A Program of a Computer (KDC-I) for Automatic Data Process of Pulse Height Spectra in Experimental Nuclear Physics

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A program for KDC-I (KYOTO DAIGAKU COMPUTER-I) was developed to analyze automatically spectra obtained from usual multichannel pulse height analyzer which stores informations of energy distribution of emitted particles in nuclear reactions. This code is able to make an automatic search of peaks in the spectrum, a proper background subtraction, and calculations of differential cross sections in lab or cm system with the statistical error.

The constitution and the performance of the code are described with several examples of operation.

Some limiting conditions for the code are : (1) the maximum number of channels to be analyzed must be less than 640, (2) standard full width at half maximum of peaks must be given, and (3) the maximum count in each channel must be less than 10^6.

I. INTRODUCTION

In many experiments in the field of nuclear physics, it often consumes large period of work to process informations stored in the memory of a multichannel pulse height analyzer (MCPHA). Usually, informations are stored in the memory as a pulse height spectrum which has more than one peak, and we need the explicit number of pulses in a single peak with proper subtraction of background counts. For final data, we must further calculate differential cross sections of the event which causes the peak in the pulse height spectrum, using other para-meters associated with the experiment. Finally, the values must be transfered to cm system from lab system.

This process of data reduction can be made automatically by an electronic computer opearated with a suitable program, and can save largely the time which may be consumed with a manual data reduction.

A simplified code for this purpose was described for a computer having rather small number of memories, for example, about 4 K words in the case of KDC-I[1]. The facilities of the code can be improved when the code is modified for a larger computer[2].

II. METHOD OF COMPUTATION

The characteristic methods in this program are in the following two points.

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(1) Background Subtraction

The complex backgrounds which could be prospected are various in kinds, for example, spurious peaks from contaminations in the target material, edge scattering of particles in the detecting system, backgrounds caused by γ-rays and neutrons, and complex combinations of each kind of the background.

Some of them are incapable of prospection in their figures, and considered to be not suitable for automatic data reduction. In many cases, however, we meet a rather uniform or monotonic shape which could be represented by an exponential-like or a smooth curve on which individual peaks are placed.

As the first approach to estimate the background by a computer, we adopted the following method, referring actual data which we have experienced. At first, we give a full width at half maximum (FWHM), Γ, of peaks which must be processed. In an actual case, the Γ is the number of channels in the MCPHA of which we know on an oscilloscope displaying the spectrum stored in the memory, at the beginning of the experiment. The computer searches the channel of minimum counts in each interval of 2Γ-channels from the top (the largest channel number) of the spectrum. If the interval has no concaved minimum, the interval is extended automatically until such a point is discovered. The group of the selected minima (MIN-1) is stored in the memory of the computer. Each two adjacent minima in the group are compared again with each other starting from the larger channel number, and the smaller minimum is chosen as a member of second minima group (MIN-2). Thus we obtain a minimum in each interval of 4Γ.

A kind of background is assumed to be a continuous curve passing through these minima (MIN-2) (On account of rather small number of memory, this code was made to connect each minimum point in adjacent interval with a straight line instead of a smooth curve). When any minimum in the group MIN-1 is below the line, the background is re-estimated regarding the minimum as the new member of MIN-2.

Another kind of background is also estimated by selecting an exponential-like curves through proper minima below which no minimum points in the intervals appear. Generally, the background is minimum or zero at the top (channel) of the spectrum and is increasing monotonously in the lower channels.

The two kinds of estimated backgrounds are always considered into calculation so that the resultant differential cross section of a peak has two values in output printing. When these values differ in each other largely, selection of two values based on experimental specifications or completely another kind of background-estimation may be necessary.

For an example, the lines of background thus estimated by the computer are shown in Fig. 1 (a) and 1 (b) for the spectrum having rather complex figure.

(2) Search of Peaks

To find peaks automatically in the spectrum, the program was so constructed that needs only the FWHM Γ of the peaks. The computer find first the edge of foot of the peak, ch(H), starting from the largest channel number and then search the channel of the maximum count in the interval of 2Γ.
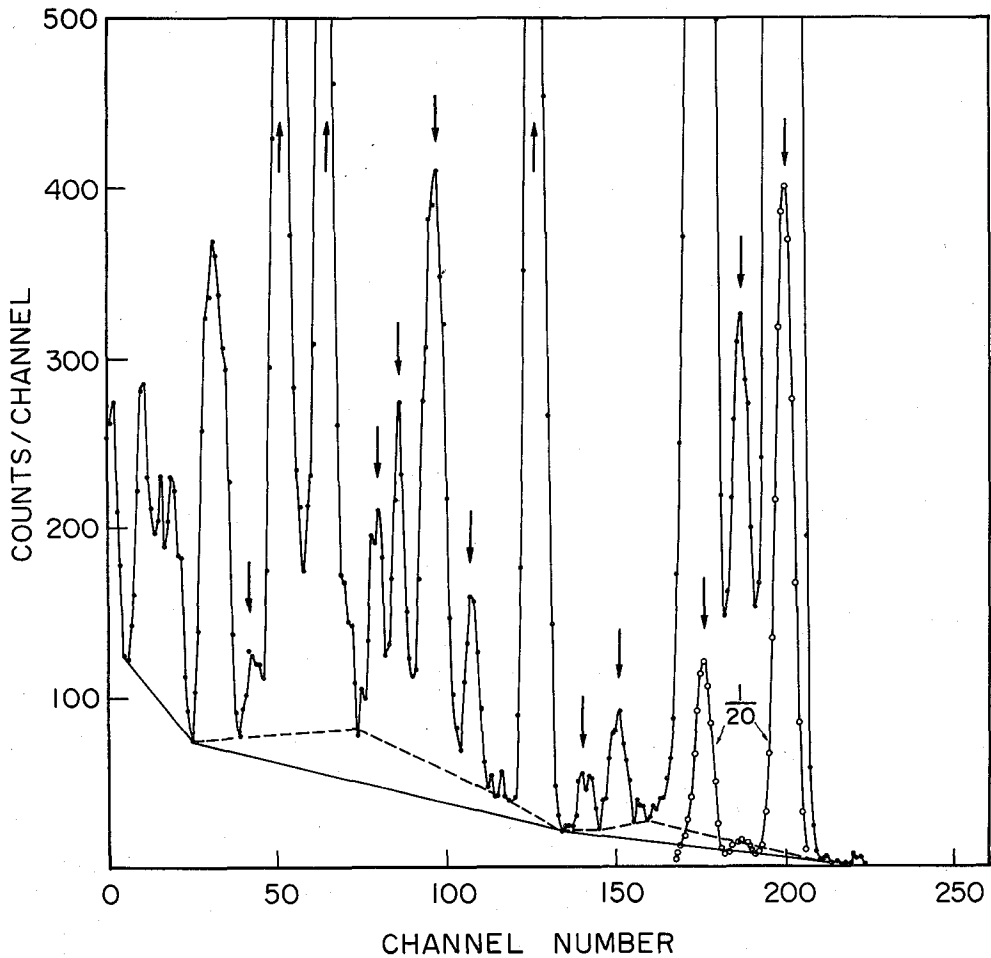
Fig. 1 (a). An example of the background estimation by the computer program. Two kinds of background estimation are made : one is an exponential-like and the other is somewhat over-estimated one. The former (solid line) seems to be preferable in this example. The spectrum shows the pulse height distribution of $Mg^{24}(\alpha, \alpha')$ Mg^{24*} at an angle of 32.5 degree. Arrows show peaks assigned by the computer (see section 5).

In the case of a single and clear peak as shown in Fig. 2 (a) and (b), this process can find the position of the peak, ch(P), easily. In the case of a distorted or complex peak as shown in Fig. 3 (a)-(c), however, the maximum point should be the lowest channel, ch(P), and some peak like that of Fig. 3 (a) would be missed. In these cases the computer searches over again peaks in the narrower interval (i.e., previous one minus one channel) until the peak is found (in the case of (a)) or the interval becomes to zero (in the case of (b)). In the extended interval of $2\Gamma+\Gamma$ starting from the channel ch(H).

When the fluctuation in counts per channel is considerably large as shown in Fig. 3 (c), a spurious maximum point may be determined. The computer cannot reject these spurious peaks automatically in some cases, but such a peak has rather small FWHM and we can select these peaks in the output print of the
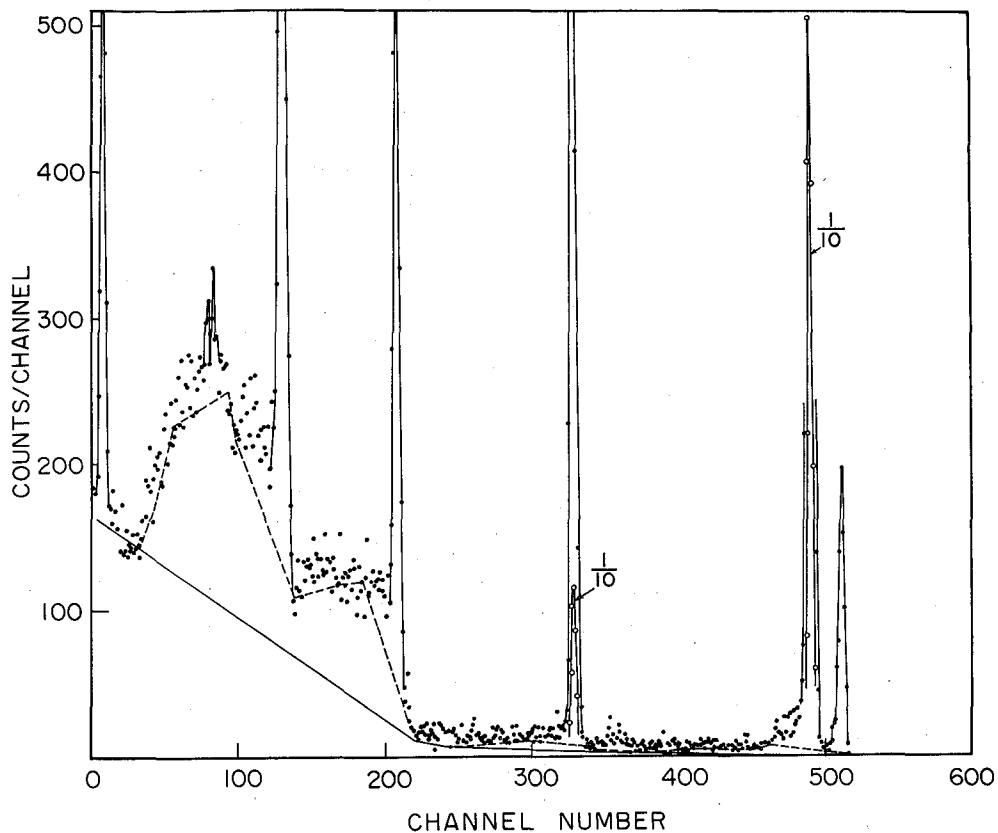
Fig. 1 (b). Another example of the background estimation. The exponential-like background (solid line) seems to be not suitable especially in lower channels. The spectrum is the pulse height distribution in C^{12} $(\alpha, \alpha')C^{12*}$ at an angle of 15.0 degree. The first peak is scattered α-particles from contaminated oxygen.
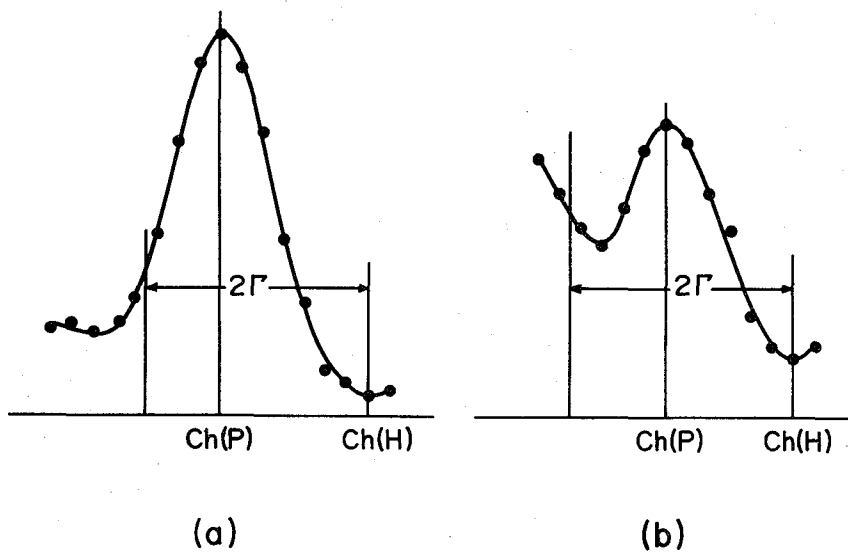

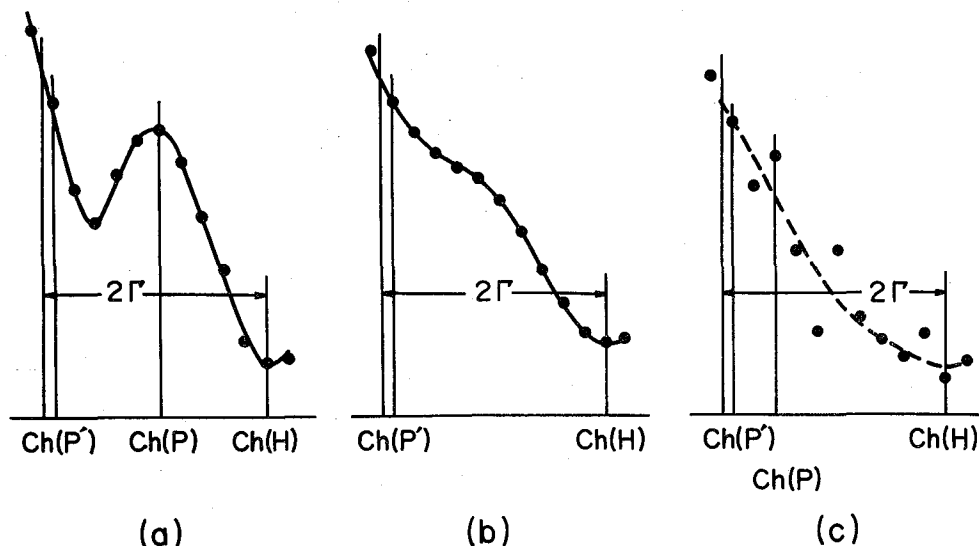
Fig. 2 (a) and (b). Examples of the peak easily assigned.

Fig. 3 (a), (b) and (c). Examples of some irregular peaks : (a) a peak having overlapped foot. (b) overlapped and disappeard peak or a peak having larger FWHM than that of standard vlaue. (c) a peak having fluctuation of counts in channels.

computer (see later section). The data in which peaks are very poor shaped or heavily overlapped are not suitable for this code. However, at least the channel of the maximum count lies near the center of a single peak, some zigzag fluctuations are tolerable in the shoulder of the peak.

After the channel ch(P) is determined, the computer begins to search the minimum, ch(T), in the next 2Γ interval starting from the channel ch(P), by the completely similar manner to the peak hunting. Additional criterion of the minimum search is whether the count in the channel ch(T) is larger or smaller than the background of the channel estimated before under statistical conditions.

Two peaks having foot overlapped each other is separated, for simplicitly, at the minimum point between two peaks. The count in this minimum is devided equally to each peak when the count is larger than one tenth of that of the peak. On the output, $H*\frac{1}{2}$ or $T*\frac{1}{2}$ is printed when the above procedure was made at ch(H) and/or ch(T) respctively. (In the case of heavy overlapping, this simplified procedure is not accurate for calculation of the total count in a peak).

(3) Counts in the Channel and Channel Number in the Computer Memory

When numerical values are treated in floating point (fl.), nine effective digit in decimal system can be stored in a word of KDC-I[1]. We use, for convenience, the first five digit to store the number of counts in a channel in fl. (0~99999), and next four digit (i. e. address part) to the channel number in an integer (0~9999). The calculation on the former part is made by the floating point calculation and that on the latter by the fixed point calculation separately.

III. FLOW CHART OF THE PROGRAM

The flow chart of the program is shown in Fig. 4. The function and constitution of each part are explained as follows :
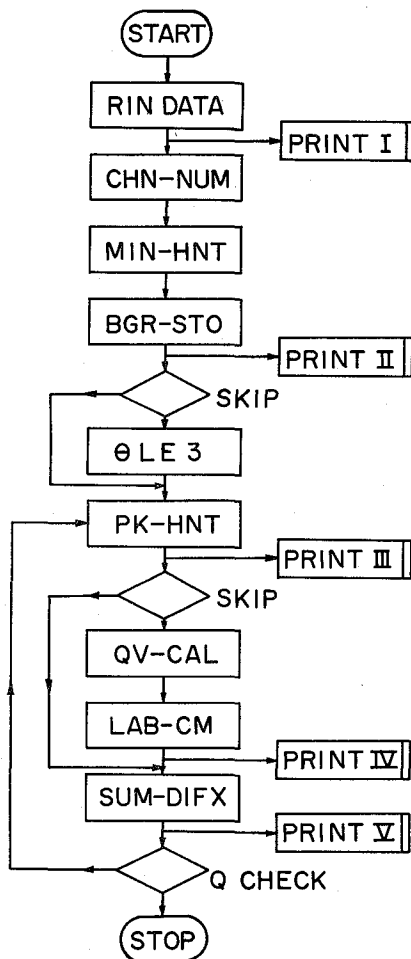

Fig. 4. The flow chart of the program.

Read-in data (RIN DATA)

This code is prepared to read in the computer memory the stored data of the MCPHA punched on a paper tape as a series of numerical values in five digit (maximum 99999 counts in each channel). At the last of the numerical series, it is necessary to punch "30 δ". The computer will start with this sign.

Though the number of words (channels) in the data are arbitrary, the maximum number of channels which can be analyzed is 640 channels (or 640 words). By a limiting condition on the memory capacity, the input data should not exceed 1450 words. If they exceed the limit, informations in higher channels than 640 th channels would be lost. When the input data having 640∼1450 words in length is fed, the computer automatically chooses the 640 words from the last word (the last channel) and exceeded data are deleted.

The read-in program can be changed to be suitable for a special output format of the read-out system of the MCPHA.

To obtain the cross sections in final form, it is necessary in the input data to give informations about the target, nuclear masses involved in the reaction and the integrated beam current etc. (The format to read-in these quantities is described in the later section). However, to find and estimate peaks in the spectrum, only the value of FWHM (Γ) is necessary. The value of Γ must be larger than or equal to 2 channels.

PRINT I

The output printer writes the following title ready after the input data were read-in : for example,

$$\text{ANG 32.50 DEG} \quad \gamma = 6 \text{ (CHM/)}.$$

The title shows the data are obtained at the lab angle of 32.5 degree and the standard FWHM of peaks to be analyzed is over six channels. If the value Γ were not given, the computer stopps here.

When an information about the lowest channel, ch(min) (see later section, "Background estimation and store"), is not given in the input data, a mark CHM/ is printed to call attention.

Channel numbering (CH-NUM)

In this program, a serial number of channels starting from the lowest channel are labeled in the address part of each memory in which the data were stored. To prevent this number is treated as a "count" of event in the channel which has occassionally zero count, all the data stored are added by a meaningless small value (e.g. 10^{-12}) in fl. The number of the last channel, ch(max), is thus counted automatically and recorded on a computer memory.

Minimum hunting (MIN-HNT)

The function of this subprogram is described in section 2.

Background estimation and store (BGR-STO)

To estimate the background, minima are combined with a straight line in two modes as described above. The one is simple connection of adjacent points by a straight line and the other is exponential-like combination. The estimated background of the latter type in each channel is stored in a memory at the first five digit as a floating point mode, and the simple connection background are stored in address part as the fix point (integer) mode. The counts of the latter backgrounds should not exceed 9999 counts per channel.

It is to be noted that when the end of the pulse height spectrum (the lowest channel) is not real spectrum, for example some series of zero count on account of gated coincidence, the background estimation may be false. To secure against the failure, ch(min) must be given properly.

PRINT II

Here the input data are checked whether the informations are complete or not concerning the reaction kinematics, i.e. masses of the incident and outgoing

particles, of the target material, and Q-value of the raction etc. When these informations are complete in the input data, the final differential cross sections can be obtained in absolute values of cm system. If one of these informations is not given, the final values are given in lab system, and M1-E/, Q/ etc. will be printed corresponding to lack of masses or Q-value etc. In this case te program skips hereafter all calculations necessary for transformation from lab tocm system.

Calculation of reaction kinematics (θ LE 3)

When informations concerning reaction kinematics are given, the energy of outgoing particles can be calculated in this subprogram. If we give initially two Q-values and two channel numbers corresponding to two peaks arbitrary chosen in the pules height spectrum, the value of ΔE/ch (energy difference per channel) is calculated assuming the linearity between the energy of particles represented by a peak and channel number. Using this value, the energy of a peak in any channel can be estimated and corresponding Q-value of the peak is calculated in the program QV-CAL.

Search of peaks (PK-HNT)

The main function of this subprogram was described in section 2.

It starts from the largest channel number and begins to scan towards the lower channel number. To prevent mistaking small fluctuations for real peaks, the foot ch(H) of the first peak is assigned only in recognition of that the count increasing at three serial channels separated each other by the interval of $\Gamma/2$ channels.

PRINT III

The channel number of the peak is printed out together with the counts in the channel and two kinds of background counts, for example,

$\sharp$ 200 (7995/E5-9).

This shows a peak was assigned at 200 th channel in which the count of the event is 7995 and the estimated background of exponential-like type is 5 and the other kind background is 9 counts. By the same manner, in the following two lines, informations about ch(H) and ch(T) are printed out.

As was already mentioned, $H*\frac{1}{2}$ or $T*\frac{1}{2}$ is printed when some overlapping of peaks occurs. Besides, notations P ? or Z may be printed for a case shown in Fig. 4 (a) and (b). In the figure, the peak is assigned as a single peak, but it may have a subpeak in lower channels (case (a). Then the notation T*P ? is printed out. In the case (b), the peak show some zigzag shape in higher channels, and the notation H*Z will be printed out.

After a peak was assigned, the FWHM of the peaks is calculated and printed, for example, as $\gamma = 6$. When the value differs from the given FWHM very much, the peak may be heavily overlapped or a spurious peak.

Calculation of Q-value (QV-CAL)

Using the channel number of the peak, ch(P), and ΔE/channel, the energy for the peak is calculated and the Q-value corresponding the peak can be obtained.

If the peak is not a peak desired, the obtained Q-value would show unreasonable value.

Calculation of G-factor and cm angle (LAB-CM)

Here are calculated the angles in cm system and the G-factors by which the differential cross section in lab system is transformed to that in cm system.

PRINT IV

The output printer writes the Q-value, the angle in cm system and the G-factor obtained in the subprogram QV-CAL and LAB-CM. If the input data were not sufficient to calculate these factors, the printing is omitted.

Summing up and calculation of differential cross sections (SUM-DIFX)

The number of counts is summed up from ch(H) to ch(T). In the same interval, the backgronds of two kinds are also calculated.

The differential cross section is calculated by usual procedure together with the statistical error.

PRINT V

The summed counts in the peak and background counts are printed out as follows, for example,

$$TT = 50457 \ (E177\text{-}249).$$

This means the summed count is 50457 (including background counts) and the exponential-like background is 177 counts and the other kind of background is 249 counts in total.

If in the input data there is no information on charge of the incident, integrated beam intencity, dimensions of the slit system of the detector or monitor counts etc., Z/, I/, S/ or M/ etc. will be printed respectively.

The differential cross section is given in unit of cm^2 when all informations are given in the input data, otherwise it is only relative value in arbitrary unit.

Following the value of the cross section, the statistical error is printed in per cent.

Two values of the cross section are calculated for two kinds of background. When the difference in two value is considerably large, one of the background estimation may be unreasonable or both background lines may be improper.

Q-check

When the limiting value of excitation of residual nucleus is given in the input data, the peak hunting is repeated until to find the peak corresponding to the outgoing particles leaving the residual nucleus just above the given height.

If the limit is not given, the program repeats to search peak until to reach the ch(min).

IV. THE FORMAT OF INPUT DATA

To obtain the differential cross section in absolute value or in cm system, parameters listed in Table I are needed before starting calculation. The absolute

Table 1. Input data and format with an example.

Absolute address	Parameter		Unit	Example	
				Value	Format
43	R	Distance from target center to detector	cm	15.0	$+15+2\|$
44	S	Aparture of the defining slit	cm^2	0.04	$+4-1\|$
45	θ_T	Target inclination to incident beam	degree	30.00	$+3000000000\|$
46	IND	For solid target : 0	—	solid	$0\|$
		For gas target : 1	—	—	—
47	T	Target thickness	mg/cm^2	1.00	$+1+1\|$
48	N	Number of atoms (gas target)	/cm^3	(none)	$-1+1\|*$
49	Z	Charge of incident paricle	e	2	$+2+1\|$
50	$M1$	Mass of incident particle	a.m.u.	α-particle	$+4+1\|$
51	$M2$	Mass of target nucleus	a.m.u.	Mg^{24}	$+24+2\|$
52	$M3$	Mass of outgoing particle	a.m.u.	α-particle	$+4+1\|$
53	$E1$	Energy of incident particle	MeV	28.4	$+284+2\|$
54	Q_o	Q-value of the reaction	MeV	0	$0\|$
55	$QX1$, ch$(X1)$	Excitation of residual nucleus (see text)	MeV	0(200)	$+000000200+0\|$
56	$QX2$, ch$(X2)$	Excitation of residual nucleus (see text)	MeV	−5.22(107)	$-522000107+1\|$
57	Q(max)	The maximum excitation of residual nucleus	MeV	−10.0	$-1+2\|$
58	θ_L	Observed angle of the detector	degree	32.5	$+3250000000\|$
59	N_m	Counts of monitor counter	—	50024	$+50024+5\|$
60	N_g	Counts of gate signal	—	104836	$+104836+6\|$
61	I	Beam current	μCoulomb	63.3	$+633+2\|$
62	A	Averaged monitor counts by beam current	—	(none)	$-1+1\|*$
63	ch(min)	The lowest channel number to be analyzed	—	4 th ch.	$+4\|$
64	Γ	Full width at half maximum	—	6 ch.	$+6\|$

* Addresses omitted to put numerical value are to be filled with $-1+1\|$, or must be jumped. In addresses of 45, 58, 63 and 54, zero $(0\|)$ must be stored instead of $-1+1\|$.

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addresses in which these parameters are stored also are listed in the table. To store these values in their proper address, standard procedure[1] in KDC-I is used, namely 0 δ 830100 ω ADDRESS//4 δ must proceed numerical values.

The numerical values must be written in fl. except the values concerning angle and channel. Special expression is used to give $QX1$ and $QX2$. The value QX is the excitation of the residual nucleus and written in fl. expression. In address part of this numeral, the channel number, at which appears the peak corresponding to the residual excitation of QX, must be written in fx. expression. For example, the expression −522000107+1 shows that the peak which appeared at 107 th channel is correponding to particles leaving the residual nucleus at the excitation of 5.22 MeV.

All parameters are not always necessary to process the pulse height spectrum. The withdrawn parameters will be printed out automatically in the output.

V. AN EXAMPLE OF OVERALL PERFORMANCE

In this section the overall performance of the program is shown with an example which is the pulse heigt spectrum shown in Fig. 1 (a). The spectrum was obtained in an experiment of Mg^{24} (α, α') Mg^{24*} at an angle of 32.5 degree. Experimental conditions are shown in Table I as examples of the input data. In this case, the exponential-like background is more preferable than the other kind.

The result in format of the output printer is shown below. (cf. section 3.)

The notation α before the letters CM shows the differential cross sections are not processed with the averaged monitor-by-beam integrator. The latter value must be a constant in ideal case throughout a serial runs under the same conditions, but sometimes shows some fluctuation. A mean ratio would be used
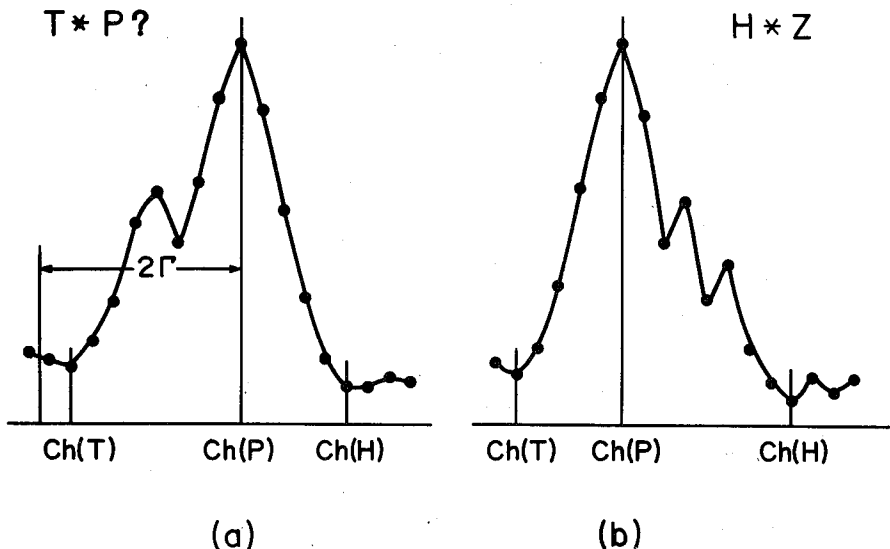

Fig. 5 (a) and (b). Some examples of a deformed peak. (a) The peak may have a sub-peak in lower channels. For this peak, the output printer writes T✳P ?. (b) The peak has zigzag slope in higher channels. The printer writes the notation H✳Z for such a case.

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to average over the individual run. When the process was made, the notation α will disappear.

<div align="center">EXAMPLE</div>

ANG 32.50DEG $\gamma = 6$

♯ 200(7995/E5-9)
210(4/E2-4)
191(153/E7-14)
T✳1/2, $\gamma = 6$
Q = -0.000 37.64DEG G = 0.7710
TT = 50457(E177-249)
I = 63
M = 50024
αCM +3895$-$25(0.4475/), +3890$-$25(0.4485/),

♯ 187(326/E8-16)
191(153/E7-14)
182(148/E9-19)
H✳1/2, T✳1/2. $\gamma = 7$
Q = -0.7346 37.72DEG G = 0.7681
TT = 2328(E227-297)
I = 63
M = 50024
αCM +1621$-$26(2.406/), +1568$-$26(2.522/),

♯ 176(2417/E11-22)
182(148/E9-19)
162(34/E14-29)
H✳1/2, T✳1/2, $\gamma = 6$
Q = -1.354 37.79DEG G = 0.7656
TT = 15995(E331-563)
I = 63
M = 50024
αCM +1205$-$25(0.8157/), +1187$-$25(0.8338/),

♯ 151(92/E17-25)
162(34/E14-29)
145(22/E18-22)
H✳1/2, P ?. $\gamma = 6$
Q = -2.760 37.96DEG G = 0.7596
TT = 882(E305-474)
I = 63
M = 50024
αCM +4397$-$27(5.982/), +3114$-$27(9.025),

♯ 140(55/E19-30)
145(22/E18-22)
134(21/E21-21)
H✳P ?, $\gamma = 5$
Q = -3.377 38.04DEG G = 0.7568
TT = 435(E237-338)
I = 63
M = 50024
αCM +1501$-$27(13.13/), +7376$-$28(28.66/),

# 126(835/E24-30)
  134(21/E21-21)
  120(40/E27-37)
  $\gamma = 6$

  Q = −4.160 38.14DEG G = 0.7530

  TT = 5270(E366-434)

  I = 63
  M = 50024

  αCM +3710−26(1.531/), +3659−26(1.561/),

# 107(160/E34-49)
  112(47/E31-45)
  104(69/E35-52)
  T✳1/2, $\gamma = 5$

  Q = −5.220 38.30DEG G = 0.7477

  TT = 954(E320-437)

  I = 63
  M = 50024

  αCM +4761−27(5.633/), +3884−27(7.213/),

# 97(410/E39-59)
  104(69/E35-52)
  90(112/E42-66)
  H✳1/2, T✳1/2, $\gamma = 7$

  Q = −5.776 38.39DEG G = 0.7447

  TT = 3433(E638-908)

  I = 63
  M = 50024

  αCM +2091−26(2.283/), +1890−26(2.609/),

# 86(264/E44-70)
  90(112/E42-66)
  82(125/E46-73)
  H✳1/2, T✳1/2, $\gamma = 7$

  Q = −6.387 38.49DEG G = 0.7413

  TT = 1524(E474-675)

  I = 63
  M = 50024

  αCM +7817−27(4.260/), +6324−27(5.523/),

# 80(210/E47-75)
  82(125/E46-73)
  74(78/E50-81)
  H✳1/2, T✳1/2, Z $\gamma = 5$

  Q = −6.718 38.54DEG G = 0.7394

  TT = 1318(E489-719)

  I = 63
  M = 50024

  αCM +6159−27(5.127/), +4451−27(7.534/),

# 65(722/E54-80)
  74(78/E50-81)
  58(174/E58-79)
  H✳1/2, T✳1/2, $\gamma = 6$

  Q = −7.548 38.69DEG G = 0.7345

  TT = 5646(E995-1409)

```
I = 63
M = 50024
αCM   +3432−26(1.752/),   +3127−26(1.982/),

♯ 51(697/E61~78)
  58(174/E58~79)
  46(111/E64~78)
  H✳1/2, T✳1/2,  γ = 5

Q = −8.318   38.4DEG   G = 0.7296

TT = 4768(E876−1084)

I = 63
M = 50024
αCM   +2853−26(1.930/),   +2701−26(2.076/),

♯ 42(127/E66~77)
  46(111/E64~78)
  39(77/E67~77)
  H✳1/2,  γ = 6

Q = −8.813   38.94DEG   G = 0.7263

TT = 870(E550~635)

I = 63
M = 50024
αCM   +2334−27(11.78/),   +1711−27(16.54/),
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VI. CONCLUSION

The program is most reliable when the pulse height spectrum to be analyzed consists of a series of independent single peaks on a monotonic background.

For peaks having poor statistics or largely deformed are not so suitable for the program especially when these peaks overlap heavily each other.

If the spectrum includes peaks of different FWHM and the shape of each peak is not regular, a peak having larger FWHM may be detected as overlapped peaks of smaller FWHM. Slight overlap of two regular peaks is permissible for analysis, but the heavy overlap of more than three peaks may be erroneous in estimation of the summed total counts of a separated peak.

The program consists of about 2550 words of instructions and it consumes about several minuits to read-in the main program and a data code. Another several minuits are necessary for the minima hunting and the background estimation. A few minuits more is needed to find a peak, to get the differential cross section and to make output printing.

Somewhat refined program for a larger and faster computer, KDC-II (HITAC 5020) has been also developed and will be reported elsewhere[2].

REFERENCES

1) *KDC-I Manual, vol.* 2(1916), Kyoto University Computation Center.
2) J. Kokame, to be published.