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APPROXIMATION OF PEAKS IN γ-SPECTRA BY GAUSSIAN-LIKE ANALYTIC FUNCTIONS

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The program processing γ-spectra named "GAMMAPEAKS", was elaborated. This program can approximate peaks in γ-spectra with different Gaussian-like functions. The common Gaussian, the variable variance Gaussian and the sectionally defined Gaussian-like function were used as approximative functions. The contrastive analysis of quality of peaks approximating using no more than three approximative functions for one extremum in γ-spectra was performed. The quantitative and qualitative data determining the precision of approximating of γ-spectra peaks by different Gaussian-like functions are shown.

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INTRODUCTION

The nuclear radiation spectrometry is an important investigating method in the nuclear physics. The nuclear γ-spectroscopy, which is a variation of the nuclear radiation spectrometry, has taken on a great applied significance last time. It is used in the geophysics, activation analysis, space and medical investigations and many other scientific studies.

When γ-spectra measured the γ-quanta emitting when nuclei energy state changed in the process of their transiting from excited state to unexcited one are registered [1, 2]. The excitation of nuclei consequent a radioactive decay or a nuclear reaction. The aim of γ-spectroscopy measurements is determining of characteristics of radiation source and its substations surrounding which can be determined when γ-spectrum processed. The tasks of applied γ-spectrometry include, for example, measurement of native radioactive elements content in substance [2, 3], investigation of radioactive environmental pollution for their danger evaluation [4 - 7], measurement of planet radioactivity [8] and others.

One uses the computer engineering for processing results of γ-spectroscopy in research centers. This allows to determine cross-sections, RFF and others significant physical parameters of nuclear reactions. One needs as definite as possible approximate the peaks in γ-spectra with analytic functions describing the γ-quanta energy distribution to determine the nuclear reaction parameters with enough precision. The form of an ideal peak in γ-spectrum describes by Gaussian distribution. Therefore, Gaussian-like analytic functions are often used for description of peaks form. These functions represent different variations of Gaussian distribution.

The author of the present article with colleagues elaborate the program named "GAMMAPEAKS" which processes the peaks in γ-spectra [9 - 11]. The algorithm performing the approximation of the peaks in γ-spectra is modified in the last version of this program. Also one added the possibility of approximation of the summary peak formed by superposition of several closely set single peaks in this version of "GAMMAPEAKS" program. This approximation uses the conjugate gradients method with no more than three Gaussian-like functions for summary peak [10]. The studying performed either on model spectra containing both single and partially superposed peaks or real spectra. The precision of peaks approximation determined by χ-square criterion by values in channels belonging to a peak.

1. PROBLEM DEFINITION

The precision of approximating of peaks in γ-spectra by three analytic Gaussian-like functions was studied. One used the following functions: the common Gaussian, the variable variance Gaussian [12] and the sectionally defined function which described the centre of a peak by common Gaussian and the edges of a peak by exponents. The analytic expressions corresponding to all of the functions are shown in the Table 1.

Table 1

The names of approximate functions and their analytic expressions

The number of the function	The function name	The analytic expression
1	The common Gaussian	$f(x)=A\exp\left\{-\frac{(x-B)^2}{2\Delta^2}\right\}.$
2	The sectionally defined function	$\begin{cases} x<\left(B-h_1^2\right), & f(x)=A\exp\left\{\frac{h_1^2\left(2(x-B)+h_1^2\right)}{2\Delta^2}\right\}, \\ \left(B-h_1^2\right)\le x<\left(B+h_2^2\right), & f(x)=A\exp\left\{-\frac{(x-B)^2}{2\Delta^2}\right\}, \\ x\ge\left(B+h_2^2\right), & f(x)=A\exp\left\{\frac{h_2^2\left(2(B-x)+h_2^2\right)}{2\Delta^2}\right\}. \end{cases}$
3	The variable variance Gaussian	$f(x)=A\exp\left\{-\frac{(x-B)^2}{C^2+D^2\sqrt{E^2(x-B-F)^2+1}+1}\right\}.$

In the analytical expression for the common Gaussian shown in the Table 1, the parameter *A* defines the peak height, the parameter *B* defines the peak centroid position, the parameter Δ – the peak variance. For the variable variance Gaussian the analytic expression has four parameters instead of the parameter Δ, the first two of which (*C* and *D*) define the Gaussian width, the parameter *E* defines the Gaussian widening and the parameter *F* – the Gaussian asymmetry. For the sectionally defined approximate function the parameters h_1 and h_2 define the slopes of the function exponents. The parameter h_1 had the fixed value equal to 2.355Δ, and the parameter h_2 was optimized during approximation and had the initial value equal to Δ=2.

2. MATERIALS AND METHODS

The conjugate gradients method was taken for optimization of the coefficients of the approximate functions. The approximating precision determined by χ-square criterion by the values in the channels belonging to a peak.

One added the possibility of approximation of the summary peak formed by superposition of several closely set single peaks in this version of "GAMMAPEAKS" program. This approximation uses the conjugate gradients method with no more than three Gaussian-like functions for summary peak.

Table 2

The parameters of the Gaussians used for building of model spectra

The number of a Gaussian in the model spectrum	The number and the index of a parameter	The value of the parameter
1	A_1	1000
1	B_1	512
1	Δ_1	25
2	A_2	1200
2	B_2	480
2	Δ_2	30
3	A_3	600
3	B_3	544
3	Δ_3	20

The approximations was performed on model and on real spectra. The model spectra were formed by isolated or partially superposed common Gaussians. However, sometimes one could not notice by eye the fact that the peak in a model spectrum was generated by superposition of the several single common Gaussians, but the search spectrum corresponding to the model spectrum revealed this fact.

The values of the parameters of Gaussians formed the model spectra are shown in the Table 2, and the numbers of Gaussians belonging to the enumerated model spectra are shown in the Table 3.

Also the approximation of peaks in a real γ-spectrum was performed. This spectrum used for approximation of peaks with poor statistics ("weak" peaks) and well marked single and partially superposed peaks.

Table 3

The numbers of model spectra and the numbers of Gaussians in these spectra

The number of the model spectrum	The numbers of the Gaussians, belonging to the peak in the spectrum
1	1
2	1 and 2
3	1 and 3
4	1, 2, and 3

Usually one uses the χ-square method to make the fitting. The χ-square method is as follows: one needs make so that the value of χ-square criterion was minimal. As is well known the value of the χ-square criterion defines by the formula

$$\sum_{i=1}^{n} \chi^2 = \sum_{i=1}^{n} \left(y_i - f\left(x_i, C_k\right)\right)^2, \qquad (1)$$

where y_i are the values of experimentally measured or calculated data, x_i – the values of the approximative function argument, C_k – the values of approximative function parameters, and $f(x_i, C_k)$ – the values of the approximative function *f* when the values of its parameter is equal to x_i.

To find the minimal values of the χ-square criterion one needs to equate all the parameters C_k derivatives of the approximative function *f* defined by the formula (1) to zero, in other words, to decide the equation

$$-2\sum_{i=1}^{n}\left(y_i - f\left(x_i, C_k\right)\right)\frac{\partial f\left(x_i, C_k\right)}{\partial C_k} = 0, \qquad (2)$$

where C_k is the approximative function parameter with index *k*. When the approximative function is the common Gaussian the value of index *k* possesses the values from 1 to 3, and accordingly with the Table 1 we have: $C_1 \equiv A$, $C_2 \equiv B$, and $C_3 \equiv \Delta$. The sectionally defined approximative function have four parameters optimized $C_1 \equiv A$, $C_2 \equiv B$, $C_3 \equiv \Delta$, and $C_4 \equiv h_2$. The variable variance Gaussian have six parameters designed by letters form *A* to *F* in the Table 1. The values of x_i constituent the formulas (1) and (2) correspond to channel numbers in a spectrum and the values of y_i – to a number of counts in spectrum channels.

Since one is impossible to decide analytically the equations the decisions of which define the coefficients constituent the analytical expressions of approximative functions when the sectionally defined function and the variable variance Gaussian are used, one needs to use the conjugate gradients method described in detail in [10]. This method represents the numerical method of fitting of calculated or experimentally measured data by different analytic functions. Also this method gives good results in the case of existence of analytical decision of above mentioned equations when the χ-square method is used, especially when the approximative function contains only one minimal value for each of its coefficients. However, sometimes happens that an approximative function has several minimal values for one or more coefficients belonging to it. In this case the result of fitting using conjugate gradients method is sensitive to the initial values of approximative function

coefficients because one may get into different minimums of values of these coefficients. Therefore, the initial values of approximative function coefficients were taken equal to results of a search of their values which fitted a peak in a spectrum with an approximative function as precisely as possible for fitting using the conjugate gradients method. In future one plans the automation of this search.

3. RESULTS AND DISCUSSION

Four model spectra built by a special computer program are shown on the Fig. 1. These spectra are highlighted by the black line. The search spectra corresponding to the model spectra are also shown on the Fig. 1. The search spectra are highlighted by the orange line.

The numerical values of the χ-square criterion used for fitting of the model spectra are shown in the Table 4.

The graphical results of approximation of peaks in a real (experimentally measured) spectrum using different Gaussian-like analytic functions are shown on the Figs. 2-4.

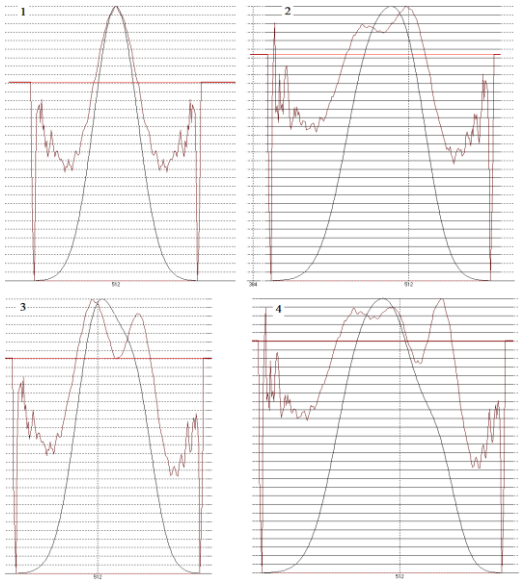

Fig. 1. The model spectra (the black line) and corresponding to them search spectra (the orange line)

Table 4

The numerical results of fitting of the model spectra

The number of the spectrum	The quantity of approximate curves	The χ-square criterion for the common Gaussian, $\times 10^4$	The χ-square criterion for the sectionally defined function, $\times 10^4$	The χ-square criterion for the variable variance Gaussian, $\times 10^4$
1	1	0.002	0.011	0.002
2	2	13.612	9.385	1.243
3	2	8.136	135.683	0.299
4	3	101.628	28.452	2.921

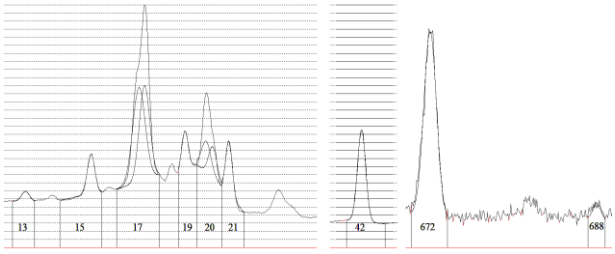

Fig. 2. The results of the approximation of some peaks in the real spectrum by the common Gaussian

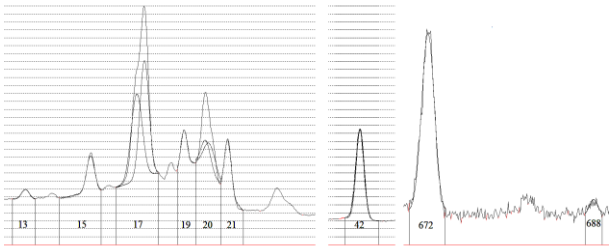

Fig. 3. The results of the approximation of some peaks in the real spectrum by the sectionally defined function

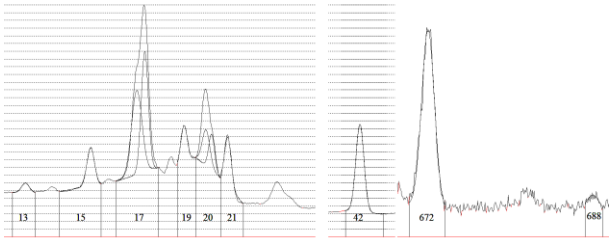

Fig. 4. The results of the approximation of some peaks in the real spectrum by the variable variance Gaussian

The results of approximation of partially superposed peaks are shown on the left of these figures, the results of approximation of an isolated peak – in the middle and the results of weak peaks approximation – on the right of these figures.

The numerical results of approximation of these peaks in the real spectrum are shown in the Table 5. The cells with minimal values of χ-square criterion are highlighted by green color, the cells with maximal χ-square criterion – by brown color and the cells with intermediate values – by yellow color.

One also needs to note that approximation of the peak No.17 in the real spectrum by two common Gaussians sometimes give the specific graphical result shown on the Fig. 5. Visually one can propose that the amplitude of the left gaussian forming this peak should have smaller numerical value than the amplitude of right gaussian in the same peak. However, as one can see from this figure the right Gaussian has the value of its amplitude smaller than the left Gaussian on the same figure (see purple lines on the Fig. 5). Nevertheless, the sum of values of these Gaussians (red line) was qualitatively similar to the experimentally measured peak (black line).

The initial and the result values of Gaussians parameters are shown in the Table 6. The values of the χ-square criterion in the case shown on the Fig. 5 (when the value of the right gaussian amplitude in the peak had less numerical value than the right Gaussian amplitude) was equal to $11281 \cdot 10^4$, and in the case shown on the Fig. 2 (when the amplitudes of both gaussians were al-

most equal) – to $78953 \cdot 10^4$ (see Table 5), that is almost seven times more than in the case shown on the Fig. 5. Of course, this result is not physical, but occurs fairly often when this peak is described by two common Gaussians.

Table 5

The numerical values of χ-square criterion of approximation of some peaks in the real spectrum. In each string the cell highlighted by green color contains the minimal χ-square criterion numerical value, the cell highlighted by brown – the maximal numerical value of the same criterion and the cell highlighted by yellow – the intermediate numerical value

The number of a peak in the spectrum	The number of approximating curves	The values of the χ-square criterion $\times 10^4$, for the function No.		
		1	2	3
13	1	39.472	39.219	39.457
15	1	215.712	616.234	215.370
17	2	78952.777	41446.816	60832.449
19	1	193.398	154.253	191.220
20	2	89559.050	32289.903	97079.860
21	1	1000.173	970.430	1321.350
42	1	60.948	7843.849	61.525
672	1	1.357	1.354	1.294
688	1	0.191	0.151	0.111

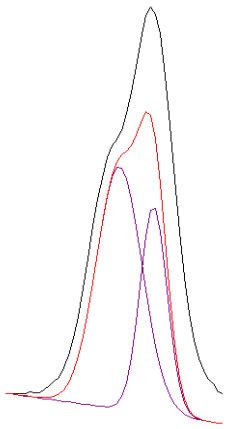

Fig. 5. The graphical result of approximation of the peak No.17 in the real spectrum by two common Gaussians. The black line on this figure represents the outline of the real spectrum peak, the purple lines – the outlines of gaussians forming the same peak, and the red line – the sum of these gaussians

Table 6

The initial and the result values of parameters of Gaussians approximating the peak No. 17 in the real spectrum

	The left Gaussian	The right Gaussian
The initial parameters values	A = 30000.000	A = 35000.000
	B = 315.000	B = 328.000
	Δ = 3.500	Δ = 3.500
The result parameters values	A = 30000.186	A = 34999.553
	B = 327.597	B = 320.512
	Δ = 3.955	Δ = 6.674

CONCLUSIONS

1. The results of approximation of model spectra formed by isolated and partially superposed common Gaussians show that in most cases the most precise fitting results occur when the variable variance Gaussians are used as the approximative functions.

2. The approximation of real spectrum peaks shows that in 66% cases the most precisely results occurs when the sectionally defined function is used for peaks approximation and in 33% cases the most precisely results are given when the variable variance Gaussian is used.

3. When two approximative function for one peak are used the most precisely results gives the using of sectionally defined functions.

4. One can see from all of the above mentioned conclusions that in more than 50% cases of peaks approximation (including superposed peaks like peaks No.17 and No.20) the best approximation results gives the using of the sectionally defined function, but for well-marked isolated peaks, such as peaks No.15 and No.42, the most precisely approximation results gives one of the two different Gaussians. The best precision of approximating of weak peaks with the poor statistics (like the peaks No.672 and No.688) gives the variable variance Gaussian.

5. One also needs to note that when the approximation of the peak No.17 in the real spectrum by two common Gaussians is performed, sometimes appears that the most precise approximation have the result when the value of the left Gaussian amplitude is bigger than the value of the right one. The χ-square criterion value in this case is appreciably less than in other cases. This result is not physical because the widths of peaks on their half-heights differ almost twice, but occurs fairly often.

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REFERENCES

1. K. Siegbahn. *Beta- and gamma-spectroscopy.* M.: "Physmathgiz", 1959 (in Russian).
2. R.M. Kogan, I.M. Nazarov, Sh.D. Fridman. *The grounds of gamma-specroscopy of natural surroundings.* M.: "Atomizdat", 1967, 366 p. (in Russian).
3. G.S. Smirnov. *The airbrushing-spectrometric method of uranic ores deposit fields. The methodical guide.* M.: "Minego USSR", 1967, 226 p.
4. E.M. Artemov et al. The surface gamma-spectrometry of radioactive contamination of land // *Atomic Energy*. 1971, v. 31, issue 1, p. 35-40.
5. A.N. Marey, R.M. Barhudarov, N.Ya. Novikova. *The global falling of Cs-137 and human.* M.: "Atomizdat", 1974, 168 p. (in Russian).
6. F.I. Pavlotskaya. *Migration of radioactive production of global fall-out on soils.* M.: "Atomizdat", 1974, 214 p. (in Russian).
7. R. Blumberg, F.F. Dyer, A. Houtzeel. Remoute gamma-spectrometry for fission product deposition studies // *Trans. Amer. Nucl. Soc.* 1969, v. 12, № 2, p. 842.

8. Yu.A. Soorkov. *The gamma-spectromatry in cosmic investigations.* M.: "Atomizdat", 1977, 240 p. (in Russian).
9. A.Yu. Berezhnoy, V.M. Mishchenko, S.N. Utenkov. The computer program "GAMMAPEAKS" for γ-spectra analysis // *Visnyk of Kharkiv National university, series Physics. "Nuclei, Particles, Fields". Kharkiv*. 2007, 4(36), 784, p. 125-128 (in Ukrainian).
10. A.Yu. Berezhnoy, S.N. Utenkov. Variable Variance Model for γ-spectra Analysis // *Problems of Atomic Science and Technology. Series "Nuclear Physics Investigations"*. 2016, № 5, p. 126-130.
11. A.Yu. Berezhnoy, Yu.V. Lyashko. Development and Comparison of the Methods of Automatical Searching of Peaks in γ-spectra // *Problems of Atomic Science and Technology. Series "Nuclear Physics Investigations"*. 2019, № 3, p. 124-128.
12. G.N. Kuptzov, B.A. Nemashkalo. *Analytical description of the form of peaks from semiconductor and scintillation detectors:* Preprint KIPT. M.: "CSIIatominform", 1987, 7 p. (in Russian).

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АППРОКСИМАЦИЯ ПИКОВ В γ-СПЕКТРАХ АНАЛИТИЧЕСКИМИ ГАУССОПОДОБНЫМИ ФУНКЦИЯМИ

А.Ю. Бережной

Разработана программа обработки γ-спектров "GAMMAPEAKS", аппроксимирующая пики различными аналитическими гауссоподобными функциями. Были использованы следующие аппроксимирующие функции: обычный гауссиан, гауссиан с переменной дисперсией и кусочно-заданная гауссоподобная функция. Проведен сравнительный анализ качества описания пиков тремя вариантами гауссоподобных функций при использовании не более трех функций одного и того же варианта на пик в γ-спектре. Приведены качественные и количественные данные, определяющие точность аппроксимации пиков в γ-спектре различными вариантами гауссоподобных функций.

АПРОКСИМАЦІЯ ПІКІВ У γ-СПЕКТРАХ АНАЛІТИЧНИМИ ГАУСОПОДІБНИМИ ФУНКЦІЯМИ

А.Ю. Бережной

Розроблено програму обробки γ-спектрів "GAMMAPEAKS", яка апроксимує піки за допомогою гаусоподібних функцій. Використовувались такі апроксимуючі фукнції: звичайний гаусіан, гаусіан зі змінною дисперсією та кусково-задана гаусоподібна функція. Проведено порівняльний аналіз якості опису піків трьома варіантами гаусоподібних функцій з використанням не більше трьох функцій однакового типу для будь-якого піку в γ-спектрі. Наведені якісні та кількісні дані, які визначають точність апроксимації піків у γ-спектрі різними типами гаусоподібних функцій.