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M. Sandoli, A. De Rosa, G. Inghima, E. Perillo, E. Rosato  
and G. Spadaccini: ASPIS: A SUITABLE CODE FOR  
PREEQUILIBRIUM SPECTRUM ANALYSIS.

M. Sandoli, A. De Rosa, G. Inghima, E. Perillo, E. Rosato and G. Spadaccini: ASPIS: A SUITABLE CODE FOR PREEQUILIBRIUM SPECTRUM ANALYSIS.

## 1. - INTRODUCTION.

In a previous report<sup>(1)</sup> it was described a computer program specially suited to spectra analysis. It was clearly stated that major difficulties in such an analysis were:

- a) poor resolution of peaks, overlapping and considerably different widths of them;
- b) presence of noticeable background.

We now present a code which is derived from the previous one in order to extract also physical informations from the background. Such a requisite is important in all the cases when the interest is in the parameters defining the background curve, rather than in those defining the peaks.

Examples of this type of spectra may be found in the preequilibrium nuclear reactions. In these experiments one obtains spectra which show distinct characteristics:

- a number of peaks which are due to particles emitted through a direct mechanism leading to discrete levels in the residual nucleus;
- a continuous distribution of particles which is interpreted as the sum of an evaporation-like emission from the compound system and a particle emission which takes place during the equilibration process of the composite system (pre-equilibrium emission).

A typical example of this kind of spectrum and of this analysis is shown in Figs. 1, 2 and 3.

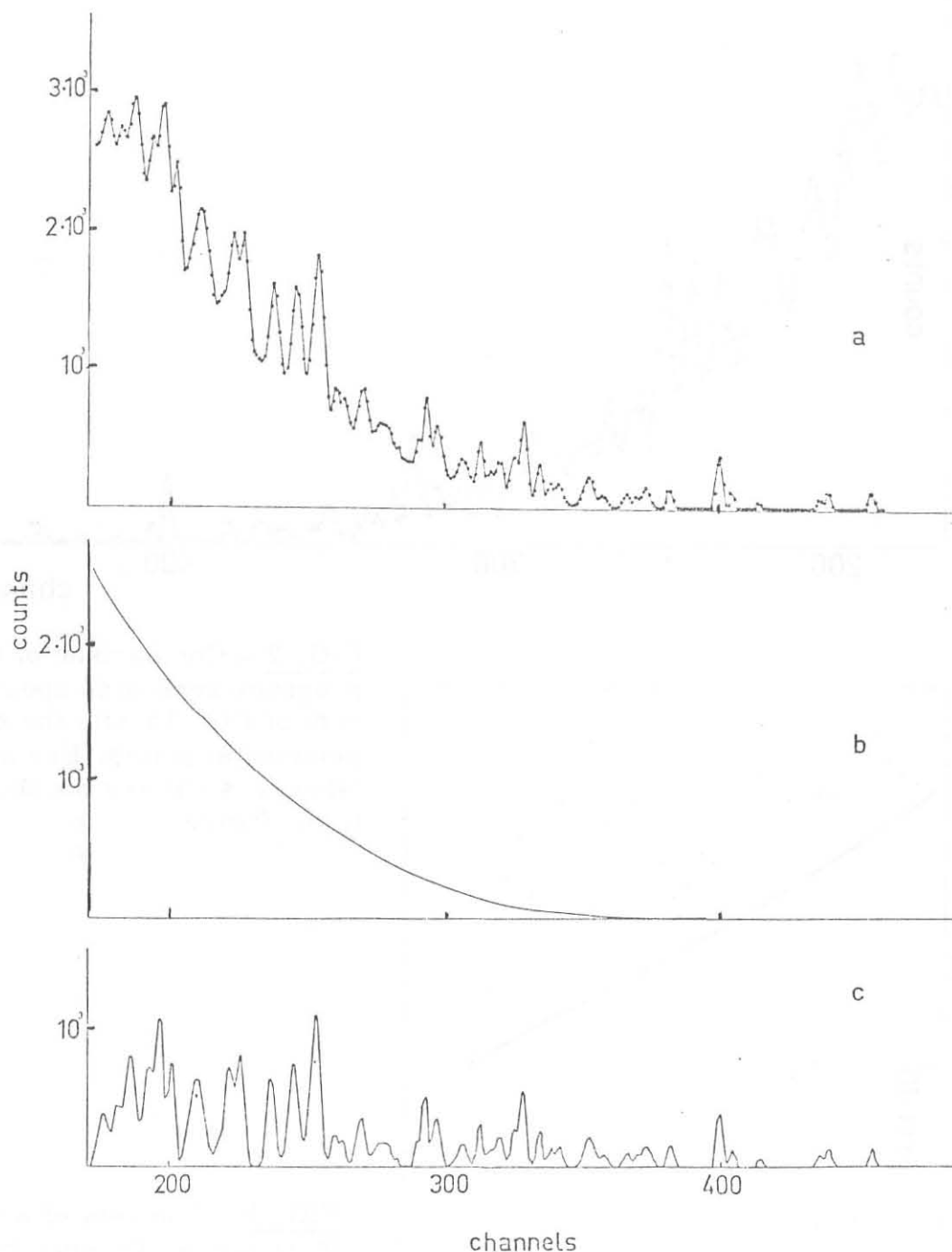


FIG. 1 - Analysis of the proton spectrum from the  $^{25}\text{Mg}({}^3\text{He}, p){}^{27}\text{Al}$  reaction at  $E({}^3\text{He}) = 13 \text{ MeV}$  and  $\theta_{\text{LAB}} = 30^\circ$ . a) Total spectrum generated by ASPIS as the sum of the continuous spectrum b) and of the discrete spectrum c). The continuous spectrum is due to evaporation-like plus preequilibrium emission mechanisms. The discrete spectrum results from a sum of gauss curves corresponding to definite final levels in  ${}^{27}\text{Al}$ .

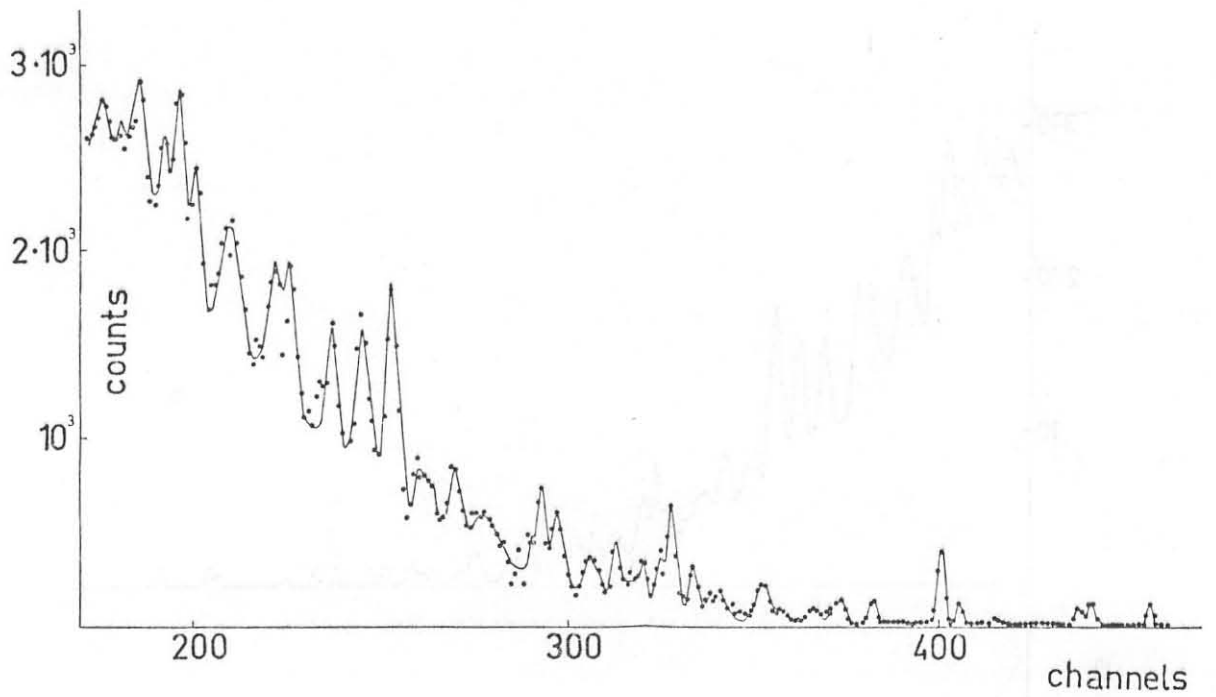


FIG. 2 - Comparison of the program-generated spectrum of Fig. 1a with the experimental points. Errors (always  $< 5\%$ ) are not shown in the figure.

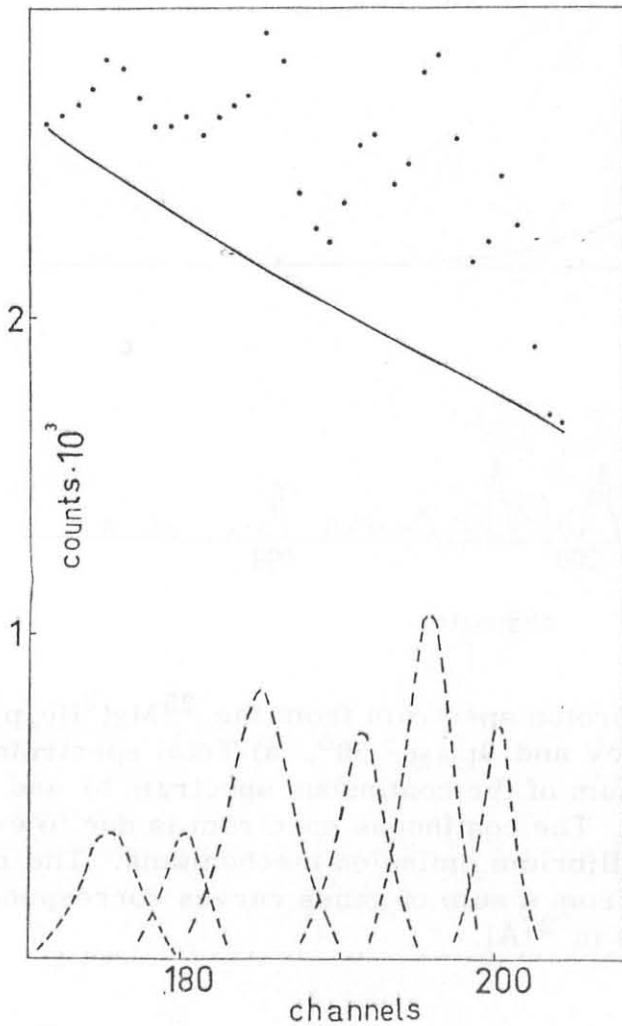


FIG. 3 - Analysis of a single region of the spectrum shown in Figs. 1 and 2. The separation of the various gauss curves (dashed lines) of the discrete spectrum is well evidenced. The solid line represents the continuous spectrum, the dots represent the experimental points.

The shape of the continuous spectrum may be quite altered due to the presence of the various peaks. So a proper determination of its shape cannot be achieved by means of procedures involving any energy average which smooths the peaks in the spectrum.

Thus it is evident that a correct subtraction of the continuous spectrum from the total spectrum is to be obtained before one tries to interpret the experimental results on the basis of any reaction mechanism (i. e. pre-equilibrium emission or evaporation).

This paper contains the description of the code ASPIS for the analysis of spectra, which is particularly suitable in the two cases mentioned above. A functional flowchart is shown in Fig. 4. The code has been widely used in the analysis of many experimental data with very good results.

Some examples are also reported in the text.

## 2. - GENERAL STRUCTURE OF THE PROGRAM.

The numerical method as the starting assumptions are those described in Sections 2 and 3 of Ref. (1).

It can be resumed as follows (see also Fig. 4):

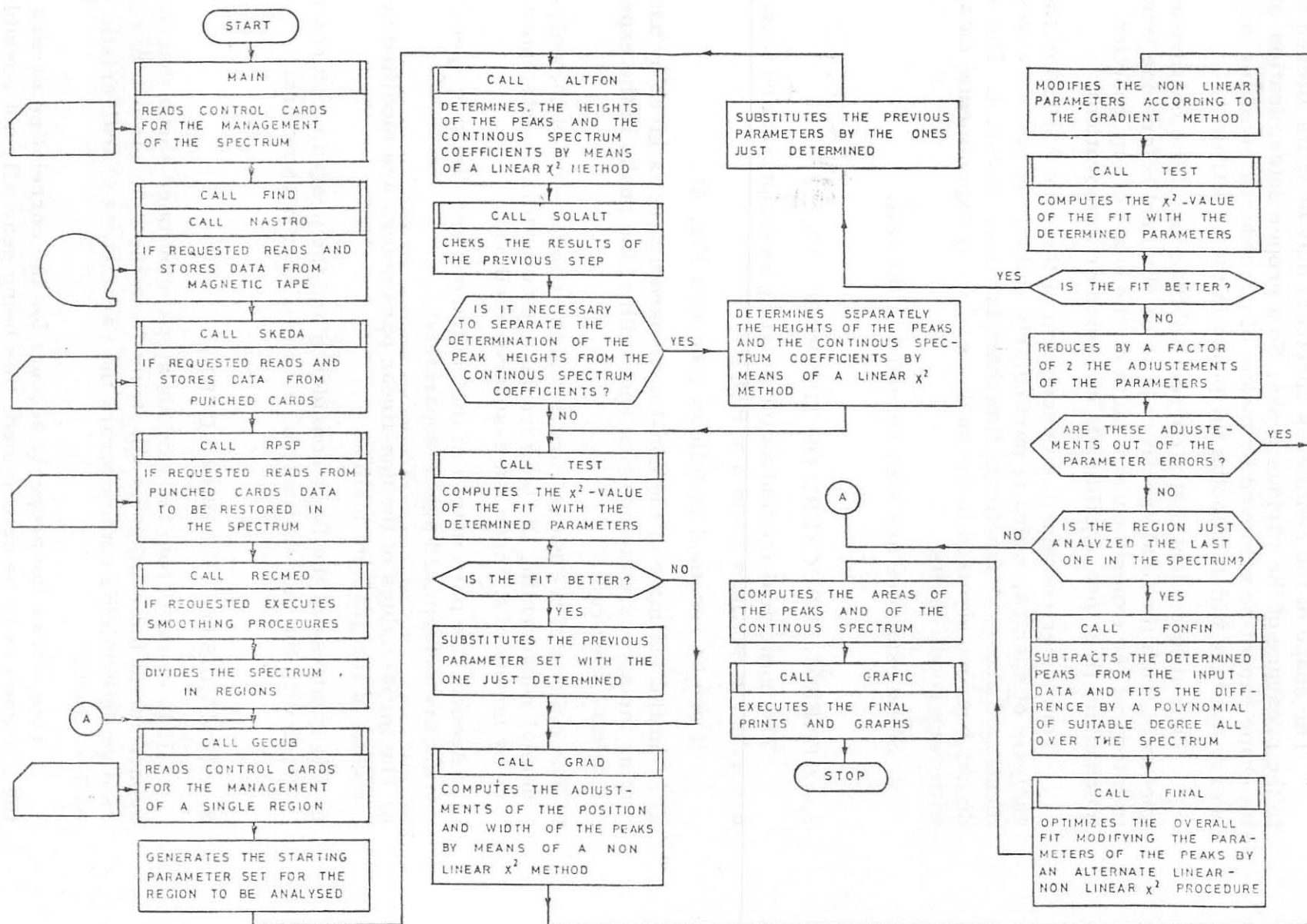
- a) An initial estimate of the non-linear parameters is given by assuming the approximate position and width of the peaks in the experimental spectrum.
- b) The heights of the gauss curves and the coefficients of the polynomial representing the background are determined contemporarily by means of a linear least-squares method.
- c) If needed, the parameters of the continuous and discrete spectrum are determined again (separately).
- d) The initial values of the non-linear parameters are modified by means of the gradient method.
- e) The goodness of the fit is considered and the program returns to step 2 with the new estimate of the non-linear parameters.

## 3. - REMARKS ON THE PROCEDURE.

It is evident from the various steps mentioned above that the separation of the continuous spectrum from the discrete one is carried on determining contemporarily the parameters characteristic of each of them.

This allows the properly account for the correlation errors of the parameters to be determined, this being generally not possible using other methods.

FIG. 4 - Functional flowchart of ASPIS.



However a too bad initial estimate of the non-linear parameters may cause a failure in the determination of the linear ones.

In this case two different results may be obtained :

- the heights of the gauss curves are overestimated, this causing the calculated continuous spectrum to become negative in some points ;
- the continuous spectrum is overestimated, this causing the disappearance of the smallest gauss curves (peaks).

If one of these bad results is obtained, a control in step 3 stops the iterative procedure. The analyses of the continuous and discrete spectrum are separated and the parameters relative to each of them are calculated separately. Thus it is possible to get over the above mentioned ambiguity. The gradient method used in the next step generally may correct the bad estimate. At this point the iterative procedure starts again and the fit is optimized, allowing a contemporary evaluation of all the linear parameters, also accounting for the correlation errors.

The separation of the two spectra in the step 3 is performed by subtracting from the total experimental spectrum a continuous spectrum represented by a polynomial of the requested degree, which is increased or decreased of a constant quantity in order to avoid the negative regions or to make all the peaks stand out from the background.

If the peaks in the spectrum are more than 10, it is necessary to separate the spectrum in regions. In this way not too big matrices are involved in the fitting procedure to avoid very large errors in the calculation of the parameters.

The analysis of the peaks is performed in each of those regions as already described. Then the peaks of all the regions are subtracted from the experimental points and the resulting spectrum is fitted with a polynomial of suitable degree. So the continuous spectrum may be obtained. Finally the parameters of the peaks in each region are readjusted in order to give the best fit of the experimental points as the sum of the continuous spectrum and all the gauss curves. This is performed following the same procedure of steps c), d) and e) of par. 2.

#### 4. - THE CODE.

The code is entirely written in Fortran V and runs on Sperry-Univac 1100 series machines. Presently it requires at least 34,5 kwords of core memory. Using overlays techniques its core occupation can be easily reduced. Also there are no difficulties in order to run the code on non-Univac computers using other Fortran dialects.

5. - CONTROL CARDS FOR PROGRAM USE.

5.1. - Control card for preliminary spectrum handling

Card 1.1.

ISPE, INIZ, IFIN, NAS, LIST, MED, IPUNC, ICON

Format (7X, A3, 7110)

ISPE	Spectrum label
INIZ	First channel to be read
IFIN	Last channel to be read
NAS = 0	Reads spectrum from punched cards (see cards 1.2)
NAS = 1	Prints spectrum list
NAS = 2	Spectrum list and no further analysis
MED = 0	No spectrum smoothing
MED = 1	Smooths the spectrum by moving average method
MED = 2	Restores the contents of some channels (see card group 1.4)
MED = 3	Performs both the previous two options (see card group 1.4)
IPUNC = 0	No output cards after spectrum analysis
IPUNC > 0	Punches output cards after spectrum analysis
ICON = 0	Last spectrum to be read from mag tape
ICON = 1	Still spectra to be read from mag tape after this

Card 1.2

KFON, NZON

Format (2110)

KFON = 0	Does not compute background in the whole region
KFON > 0	Computes background as KFON-degree polynomial in the region
NZON	Number of spectrum regions to be analysed

Card 1.3

AN(I), I = INIZ, IFIN (only if NAS = 0 in card 1.1)

Format (4X, 10F6.0)



AN            Content of the I-th channel (there must be sufficient cards  
1. 3 in order to contain the whole spectrum)

Card 1. 4. 1

NSK (only if MED = 2 or 3 in card 1. 1.)

Format (I8)

NSK            Total number of channels to be restored

Card 1. 4. 2

L(I), IAN(I), I = 1, NSK (only if MED = 2 or 3 in card 1. 1)

Format (4(2I10))

L(I)            Channel number

IAN(I)         Content of the L(I)-th channel

5. 2. - Control cards for various spectrum regions analysis  
(one set of cards for each region)

Card 2. 1

AA

Format (80A1)

AA            Alphanumeric string for region identification (max 80  
chars.)

Card 2. 2

NNMIN, NNMAX, NNPIC, NF, IILOG, INT, ICON, KPU

Format (8I10)

NNMIN         First channel of the region to analyse

NNMAX         Last channel of the region

NNPIC         Number of peaks in the region ( ≤ 10)

NF             Background polynomial degree

IILOG = 0      No plot on line-printer

IILOG = 1      Linear plot

IILOG = 2      Semilogarithmic plot

IILOG = 3      Both linear and semilogarithmic plots

INT = 0      Prints the calculated background between NNMIN and NNMAX  
INT = 1      As above between INTMI and INTMA (see card 2. 4)  
ICON = 0     Another region in the spectrum to be analysed after this  
ICON = 1     No other region to be analysed  
KPU = 0      No output cards for complete plotting of the experimental and fitted spectrum along with gaussian peaks and computed background  
KPU = 1      Punches output cards for complete spectrum plotting

Card 2. 3

IBAR(I), LAR(I), I = 1, NPIC

Format (10(14, 13, 1X)

IBAR          Rough peak position

LAR          Rough FWHM of the peak

Card 2. 4

INTMI, INTMA (only if INT = 1 in card 2. 2)

Format (2I10)

INTMI          Starting channel for background integration

INTMA          Final channel for background integration

5. 3. - Output cards

Fitted peaks data (only if IPUNC > 0 in control card 1. 1.)

ISPE, XY, NDIS, BARC, DBARM, ARE, DARE (one card for each peak)

Format (5X, A3, F8. 0, 3X, I3, 2X, 2F8. 3, 2F9. 0)

ISPE          Spectrum label

XY            Value of IPUNC (can be used to record supplementary information, e. g. incident beam energy)

NDIS          Progressive number of the peak in the spectrum

BARC          Computed position of the peak center of mass

DBARM        Absolute error on BARC

ARE          Computed area of the peak

DARE         Absolute error on ARE

Overall fit data (only if KPU  $\geq$  0 in control card 2. 2)

L, FON, GASC, FUNC, AN

Format (I4, 4(5X, E12. 5)

L	Relative channel number starting from NNMIN until NNMAX
FON	Computed background value
GASC	Sum of the computed peak value
FUNC	Overall computed spectrum
AN	Experimental value

#### 6. - AN EXAMPLE

As an example of analysis it has been chosen a particle spectrum from the reaction  $^{25}\text{Mg}({}^3\text{He}, p){}^{27}\text{Al}$  at  ${}^3\text{He}$  energy  $E({}^3\text{He}) = 13 \text{ MeV}^{(2)}$  (see Figs. 1, 2 and 3).

#### REFERENCES.

- (1) - M. Sandoli, G. Inghima, E. Perillo, E. Rosato and G. Spadaccini, Report INFN/BE-75/3 (1975).
- (2) - A. De Rosa, G. Inghima, E. Perillo, M. Sandoli, R. Bonetti, L. Colli-Milazzo and F. Shahin, Mansoura Sc. Bull. 6 (1979).