DEVELOPMENT AND COMPARISON OF THE METHODS OF AUTOMATICAL SEARCHING OF PEAKS IN γ–SPECTRA

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We elaborated the program of γ-spectra processing called "GAMMAPEAKS" which approximates peaks in specters by gauss functions. We included two new algorithms which mark peaks in spectra to the new program version. The peaks marking algorithms are based on statistical methods of searching of extremes in functions. The algorithms developed are possible to mark peaks in spectra with sufficient accuracy.

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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.

We developed the program of γ-specters processing which is named "GAMMAPEAKS". This program is possible to search and mark peaks in specters automatically. Our program initially used for this purpose differential method based on the calculation of the second derivative of the values in channels of specter processed. Results showed that some poor peaks may be omitted by their automatical searching. The results also showed that some specter's sites that obviously belong to background can be determined as peaks. The extra processing of complicated specters in the manual mode which are included in the developed program requires appreciable time resources for marking of "omitted" peaks and unneeded sites unmarking. To improve the automatical peaks marking we added in the "GAMMAPEAKS" program two additional statistical methods of automatical marking of peaks in specters. The current article is devoted to discussion of these methods.

2. PROBLEM DEFINITION

Statistical automatical peaks marking methods often use so-called "sliding window" representing the site of specter on which the convolution of channels belonging to this site with the negative smoothed second derivative was performed. The overall view of the negative smoothed second derivative is shown on the Fig.1.

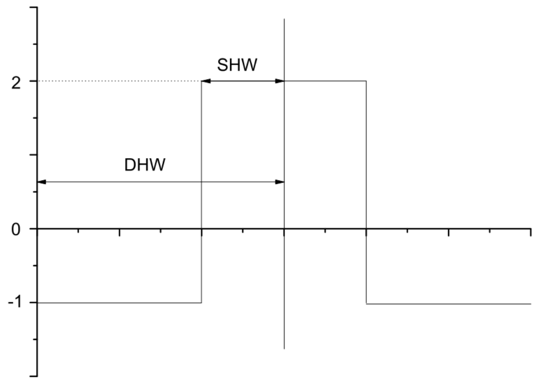


Fig.1. *The overall view of the negative smoothed second derivative. The designations: DHW – the negative smoothed second derivative half-width, SHW – the negative smoothed second derivative salient (the "step") half-width*

In our program for peaks searching so-called "searching specters" were formed in our program. These searching specters represented the transformed initial specters. Channels in searching specter contained the results of processing of count values in channels of initial specter by certain algorithms.

To build the searching specter in the first of the statistical method of peaks searching after performing of convolution the specter site limited by the sliding window with the negative smoothed second derivative the calculation of variance on this site was performed. Also one performed the calculation of the value specified by the formula:

$$\overline{y^2_{sqr}} = \frac{\sum\limits_{i=1}^{n} y_i^2}{n}, \qquad (1)$$

where n is the length of sliding window, y_i represents the value of the convolution of count values in initial specter channel with the negative second smoothed derivative.

Each channel of the searching specter built by the first statistical peaks searching method has got the value of the ratio of square root of variance value to the square root of the value counted by the formula (1), multiplied by 1000. The number of a searching specter channel coincided with the number of a channel in initial specter which was equal to the position of the center of sliding window. If the left or the right edge of the sliding window overran the edge of initial specter, the value of the channel in sliding window was taken to be equal to the value of the first or of the last channel of initial specter respectively. In the case when all the values in initial specter channels had the same values all the channels of searching specter also got identical values depending on negative smoothed second derivative step value. The overall view of the searching specter built by this way is shown on the Fig.2.

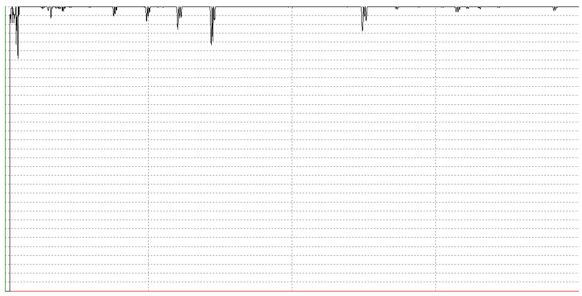


Fig.2. *The general view of a searching specter built by the first statistical method*

In the case of the using of the second statistical method of automatical peaks marking after performing the convolution of initial specter site limited by sliding window with negative smoothed second derivative one counted the value of variance on the sliding window and entered this value as the intermediate value in the searching specter. As is well known the variance defines in the following way:

$$D = \frac{1}{n-1} \sum_i (y_i - \bar{y})^2 , \qquad (2)$$

where n is the number of values, by which the variance counts, y_i represents the value in the i-th channel and $\bar{y}$ represents the mean value on the interval of n channels. This expression may be rewritten in the such way:

$$D = \tfrac{1}{n-1} \left(\sum_i y_i^2 - 2 \sum_i \bar{y} y_i + \sum_i \bar{y}^2 \right) = = \tfrac{1}{n-1} \left(\sum_i y_i^2 - 2\bar{y} \sum_i y_i + n\bar{y}^2 \right) = = \tfrac{1}{n-1} \left(\sum_i y_i^2 - 2n\bar{y}^2 + n\bar{y}^2 \right) = = \tfrac{n}{n-1} \left(\overline{y_{sqr}^2} - \bar{y}^2 \right) , \qquad (3)$$

where $\overline{y_{sqr}^2}$ represents the value defined by the formula (1). The formula (3) simplifies counting of variance.

Next one passed sliding window through the intermediate searching specter. Then one counted the variance and the arithmetical mean on the site of the intermediate searching spectrum limited by the sliding window. After this one counted the ratio of the square root variance value to the square root arithmetical mean value. The value of this ratio entered as the final value in the channel of searching spectrum. The overall view of the searching spectrum built by this way is shown on the Fig.3.

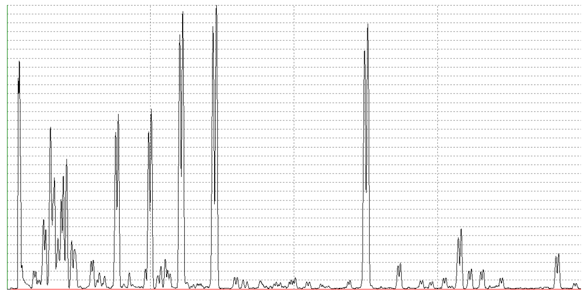


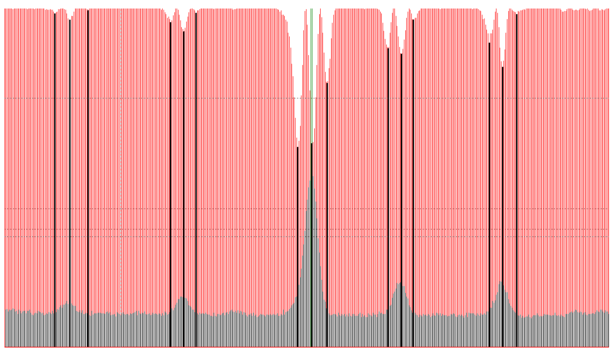
Fig.3. *The general view of a searching spectrum built by the second statistical method*

When values in an initial spectrum channels were identical the values in the corresponding channels in a searching spectrum also were identical and they were equal to zero. The criterion of belonging of a channel in an initial spectrum to a peak or to a background formulated this way: if a value in a channel of a searching spectrum differed from the values in a searching spectrum built from an initial spectrum with identical values in channels less by module than a specified level (a sensitivity), so the channel in the initial spectrum was counted to belong to a background, in the opposite case – to a peak.

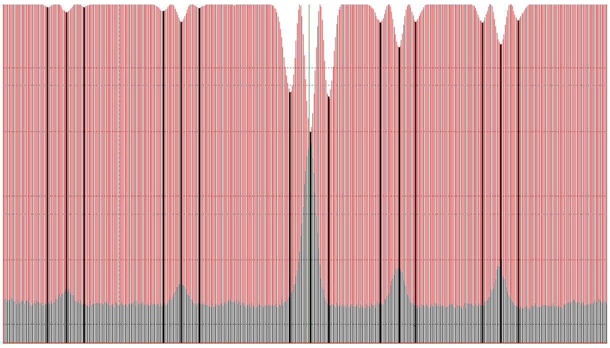
3. RESULTS AND DISCUSSION

We present some illustrations showing the results of corresponding of searching and initial spectra in this section. Searching spectra are highlighted by the red color, initial ones – by the black color.

On the Fig.4 the sites of searching spectra built by the first statistical method and the corresponding initial spectra sites in a region of isolated peaks in the initial spectrum when the value of the step of the negative smoothed second derivative was equal to 6 channels (a) and to 12 channels (b) are shown.



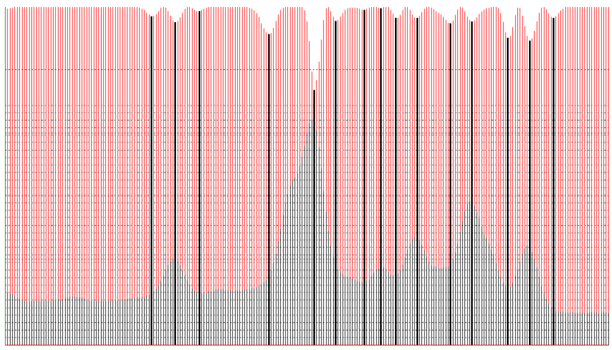
a



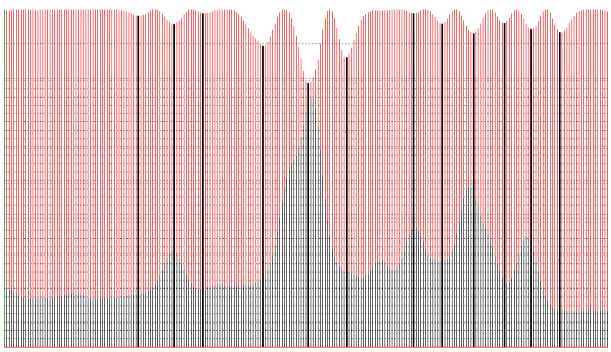
b

Fig.4. *The results of comparison of searching spectrum built by the first method (red histogram) and initial spectrum (black histogram) in the region of isolated peaks in the initial spectrum when the negative smoothed second derivative step width was equal to 6 channels (a) and to 12 channels (b)*

The initial spectrum resolution was equal to 8192 channels. One can qualitatively determine that on each enough well expressed peak in an initial spectrum accounts for 3 minimums in the corresponding searching spectrum. The central of these minimums in the searching spectrum corresponds to the maximum, when the first and the last ones – to the edges of a peak in the initial spectrum.



a



b

Fig.5. *The results of comparison of searching spectrum built by the first method (red histogram) and initial spectrum (black histogram) in the region of overlapped peaks in the initial spectrum when the negative smoothed second derivative step width was equal to 6 channels (a) and to 12 channels (b)*

On the Fig.5 the sites of the same spectra in a region of overlapping peaks in the initial spectrum when the value of the step of negative smoothed second derivative was equal to 6 channels (a) and to 12 channels (b) are shown. One can see that each initial spectrum peak also accounts for 3 minimums in a searching spectra but in these regions in both cases some relatively small peaks are recognized by the first statistical method poorly (for they were fine recognition one needs to decrease the sensitivity value).

On the Fig.6 the sites of searching spectra built by the first statistical method and initial spectra sites in the region of overlapped peaks in the initial spectrum when the negative smoothed second derivative step was equal to 2 channels are shown. In this case the peaks edges and centers in an initial spectrum accounts for maximums in a searching spectrum. One can also see that in this case sometimes is possible to reveal the overlapped peaks which are not seen by naked eye.

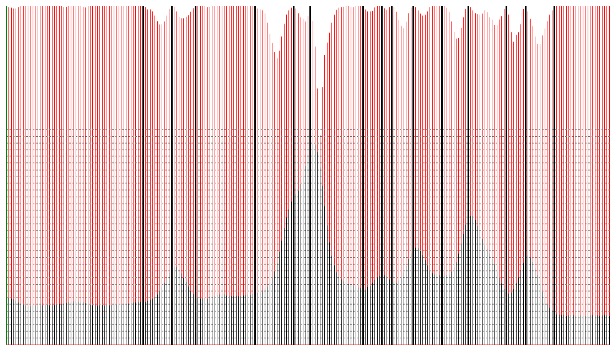
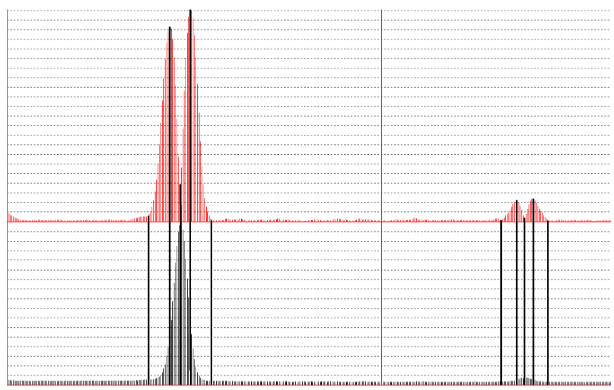
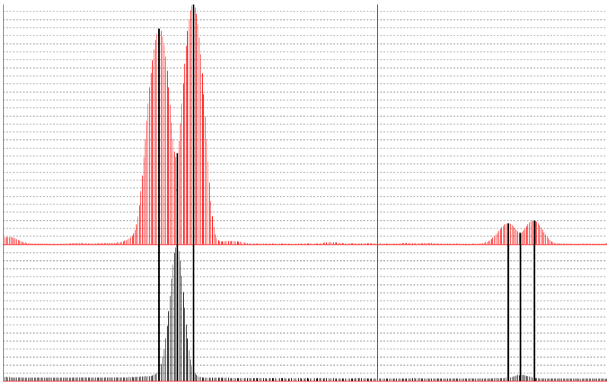


Fig.6. *The results of comparison of searching spectrum built by the first method (red histogram) and initial spectrum (black histogram) in the region of overlapped peaks in the initial spectrum when the negative smoothed second derivative step width was equal to 2 channels*

On the Fig.7 the sites of searching spectra built by the second statistical method and initial spectra sites in a region of isolated peaks in the initial spectrum when the value of the step of the negative smoothed second derivative was equal to 6 channels (a) and to 12 channels (b) are shown.

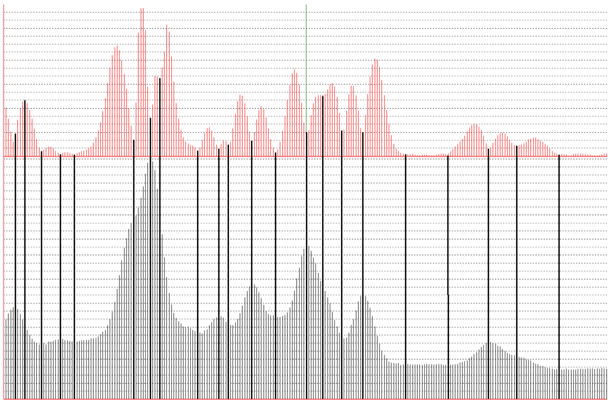


a

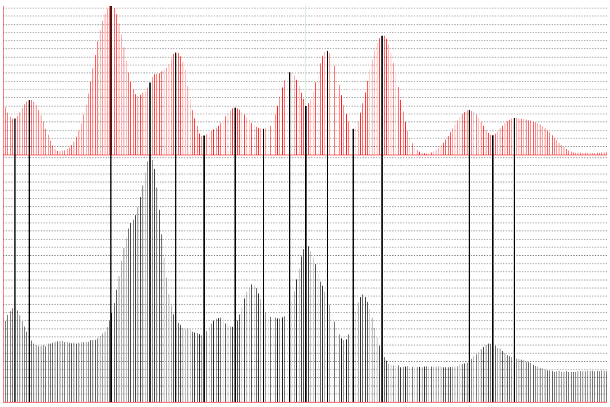


b

Fig. 7. *The results of comparison of searching spectrum built by the first method (red histogram) and initial spectrum (black histogram) in the region of isolated peaks in the initial spectrum when the negative smoothed second derivative step width was equal to 2 channels (a) and to 6 channels (b)*



a



b

Fig. 8. *The results of comparison of searching spectrum built by the first method (red histogram) and initial spectrum (black histogram) in the region of overlapped peaks in the initial spectrum when the negative smoothed second derivative step width was equal to 2 channels (a) and to 6 channels (b)*

On the Fig.8 the sites of the same spectra in a region of overlapped peaks for the same negative smoothed second derivative step values are shown.

One can see that when the second statistical method is used in the case of isolated peaks (see Fig.7) the corresponding site of a searching spectrum has well observable rising which has a groove, so that extremes of this rising corresponds to the edges of a peak in an initial spectrum and the center of the groove falls on the maximum of peak in the initial spectrum.

One can also see that in the case of using the same method in the region of overlapped peaks (see Fig.8) in the case (b) the extremes of peaks in an initial spectrum correspond either to the extremes or to the edges of a peak in an initial spectrum. In the case (a) minimums in a searching spectrum corresponds either to the maximums or to the edges of peaks in an initial spectrum. The same situation is observed in the case of isolated peaks of a searching spectrum are processed (see Fig.7,a). As to comparison of an initial and a searching spectra when the negative smoothed second derivative step width is equal to 12 channels (see Fig.8,b) one can see that relatively small peaks are recognized poorly (for their enough fine recognition one needs to decrease the sensitivity value). Thus one can make a conclusion that the width of the step in the negative smoothed second derivative is smaller the more narrow peaks can be recognized by using of the second statistical method. The same situation is observed when the first statistical method is used (see Fig.6).

4. CONCLUSIONS

1. The first of statistical methods observed give appreciable good results of peaks marking when the negative smoothed second derivative step width is taken from 2 channels to the average full FWHM of a peak in a spectrum.

2. The second of statistical methods observed give appreciable good results of peaks marking when the negative smoothed second derivative step width is taken from 2 channels to the half of an average FWHM of a peak in a spectrum.

3. The less width of the step of the negative smoothed second derivative is taken the better in most cases is the result of using of the both statistical method.

4. Both the statistical methods of peaks searching and marking may give the enough good results when they are used not only for γ–spectra processing, but when the discrete spectrum of values of an arbitrary analytical function having extremes is processed.

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РАЗРАБОТКА И СРАВНЕНИЕ МЕТОДОВ АВТОМАТИЧЕСКОГО ПОИСКА ПИКОВ В γ–СПЕКТРАХ

А. Ю. Бережной, Ю. В. Ляшко

Разработана программа обработки γ-спектров «GAMMAPEAKS», аппроксимирующая пики гауссовыми функциями. В настоящей версии программы использованы два новых алгоритма автоматической разметки пиков в спектрах. Эти алгоритмы основаны на статистических методах поиска экстремумов в функциях. Созданные алгоритмы позволяют с достаточно хорошей точностью проводить автоматическую разметку пиков в обрабатываемых спектрах.

РОЗРОБКА І ПОРІВНЯННЯ МЕТОДІВ АВТОМАТИЧНОГО ПОШУКУ ПІКІВ У γ–СПЕКТРАХ

А. Ю. Бережной, Ю. В. Ляшко

Розроблено програму обробки γ-спектрів «GAMMAPEAKS», що апроксимує піки за допомогою гауссових функцій. У теперешній версії програми використано два нових алгоритми, які виконують автоматичну розмітку піків у спектрах. Ці алгоритми основані на статистичних методах пошуку екстремумів у функціях. Створені алгоритми дають змогу з достатньо задовільною точністю розмічати піки в спектрах, які обробляються.