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ANALYSIS OF SEARCH SPECTRA AND METHODS OF PEAKS LOCATION DETERMINATION IN γ-SPECTRA

A.Yu. Berezhnoy, Yu.V. Lyashko
National Science Center "Kharkov Institute of Physics and Technology", Kharkiv, Ukraine
E-mail: aberezhnoy80@gmail.com

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 "weak" 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 there was no convolution with gaussian before creation of a search spectrum.

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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 by the author of current work. In this program there is 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 "GAMMA-PEAKS" 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 "weak" 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 weak 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 we used for this purpose the so-called "smoothing filters" [4–6]. In the current work we replaced these smoothing filters with convolution of an initial spectrum with an ideal gaussian of small amplitude and variance. We made possible to set values of the amplitude and the variance of this gaussian from the keyboard.

2. MATERIALS AND METHODS

As shown in Fig. 1, the negative smoothed second derivative of gaussian has a step appearance with a jut in its central part. One was possible to change quality of peaks search in a γ-spectrum setting half-width of the jut of this step. Full width of a step was equal threefold width of its jut.

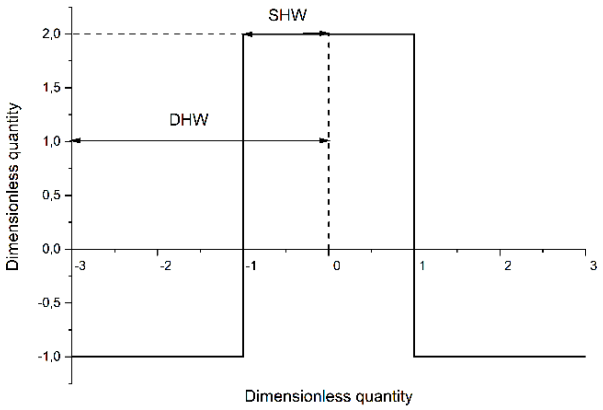

Fig. 1. The general view of the negative smoothed second derivative of gaussian. The designations: DHW – the negative smoothed second derivative half-width, SHW – the negative smoothed second derivative jut (the "step") half-width

In the manual to the program of γ-spectra processing called "AnGamma" for creation of a search spectrum the convolution of an initial spectrum with a negative smoothed second derivative was defined by the formula

$$C_j = \frac{\sum_i Y_i L_i}{\sqrt{\sum_i Y_i L_i^2}}, \quad (1)$$

where C_j – channel count in a search spectrum channel; Y_i – channel count in an initial spectrum channel; L_i – value of a negative smoothed second derivative of gaussian in i-th channel. Summation performed on an initial spectrum site on which convolution was made.

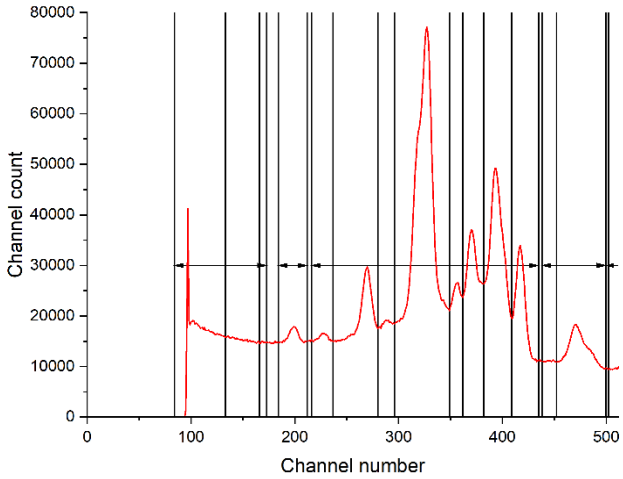

Fig. 2a. The site of the initial spectrum with good statistics (the beginning of the spectrum) and the results of peak search when the jut half-width was equal to 1 channel

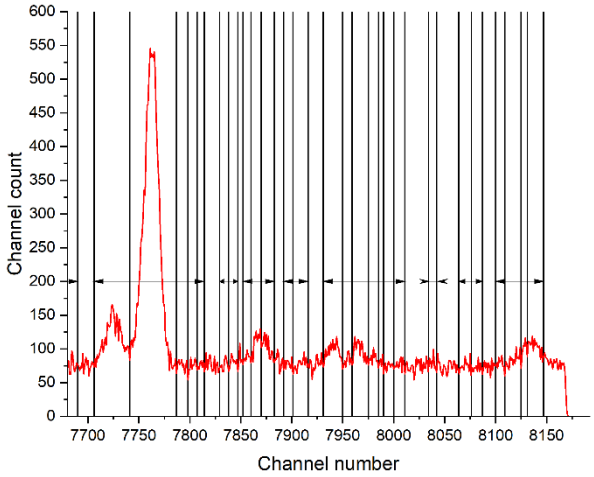

Fig. 2b. The site of the initial spectrum with "weak" (poor) statistics (the end of the spectrum) and the results of peak search when the jut half-width was equal to 1 channel

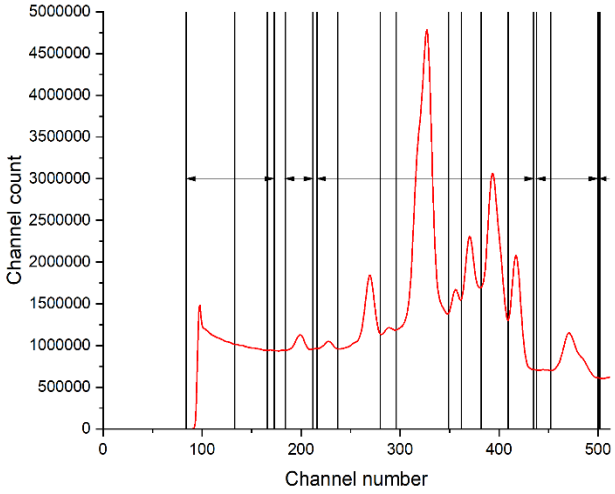

Fig. 3a. The result of convolution of the site of initial spectrum having good statistics with a gaussian and the results of peak search when the jut half-width was equal to 1 channel

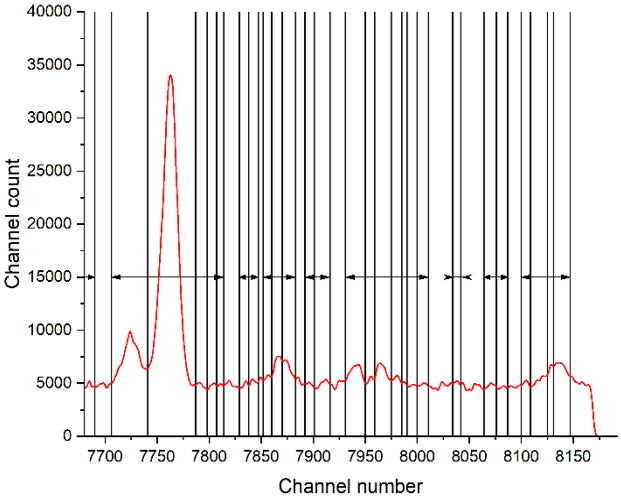

Fig. 3b. The result of convolution of the site of initial spectrum having "weak" statistics with a gaussian and the results of peak search when the jut half-width was equal to 1 channel

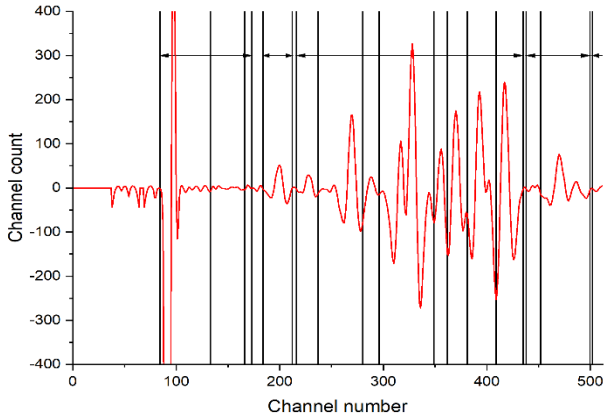

Fig. 4a. The site of the search spectrum corresponding to the site of initial spectrum with good statistics when the jut half-width was equal to 1 channel

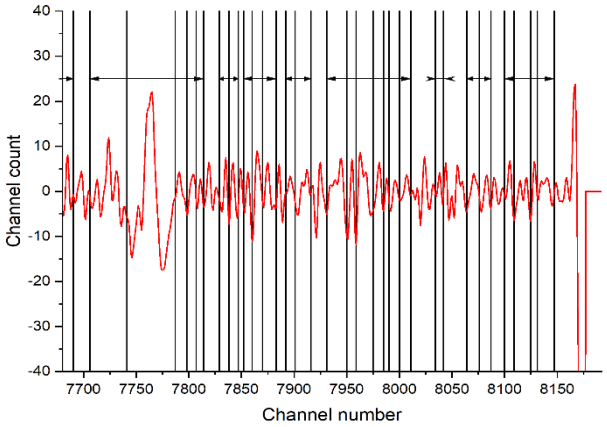

Fig. 4b. The site of the search spectrum corresponding to the site of initial spectrum with "weak" statistics when the jut half-width was equal to 1 channel

The width of this site was equal to the width of a negative smoothed second derivative of gaussian the center of which was equal to the center of this spectrum site. However, in this formula there was a mistake which was revealed when this formula was verified with formulas from the manual to the program of γ-spectra processing called "GammaVision" [7]. One revealed by the formulas given in this manual that the formula (1) should have the following form:

$$C_j = \frac{\sum_i Y_i L_i}{\sqrt{Y_j \sum_i L_i^2}}, \qquad (2)$$

where Y_j – channel count in the j-th channel of an initial spectrum.

One also written in that manual that the channel of an initial spectrum considered belonging to a peak if the value of C_j was less than a definite numerical value that was taken equal to -2 in that manual. This value was negative because the "GammaVision" program operated with a positive smoothed second derivative of gaussian.

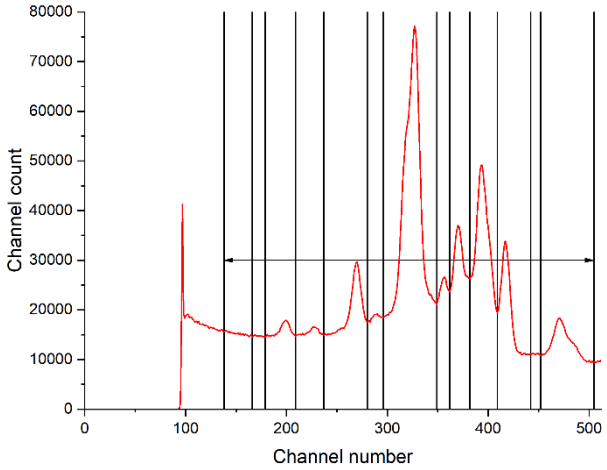

Fig. 5a. The site of the initial spectrum with good statistics and the results of peak search when the jut half-width was equal to 3 channels

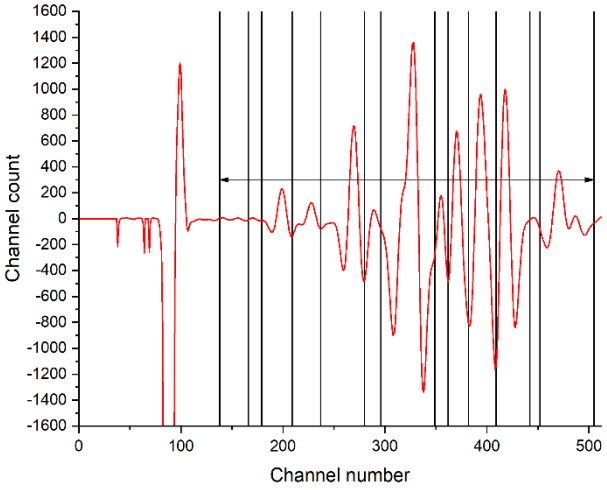

Fig. 6a. The site of the search spectrum corresponding to the site of the initial spectrum with good statistics and the results of peak search when the jut half-width was equal to 3 channels

The "GAMMAPEAKS" program used the negative smoothed second derivative to create a search spectrum, therefore the value of C_j should be bigger than 2 for the program considered that the channel belongs to the peak.

The algorithm of peaks search in the "GAMMA-PEAKS" program was built such way: first the program performed search of the peak centers for what in search spectrum was performed the search of channels in which numerical value was not less than 2. The channel with the highest value in group of channels of the search spectrum was considered as the center of a peak if the value in that channel was bigger than in adjacent channels. After that the program took the values in the adjacent search spectrum channels from the found peak center channels moving in both directions from centers and when the value in the channel of search spectrum became negative and bigger than -2 and also bigger than value in the previous adjacent channel of search spectrum, this chan-nel was considered as peak border in initial spectrum.

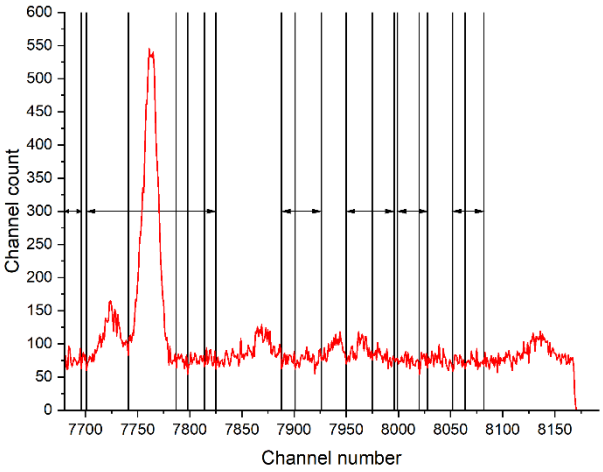

Fig. 5b. The site of the initial spectrum with "weak" statistics and the results of peak search when the jut half-width was equal to 3 channels

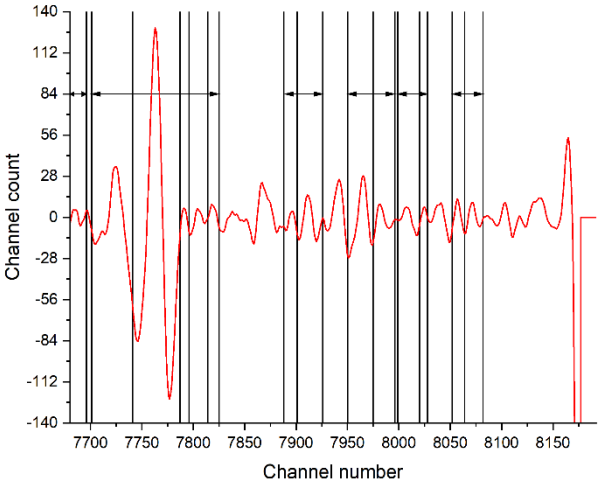

Fig. 6b. The site of the search spectrum corresponding to the site of the initial spectrum with "weak" statistics and the results of peak search when the jut half-width was equal to 3 channels

However, if two peaks bordered closely (the right border of one peak considered equal to the left border of the following peak), the program made a little correction to the peak borders.

3. RESULTS AND DISCUSSION

As the analyzed material the real uranic ore sample γ-spectrum measured on the germanium detector has been taken. For smoothing the convolution of initial spectrum with gaussian having amplitude equal to 18 and the variance equal to 2 was performed. For creation of a search spectrum the convolution of smoothed spectrum with negative smoothed second derivative of gaussian which had the jut half-width value equal to 1 channel was performed. The value of sensibility for determining of peak or background has been set equal to 2. All channels on search spectrum which had value less than the sensibility value considered belonging to background, all the channels which had values bigger or equal to the sensibility value considered belonging to the peaks on initial spectrum.

Sites of the test initial spectrum are shown in Figs. 2a and 2b. In Fig. 2a the initial site of spectrum containing peaks with good statistics is shown and in Fig. 2b is shown the site of the same spectrum with weak statistics (final site of γ-spectrum). Arrows shows borders of the determined groups of peaks. In each group there were at least one peak but if the group contained several peaks the right border of one peak was equal to the left border of next peak in the group. The sites of smoothed spectrum corresponding to the sites of initial spectrum with good statistics and weak statistics are shown in Figs. 3a and 3b. One can see from these figures that the convolution of initial spectrum with ideal gaussian well smooths a spectrum, especially on sites with weak statistics (see Fig. 3b). The sites of a search spectrum corresponding to the site of the initial spectrum with good statistics and with weak statistics are shown in Figs. 4a and 4b. One can see comparing Fig. 3a with Fig. 4a that where on smoothed spectrum one peak is observed, on the search spectrum several peaks limited to the same site as the peak in Fig. 3a are observed. In particular, the peak on smoothed spectrum having borders from 296 to 348 channel number represents superposition of three or four gaussians that is observed on the search spectrum (see Fig. 4a). On the site of the smoothed spectrum having weak statistics (see Fig. 3b) the peak having borders from 7706 to 7740 channel number also represents superposition not less than three gaussian at one peak on initial spectrum (see Fig. 4b). So, one can see that the convolution of initial spectrum with ideal gaussian and the following convolution of the received spectrum with the negative smoothed second derivative of gaussian allows well determine peaks from atoms of different elements.

In the Figs. 5a and 5b the sites of the initial spectrum marked by means of a search spectrum which constructed by convolution of smoothed spectrum with the negative smoothed second derivative of gaussian the half-width of the jut of which was set equal to 3 channels are shown. In Figs. 6a and 6b the sites of this search spectrum are shown. One can see from these figures that with such half-width jut value of negative smoothed second derivative it is impossible to see that several peaks in search spectrum are superposed on one gaussian in initial and smoothed spectra as it is observed in Figs. 4a and 4b.

CONCLUSIONS

1. The convolution of an initial γ-spectrum with an ideal gaussian having small amplitude and small variance well smooths the initial spectrum especially on its sites which have a weak statistic.

2. A search spectrum constructed by the convolution of the smoothed spectrum with the negative smoothed second derivative of gaussian allows determine how many singlets superpose on a peak in the initial spectrum.

3. The lower is the value of negative smoothed second derivative of gaussian the better one can determine how many singlets superpose on a peak in the initial spectrum.

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АНАЛІЗ ПОШУКОВИХ СПЕКТРІВ І МЕТОДІВ ВИЗНАЧЕННЯ РОЗТАШУВАННЯ ПІКІВ У γ-СПЕКТРАХ

А.Ю. Бережной, Ю.В. Ляшко

У програмі обробки γ-спектрів «GAMMAPEAKS» розроблено алгоритм автоматичного пошуку піків у γ-спектрах, заснований на використанні згортки ділянок спектра з від'ємною згладженою другою похідною від ґавсіана. У новій версії цієї програми перед побудовою пошукового спектра проводилася згортка початкового спектра з ідеальним ґавсіаном невеликої амплітуди та дисперсії. У результаті цієї згортки початковий спектр на ділянках зі «слабкою» статистикою був добре згладжений, що полегшувало пошук піків на пошуковому спектрі. Пошуковий спектр будувався шляхом згортки здобутого γ-спектра з від'ємною згладженою другою похідною від ґавсіана, що має вигляд сходинки. Результат пошуку піків виявив, що програма «GAMMAPEAKS» розмічає піки точніше, ніж попередні версії цієї програми, в яких не було згортки з ґавсіаном перед побудовою пошукового спектра.