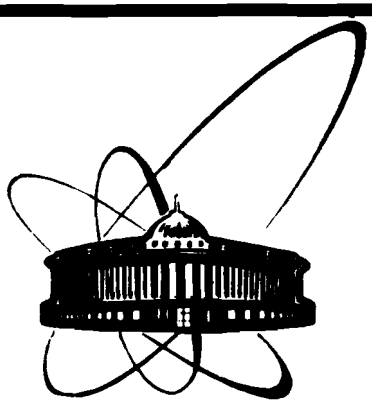

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GSAP: FORTRAN CODE FOR GAMMA-SPECTRUM ANALYSIS

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PROGRAM SUMMARY

Title of program: GSAP

Catalogue number:

Program obtainable from: CPC Program Library, Queen's University of Belfast, Northern Ireland

Computer: EC-1055 M (IBM compatible)

Installation: Joint Institute for Nuclear Research, Dubna, Moscow Region, U.S.S.R.

Operating system: OS/360

Programming language used: FORTRAN IV (H)

High speed store required: 128 Kwords at execution time

Number of bits per word: 32

Overlay structure: None

Number of magnetic tapes required: None

Other peripherals used: Card reader, line printer

Number of cards in combined program and test deck: 716

Card punching code: EBCDIC

Keywords: Automatic peak detection, doublet resolution, Gaussian fit, gamma-ray spectroscopy, neutron activation analysis, fragmentation, spallation, fission.

Nature of physical problem

The program performs fully automatic detection and evaluation of peaks in gamma-ray spectra measured with semiconductor detectors and stored in digital form.

Method of solution

Automatic peak detection is accomplished by convoluting the experimental spectrum with Gaussian second derivative digital filter. The sensitivity of the searching procedure may be chosen beforehand. The detected peaks are arranged into multiplets and corresponding fitting interval is found. Each multiplet is unfolded using standard non-linear least squares fit assuming Gaussian peak shape and linear background. The number of free adjustable parameters may be chosen depending on the spectrum complexity and particular goal of the evaluation. The results are printed in concise form including statistical errors of the peak parameters. All quantities enabling one to judge the fit quality are also given. The result of the fit is presented in graphical form too.

Unusual features of the program

The present program works in fully automatic mode. The only input parameters are the measured spectrum, its starting and final points, energy calibration, peak FWHM calibration and three parameters controlling the peak search routine. The number of fitted peak parameters may be restricted. The restriction of the free parameter

number is also performed automatically whenever the fitting procedure fails. In an extreme case, no least-squares fit is performed and only first parameter guesses are given.

Restrictions on program complexity

The dimensions, such as 4096 spectral points, are easily changed.

Typical running time

On an EC-1055M compilation (H) takes 53 CPU seconds. A 4096 channel spectrum with 53 peaks is processed in 12 CPU seconds.

LONG WRITE-UP

1. Introduction

Gamma-ray spectroscopy is of great importance for basic research in nuclear physics as well as for such applications as neutron activation analysis. In recent years a considerable experimental effort has been also devoted to the investigation of nuclear reactions induced by high-energy projectiles which yield a large number of heavy target residues. An experimental study of these interactions is particularly based on the foil stack activation technique and successive Ge(Li) gamma-ray spectroscopy. This experimental technique is unique as regards the identification of a variety of nuclides, the products of spallation, fission and fragmentation.

A large number of those forms a good statistical basis for obtaining pertinent characteristics of such processes.

The gamma-ray spectra measured using semiconductor detectors with high energy resolution exhibit complex structure comprising great number of discrete peaks superposed on varying background. Due to statistical nature of the gamma-ray emission and detection too, the measured spectra are subjected to considerable statistical fluctuations obscuring the physical information. For these reasons, the evaluation of the gamma-ray spectra is not an easy task which is commonly solved with computer aid. The capabilities of the present measuring devices are enormous, so that many gamma-ray spectra are commonly obtained in the course of one experiment. Fast and possibly automatic evaluation of the measured gamma-ray spectra is therefore necessary to obtain physical information needed and to control the progress of the experiment.

Many dedicated computer programs have been published for the gamma-ray spectra evaluation [1,2] , but most of them are too complex and not easily obtainable. We developed new computer code GSAP for fully automatic evaluation of the gamma-ray spectra measured with the semiconductor detectors and stored in a digital form. The main advantages of the present program are:

i/ simplicity and robustness of the algorithms used,
ii/ fully automatic performance with minimum amount of input information needed,
iii/ low amount of high speed storage required,
iv/ overall simplicity of the program code.

2. Outline of mathematical method

The program GSAP is intended for fully automatic evaluation of the gamma-ray spectra recorded using semiconductor detectors and stored digitally in the memory of a multichannel analyser. The program may be in principle applied also to any other spectra with pronounced peak structure (X-ray spectra, energy spectra of charged particles, etc.).

The program is based on known and well examined mathematical procedures ensuring fast and stable evaluation with minimum of computational fails. In the program GSAP, the evaluated spectrum is divided into peak multiplets which are processed separately. Any peak multiplet comprises one peak or a group of overlapping peaks and is separated from preceding and following multiplets by more than a prescribed distance. The program performs automatic search for spectral peaks starting from the spectrum beginning (or from any other specified point). Whenever a peak multiplet is identified, the peak parameters are immediately determined by non-linear squares fit. After the current multiplet is processed, the search continues until next multiplet is found or the spectrum end is reached.

The gamma-ray spectrum generally consists of well pronounced spectral peaks superimposed on slowly varying background. The gamma-ray spectrum, when recorded by multichannel analysers, formally represents a vector $S(k)$ $(k=1,\ldots,N)$ of count numbers registered in separate channels numbered by index k. Due to statistical nature of the gamma-ray emission and photon detection

as well, the count numbers $S(k)$ are subjected to statistical fluctuations. In the present program , the count numbers $S(k)$ are assumed to be statistically independent and Poisson distributed [3]. The presence of the spectral background as well as the statistical scatter of the experimental data seriously complicate automatic peak search, especially in the case of weak peaks.

In the present program , the peak search is accomplished by convoluting the experimental spectrum with a zero area digital filter [3]:

$$C(k) = \frac{2\,(PP^2 - k^2)}{\sqrt{\pi}\cdot PP^3}\cdot \exp\left[-\frac{k^2}{2\cdot PP^2}\right], \qquad (1)$$

where PP = FWHM/2.355 (FWHM - local full width at half maximum of the peak). Due to the large dynamic range of the gamma-ray spectra, and the energy-dependent resolution of the semiconductor detectors, there is a considerable variation of the peak FWHM throughout the spectrum. In the present program, the FWHM is supposed to be a linear function of the channel number. Two coefficients (AM,BM) of the linear function are determined from the input data. The peak search begins with digital filter $C(k)$ calculated for some initial FWHM value. At each subsequent channel, the current FWHM is calculated and compared with initial one. Whenever the current FWHM exceeds the initial one by more than 10%, the digital filter $C(k)$ is recalculated using the current FWHM. The current FWHM becomes a new initial value. It was shown in [4] that the digital filter (1) offers high searching effectivity and, at the same time, it is not

sensitive to local background non-linearities which may give rise to incorrect decisions in some situations.

The peak search starts from some specified spectrum point. For each i-th channel, the following two sums are calculated

$$SC(i) = \sum_{l=-m}^{m} C(l) \cdot S(i-l) , \qquad (2a)$$

$$SCC(i) = \sum_{l=-m}^{m} C(l)^2 \cdot S(i-l) . \qquad (2b)$$

Here, summation limit $m \geq 1.5 FWHM$ is chosen from the condition $abs(C(m)) \leq 0.005 \cdot C(0)$. The convolution (2a) achieves the local maximum at the peak position. In the present program, a peak in the vicinity of i-th channel is declared if the following two conditions are fulfilled

$$SC(i) > SENS \cdot (SCC(i))^{1/2}$$
$$SC(i+1) < SC(i) > SC(i-1) , \qquad (3)$$

where the search sensitivity SENS is an input parameter. For SENS = 3 the probability of the peak detected by the above procedure to be fraudulent is about 3%.

The peak centroid representing the peak position is estimated as weighted average

$$PP(j) = \frac{\sum_{l=i-1}^{i+1} SC(l) \cdot l}{\sum_{l=i-1}^{i+1} SC(l)} \qquad (4)$$

and stored in an auxiliary array $PP(j)$, where j is the peak index in the current multiplet. The maximum value of the convolution SC achieved at the peak position is approximatelly equal to the peak amplitude. The amplitude

estimates for the current multiplet are stored in an auxiliary array $A(j)$. It should be mentioned that for well isolated peaks, the above centroid estimate lies, as a rule, very close to the true value. In the case of two or more overlapping peaks, however, the estimated peak centroids are biased due to peak mutual interferences. The following simple procedure is employed for correcting the biases. For the sake of simplicity, the j-th peak centroid is assumed to be influenced only by its closest neighbours from the left ((j-1)-th peak) and from the right-hand side ((j+1)-th peak). Then the raw centroid estimate $PP(j)$ is corrected by the preseription

$$PP_{cor}(j) = \frac{A(j+1) \cdot K_{j+1} + A(j-1) \cdot K_{j-1}}{A(j)} , \qquad (5)$$

where

$$K_{j\pm1} = D_{j\pm1} \cdot \exp\left[\frac{D_{j\pm1}^2}{4 \cdot FP^2}\right] \cdot \left[1 - \frac{D_{j\pm1}^2}{6 \cdot FP^2}\right]$$

and $D_{j\pm1} = PP(j) - PP(j\pm1)$ is the approximate distance between the relevant peaks. $A(j)$, $A(j+1)$ and $A(j-1)$ are the respective peak amplitudes as estimated in the searching procedure.

The peak search continues until the separation between two subsequent peaks exceeds a critical limit given as a product of chosen factor PMAX and the local FWHM

$$PP(np+1) - PP(np) > PMAX \cdot FWHM . \qquad (6)$$

The parameter PMAX is usually chosen in the interval 2-4 depending mainly on the overall spectrum complexity.

If the above condition is fulfilled, the current multiplet is closed and the np-th peak is declared to be its last peak. The searching procedure is temporarily left and the peak multiplet is evaluated using common non-linear least-squares routine. The limits of the interval of fitting, jy1 and jy2, are given by local spectrum minima which are found by scanning the spectrum intervals $(PP(1)-PMAX\cdot FWHM,\ PP(1)-FWHM)$ and $(PP(np)+FWHM,\ PP(np)+PMAX\cdot FWHM)$ on the respective left and right hand wings of the multiplet.

The spectrum in the fitting interval $jy1 \le k \le jy2$ is approximated by the expression

$$F(k,\bar{P}) = \sum_{j=1}^{np} P(j)\cdot \exp\left(-\frac{(k - P(j+np))^2}{2\cdot P(2np+3)^2}\right) + P(2np+1) + P(2np+2)\cdot k, \qquad (7)$$

where the vector of adjustable parameters P comprises: the peak amplitudes $P(j)$ and positions $P(j+np)$ $(j=1,\ldots,np)$, the coefficients $P(2np+1)$, $P(2np+2)$ of the linear background and the common peak width $P(2np+3) = FWHM/2.355$.

In many instances of practical importance, the fitting procedure becomes more stable and faster if only limited number of parameters is adjusted. In the present program, the number of free parameters is determined by control parameter PR specified in the input data. The following choices are possible:

PR value	Free parameters $(j=1,\ldots np)$	Total number of free parameters, jj
1	$P(j)$	np
2	$P(j)$, $P(j+np)$	2np
3	$P(j)$, $P(j+np)$, $P(2np+1)$, $P(2np+2)$	2np+2
4	$P(j)$, $P(j+np)$, $P(2np+1)$, $P(2np+2)$, $P(2np+3)$	2np+3

The optimal values of the adjustable parameters are obtained by minimization of the functional

$$CH = \sum_{k=jy1}^{jy2} \left(S(k) - F(k,\bar{P})\right)^2 \cdot S(k)^{-1/2}. \qquad (8)$$

In the present program, the standard Gauss-Jordan minimization procedure with only a slight modification is used. To ensure better stability and convergence of the minimization process, especially in the case of close, overlapping peaks, the diagonal elements of the inverted matrix are modified using following semiempirical procedure

$$G(i,i) = G(i,i)\cdot\left(1.0 + DX\cdot\exp(-float(it))\right) \qquad (9)$$

$$DX = 0.05 + 0.1\cdot\left(1.0 - \exp(-0.01\cdot CHNO)\right),$$

where CHNO is the normalized value of the functional (8) calculated for the starting values of the adjustable parameters (for initial parameter guesses see lower) as

$$CHNO = CH/PW, \qquad (10)$$

where PW=jy2-jy1-jj+1 is the number of degrees of freedom (jj is the number of adjustable parameters).

The correction (9) is an increasing function of CHNO and it converges rapidly to unity with increasing iteration number, it.

The initial values of peak positions $P(j+np)$ are obtained directly from the peak searching procedure (see above). The parameters $P(2np+1)$ and $P(2np+2)$ of the linear background are estimated as

$$P(2np+2) = \left(S(jy2) - S(jy1)\right) / (jy2-jy1) \qquad (11)$$
$$P(2np+1) = S(jy2) - P(2np+2) \cdot jy2 \quad .$$

The peak amplitudes are estimated using known peak positions and approximate background coefficients according to

$$P(j) = S(jp) - P(2np+1) - P(2np+2) \cdot jp \qquad (12)$$
$$jp = \mathrm{int}(P(j+np)) \quad .$$

The parameter $P(2np+3)$, common to all peaks within multiplet is estimated as

$$P(2np+3) = AR/(\sqrt{2\pi} \cdot AM), \qquad (13)$$

where

$$AM = \sum_{j=1}^{np} P(j)$$

and

$$AR = \sum_{k=jy1}^{jy2} \left(S(k) - P(2np+1) - P(2np+2) \cdot k\right)$$

is the multiplet net area.

In each iterative step, the value of the functional (8) is calculated with the current parameter values.

The iterative process is finished if the increments of all parameters are less than 1% of current parameter value or if the CH values in two subsequent steps differ by less than 5%. The maximum number of iterative steps is set to 7. In the cases of large multiplets with strongly overlapping peaks the iterative process need not converge. In such situation, the computation is aborted and the program tries to evaluate current multiplet with restricted number of free parameters. In an extreme case, only starting parameter estimates are given as a result.

After the iterative process is finished, the overall quality of the fit is examined. First, the final value of normalized functional (8), CHN, is calculated as in (10). Significant differences of CHN from the expected value of unity may indicate an incorrect fit. Further, the normalized residua are calculated in each channel of the fitting interval according to

$$R(k) = \left(S(k) - P(k, \overline{P}_{min})\right) \cdot S(k)^{-1/2} \quad . \qquad (14)$$

The extreme values of the residua are identified and the correlation function RH is determined as

$$RH = \left(\sum_{k=jy1}^{jy2-1} R(k) \cdot R(k+1) \right) / PW \quad . \qquad (15)$$

High values of RH indicate an incorrect fit. According to [5] the RH-test may be more sensitive than the standard one based on CH.

By inspecting the spectrum of normalized residua $R(k)$, the regions of erroneous fit may be easily identified. In many instances, high positive residua

manifest the presence of another peak which was not found by the searching procedure. If max $R(k) > RES$ (where RES is an input parameter), a new line is assumed automatically at the channel corresponding to the maximum residuum and the whole fitting process is repeated with increased peak number. The number of additional peaks is restricted to 2 in the present program.

The final results of the multiplet evaluation are printed on the line-printer. The output includes the following items:

np - number of peaks in the multiplet,

jy1, jy2 - first and last channel of the fitting interval,

B1, B2 - the values of calculated background at the beginning and the end of the interval,

it - number of iterations performed,

CHNO, CHN - starting and final values of normalized functional CH (8),

RH - final value of the functional (15).

For j-th peak evaluated, the output comprises:

$PKENRG_j$ - position of j-th peak in energy units
$PKENRG_j = P(2np+1) + P(2np+2) \cdot P(j+np)$;

$PKENER_j$ - statistical error in the peak position calculated as
$PKENER_j = \left(G^{-1}(j+np, j+np)\right) \cdot CHN^{1/2}$, (16)
where G^{-1} is pertinent diagonal element of the inverted matrix ;

$PKAREA_j$ - area of j-th peak calculated as
$PKAREA_j = \sqrt{2\pi} \cdot P(2np+3) \cdot P(j)$; (17)

$PKARER_j$ - statistical error in peak area calculated similarly as in (16).

In addition, the results of the fit are shown in graphical form using the subroutine PLOT. The experimental spectrum in the fitting interval is depicted together with the calculated values. The channel numbers and the normalized residua are also given.

3. Specifications

The following principal arrays are employed in the program GSAP:

S(4100) - experimental spectrum (counts per channel)

C(30) - digital filter (1) for the peak searching procedure

CC(30) - squared values of the digital filter C

G(20,20) - matrix of coefficients of the linear equation system of least-squares problem

Q(20) - right hand side vector of the linear equations system

D(20) - the vector of derivatives of the spectrum functional representation (7)

PP(20) - the peak positions within one multiplet estimated in searching procedure and corrected using (5)

A(30) - peak amplitudes estimated in the searching procedure

P(30) - current values of adjuetable parameters. The array is arranged in the following manner:
j=1,...,np - peak amplitudes
j= np+1,...,2np - peak positions
j= 2np+1, 2np+2 - coefficients of the linear background
j= 2np+3 - peak FWHM/2.355

IKS(17) - job name

IJ(50) - evaluated spectra indexes

IS(4140) - auxiliary integer array for temporary storage of the experimental spectrum

ISS(140) - auxiliary integer array

IC(3) - auxiliary array of symbols needed by the procedure plot

IY(120) - buffer array for the PLOT subroutine. It comprises the arranged set of symbols to be printed in current line

JY(3) - auxiliary integer array for the PLOT subroutine.

4. Program structure

The program comprises main body GSAP and two subroutines OHIO and PLOT.

GSAP

The main program performs all input and most of the output operations. It sets the digital filter for the peak searching procedure, performs the peak search, arranges the peaks into multiplets and finds the fitting interval borders. It accomplishes least-squares non-linear fit of each multiplet.

OHIO(N,A,EPS,KN)

This subroutine performs the inversion of the A(N,N) matrix. The inverted matrix is stored in the same array A. N - matrix order, EPS - mashine precision, KN - control parameter (KN>0 - normal performance, KN<0 - singular matrix).

PLOT(A,IB,IC,AA,AB,KX,AX,IY,JY)

This subroutine prints one-dimensional histogram of experimental and calculated spectrum in the fitting interval. Also shown are the channel numbers and the normalized residua (14). The following symbol convention is used:

S - experimental spectrum,

F - calculated spectrum, and

B - background.

The subroutine parameters have the following meaning:

A(3) - numerical values of the experimental and calculated spectrum and the calculated background;

IB, IC(3) - graphical symbols (see above) ;

AA - lower limit of the histogram;

AB - range of the histogram;

KX - current channel number;

AX - normalized residuum in KX-th channel;

IY(3)- auxiliary integer array;

IY(120) - auxiliary buffer array. This array has to be initialized by calling the PLOT subroutine with KX=0.

5. Test data

Test data comprises 210 channels containing a part of the gamma-ray spectrum of ^{57}Co calibration source with the peak energies of 122.06 keV and 136.47 keV.

The second data sample consists of a lower energy part of the gamma-ray spectrum of products from the reaction ^{12}C + ^{nat}Ni measured at 3.65 AGeV at the Dubna synchrophasotron.

6. Applications

Among others, the program GSAP has been also successfully applied in gamma-ray spectra processing from activity measurements of irradiated targets of Cu, Ni, Co, Mn, Ta, Pb, Ag, Au, U and Th with relativistic projectiles (protons, deuterons and ^{12}C-ions) at the Dubna synchrophasotron [6].

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GSAP - программа для анализа гамма-спектров

Программа GSAP осуществляет автоматическую обработку гамма-спектров, измеренных полупроводниковыми детекторами. После ввода экспериментального спектра, калибровочных значений энергий и полуширин, а также параметров, контролирующих процесс поиска пиков, программа начинает поиск гамма-пиков. Обнаруженные пики группируются в мультиплеты, которые фитируются по методу нелинейного МНК в предположении гауссовской формы пиков и нелинейного фона. Программа работает до тех пор, пока не будут найдены параметры всех мультиплетов. По окончании работы программа распечатывает найденные параметры пиков, при этом результаты фитирования представляются в графической форме.

Работа выполнена в Лаборатории высоких энергий ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1989

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GSAP: Fortran Code for Gamma-Spectrum Analysis

The program GSAP performs fully automatic evaluation of gamma-ray energy spectra measured with semiconductor detectors. After the input data comprising experimental spectrum, energy and FWHM calibrations and parameters controlling the peak search are supplied, the program starts peak searching from the spectrum beginning. The detected peaks are arranged into multiplets which are unfolded by standard non-linear least-squares fit assuming Gaussian peak and linear background. The program proceeds until all multiplets are processed. The determined peak parameters are printed and the result of each particular fit is shown in the graphical form.

The investigation has been performed at the Laboratory of High Energies, JINR.

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