoothed second derivative of gaussian is developed. In the new version of this program before creation of a search spectrum the convolution of an initial spectrum with an ideal gaussian of small amplitude and variance was carried out. As a result of this convolution the initial spectrum on sites with "poor" statistics was well smoothed that facilitated search of peaks on a search spectrum. The search spectrum was under construction by convolution of the received γ-spectrum from the negative smoothed second derivative of gaussian that looks like a step. The search result of peaks shows that the "GAMMAPEAKS" program marks peaks more precisely, than the previous versions of this program in which were not used formulas based on Student's test.

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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.

The computer program "GAMMAPEAKS" [1 – 3] is developed for processing of γ-spectra. This program has a possibility of automatic search of peaks in a spectrum. For these purposes the program creates a so-called "search spectrum" by which borders of peaks in the γ-spectrum processed by the program are determined. The search spectrum constructed by the convolution of the site of a γ-spectrum with a negative smoothed second derivative of gaussian. In the new version of the "GAMMAPEAKS" program the convolution of an initial γ-spectrum with an ideal gaussian of small amplitude and small variance was added. A result of this convolution was the spectrum in which sites of an initial spectrum having "poor" statistics were smoothed well. Then this smoothed initial spectrum was used for creation of a search spectrum which was constructed by convolution of a smoothed spectrum with a negative smoothed second derivative of gaussian.

1. PROBLEM DEFINITION

One knows that the spectra measured even when used good multichannel detectors sometimes contain sites with poorly expressed peaks having poor statistics. In the previous versions of the "GAMMAPEAKS" program some of such peaks were not marked after automatic peaks search. In order to find them automatically, it is necessary to smooth an initial γ-spectrum before creation of a search spectrum. Earlier for this purpose the so-called "smoothing filters" [4 – 6] were used. In the current work these smoothing filters with convolution of an initial spectrum with an ideal gaussian of small amplitude and variance were replaced. We made possible to set values of the amplitude and the variance of this gaussian manually. To build a "search spectrum" the formulas of a test of validity called Student's test were used from a theory of mathematical statistics [7].

2. MATERIALS AND METHODS

Tests of validity are used for testing statistical hypotheses. One of such tests is a Student's test [7]. It uses when sample averages have the normal distribution. The Student's test describes by the formula

$$t = \frac{\bar{X} - m}{s_X/\sqrt{n}}, \qquad (1)$$

where m is a some (expected) value; n – number of sample elements; $\bar{X}$ – arithmetic mean value of sample elements; s_X – standard deviation of X_i, determined by the formula

$$s_X = \sqrt{\frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{n-1}}. \qquad (2)$$

Student's test can be used for building a search spectrum for searching of peaks in γ-spectrum.

Convolution of the part of the smoothed γ-spectrum with the negative smoothed second derivative of ideal Gaussian was made for creation of the search spectrum. This derivative has a step appearance (Fig. 1).

$$t = \frac{\bar{X}}{s_X/\sqrt{n}}\,. \qquad (3)$$

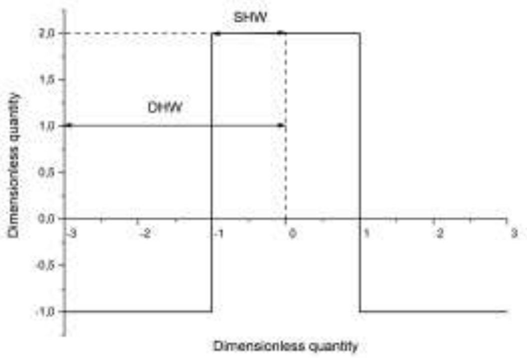

Fig. 1. The general view of the negative smoothed second derivative of gaussian. The designations: DHW – the negative smoothed second derivative half-width; SHW – the negative smoothed second derivative jut (the "step") half-width

Mean value of this smoothed negative second derivative of ideal Gaussian distribution is equal to zero. When $m = 0$ (a zero hypothesis), the formula for Student's test should have the following form:

It was supposed that after the convolution of a smoothed spectrum with the sectionally defined function describing the smoothed negative second derivative of the ideal Gaussian a value in the resulting search spectrum was modulo less than a definite numerical value that was set manually, the channel considered belonging to background, otherwise – to a peak. The search spectrum was under construction as follows: length of the sliding window on which the convolution was performed was set equal to the smoothed negative second derivative of ideal Gaussian, the sliding window moved on the spectrum from the first to the last spectrum channel, and the value in the channel of the search spectrum is calculated by the formula

$$X_i = \sum_{j=1}^{w} L_j Y_j, \qquad (4)$$

where L_j is the value of sectionally defined function describing the negative smoothed second derivative of the ideal Gaussian; Y_j is a number of counts in the j-th channel of initial spectrum; w is the width of the sliding window on which convolution was performed. L_j was defined by the formula

$$L_j = \begin{cases} -1, \text{ для } j < i - uw \\ \;\;2, \text{ для } i - uw \le j \le i + uw, \\ -1, \text{ для } j > i + uw \end{cases} \qquad (5)$$

where j is a number of a channel in the sliding window on which the convolution was performed; uw is a half-width of a jut of the negative smoothed second derivative of an ideal Gaussian. In this case the standard deviation of X_i defines by the formula:

$$s_X = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}\left(L_iY_i - \sum_{i=1}^{n}\frac{L_iY_i}{n}\right)^2} =$$
$$= \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(L_iY_i - \overline{L_\iota Y_\iota})^2}. \qquad (6)$$

After transformations we have:

$$s_X =$$
$$= \sqrt{\frac{1}{n-1}\left(\sum_i (L_iY_i)^2 - 2\overline{L_\iota Y_\iota}\sum_i (L_iY_i) + \sum_i (\overline{L_\iota Y_\iota})^2\right)} =$$
$$= \sqrt{\frac{1}{n-1}\left(\sum_i (L_iY_i)^2 - 2n(\overline{L_\iota Y_\iota})^2 + n(\overline{L_\iota Y_\iota})^2\right)} =$$
$$= \sqrt{\frac{n}{n-1}\left(\sum_i \frac{(L_iY_i)^2}{n} - (\overline{L_\iota Y_\iota})^2\right)} =$$
$$= \sqrt{\frac{n}{n-1}\left(s_{L_iY_i}^2 - (\overline{L_\iota Y_\iota})^2\right)}, \qquad (7)$$

where $s_{L_iY_i}$ is the quadratic mean of L_iY_i described by the formula:

$$s_{L_iY_i} = \sqrt{\frac{\sum_i (L_iY_i)^2}{n}}. \qquad (8)$$

3. RESULTS AND DISCUSSION

In the new version of the «GAMMAPEAKS» program the support of the new format of the spectra which are written down in the file with ".CNF" extension was added (the "Genie 2000" program from "Canberra"). The results received in this article were tested generally on the spectra written in files having this format.

Search of peaks was performed by search spectra which were constructed by the Student's test based on formula (1), in which $\bar{X}$ is a mean value of $X_i = \sum_{j=1}^{w} L_j Y_j$ (formula (4) and comments to it). However, Y_j was not the number of counts in the channel of the initial spectrum, but the value in the smoothed spectrum which was constructed by convolution of the initial spectrum with ideal Gaussian, the height and the variance of which were set manually through entry fields in the window of parameters of peaks search window in the program. It turned out that changing of amplitude of ideal Gaussian which used to smooth the initial spectrum did not change the search spectrum neither qualitative nor quantitatively. The variance of ideal Gaussian with which the convolution of the spectrum was performed was set numerically equal to 2. Also, in the window of parameters of peaks search in the program we used a "sensitivity" parameter the numerical value of which in the search spectrum defined the criterion of accessory of certain channels to peak or to the background. It turned out that for good peaks search this parameter needs to be set numerically equal to 0.15 or less. The half-width of the negative smoothed second derivative of ideal Gaussian was set numerically equal to 1 because this value peaks were marked most precisely.

As the example for analysis the real γ-spectrum of uranium ore, measured on VCG (of the very clean germanium) detector, which had the program «Genie 2000» to processing spectra was taken. The fragments of initial spectrum with good and poor statistics are shown on the Figs. 2a and 2b. On the Figs. 3a and 3b the sites of spectrum smoothed by convolution of the initial spectrum with ideal Gaussian are shown. One can see that the convolution of initial spectrum with ideal Gaussian distribution smooths the initial spectrum good, especially on sites with poor statistics (see Fig. 3b). Peaks search was performed with sensitivity numerically equal to 0.05. The sites of the search spectrum with good and poor statistics respectively are shown in Figs. 4a and 4b.

Apparently from Figs. 2a, 2b: 3a, 3b and 4a, 4b, the program enough precisely marks peaks in the spectrum. The new algorithm was also tested on peaks search in the γ-spectrum on the sample of uranium ore, measured on the germanium detector, and one revealed that when the sensitivity was numerically equal to 0.02 the new algorithm marks peaks with good statistics not worse, than the algorithm in the previous version of the program which was described in [8].

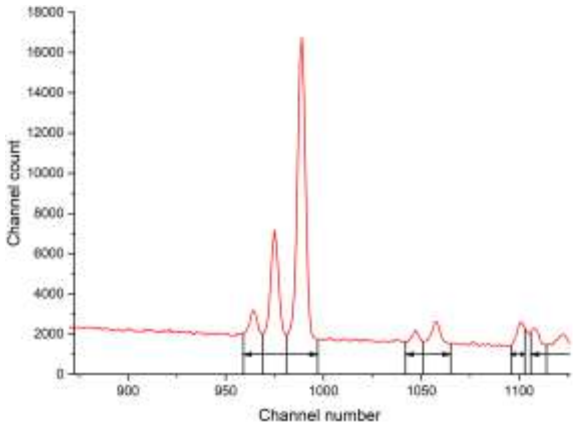

Fig. 2a. The site of the initial spectrum with good statistics (near the beginning of the spectrum) and result of peaks marking

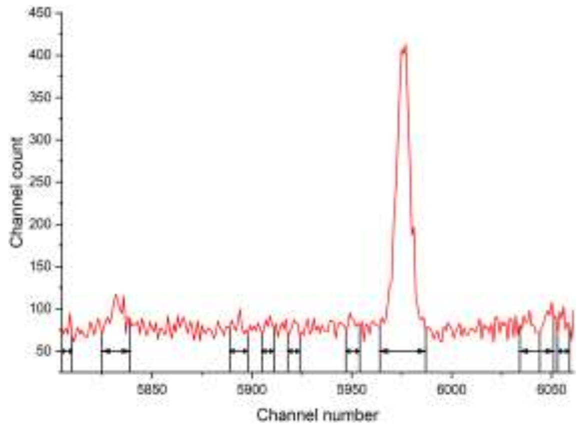

Fig. 2b. The site of the initial spectrum with "poor" statistics (at the end of the spectrum) and result of the peaks marking

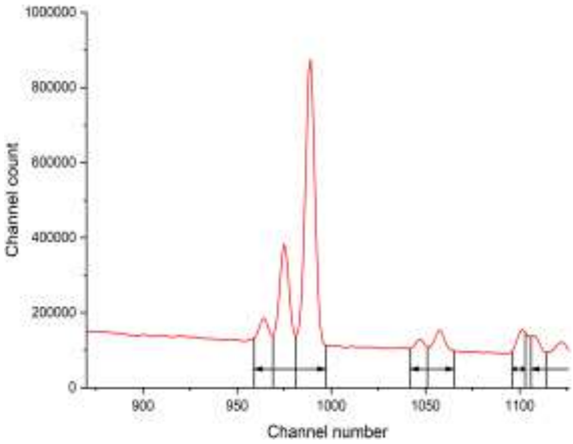

Fig. 3a. Result of convolution with ideal Gaussian of the site of the initial spectrum with good statistics and result of the peaks marking

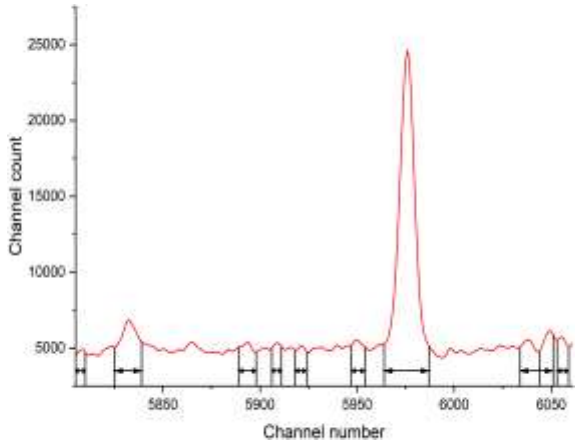

Fig. 3b. Result of convolution with ideal Gaussian of the site of the initial spectrum with "poor" statistics and result of the peaks marking

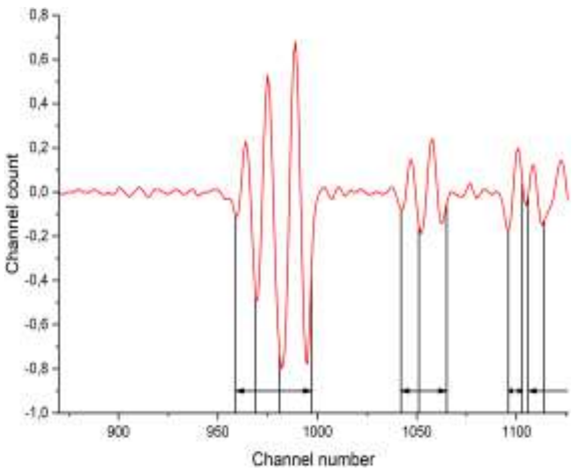

Fig. 4a. Site of the search spectrum, corresponding to the site of the initial spectrum with good statistics

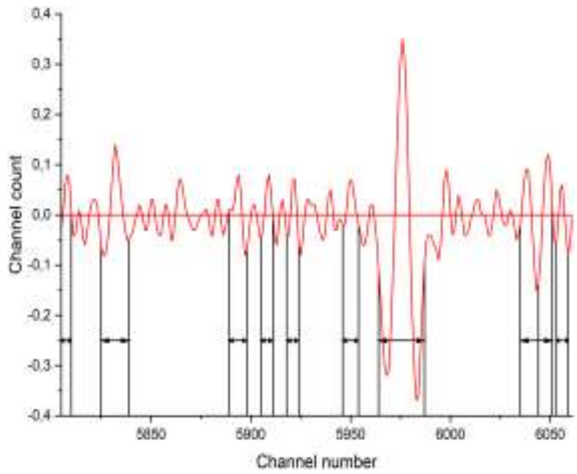

Fig. 4b. Site of the search spectrum, corresponding to the site of the initial spectrum with "poor" statistics

However, on the sites of the spectrum with "poor" statistics the peaks marking with the new algorithm (Fig. 5a) differs from the marking of peaks in the same spectrum when the old algorithm was used (Fig. 5b). It is connected with that the search spectrum has other appearance (Fig. 6a) than when the old algorithm was used (Fig. 6b) and also partially with the fact that new correction of borders of peaks in which features of the initial spectrum were considered was entered into the new algorithm of the marking of peaks in the spectrum. Further the improvement of this adjustment is planned.

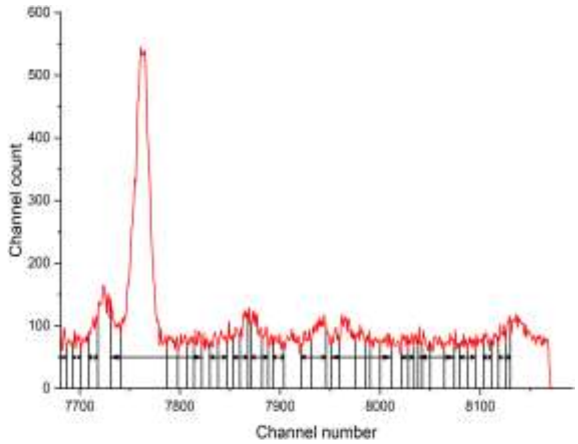

Fig. 5a. The site of the initial spectrum with "poor" statistics marked using the new algorithm of peaks search

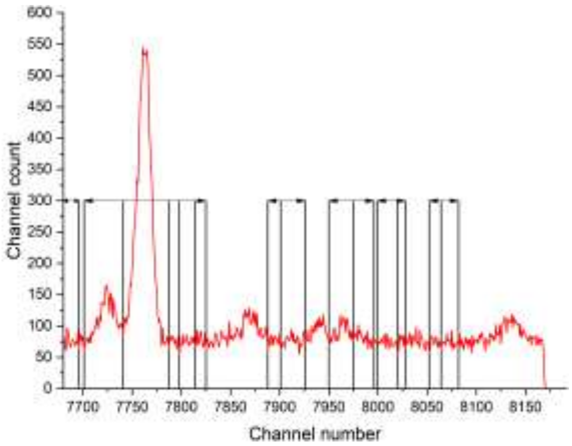

Fig. 5b. The site of the initial spectrum with "poor" statistics marked using the old algorithm of peaks search

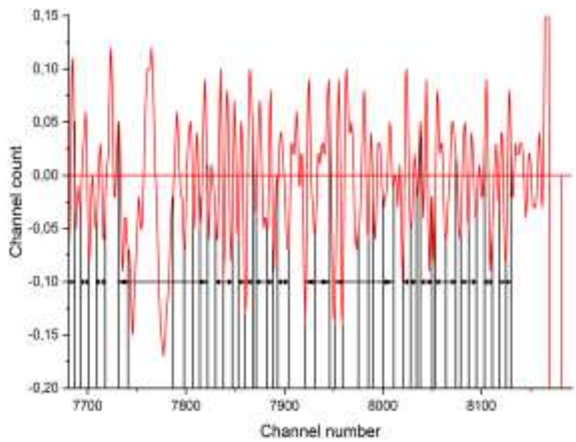

Fig. 6a. The site of the search spectrum with "poor" statistics marked using the new algorithm of peaks search

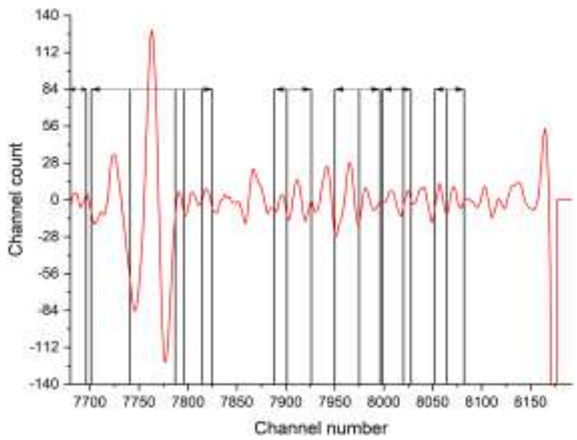

Fig. 6b. The site of the search spectrum with "poor" statistics marked using the old algorithm of peaks search

4. CONCLUSIONS

1. Changing of amplitude of ideal Gaussian by convolution of which the initial spectrum was smoothed does not change the spectrum which constructed after smoothing of the initial spectrum.

2. The sensitivity used for the marking of peaks in the search spectrum should be numerically equal to 0.15 or less. In some spectra its numerical value is better to set less than 0.1.

3. For enough good marking of peaks in the spectrum, the half-width of the negative smoothed second derivative of ideal Gaussian should be taken numerically equal to 1. At this value two next peaks do not merge in one that can be observed when this value is bigger than 1.

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