# Beam Optics Studies Using the Monte Carlo Method *

A. A. SUAREZ, E. MAZZILLI and F. A. B. COUTINHO

Divisão de Física Nuclear e Serviço de Cálculo Analógico e Digital,
Instituto de Energia Atômica, São Paulo, SP

(With 16 text-figures)

## I — INTRODUCTION

Due to optical aberrations, a beam of monoenergetic charged particles focused by a spectrometer will appear as a line of a certain finite width $\Delta(B\varrho)$. For convenience $\Delta(B\varrho)$ refers to the full width at half the height of the line. This quantity is experimentally well defined, whereas theoretical calculations usually yield the width at the bottom of the line $\Delta^{o}(B\varrho)$ with a much better definition.

The relative line width $R = \Delta(B\varrho)/B\varrho$ is a constant for given a spectrometer with fixed geometry and is a good measure of its resolution.

For some spectrometers, this quantity and the line profile can be quite well established theoretically. This happens for instance in semicircular spectrometers and in several kinds of double focusing spectrometers [1].

However, when one is involved in coupling complicated particle optics elements, an expression giving the resolution of the system in second or higher order approximations is not always available.

Thus, in order to get an idea of the line profile and resolution, orbits originated from a source with location, size and momentum distribution specified, have randomly been generated by a Monte Carlo method. In this way the resolution function is obtained by recording the number of such orbits of various momenta which enter a specified detector.

The size of this detector is adjustable and its location can be varied about the image point.

At the same time the line profile is recorded in the radial and axial directions for particles which the same momentum.

Another important quantity is the solid angle seen by the source through the defining entrance slits. This parameter, as well as the transmission, which gives the fraction of all monokinetic electrons leaving the source which are counted in the detector, are also obtained with such program.

Multi-strips source arrangements can also be simulated by the program testing the high voltage distribution applied on the sources and estimating the overall transmission which can be obtained by using this trick.

In order to facilitate the programming work, the spectrometers were divided in two types, according to whether the source of charged particles was immersed or not in the magnetic field of the spectrometer. They were named type I and type II respectively.

## II — OUTLINE OF THE METHOD

The programs were developed in FORTRAN II-D for an IBM/360-44 or IBM-1620-

* Received August 28, 1970; presented by José Goldemberg.

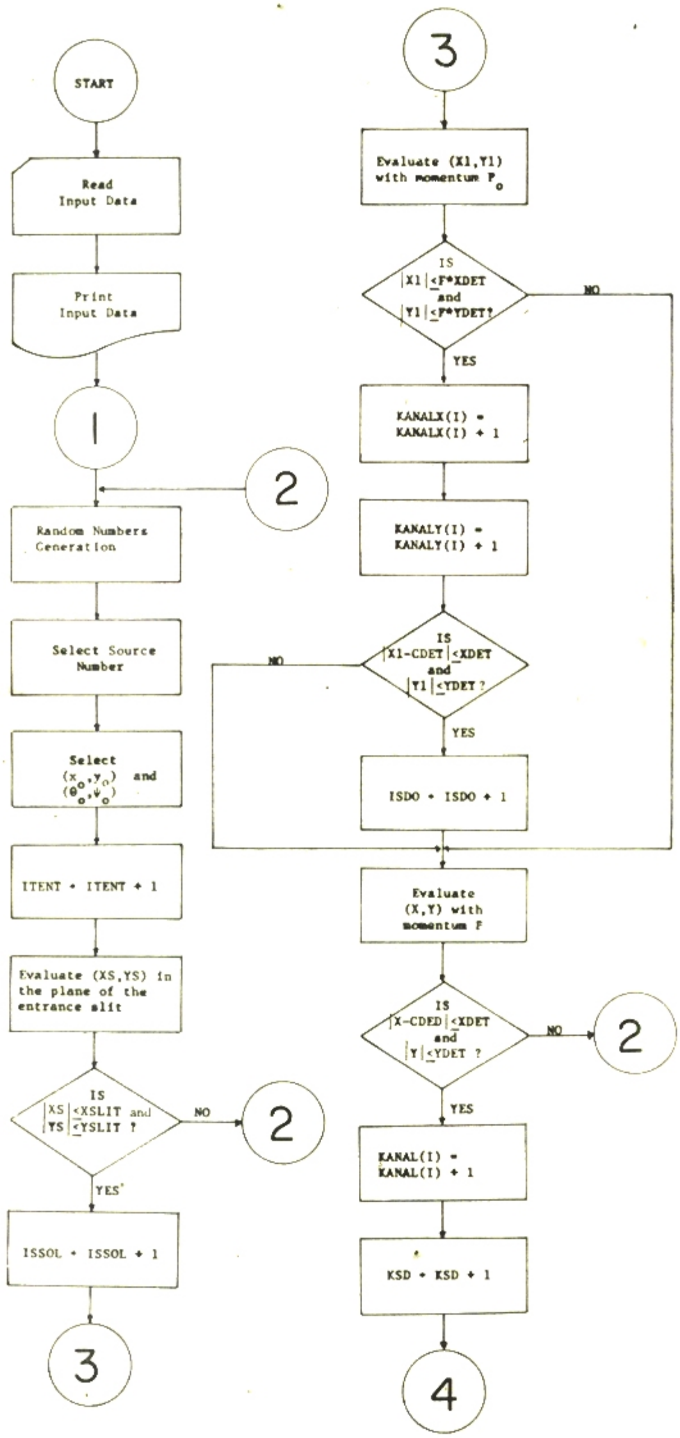


Fig. 1A – Routine for Spectrometer Type I.

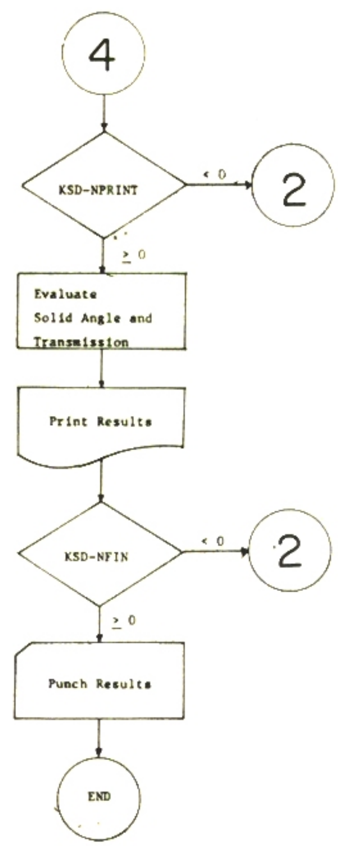


Fig. 1B – Routine for Spectrometer Type I.

-II digital computer, using the Monte Carlo method.

The flowcharts are shown in figures 1 and 2 and a general description of the method will be given.

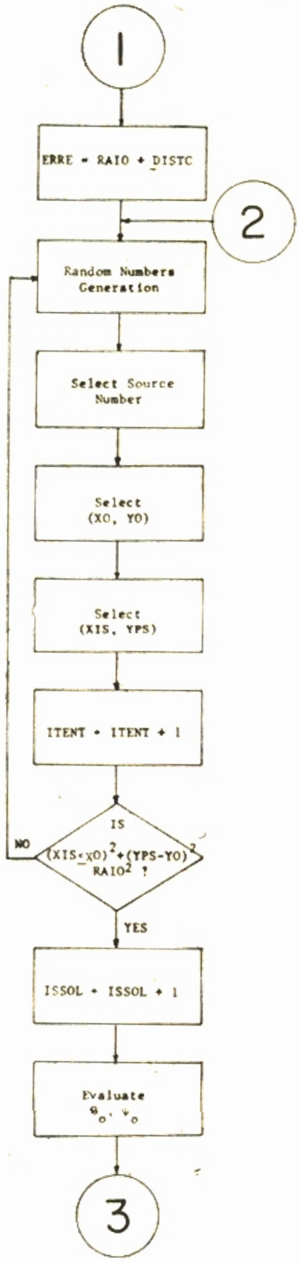


Fig. 2 – Selection of $\theta_o$ and $\psi_o$ for Spectrometer Type II.

The input data are the transfer coefficients, i.e., the coefficients which connect the radial or axial exit coordinates with the input coordinates of the particles [2]; the characteristics of the source, detector and spectrometer; the transfer coefficients corresponding to the entrance slit and the desired number of particles reaching the detector.

The two programs differ only by the way in which $\theta_o$ and $\psi_o$ are selected and as the solid angle is calculated. In the first type, $\theta_o$ is uniformly selected in the interval $|\theta_o| \leq$ TOM and $\psi_o$ from the interval $|\psi_o| \leq$ FOM.

The radial and axial displacements of the particle are then evaluated in the slit position by using the corresponding transfer coefficients. By determining the acceptance of the particles in the spectrometer slit, the solid angle is calculated as a fraction of the solid angle determined by TOM and FOM.

For the second type of spectrometers use is made of the dimensions of the source (or sources) in order to calculate the radius R of a circle centered in the outermost point of the source arrangement which encompasses the spectrometer entrance slit.

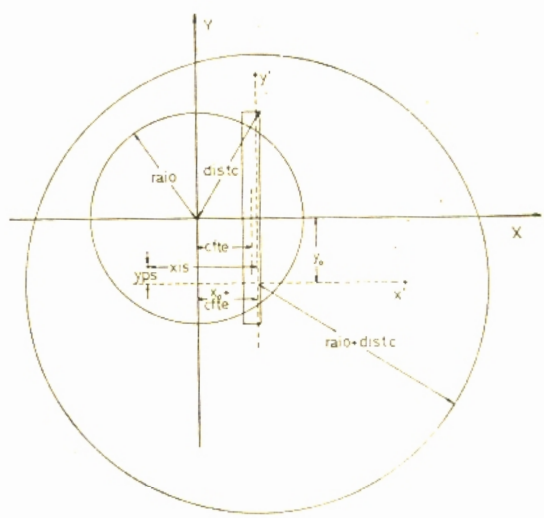


Figure 3

In this circle, points $(x_r, y_r)$ are taken which, when inside the entrance slit of the spectrometer, will enable us to evaluate $\theta_o$ and $\psi_o$ and also the solid angle according to the method suggested by I. R. Williams [3].

The starting point $(x_o, y_o)$, the source number identification, the point $(x_r, y_r)$ and the momentum of the particle are sampled from an uniform distribution randomly generated. Finally the computer evaluates the resulting coördinates (x,y) of the particle after having passed through the spectrometer. If it reaches the detector, a record is made in a channel labelled according to its momentum.

By using the same run, i.e., the same initial conditions, the line profile can be determined by considering all particles, with the same momentum, and by using the relation which connects ($x_o$, $y_o$, $\theta_o$, $\psi_o$, $\delta$) to (x,y) for calculating the resulting coordinates of the particle. Records are then made in channels along the axial and radial directions.

New random numbers are then taken and the procedure is repeated until the detector counter registers N counts; afterwards the solid angle $\Omega$, the transmission T and their standard deviations are evaluated, and printed as well as the resolution function and the axial and radial profiles of the line.

## III — ILLUSTRATION OF THE METHOD

As an illustration of the method outlined above, the resolution function and the line profile following the axial and radial directions were calculated for two beta spectrometers.

The first example is relative to the simplest spectrometer: the semicircular spectrometer with an homogeneous magnetic field.

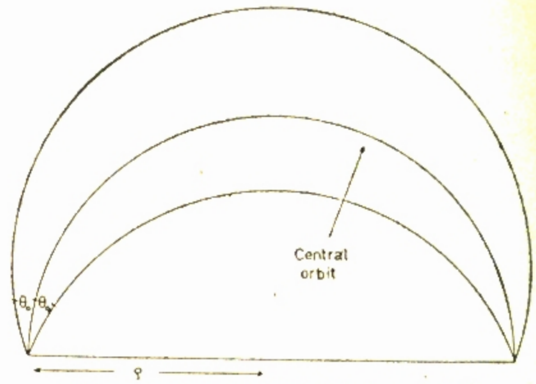


Fig. 4 — Semicircular Spectrometer — Type I.

This kind of spectrometer has been studied extensively by several authors [1].

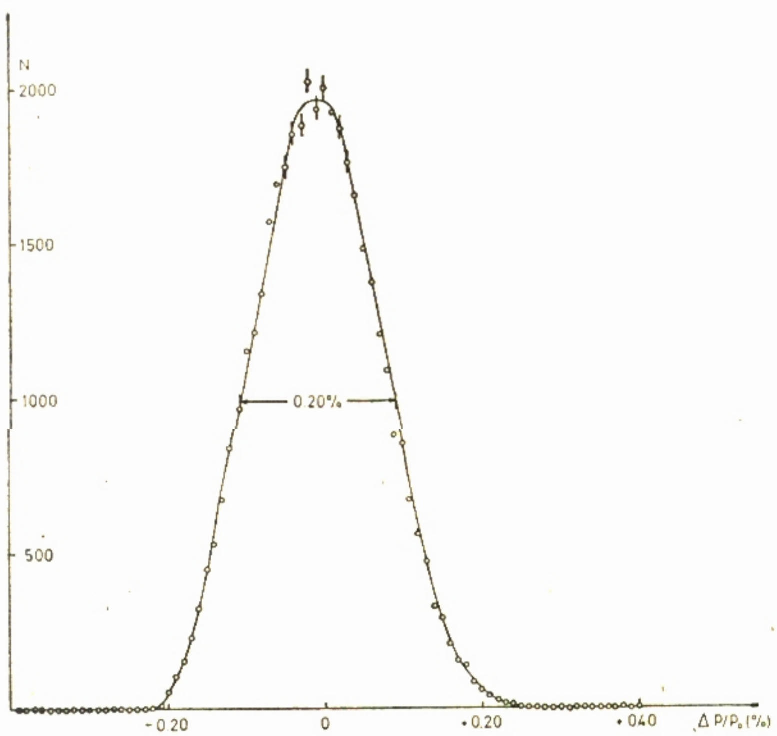


Fig. 5 — Semicircular Spectrometer — Resolution Function.

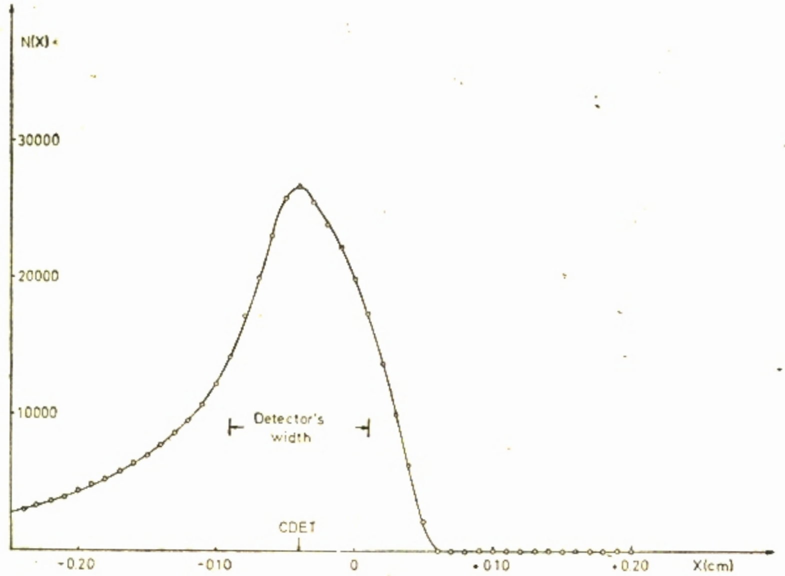


Fig. 6 — Semicircular Spectrometer — Radial Line Profile.

GEOFFRION [4] has particularly made a detailed study of the optimum conditions when a very long source and a correspondingly sized GM counter slit are used with fixed geometry. To illustrate the program developed, this spectrometer was simulated using the parameters utilized by GEOFFRION AND GIROUX [5] and the results are compared in TABLE I and figures 5, 6 and 7.

TABLE I

| Parameters of the spectrometer a) | GEOFFRION AND GIROUX spectrometer [5] | Monte Carlo Method (present work) |
|---|---|---|
| mean radius | 30.5 | 30.5 |
| source and detector width | 0.1 | 0.1 |
| source, detector and slit height | 5.5 | 5.5 |
| slit width | 2.4 | 2.4 |
| slit position | 90° | 90° |
| solid angle | 0.07 % | (0.0706 ± 0.0001) % |
| transmission | — | (0.02815 ± 0.00008) % |
| resolution | 0.25 % b)<br>0.23 % c) | 0.20 % d)<br>— |

a) all dimensions are given in cm
b) theoretical limit of resolution for these geometrical characteristics
c) experimental resolution obtained with F line of thorium
d) instrumental resolution obtained by Monte Carlo method

As can be seen from TABLE I, the results compare quite well with the experiment. Even for the resolution which seems smaller, this is not the case when the natural line width

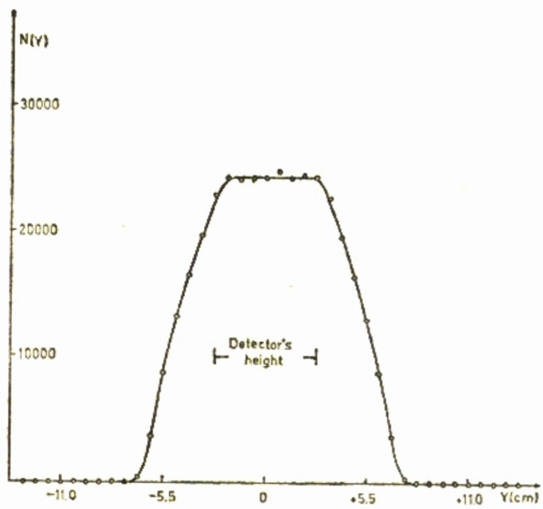


Fig. 7 — Semicircular Spectrometer — Axial Line Profile.

is taken in account. The natural line width of the F line of ThB is according K. SIEGBAHN — vol 2 [1] 65 ev which means a momentum resolution of 0,025%. This added to the instrumental resolution obtained by the Monte Carlo method agrees with the experimental resolution as well as the solid angle calculation does.

Those spectrometers which have the source outside the magnetic field uses the program shown in figure 2. This type of spectrometer is quite convenient when the resolving power is the main characteristic desired and when the access to the source is necessary. On the other hand, the solid angle as well as the transmission are quite small.

In figure 8 is shown an example of this kind of spectrometer which was built in the IEAR-1 research reactor and the simulation presented here corresponds to its parameters.

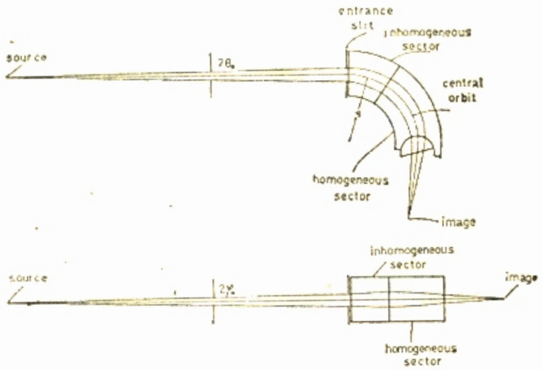


Fig. 8 — Sector Spectrometer — Type II.

TABLE II gives its parameters and also the results obtained with the Monte Carlo simulation which are illustrated in figures 9, 10 and 11.

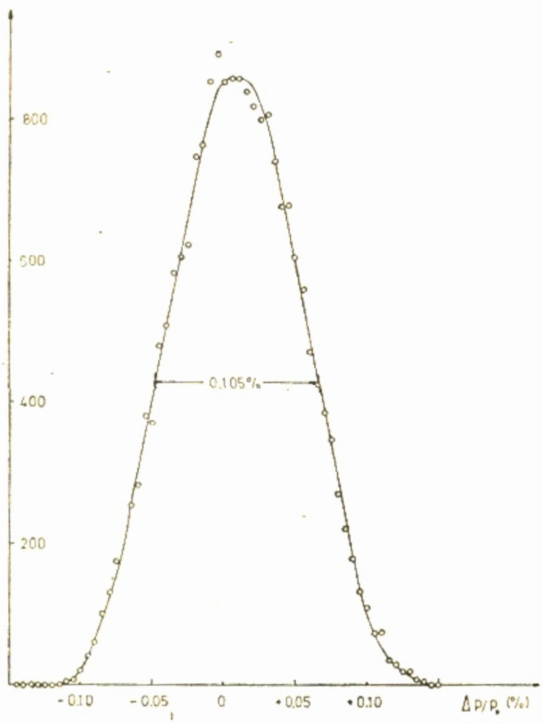


Fig. 9 — Sector Spectrometer — Resolution Function.

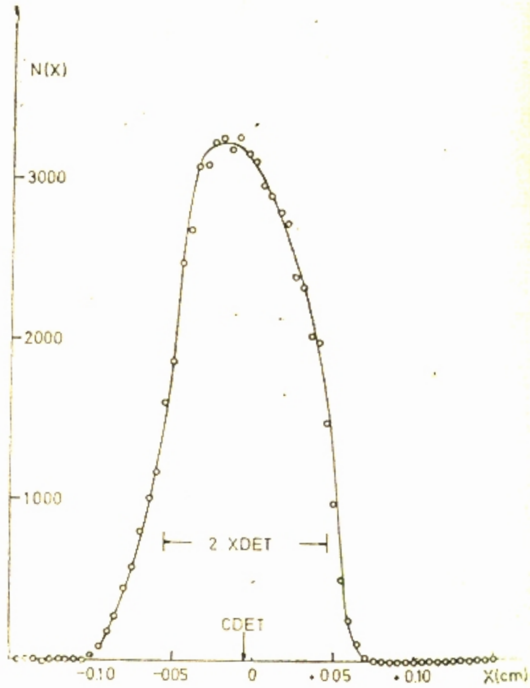


Fig. 10 — Sector Spectrometer — Radial Line Prolife.

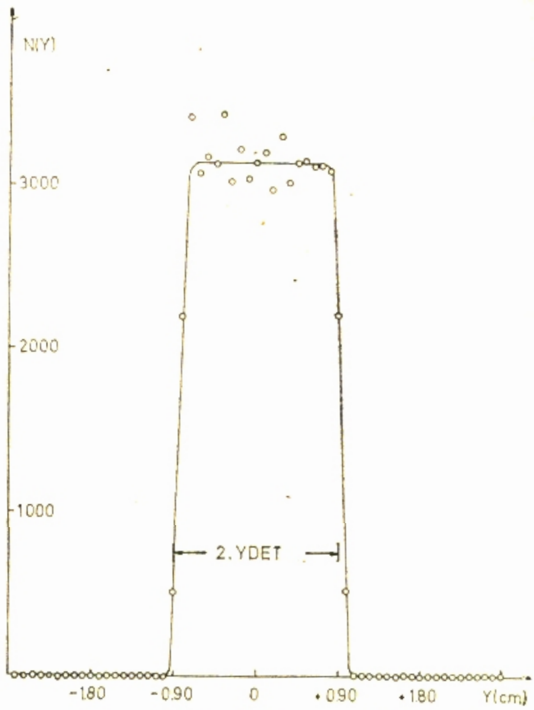


Fig. 11 — Sector Spectrometer — Axial Line Prolife.

In order to increase the luminosity under the limited transmission, it is often desired to enlarge the source area without any impair-

TABLE II

| Parameters and results of the spectrometer type II a) | One source | Seven sources |
|---|---|---|
| mean radius | 50 | 50 |
| overall angular deflection | 95° | 95° |
| source width | 0.60 | 0.865 |
| source height | 6.80 | 6.80 |
| source area | 4.08 | 35.65 |
| detector width | 0.10 | 0.10 |
| detector height | 1.80 | 1.80 |
| $\gamma$ b) | — | 46.15° |
| solid angle | $(0.951 \pm 0.004) \times 10^{-5}$ | $(0.984 + 0.003) \times 10^{-5}$ |
| transmission | $(0.817 \pm 0.007) \times 10^{-5}$ | $(0.812 \pm 0.003) \times 10^{-5}$ |
| luminosity c) | $(3.33 \pm 0.01) \times 10^{-5}$ | $(28.95 \pm 0.09) \times 10^{-5}$ |
| resolution d) | 0.105 % | 0.116 % |

a) all dimensions are given in cm
b) angle between the focal plane and the central orbit
c) source area times transmission
d) instrumental resolution obtained by the Monte Carlo method

ment of the resolution. The multi-strip source technique developed by K. BERGKVIST [6] for the double focussing spectrometer of K. Siegbahn is the best method to increase the source area. He used many source strips and applied an appropriate voltage to each strip.

The principle of the multi strip source technique is illustrated in figure 12. Suppose particles are emitted from two sources at $x = 0$ and $x_o = a$ both on the median plane. When the momenta of the particles from both sources are the same, they are focused at $x = 0$ $(x \mid x_o)a$* respectively, in the first order approximation. When the energy of the particles leaving the second source is appropriate, both sources are focused at the same point. Therefore, if one applies an suitable voltage to the second source, particles of the same energy coming from the two sources are focused at the same point. Whens n strips of sources are used and suitable potentials are applied to each strip, the luminosity is n times larger than for the case of single strip with the same resolution.

However, when use is made of a wide source arrangement the focal plane makes a angle $\gamma$ with the central orbit.

* $(x \mid x_o)$ is the radial magnification of the spectrometer.

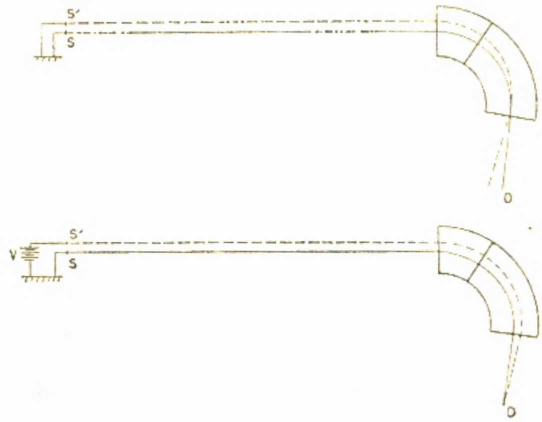


Fig. 12 — Multi-Strip Source Arrangement.

In this case, in order to get the image perpendicular to the central orbit, the source is positioned making an angle $\gamma$ with the central orbit.

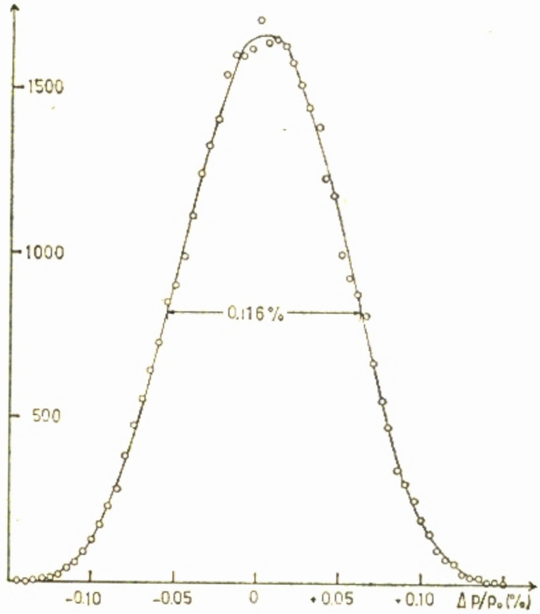


Fig. 13 — Sector Spectrometer with Multi-Strip Source Arrangement — Resolution Function.

Figure 13 shows the resolution function obtained for this spectrometer using 7 sources with voltage compensation. As it can be seen, the resolution does not get worse by use of several strips. In the same way in figures 14 and 15 are displayed the radial and axial line profiles where the voltage distribution can also be checked.

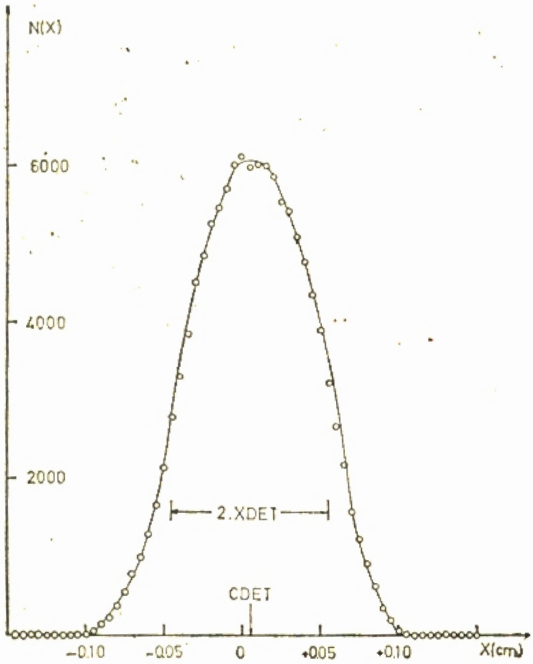


Fig. 14 — Sector Spectrometer with Multi-Strip Source Arrangement — Radial Line Profile.

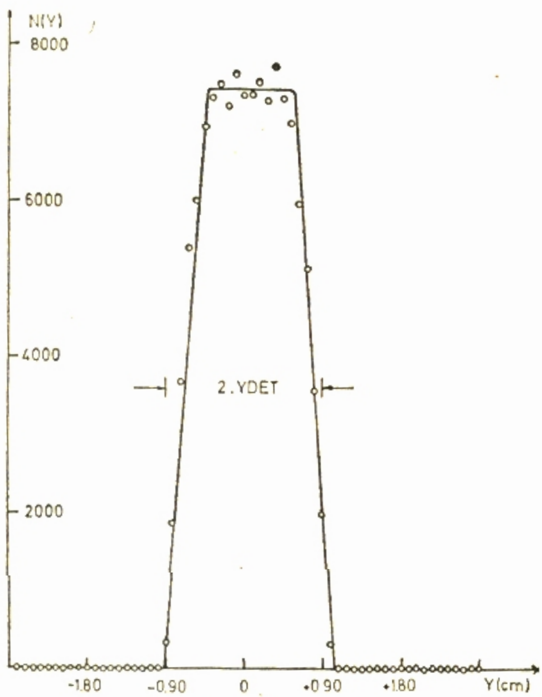


Fig. 15 — Sector Spectrometer with Multi-Strip Source Arrangement — Axial Line Profile.

Finally, in TABLE II a comparison of the characteristics of this new arrangement with the one source arrangement is made.

## IV. COMPUTATIONAL ASPECTS

1. Modifications of the RESOL program and ACC function for IBM-1620-II.

   a) The initial random number IU must contain 10 digits ending by 1, 3, 7 or 9 in the unit position.

   b) Sense switch conditions. Due to the low speed of the 1620 computer, the sense switches 1 and 2 are used for punching of intermediate results to be used as input data in a further processing run.

   c) The ACC function must be replaced by a new one (see list).

   d) The control card *FANDK1010 must be used in the main program and in the ACC subprogram.

2. Number of core storage positions required.

   a) /360-44 — Main: 9656 bytes
      — ACC: 504 bytes

   b) 1620-II — Main: 22400 cores
      — ACC: 322 cores

## ACKNOWLEDGEMENTS

The authors wish to thank PROFESSOR MARCELLO DAMY DE SOUZA SANTOS, for his stimulating interest in and encouragement during the execution of this work. For the computations they gratefully acknowledge the *Departamento de Matemática, Faculdade de Filosofia, Ciências e Letras — Universidade de São Paulo*, for the use of IBM/360 Computer.

## SUMMARY

A computer program using the Monte Carlo method was developped to calculate the line profile and resolution of magnetic spectrometers for charged particles (flat type). The program gives also informations about the solid angle and transmission of the spectrometer as well as the particle distribution in focal plane.

**RESUMO**

Um programa para computador usando o método de Monte Carlo foi desenvolvido para calcular o perfil de linhas e resolução de espectrômetros magnéticos para partículas carregadas (tipo plano). O programa dá também informação sôbre o ângulo sólido e a transmissão do espectrômetro, bem como a distribuição das partículas no plano focal.

**BIBLIOGRAPHY**

[1] "α,β *and* γ *Ray Spectroscopy*", editor K. SIEGBAHN – two volumes.

[2] SUAREZ, A. A., AND F. A. B. COUTINHO, (1967), Matrix Representation for the Calculation of the Second Order Aberrations in Particle Optics for Homogeneous and Inhomogenous (n = 1) Magnetic Fields, *IEA Publication*, n.° 144.

[3] WILLIANS, I. R., ORNL-4099.

[4] GEOFFRION, C., (1949), *Rev. Sci. Instr.*, **20**, 638.

[5] GEOFFRION, C., AND G. GIROUX, (1956), *Can. J. Phys.*, **34**, 920.

[6] BERGKVIST, K. E., (1964), *Ark. Fysik*, **27**, 383.

```
C**** RESOLT
C** RESOLUTION,TRANSMISSION AND SOLID ANGLE CALCULATIONS
C  FOR CHARGED PARTICLES SPECTROMETERS
C** FOR IBM /360
C**** INPUT DATA
C** NOME ... IDENTIFICATION
C** N ... NUMBER OF CHANNELS FOR THE RESOLUTION FUNCTION
C** NX ... NUMBER OF CHANNELS FOR THE RADIAL PROFILE ANALYSIS
C** NY ... NUMBER OF CHANNELS FOR THE AXIAL PROFILE ANALYSIS
C** NPRINT ... DESIRED NUMBER OF PARTICLES REACHING THE
C  DETECTOR FOR INTERMEDIATE PRINTINGS
C** NFIM ... FINAL DESIRED NUMBER OF PARTICLES REACHING THE
C  DETECTOR
C** 2 * XDET ... DETECTOR WIDTH
C** 2 * YDET ... DETECTOR HEIGHT
C** CDET ... DETECTOR CENTER
C** XSLIT AND YSLIT ... DIMENSIONS OF SPECTROMETER SLIT
C** F*XDET AND F*YDET... RANGE OF RADIAL AND AXIAL PROFILES
C  ANALYSIS
C** 2 * DM ... RANGE OF MOMENTUM ANALYSIS
C** IU ... STARTING RANDOM NUMBER
C** KANAL,KANALX,KANALY ... RESOLUTION,RADIAL AND AXIAL
C  CHANNEL COUNTERS
C** NF ... NUMBER OF SOURCES
C** CFTE... CENTERS OF THE SOURCES
C** XX0,XT0,ETC... TRANSFER COEFFICIENTS
C** X0M... SOURCE HALF-WIDTH
C** Y0M... SOURCE HEIGHT
C** T0M... HIGHEST ALLOWABLE VALUE FOR STARTING POLAR ANGLE
C** T0M... HIGHEST ALLOWABLE VALUE FOR STARTING AZIMUTHAL
C  ANGLE
C** NS... NUMBER OF STORIES
C** NES... NUMBER OF PARTICLES PASSING THE ENTRANCE SLIT
C** NSM... NUMBER OF PARTICLES WITH SAME MOMENTUM REACHING
C  THE DETECTOR
C** NRM... NUMBER OF PARTICLES WITH RANDOM MOMENTA REACHING
C  THE DETECTOR
C** NS,NES,NSM,AND NRM ARE ZERO AT FIRST RUNNING
      FX(W,XX0,XT0,XD,XX02,XX0T0,XX0D,XT02,XT0D,XD2,XY02,
     1XY0F0,XF02)=XX0*X0+XT0*T0+XD*W+XX02*X0**2+XX0T0*X0*T0
     2+XX0D*X0*W+XT02*T0**2XT0D*T0*W+XD2*W**2+XY02*Y0**2+
     3XY0F0*Y0*F0+XF02*F0**2
```

```
      FY (W,YY0,YF0,YX0Y0,YT0Y0,YX0F0,YT0F0,YY0D,YF0D)=YY0
     1*Y0+YF0*F0+YX0Y0*X0*Y0+YT0Y0*T0*Y0*YX0F0*X0*F0+YT0F0*
     2T0*F0+YY0D*Y0*W+YF0D*F0*W
      DIMENSION NOME(40),AC(6),KANAL(200),KANALX(200),
     1KANALY(200,CFTE(20),Y0M(20)
      READ 500,NOME
      READ 2200,N,NX,NY,NPRINT,NFIM
      PRINT2200,N,NX,NY,NPRINT,NFIM
      READ 100,XDET,YDET,CDET
      PRINT100,X,XDET,YDET,CDET
      READ 100,XSLIT,YSLIT
      PRINT100,XSLIT,YSLIT
      READ 100,F,DM
      PRINT100,F,DM
      READ 300,IU
      PRINT300,IU
      READ 400,(KANAL(I),I=1,N)
      PRINT400,(KANAL(I),I=1,N)
      READ 400,(KANALX(I),I=1,NX)
      PRINT400,(KANALX(I),I=1,NY)
      READ 400,(KANALY(I),I=1,NY)
      PRINT400,(KANALY(I),I=1,NY)
      READ 200,NF
      PRINT200,NF
      READ 100,(CFTE(I),I=1,NF)
      PRINT100,(CFTE(I),I=1,NF)
      READ 100,XX0,XT0,XD,XX02,XX0T0,XX0D,XT02,XT0D,XD2,
     1XY02,XY0F0,XF02
      PRINT100,XX0,XT0,XD,XX02,XX0T0,XX0D,XT02,XT0D,XD2,
     1XY02,XY0F0,XF02
      READ 100,YY0,YF0,YX0Y0,YX0F0,YT0Y0,YT0F0,YY0D,YF0D
      PRINT100,YY0,YF0,YX0Y0,YX0F0,YT0Y0,YT0F0,YY0D,YF0D
      READ 100,SXX0,SXT0,SXD,SXX02,SXX0T0,SXX0D,SXT02,SXT0D
     1,SXD2,SXY02,SXY0F0,SXF02
      PRINT100,SXX0,SXT0,SXD,SXX02,SXX0T0,SXX0D,SXT02,SXT0D
     1,SXD2,SXY02,SXY0F0,SXF02
      READ 100,SYY0,SYF0,SYX0Y0,SYX0F0,SYT0Y0,SYT0F0,SYY0D,
     1SYF0D
      PRINT100,SYY0,SYF0,SYX0Y0,SYX0F0,SYT0Y0,SYT0F0,SYY0D.
     1SYF0D
      READ 100,(Y0M(JJ),JJ=1,NF)
      PRINT100,(Y0M(JJ),JJ=1,NF)
C** T0M AND F0M ARE GIVEN IN RADIANS
      READ 100,T0M,F0M,X0M
      PRINT100,T0M,F0M,X0M
      READ 9944,NS,NES,NSM,NRM
      PRINT 9944,NS,NES,NSM,NRM
       PI=3.141592654
      ANF=NF
      BN=N
      BNX=NX
      BNY=NY
      PRINT 1500,NOME
      PRINT 1600
    2 DO 5 I=1,6
      AC(I)=2.*ACC(IU)-1.
    5 CONTINUE
      III=(AC(1)+1.)*ANF/2.+1.
```

```
      X0=AC(2)*X0M+CFTE(III)
      Y0=AC(3)*Y0M(III)
      T0=AC(4)*T0M
      F0=AC(5)*F0M
      NS=NS+1
   71 DD=-XX0*CFTE(III)/XD-XX02*CFTE(III)**2/XD
      XS=FX(DD,SXX0,SXT0,SXD,SXX02,SXX0T0,SXX0D,SXT02,SXT0D
     1,SXD2,SXY02,SXY0F0,SXF02)
      YS=FY(DD,SYY0,SYF0,SYX0Y0,SYT0Y0,SYX0F0,SYT0F0,SYY0D,
     1SYF0D)
      IF(ABS(XS)-XSLIT)141,141,2
  141 IF(ABS(YS)-YSLIT)142,142,2
  142 NES=NES+1
      X1=FX(DD,XX0,XT0,XD,XX02,XX0T0,XX0D,XT02,XT0D,XD2,
     1XY02,XYCF0,XF02)
      Y1=FY(DD,YY0,YF0,YX0Y0,YT0Y0,YX0F0,YT0F0,YY0D,YF0D)
      IF(ABS(X1-CDET)-XDET)50,50,51
   50 IF(ABS(Y1)-YDET)52,52,51
   52 NSM=NSM+1
   51 IF(ABS(X1)-F*XDET)30,30,32
   30 IF(ABS(Y1)-F*YDET)31,31,32
   31 X1=X1+F*XDET
      NCX=X1*BNX/(2.*F*XDET)+1.
      KANALX(NCX)=KANALX(NCX)+1
      Y1=Y1+F*YDET
      NCY=Y1*BNY/(2.*F*YDET)+1.
      KANALY(NCY)=KANALY(NCY)+1
   32 D=AC(6)*DM+DD
      X =FX(D ,XX0,XT0,XD,XX02,XX0T0,XX0D,XT02,XT0D,XD2,
     1XY02,XY0F0,XF02)
      Y =FY(D ,YY0,YF0,YX0Y0,YT0Y0,YX0F0,YT0F0,YY0D,YF0D)
      IF(ABS(X-CDET)-XDET)16,16,2
   16 IF(ABS(Y)-YDET)17,17,2
   17 NRM=NRM+1
        D1=DM+DM*AC(6)
      NC=D1*BN/(2.*DM)+1.
      KANAL(NC)=KANAL(NC)+1
      IF(NRM-NRM/NPRINT*NPRINT)2,20,2
   20 TENT=NS
      SD0=NSM
      SSOL=NES
      OMEGA=T0M*F0M*SSOL/(PI*TENT)
      ERROM=SQRT(1./SSOL+1./TENT)
      TRANS=T0M*F0M*SD0/(PI*TENT)
      ERROT=SQRT(1./SD0+1./TENT)
   26 PRINT 1300,NS,NES,NSM,NRM,OMEGA,ERROM,TRANS,ERROT
      PRINT 600,(I,KANAL(I),I=1,N)
      PRINT 600,(I,KANALX(I),I=1,NX)
      PRINT 600,(I,KANALY(I),I=1,NY)
      IF(KSD-NFIM)2,24,24
   24 PUNCH 2200,N,NX,NY,NPRINT,NFIM
      PUNCH 100,XDET,YDET,CDET
      PUNCH 100,XSLIT,YSLIT
      PUNCH 100,F,DM
      PUNCH 300,IU
      PUNCH 400,(KANAL(I),I=1,N)
      PUNCH 400,(KANALX(I),I=1,NX)
      PUNCH 400,(KANALY(I),I=1,NY)
```

```
      PUNCH 200,NF
      PUNCH 100,(CFTE(I),I=1,NF)
      PUNCH100,XX0,XT0,XD,XX02,XX0T0,XX0D,XT02,XT0D,XD2,
     1XY02,XY0F0,XF02
      PUNCH100,YY0,YF0,YX0Y0,YX0F0,YT0Y0,YT0F0,YY0D,YF0D
      PUNCH100,SXX0,SXT0,SXD,SXX02,SXX0T0,SXX0D,SXT02,SXT0D
     1,SXD2,SXY02,SXY0F0,SXF02
      PUNCH100,SYY0,SYF0,SYX0Y0,SYX0F0,SYT0Y0,SYT0F0,SYY0D,
     1SYF0D
      PUNCH 100,(Y0M(JJ),JJ=1,NF)
      PUNCH 100,T0M,F0M,X0M
      PUNCH 9944,NS,NES,NSM,NRM
  302 CALL EXIT
   12 FORMAT(2E18.10)
  100 FORMAT(5E14.8)
  200 FORMAT(5I3)
  300 FORMAT(4I10)
  400 FORMAT(12I6)
  500 FORMAT(40A2)
  600 FORMAT(1H0,10(I3,1X,I5,2X))
 1300 FORMAT(4H0NS=I10/5H NES=I10/5H NSM=I10/5H NRM=I10/
     17H0OMEGA=E14.8,5X,15H PERCENT ERROR=E14.8/
     214H TRANSMISSION=E14.8,5X,15H PERCENT ERROR=E14.8)
 1500 FORMAT(1H ,40A2//)
 1600 FORMAT(/,10(1H ,7HCHANNEL,1X,6HCOUNTS)/)
 2200 FORMAT(3I3,3I6)
 9944 FORMAT(5I10)
        END
```