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EUROPEAN ATOMIC ENERGY COMMUNITY - EURATOM

NEUTOF - A PROGRAM TO CORRECT NEUTRON TIME OF FLIGHT SPECTRA

by

G. VERDAN

1966

Joint Nuclear Research Center
Ispra Establishment - Italy

Reactor Physics Department
Experimental Neutron Physics

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Thanks to the free parameter choice it can be used for many inelastic and elastic neutron scattering problems.
In the optional second section of the main program the generalized frequency distribution of the investigated solid can be calculated.
The programs written in FORTRAN II are listed in chapter 3.

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C O N T E N T S

SUMMARY

Under special consideration of the finite energy width of the incident neutrons and of the finite chopper burst-time a correction computer program is being developed.

Thanks to the free parameter choice it can be used for many inelastic and elastic neutron scattering problems.

In the optional second section of the main program the generalized frequency distribution of the investigated solid can be calculated.

The programs written in FORTRAN II are listed in chapter 3.

I. INTRODUCTION : (°)

The programs in question have been developed in order to correct the neutron time-of-flight data carried out at the Ispra I cold neutron facility [1].

Thanks to a free parameter choice and the exchange possibility of single program parts, this program can also be used for other similar neutron time-of-flight facilities.

Since present investigatements deal mainly with lattice dynamics of solids with impurities [2], [3] , [4] , [5] , the main program NEUTOF PART II calculates in an optional second part the generalized frequency distribution.

The general lay out of the cold neutron time of flight facility is given in Fig. 1.

2. THEORY :

2.1. Corrections in case of monoenergetic incident neutrons and a negligible short burst-time.

2.1.1. The neutron time-of-flight-spectrum

In order to get the real neutron time-of-flight-spectrum, the measured data have to be corrected for background, sample-thickness, air attenuation in the flight path and the counter efficiency.

Background

The slow neutron background in the reactor hall and the epithermal neutron transmission of the chopper lead to a necessery background correction.

$$IC_1(N) = I_A(N) - I_B(N) \tag{1}$$

where $IC_1(N)$ is the background corrected intensity,
$I_A(N)$ the measured intensity value at the analyzer and
$I_B(N)$ the background intensity.

The index N is the analyzer channel number which defines the time-of-flight : $t(N)$ defined in equation (8).

Sample - thickness

As for reasons of intensity the sample has finite thickness, the measured intensity of the scattered neutrons is not exactly proportional to the partial differential scattering cross section.

(°) Manuscript received on March 7, 1966

Absorption and scattering of the incoming neutrons on the one hand, as well as absorption of the scattered neutrons on the other hand falsify the exact proportionality between I scattering and $d^2\sigma/dt\,d\Omega$.

In the case of a geometrical arrangement according to Fig. 2 one obtains :

(2) $$IC_2(N) = IC_1(N) \cdot S(N)$$

with

(3) $$S(N) = Y(N)/[1-\exp(-Y(N))]$$

(4) $$Y(N) = VN \cdot d_1 \cdot [k \cdot \sigma_t(E_i) + l \cdot \sigma_a(E(N))]$$

(5) $$k = 1/\sin\beta$$
$$l = 1/\sin(\alpha-\beta)$$

(6) $$\sigma_a(E(N)) = f \cdot (25.3/E(N))^{1/2}$$

(7) $$E(N) = EBE \cdot (TBE/t(N))^2$$

(8) $$t(N) = N \cdot W + D - t_0$$

where $S(N)$ is the correction factor, VN the number of atoms per ccm. of the sample, $\sigma_t(E_i)$ the total cross section of the incident neutrons in the sample,

$\sigma_a(E(N))$ the absorption cross section of the sample at the neutron energy $E(N)$,

f = $\sigma_a(25.3\,meV)$

EBE : the energy of the reference neutrons

TBE : the time-of-flight of the reference neutrons between sample and detectors

N : the channel number at the analyzer

W : the channel width

D : the preset delay at the analyzer

and to : the time-of-flight of the incident neutrons between chopper and sample.

Air attenuation in the flight path

As the flight path of the facility is not evacuated, part of the scattered neutrons are being absorbed or scattered in the flight path.

The appropriate correction yields :

(9) $$IC_3(N) = IC_2(N)/A(N)$$

with

(10) $$A(N) = \exp[-(g\cdot\{0.2\times\sigma_{to} + 0.8\times\sigma_{tN}\})]$$

(11) $$g = n_A \cdot L$$

where n_A is the number of "air molecules" per ccm in the flight path

L: the flight path length,

σ_{to}: the total neutron cross section of the oxygen molecules and

σ_{tN}: the total neutron cross section of the nitrogen molecules.

Counter efficiency

The calculations are valid for a "two or one layer" BF_3 - counter bank of a geometrical arrangement, given in Fig. 3.

With simple geometrical arguments one obtains for the counter efficiency :

(12) $$C(N) = 1 - \left[\frac{a}{R}\left\{\int_0^R \exp[-2\times\Sigma(N)\sqrt{2Rx-x^2}]\,dx\right.\right. + \left.\left.\frac{b}{R}\left\{\int_0^R \exp[-2\times\Sigma(N)(\sqrt{2Rx-x^2}+\sqrt{R^2-x^2})]\,dx\right\}\right]$$

with

(13) $$\Sigma(N) = dp\cdot(25.3/E(N))^{1/2}$$

where a is the "one" layer", b the "two layer" solid angle portion of the counter bank with the condition a + b = 1

$\Sigma(N)$ the "macroscopic cross section" of the $Be^{10}(n,\alpha)Li^7$ reaction at the neutron energy $E(N)$

and dp = Σ(25.3 meV).

Finally one obtains for the "true" corrected neutron intensity:

(14) $$IC(N) = IC_3(N)/C(N)$$
$$= IC_1(N)\times S(N)/(C(N)\times A(N))$$

or

(15) $$IC(N) = (I_A(N) - I_B(N))\times S(N)/(C(N)\times A(N))$$

2.1.2. The generalized frequency distribution

If necessary, with the present program one can calculate in an optional second section the generalized frequency distribution. If the sample or its impurity (e.g. hydrogen) has an almost entirely incoherent scattering cross section, one can easily calculate the partial differential cross section as it was shown by Zemach and Glauber [6]. Following this formalism Kley et al.[4] found for the incoherent inelastic neutron cross section of one phonon precesses in the band mode region :

(16) $$d^2\sigma/d\epsilon\cdot d\Omega = \frac{1}{8\pi}\times\frac{k_f}{k_i}\times\frac{K^2}{\epsilon}\times[\exp(\epsilon/T)-1]^{-1}\times g(\epsilon) \times \sum_\nu \sigma_\nu^{inc}\times e^{-2W_\nu}\times|C_\nu(\epsilon)|^2 = F(\epsilon)\times G(\epsilon)$$

with

(17) $$F(\epsilon) = \frac{1}{8\pi}\times\frac{k_f}{k_i}\times\frac{K^2}{\epsilon}\times[\exp(\epsilon/T)-1]^{-1}$$

(18) $$G(\epsilon) = g(\epsilon)\times\sum_\nu \sigma_\nu^{inc}\times e^{-2W_\nu}\times|C_\nu(\epsilon)|^2$$

where : $G(\epsilon)$ is the generalized frequency distribution function

$g(\epsilon)$ the "normal" frequency distribution.

The signification of all other symbols in formula (16) is given in [4].

Since $JC(N)$ is proportional to $\frac{\partial\epsilon}{\partial t}\times\frac{d^2\sigma}{d\epsilon\cdot d\Omega}$

one obtains

(19) $$G(\epsilon) \sim JC(N)/F'(N)$$

with

(20) $$F'(N) = \frac{\partial\epsilon(N)}{\partial t}\times F(\epsilon(N))$$

where $\frac{\partial\epsilon(N)}{\partial t}$ is the time to the energy scale convertion factor

Neglecting all the unimportant factors of proportionality one obtains under consideration of:

$$k_i \sim E_i^{1/2}$$
$$k_f \sim (E_i + \epsilon(N))^{1/2}$$
$$k^2 \sim 2E_i + \epsilon(N) - 2(E_i^2 + E_i \times \epsilon(N))^{1/2} \times \cos\alpha$$

and using (17), (20).

(21) $$F'(N) = \frac{(E_i + \epsilon(N))^{3/2}}{E_i^{1/2}} \times \frac{1}{t(N)} \times \frac{(2E_i + \epsilon(N) - 2[E_i^2 + E_i \times \epsilon(N)]^{1/2}}{\epsilon(N)}$$
$$\times \cos\alpha \times \frac{1}{\exp(\epsilon(N)/T) - 1}$$

where E_i is the energy of the incident neutrons

$\epsilon = E_{final} - E_i$:
the energy transfered to the neutron upon scattering

α : the scattering angle (see Fig. 2).

T : the temperature of the sample in unities of energy

$t(N)$: the time-of-flight (see formula (8)).

In order to have also the possibility to calculate the normal frequency distribution function g (E) in case of a monoatomic cubic incoherent scatterer (e.g. Vanadium), the program replaces $F'(N)$ in formula (19) by F" (N) as given in (22).

(22) $$F''(N) = F'(N) \times \exp(-2W(N))$$

with

(23) $$\begin{aligned} W(N) &= a'(T) \times k^2(N) \\ &= a(T)[2E_i + \epsilon(N) - 2(E_i^2 + E_i\,\epsilon(N))^{1/2} \times \cos\alpha] \end{aligned}$$

where $W(N)$ is the Debye Waller exponent

$a(T)$: is the temperature dependent prefactor of the Debye Waller exponent (Apart from numerical factors the mean square amplitude $\langle \bar{x}^2 \rangle_T$).

By taking $a(T) = 0$ one obtains $F'(N)$ according to (21), as it is necessary to get the generalized frequency distribution function (19).

2.2. Corrections in case of finite energy width of the incident neutrons and finite chopper-burst-time.

In case of replacing E_i by $\overline{E_i}$; $\epsilon(N)$ by $\overline{\epsilon(N)}$ and $F''(N)$ by $\overline{F''(N)}$ the formulas given in chapter 2.1. are valid without any restrictions, also for finite energy width of the incident neutrons and finite chopper-burst-time.

2.2.1. A method to determinate the spectrum of the incident neutrons

By measuring the time of flight spectrum of a completely incoherent scattered (e.g. Vanadium) one can calculate from the "elastic" part of the spectrum the incident neutron distribution.

Following the derivation of Zemach and Glauber [6] the cross section for elastic scattering in the case of a small Debye Waller exponent W is given by :

$$\left(\frac{d\sigma}{d\Omega}\right)_{el} \sim \sigma^{inc} \times \exp(-2W) \tag{24}$$

therefore

$$I_i(N) \sim IC(N) \times \exp(+2W) \tag{25}$$

The energy dependence of the Debye Waller exponent is given in the first approximation by fromula (23). Especially for elastic scattering one obtains :

$$W_e = 2E_i \times a(T)(1 - \cos\alpha) \tag{26}$$

$a(T)$ is a temperature and material dependent factor (essentially the mean square amplitude of the lattice vibrations).

In the NEUTOF - SPECIAL Program (see 3.1.) the distribution $I_i(N)$ of the incident neutrons is calculated according to formulas (25) and (26).

2.2.2. The mean energy and time-of-flight values

If the incident neutron distribution $I_i(t_o)$ as well as the burst function[1] T (to,ts) are known, the mean value $\bar{f}$ (t) of a arbitrary to and ts dependent function f (t, t_o, ts) can be calculated as follows:

$$\bar{f}(t) = \iint_{t_o, t_s} I_i(t_o) \cdot T(t_o, t_s) \cdot f(t, t_o, t_s)\, dt_o\, dt_s \times \Big/ \iint_{t_o, t_s} I_i(t_o) \times T(t_o, t_s)\, dt_o\, dt_s \tag{27}$$

by replacing f (t, to, ts) by the transfer energy function

$$\epsilon(t, t_o, t_s) = EBE \times \left(TBE_1^2 / (t - t_o - t_s)^2 - TBE_2^2 / t_o^2 \right) \tag{28}$$

one obtains from (27) the value of the average energy transfer $\bar{\epsilon}$(t).

On the other hand by replacing f (t, to, ts) by the incident energy

$$E_i(t_o) = EBE \times TBE_2^2 / t_o^2 \tag{29}$$

---

1) The burst function is the time dependence of the neutron transmission through the chopper as a function of the incident neutron velocity $v_i \sim \frac{1}{t_o}$, and the chopper slits position (ts). (See Fig. 4.) Generally the burst function of the chopper is a determinated function dependent on to and ts. However in our case this function is independent on to and can be approximated by the function T (ts) = $1/BB$ for $-BB/2 \leq ts \leq +BB/2$, what simplifies considerably the numerical calculations.

one obtains from (27) the average energy value of the incident neutrons $\overline{E_i}$.

The average final energy value of the neutrons is therefore given by

$$\overline{E_{final}}\,(N) = \overline{\epsilon}(N) + \overline{E_i} \tag{30}$$

Finally by setting to on the place of f (t,to,ts) one obtains the average value of the time-of-flight of the incident neutrons between the chopper and the sample : $\overline{t_o}$.

The meaning of the different symbols used in (28) and (29) are:

EBE : Energy of the reference neutrons

TBE_1 : Time-of-flight of the reference neutrons from the sample to the counters.

TBE_2 : Time-of-flight of the reference neutrons from the chopper to the sample.

t : total time-of-flight from the chopper to the counters.

to : time-of-flight of the incident neutrons, between the chopper and the sample.

ts : time-variable of the burst-function.

2.2.3. The mean value of the F-factor

By replacing E_i and $\epsilon(N)$ in formulas (21),(22) and (23) by their mean values $\overline{E_i}$ and $\overline{\epsilon}(N)$, one also obtains a mean value for the F-factor. In a large energy range (5 - 60 meV) these results are sufficient precise. Above this range (60 - 200 meV) the F-factor calculated in this way is generally too small, because of overestimation of the higher energy contribution. In order to overcome this difficulty the mean F-factor $\overline{F''}(t)$ is calculated according to formula (27), by replacing f (t,to,ts) by F" (t(N)) of formula (22).

At this place it is to be pointed to the fact that the calculations of paragraphs 2.2.2. and 2.2.3. are not real resolution corrections, though the finite resolution influences much the results.

The mean values $\bar{\varepsilon}(N)$, $\bar{E}i$, $\bar{\tau}o$ and $\bar{F}''(N)$ are calculated by the NEUTOF PART I Program, given in section 3.2.
Finally the main program NEUTOF PART II (see section 3.3.) calculates the corrected neutron spectrum IC(N) and in the optional second section the generalized frequency distribution G(E), the normalized generalized frequency distribution as a function of the energy GN(E), and the normalized generalized frequency distribution as a function of the frequency. GN(ν).

3. PROGRAMS

The only reason of this chapter is to give some directions of use for the three programs. Therefore no particular explanations to the coding system are given.
The reader should note, that because of practical reasons the symbols used in the FORTRAN programs are not throughout the same as those of chapter 2.
All the programs are written in FORTRAN II Version 3 for the IBM 7090 Data Processing System.

3.1. NEUTOF - SPECIAL Program

NEUTOF - SPECIAL is a program to calculate the corrected time-of-flight spectrum of elastically scattered neutrons.
Therefore it can be used to calculate the spectrum of the incident neutrons $I_i(N)$ according to the equations (15), (25) and (26).

The sequence of the Input Data and the signification of the several symbols are given in Table[1) I.

---

1) For further informations on Format Statements please refer to the program Listing.

For control purposes the detailed intermediate and final results are printed.
Only the main results Ii(N) are punched in cards for Input use to the NEUTOF PART I program.

Table I. Input Data Sequence for the NEUTOF SPECIAL Program

DATA SYMBOL	SIGNIFICATION
A1(1), B1(1) . . . . A1(15),B1(15)	A1(N) : Energy in channel N B1(N) : Total neutron cross section of oxygen molecules at the energy A1(N)
A2(1), B2(1) . . A2(18),B2(18)	A2(N) : Energy in channel N B2(N) : Total neutron cross section of nitrogen molecules at the energy A2(N). A1,B1,A2,B2 are used to calculate A(N)
M	Number of channels of the spectrum
TBE	Time-of-flight of the reference neutrons from the chopper to the counters.
W	Channel width
D	Delay at the analyzer
TOP	Delay of the pick - up
The Data from M to TOP are given as ordinary whole numbers.	
VN	Number of atoms per ccm. of the sample in 10^{23} - units.
STNO	Total neutron cross section of the incident neutrons in the sample
D1	Thickness of the sample
F	Absorption neutron cross section, at 25.3 meV of the sample
EBE	Energy of the reference neutrons
A	"One-layer" solid angle portion of the counter bank.
B	"Two-layer" solid angle portion of the counter bank. A + B = 1

Cont. Table I

DATA SYMBOL	SIGNIFICATION
R	Radius of the BF_3 detectors
VK	$1/\sin\alpha$ see Fig. 2.
VI	$1/\sin(\alpha-\beta)$ see Fig. 2.
VH	Normalisation factor of the measured spectrum
VI	Normalisation factor of the background spectrum
CFA	$\cos\alpha$ see Fig. 2.
The Data from VN to CFA are given as ordinary floating point numbers.	
AT	Temperature dependent pre-factor of the Debye-Waller exponent (see (23),(26))
DP	Macroscopic cross section of the $B^{10}(n,\alpha)\,Li^7$ reaction in the BF_3 detectors in cm^{-1} at 25.3 meV.
G	"Air molecules" per qcm in the flight path = number of "air molecules" per ccm x flight path length
The Data from AT to G are given as a decimal fraction times a power of ten	
The Data from M to G are read into the program by the SUBROUTINE LECDO.	
IO(1) .... IO(12) .... IO(M)	IO(N) : Background Intensity in channel N
IN(1) .... IN(12) ....IN(M)	IN(N) : Measured Intensity in channel N

Note : All times are given in microseconds, the distances in centimeters, the energies in millielectronvolts and the cross sections in barns.

```
      COMMON NID,NFD,CN,NC
      DIMENSION AN(600),CM(600),EN(600),IN(600),IO(600),CN(600),SN(600),
     1TN(600),VIC(600),TOV(600),A1(20),B1(20),A2(20),B2(20),NC(30),CN(30
     2)
      FINTF(X)=EXPF(PSR*SQRTF(X*(2.-X)))*(A+B*EXPF(PSR*SQRTF(1.-X*X)))
      REWIND 10
      I1=15
      I2=18
      READ INPUT TAPE 5,60,(A1(I),B1(I),I=1,I1)
      READ INPUT TAPE 5,60,(A2(I),B2(I),I=1,I2)
      I11=I1-1
      I21=I2-1
      WRITE OUTPUT TAPE 6,59
      NID=5
      NFD=18
      CALL LECDO
      M=NC(1)
      TBE=NC(2)
      W=NC(3)
      D=NC(4)
      TOP=NC(5)
      VN=CN(6)
      STNO=CN(7)
      D1=CN(8)
      F=CN(9)
      EBE=CN(10)
      A=CN(11)
      B=CN(12)
      R=CN(13)
      VK=CN(14)
      VL=CN(15)
      VH=CN(16)
      VI=CN(17)
      CFA=CN(18)
      AT=CN(19)
      DP=CN(20)
      G=CN(21)
      M1=1
      READ INPUT TAPE 5,79,(IO(N),N=1,M)
      READ INPUT TAPE 5,79,(IN(N),N=1,M)
      AF=EBE*TBE**2.
      D2=D-TOP
      DO 5 N=1,M
      TN(N)=FLOATF(N)*W+D2
      IF(TN(N))241,241,240
  240 EN(N)=AF/(TN(N)**2.)
      IF((EN(N)-A1(1))*(EN(N)-A1(I1)))13,14,14
   13 SA=F*SQRTF(25.3/EN(N))
      SNUM=(VK*STNO+VL*SA)*0.1*VN*D1
      SN(N)=SNUM/(1.-EXPF(-SNUM))
      SIG=SA*DP/F
```

```
      PSR=-2.*SIG*R
      NI=100
      H=1./FLOATF(NI)
      FPAIR=0.
      FIMP=0.
      DO 1 I=1,NI,2
    1 FIMP=FIMP+FINTF(H*FLOATF(I))
      DO 2 I=2,NI,2
    2 FPAIR=FPAIR+FINTF(H*FLOATF(I))
      CM(N)=1.-H*(FINTF(0.)-FINTF(1.)+2.*FPAIR+4.*FIMP)/3.
      DO 16 I=1,I11
      IF((EN(N)-A1(I))*(EN(N)-A1(I+1)))15,15,16
   15 STO=(B1(I)*A1(I+1)-A1(I)*B1(I+1)+EN(N)*(B1(I+1)-B1(I)))/(A1(I+1)-A
     11(I))
      GO TO 17
   16 CONTINUE
   17 DO 19 I=1,I21
      IF((EN(N)-A2(I))*(EN(N)-A2(I+1)))18,18,19
   18 STN=(B2(I)*A2(I+1)-A2(I)*B2(I+1)+EN(N)*(B2(I+1)-B2(I)))/(A2(I+1)-A
     12(I))
      GO TO 202
   19 CONTINUE
  202 AN(N)=EXPF(-G*(0.2*STO+0.8*STN))
      QN(N)=SN(N)*EXPF(4.*AT*EN(N)*(1.-CFA))/(CM(N)*AN(N))
      VIC(N)=QN(N)*(VH*FLOATF(IN(N))-VI*FLOATF(IO(N)))
      GO TO 5
  241 EN(N)=0.999999E38
   14 WRITE OUTPUT TAPE 6,71,N,EN(N)
      M1=N+1
    5 CONTINUE
      WRITE OUTPUT TAPE 6,66,(N,IN(N),IO(N),SN(N),CM(N),AN(N),QN(N),TN(N
     1),EN(N),VIC(N),N=M1,M)
      JJ=XINTF(D/W)
      DO 20 N=M1,M
      I=N+JJ
   20 TOV(I)=VIC(N)
      ND=M+JJ
      WRITE OUTPUT TAPE 10,62,(TOV(N),N=1,ND)
      END FILE 10
      CALL EXIT

   59 FORMAT (///)
   60 FORMAT (2X2F10.2)
   62 FORMAT (2H 9,5E14.6)
   66 FORMAT (1H0,9XI3,2I7,4E13.4/52XE14.5,E13.4,E15.6)
   71 FORMAT (10XI3,E20.5)
   79 FORMAT (12I6)
      END(1,0,0,0,0,0,1,0,0,0,0,0,0,0,0)
```

```
      SUBROUTINE LECDO
      COMMON NID,NFD,CN,NC
      DIMENSION C1(30),C2(5,30),CN(30),NC(30)

      DO 91 N=1,30
      IF(N-NID)241,241,242
  242 IF(N-NFD)243,243,244
  241 READ INPUT TAPE 5,9953,IND,JND,C1(N),NC(N),(C2(M,N),M=1,5)
      GO TO 245
  243 READ INPUT TAPE 5,9950,IND,JND,C1(N),CN(N),(C2(M,N),M=1,5)
      GO TO 245
  244 READ INPUT TAPE 5,9952,IND,JND,C1(N),CN(N),(C2(M,N),M=1,5)
  245 IF(N-IND)92,93,92
   93 IF(N-JND)91,95,92
   92 WRITE OUTPUT TAPE 6,951
      CALL EXIT

   91 CONTINUE
   95 WRITE OUTPUT TAPE 6,961
      IF(NID)92,246,247
  247 WRITE OUTPUT TAPE 6,9963,(N,C1(N),NC(N),(C2(M,N),M=1,5),N=1,NID)
  246 IF(NFD-NID)92,2411,249
  249 NID=NID+1
      WRITE OUTPUT TAPE 6,9960,(N,C1(N),CN(N),(C2(M,N),M=1,5),N=NID,NFD)
      IF(JND-NFD)92,2410,2411
 2411 NFD=NFD+1
      WRITE OUTPUT TAPE 6,9962,(N,C1(N),CN(N),(C2(M,N),M=1,5),N=NFD,JND)
 2410 WRITE OUTPUT TAPE 6,961
      RETURN

  951 FORMAT (1H0//10X27HCHECK NUMBERING OF THE DATA)
  961 FORMAT (1H0/1H0)
 9950 FORMAT (I2,2XI2,6XA6,3XF15.6,6X5A6)
 9952 FORMAT (I2,2XI2,6XA6,3XE13.6,8X5A6)
 9953 FORMAT (I2,2XI2,6XA6,3XI9,12X5A6)
 9960 FORMAT (1H0,I2,10XA6,3H = ,F15.6,16X5A6)
 9962 FORMAT (1H0,I2,10XA6,3H = ,E13.6,18X5A6)
 9963 FORMAT (1H0,I2,10XA6,3H = ,I9,22X5A6)
      END(1,0,0,0,0,0,1,0,0,0,0,0,0,0,0)
```

3.2. NEUTOF - PART I Program

The NEUTOF PART I program calculates the mean values $\bar{\epsilon}(N)$, $\bar{E_i}$, $\bar{t_0}$ and $\bar{F''}(N)$ according to the equations (27), (28) and (29).

One can calculate in the same run the $\bar{F''}(N)$ values for more than one temperature.

All final results are printed. Only the set of values for $\bar{\epsilon}(N)$ and $\bar{F''}(N)$ are punched into cards for Input use to the NEUTOF PART II program.

The sequence of the Input Data and the signification of the several symbols are given in Table II.

Table II. Input Data Sequence for the NEUTOF PART I Program

DATA SYMBOL	SIGNIFICATION
NA	First used channel in the incident neutron time-of-flight spectrum.
NB	Last used channel in the incident neutron time-of-flight spectrum
ND	Last read channel in the incident neutron time-of-flight spectrum
NK	NK - 1 : Number of calculated series (different temperatures)
LO	Number of steps in the ts-integration
W	see Table I
TOP	see Table I
The Data from NA to TOP are given as ordinary whole numbers	
BB	Burst-width
TBE 1	Time-of-flight of the reference neutrons from the sample to the counters
TBE 2	Time-of-flight of the reference neutrons from the chopper to the sample

Cont. Table II

DATA SYMBOL	SIGNIFICATION
EBE	see Table I
CFA	see Table I
The Data from BB to CFA are given as ordinary floating point numbers.	
The Data from NA to CFA are read into the program by the SUBROUTINE LECDO	
TT(1) . . TT(NK)	TT(N) : Temperature in energy units for series number N.
A(1) . . A(NK)	A(N) : Same signification as AT in the NEUTOF-SPECIAL program. see Table I
TOV(1) . . TOV(ND)	TOV(N) : Incident neutron intensity as calculated and punched into cards by the NEUTOF-SPECIAL program.
NAO	First calculated channel
NBO	Last calculated channel

```
      COMMON NID,NFD,CN,NC
      DIMENSION CN(30),NC(30),TOV(400),TT(5),A(5),TO(300),EO(300),TS(30)
     1,F(5),FP(5,400)
      FAKTF(P,Q,R)=SQRTF(P/Q)*(P+Q-2.*CFA*SQRTF(P*Q))/(P-Q)*R
      FPOPF(U,V)=EXPF(-2.*U*(E1+E2-2.*CFA*SQRTF(E1*E2)))/(EXPF((E1-E2)/V
     1)-1.)
      REWIND 10
      NID=7
      NFD=12
      CALL LECDO
      NA=NC(1)
      NB=NC(2)
      ND=NC(3)
      NK=NC(4)
      LO=NC(5)
      W=NC(6)
      TOP=NC(7)
      BB=CN(8)
      TBE1=CN(9)
      TBE2=CN(10)
      EBE=CN(11)
      CFA=CN(12)
      READ INPUT TAPE 5,50,(TT(K),K=1,NK)
      READ INPUT TAPE 5,51,(A(K),K=1,NK)
      READ INPUT TAPE 5,51,(TOV(K),K=1,ND)
      READ INPUT TAPE 5,52,NAO,NBO
      WRITE OUTPUT TAPE 6,70,(K,TT(K),A(K),K=1,NK)
      WRITE OUTPUT TAPE 6,71,(TOV(N),N=NA,NB)
      C1=EBE*TBE1**2.
      C2=EBE*TBE2**2.
      S1=0.
      S2=0.
      S3=0.
      DO 1 N=NA,NB
      S1=S1+TOV(N)
      TO(N)=(FLOATF(N)*W-TOP)*TBE2/(TBE1+TBE2)
      EO(N)=C2/(TO(N)**2.)
      S3=S3+TO(N)*TOV(N)
    1 S2=S2+EO(N)*TOV(N)
      EOM=S2/S1
      TOM=S3/S1+TOP
      WRITE OUTPUT TAPE 6,60,S1,S2,EOM,TOM
      VLO=LO
      DO 2 N=1,LO
      VN=N
    2 TS(N)=(VN-0.5)*BB/VLO-BB/2.
      T=W-TOP-TO(NB)-BB/2.
      IF(NAO-1)200,200,201
  200 IF(T)20,20,30
   20 XX=-T/W
      NRA=XINTF(XX)+1
```

```
      DO 3 N=1,NRA
      WRITE OUTPUT TAPE 6,61
      DO 4 M=1,NK
    4 FP(M,N)=0.999999E38
    3 CONTINUE
      NRA=NRA+1
      GO TO 40
   30 NRA=1
      GO TO 40
  201 NRA=NAC
   40 WRITE OUTPUT TAPE 6,72
      DO 5 N=NRA,NBO
      T=FLOATF(N)*h-TOP
      DO 100 K=1,NK
  100 F(K)=0.
      DO 6 L=1,LO
      TZ=T-TS(L)
      DO 7 M=NA,NB
      E1=C1/((TZ-TC(M))**2.)
      ET1=E1*TOV(M)
      DE=E1/(TZ-TO(M))
      E2=EO(M)
      F1=FAKTF(E1,E2,DE)*TOV(M)
      DO 8 K=1,NK
      TK=TT(K)
      AK=A(K)
      IF(K-1)41,41,42
   41 F(K)=ET1+F(K)
      GO TO 8
   42 F(K)=F(K)+F1*FPOPF(AK,TK)
    8 CONTINUE
    7 CONTINUE
    6 CONTINUE
      DO 9 K=1,NK
    9 FP(K,N)=F(K)/(VLO*S1)
      FP(1,N)=FP(1,N)-EOM
    5 WRITE OUTPUT TAPE 6,62,N,(FP(K,N),K=1,NK)
      DO 10 K=1,NK
      WRITE OUTPUT TAPE 10,63,K
   10 WRITE OUTPUT TAPE 10,51,(FP(K,N),N=NAO,NBO)
      END FILE 10
      CALL EXIT

   50 FORMAT (1XF8.3,4F12.3)
   51 FORMAT (2X5E14.6)
   52 FORMAT (2I6,60X)
   60 FORMAT (1H0///2X2E14.6//2X6HEOM = ,E11.4//2X6HTOM = ,E11.4//1H0)
   61 FORMAT (//)
   62 FORMAT (2XI3,5E17.6)
   63 FORMAT (I2,70X)
   70 FORMAT (1H0//4X1HK,9X7HTEMP=TT,14X6HDWF=AK///(4XI1,2E19.6))
   71 FORMAT (1H0//30X6HTOV(N)///(2X10E12.4))
   72 FORMAT (4X1HN,8X6HEPS(N),13X4HF(2),13X4HF(3),13X4HF(4),13X4HF(5)//
     1/1H0)
      END(1,0,0,0,0,0,1,0,0,0,0,0,0,0,0)
```

SUBR, LECDO see page 16

3.3. NEUTOF-PART II Program

The NEUTOF PART II program calculates in the first section the corrected time-of-flight spectrum of inelastically scattered neutrons.
In an optional second section, the generalized frequency distribution G (ϵ), the normalized generalized frequency distribution as a function of the oscillator energy, GN (ϵ), as well as the normalized generalized frequency distribution as a function of the frequency GN (ν) can be obtained.

Some intermediate and all final results are printed.
The main results of the first section $\bar{\epsilon}(N)$ and $IC(N)$, and those of the optional second section ν, GN(ν) are punched into cards.
One can calculate in the same run more than one series.

The sequence of the Input Data and the signification of the several symbols are given in Table III.

Table III. Input Data Sequence for the NEUTOF PART II Program

DATA SYMBOL	SIGNIFICATION
A1(1), B1(1) . . A1(15),B1(15)	see Table I.
A2(1), B2(1) . . A2(18),B2(18)	see Table I.
Special Identification Card with Text (see LECDO 3 - Listing)	
M	see Table I
NA	First calculated channel in the second section
NB	Last calculated channel in the second section
ND	Last read channel of the $\bar{\epsilon}(N)$ and $\bar{F}''(N)$ values punched on cards by the NEUTOF PART I program

Cont. Table III

DATA SYMBOL	SIGNIFICATION
NK	NK - 1 : Number of calculated series per run
W	see Table I
D	see Table I
TOM	: $\overline{t_o}$ calculated by the NEUTOF PART I program
The Data from M to TOM are given as ordinary whole numbers.	
VN	)
STNO	)
D1	)
F	) see Table I
A	)
B	)
R	)
EOM	: $\overline{E_i}$ calculated by the NEUTOF - PART I program
VK	) see Table I
VL	)
The Data from VN to VL are given as ordinary floating point numbers.	
DP	) see Table I
G	)
VK1	Time to energy scale convertion factor : VK1 = Mass of the neutron x (flight path length)^2 in meV/ μsec - units.
The Data from DP to VK1 are given as a decimal fraction times a power of ten	

Cont. Table III

DATA SYMBOL	SIGNIFICATION
The Data from the Identification Card to VK1 are read into the program by the SUBROUTINE LECDO 3.	
K	Identification number at the top of each card set punched by the NEUTOF PART I program. K = 1 : Identification for the $\bar{\varepsilon}(N)$ card set. K $\neq$ 1 : Identification number for the $\bar{F}''(N)$ card set.
FP(K,1) . . FP(K,ND)	FP(L,N) : N^{th} - value of the L^{th} card set calculated and punched by the NEUTOF PART I program. FP(1,N) = $\bar{\varepsilon}(N)$ FP(L,N) = $\bar{F}''(N)$ if L $\neq$ 1
Cyclic repetition of the set of cards (K, FP) with 1 $\leq$ K $\leq$ NK	
IO(1) ..... IO(12) ....IO(M)	see Table I
Special Identification Card with Text (see LECDO 3 - Listing)	
KEY	If KEY = 1 : the program calculates only the first section if KEY = 2 : the program calculates the first and the second section if KEY = 3 : the program calculates only the second section with IC(N) = IN(N)
KK	KK - 1 : Number of the series
The Data from KEY to KK are given as ordinary whole numbers	
VH	) see Table I
VI	)
AT	AT = A(KK)) see Table II
TT	TT = TT(KK))

Cont. 2. Table III.

DATA SYMBOL	SIGNIFICATION
The Data from VH to TT are given as ordinary floating point numbers.	
The Data from KEY to TT are read into the program by the SUBROUTINE LECDO 3.	
IN(1) ....IN(12) ....IN(M)	see Table I
Cyclic repetition of the set of cards (Special Id. Card, KEY, KK,VH, VI,AT,TT,IN (1-M)) with 2 $\leq$ KK $\leq$ NK	
Card 99	Card to stop the program (Transfer to Call Exit)

```
      COMMCN LU,VU,TITRE
      DIMENSION AN(300),CN(300),EN(300),FN(300),GP(300),GPN(300),GPNN(30
     10),GPT(300),IN(300),IO(300),QN(300),SN(300),TN(300),VIC(300),XNU(3
     200),W1(300),W2(300),FP(5,400),F1(5,400),A1(20),B1(20),A2(20),B2(20
     3),LU(20),VU(40),TITRE(8)
       FINTF(X)=EXPF(PSR*SQRTF(X*(2.-X)))*(A+B*EXPF(PSR*SQRTF(1.-X*X)))
      REWIND 10
      I1=15
      I2=18
      READ INPUT TAPE 5,60,(A1(I),B1(I),I=1,I1)
      READ INPUT TAPE 5,60,(A2(I),B2(I),I=1,I2)
      WRITE CUTPUT TAPE 6,61,(I,A1(I),B1(I),I=1,I1)
      WRITE CUTPUT TAPE 6,61,(I,A2(I),B2(I),I=1,I2)
      I11=I1-1
      I21=I2-1
      WRITE CUTPUT TAPE 6,59
      CALL LECDO
      M=LU(1)
      NA=LU(2)
      NB=LU(3)
      ND=LU(4)
      NK=LU(5)
      W=LU(6)
      D=LU(7)
      TOM=LU(8)
      VN=VU(9)
      STNO=VU(10)
      D1=VU(11)
      F=VU(12)
      A=VU(13)
      B=VU(14)
      R=VU(15)
      EOM=VU(16)
      VK=VU(17)
      VL=VU(18)
      DP=VU(19)
      G=VU(20)
      VK1=VU(21)
      MDW=XINTF(D/W)
      ND1=ND-MDW
      MD1=MDW+1
      DO 20 K=1,NK
      READ INPUT TAPE 5,81,KK
      IF(KK-K)300,301,300
  300 WRITE OUTPUT TAPE 6,82,KK
      CALL EXIT
  301 READ INPUT TAPE 5,80,(FP(K,N),N=1,ND)
      DO 30 M6=MD1,ND
      N=M6-MDW
   30 F1(K,N)=FP(K,M6)
```

```
   20 WRITE OUTPUT TAPE 6,83,KK,(F1(K,N),N=1,ND1)
      READ INPUT TAPE 5,79,(IO(N),N=1,M)
      M1=1
      IS=0

   99 CALL LECDO

      KEY=LU(1)
      KK=LU(2)
      VH=VU(3)
      VI=VU(4)
      AT=VU(5)
      TT=VU(6)
      READ INPUT TAPE 5,79,(IN(N),N=1,M)
      IF(IS)1000,1000,1001
 1000 IS=1
C     FIRST SERIES, FIRST SECTION TERMINATED BY STATEMENT NO 5

      DO 5 N=1,M
      TN(N)=FLOATF(N)*W+D-TOM
      IF(TN(N))241,241,240
  240 EN(N)=F1(1,N)+EOM
      IF((EN(N)-A1(1))*(EN(N)-A1(I1)))13,14,14
   13 IF(3-KEY)40,40,46
   46 SA=F*SQRTF(25.3/EN(N))
      SNUM=(VK*STNC+VL*SA)*0.1*VN*D1
      SN(N)=SNUM/(1.-EXPF(-SNUM))
      SIG=SA*DP/F
       PSR=-2.*SIG*R
      NI=100
      H=1./FLOATF(NI)
      FPAIR=0.
      FIMP=0.
      DO 1 I=1,NI,2
    1 FIMP=FIMP+FINTF(H*FLOATF(I))
      DO 2 I=2,NI,2
    2 FPAIR=FPAIR+FINTF(H*FLOATF(I))
      CN(N)=1.-H*(FINTF(0.)-FINTF(1.0)+2.*FPAIR+4.*FIMP)/3.
      DO 16 I=1,I11
      IF((EN(N)-A1(I))*(EN(N)-A1(I+1)))15,15,16
   15 STO=(B1(I)*A1(I+1)-A1(I)*B1(I+1)+EN(N)*(B1(I+1)-B1(I)))/(A1(I+1)-A
     11(I))
      GO TO 17
   16 CONTINUE
   17 DO 19 I=1,I21
      IF((EN(N)-A2(I))*(EN(N)-A2(I+1)))18,18,19
   18 STN=(B2(I)*A2(I+1)-A2(I)*B2(I+1)+EN(N)*(B2(I+1)-B2(I)))/(A2(I+1)-A
     12(I))
      GO TO 202
   19 CONTINUE
  202 AN(N)=EXPF(-G*(0.2*STO+0.8*STN))
      QN(N)=SN(N)/(CN(N)*AN(N))
      VIC(N)=QN(N)*(VH*FLOATF(IN(N))-VI*FLOATF(IO(N)))
      GO TO 42
   40 VIC(N)=IN(N)
```

```
   42 IF(KEY*(KEY-1)*(N-NA+1)*(N-NB-1))12,5,5
   12 IF(F1(1,N))5,500,500
  500 M2=N
      GO TO 5
  241 EN(N)=0.99999E38
   14 WRITE OUTPUT TAPE 6,71,N,EN(N)
      M1=N+1
    5 CONTINUE
      WRITE OUTPUT TAPE 6,66,(N,IN(N),IO(N),SN(N),CN(N),AN(N),QN(N),TN(N
     1),EN(N),F1(1,N),VIC(N),N=M1,M)
       M4=M2+1
       M3=M4-NA
      IF(KEY-1)320,320,101
C     OTHER THAN FIRST SERIES
 1001 DO 1002 N=M1,M
      IF(3-KEY)43,43,44
   43 VIC(N)=IN(N)
      GO TO 1002
   44 VIC(N)=QN(N)*(VH*FLOATF(IN(N))-VI*FLOATF(IO(N)))
 1002 CONTINUE
      WRITE OUTPUT TAPE 6,64,(N,IN(N),IO(N),F1(1,N),VIC(N),N=M1,M)
      IF(KEY-1)320,320,101
  101 SOM=0.
      DO 22 N=NA,NB
      FN(N)=F1(KK,N)
      GP(N)=VIC(N)/FN(N)
      GPT(N)=GP(N)/(TN(N)**3.)
   22 SOM=SOM+GPT(N)
      SOM=VK1*W*SOM
      F2=1.E-12/SOM
      F3=4.14E-24/SOM
      DO 23 N=NA,NB
      XNU(N)=F1(1,N)/4.14E-12
      GPN(N)=GP(N)*F2
   23 GPNN(N)=GP(N)*F3
      WRITE OUTPUT TAPE 6,59
      WRITE OUTPUT TAPE 6,68,(N,GP(N),GPT(N),F1(1,N),GPN(N),XNU(N),GPNN(
     1N),N=NA,NB)
       DO 501 J=1,M3
       I=M4-J
       W1(J)=XNU(I)
  501 W2(J)=GPNN(I)
      WRITE OUTPUT TAPE10,73,M2,NA,(TITRE(I),I=1,8)
       WRITE OUTPUT TAPE10,63,(W1(N),W2(N),N=1,M3)
  320 WRITE OUTPUT TAPE10,72,(TITRE(I),I=1,8)
      WRITE OUTPUT TAPE 10,62,(F1(1,N),VIC(N),N=1,M)
  100 WRITE OUTPUT TAPE 6,70
      GO TO 99

   59 FORMAT (///)
   60 FORMAT (2X2F10.2)
   61 FORMAT (1H0/(10XI2,2F7.2))
   62 FORMAT(2H 1,E16.5,3E18.5)
   63 FORMAT(2H 2,E16.5,3E18.5)
```

```
64 FORMAT (1H0,11X1HN,2X5HIN(N),2X5HIO(N),5X6HEPS(N),10X5HIC(N)//(1H
  1,9XI3,2I7,E14.4,E16.6))
66 FORMAT (1H0,9XI3,2I7,4E13.4/38XE14.5,2E13.4,E15.6)
68 FORMAT (1H0,10X1HN,6X4HG(N),9X5HGT(N),11X6HEPS(N),8X7HGN(EPS),12X5
  1HNU(N),8X6HGN(NU)//(1H ,8XI3,2E13.4,5X2E13.4,5X2E13.4))
70 FORMAT (1H1)
71 FORMAT (10XI3,E20.5)
72 FORMAT(24X8A6)
73 FORMAT(2I6,12X8A6)
79 FORMAT (12I6)
80 FORMAT (2X5E14.6)
81 FORMAT (I2,70X)
82 FORMAT (1H0//11HTHE SET F1(,I2,32H,N) IS NOT ON THE RIGHT POSITION
  1)
83 FORMAT (1H0//2X5HKK = ,I2//(1H ,10E12.4))
   END(1,0,0,0,0,0,1,0,0,0,0,0,0,0,0)
```

```
      SUBROUTINE LECDO
C     LECDO 3

      COMMON LU,VU,TITRE
      DIMENSION LU(20),VU(40),TITRE(8),COM(6,40)

      WRITE CUTPUT TAPE 6,1
      READ INPUT TAPE 5,2,LEC1,LEC2,LEC3,LEC4,(TITRE(I),I=1,8)
      WRITE CUTPUT TAPE 6,3,(TITRE(I),I=1,8)
      IF(LEC1-98)51,51,100
   51 IF(LEC2)200,53,54
   54 IF(LEC3)200,56,50
   50 DO 55 N=1,LEC3
      READ INPUT TAPE 5,7,I,J,COM(1,N),LU(N),(COM(M,N),M=2,6)
      IF((N-I)*(N-I)+(LEC2-J)*(LEC2-J))200,55,200
   55 CONTINUE
      WRITE CUTPUT TAPE 6,8,(N,COM(1,N),LU(N),(COM(M,N),M=2,6),N=1,LEC3)
   56 IF(LEC4-LEC3)200,57,58
   58 LEC3=LEC3+1
      DO 59 N=LEC3,LEC4
      READ INPUT TAPE 5,9,I,J,COM(1,N),VU(N),(COM(M,N),M=2,6)
      IF((N-I)*(N-I)+(LEC2-J)*(LEC2-J))200,59,200
   59 CONTINUE
      WRITE CUTPUT TAPE 6,10,(N,COM(1,N),VU(N),(COM(M,N),M=2,6),N=LEC3,L
     1EC4)
      IF(LEC2-LEC4)200,53,57
   57 LEC4=LEC4+1
      DO 61 N=LEC4,LEC2
      READ INPUT TAPE 5,11,I,J,COM(1,N),VU(N),(COM(M,N),M=2,6)
      IF((N-I)*(N-I)+(LEC2-J)*(LEC2-J))200,61,200
   61 CONTINUE
      WRITE CUTPUT TAPE 6,12,(N,COM(1,N),VU(N),(COM(M,N),M=2,6),N=LEC4,L
     1EC2)
      GO TO 53
   53 WRITE CUTPUT TAPE 6,1
      RETURN

C     FORMAL PROCEDURES BEFORE EXIT
  100 CONTINUE
      END FILE 10
      CALL EXIT

  200 WRITE CUTPUT TAPE 6,6
      CALL EXIT

    1 FORMAT (///)
    2 FORMAT (I2,2XI2,4XI2,4XI2,6X8A6)
    3 FORMAT (1H0,10X8A6)
    6 FORMAT (1H0//10X27HCHECK NUMBERING OF THE DATA)
    7 FORMAT (I2,2XI2,6XA6,3XI9,12X5A6)
    8 FORMAT (1H0,I2,10XA6,3H = ,I9,22X5A6)
    9 FORMAT (I2,2XI2,6XA6,3XF15.6,6X5A6)
   10 FORMAT (1H0,I2,10XA6,3H = ,F15.6,16X5A6)
   11 FORMAT (I2,2XI2,6XA6,3XE13.6,8X5A6)
   12 FORMAT (1H0,I2,10XA6,3H = ,E13.6,18X5A6)
      END(1,0,0,0,0,0,1,0,0,0,0,0,0,0,0)
```

Acknowledgment.

The author wishes to thank Mr. J. Rousseaux for the use of the Subroutine LECDO and for his help to prepare the computer programs.

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EUR 522 d

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5. FIGURES

see next pages

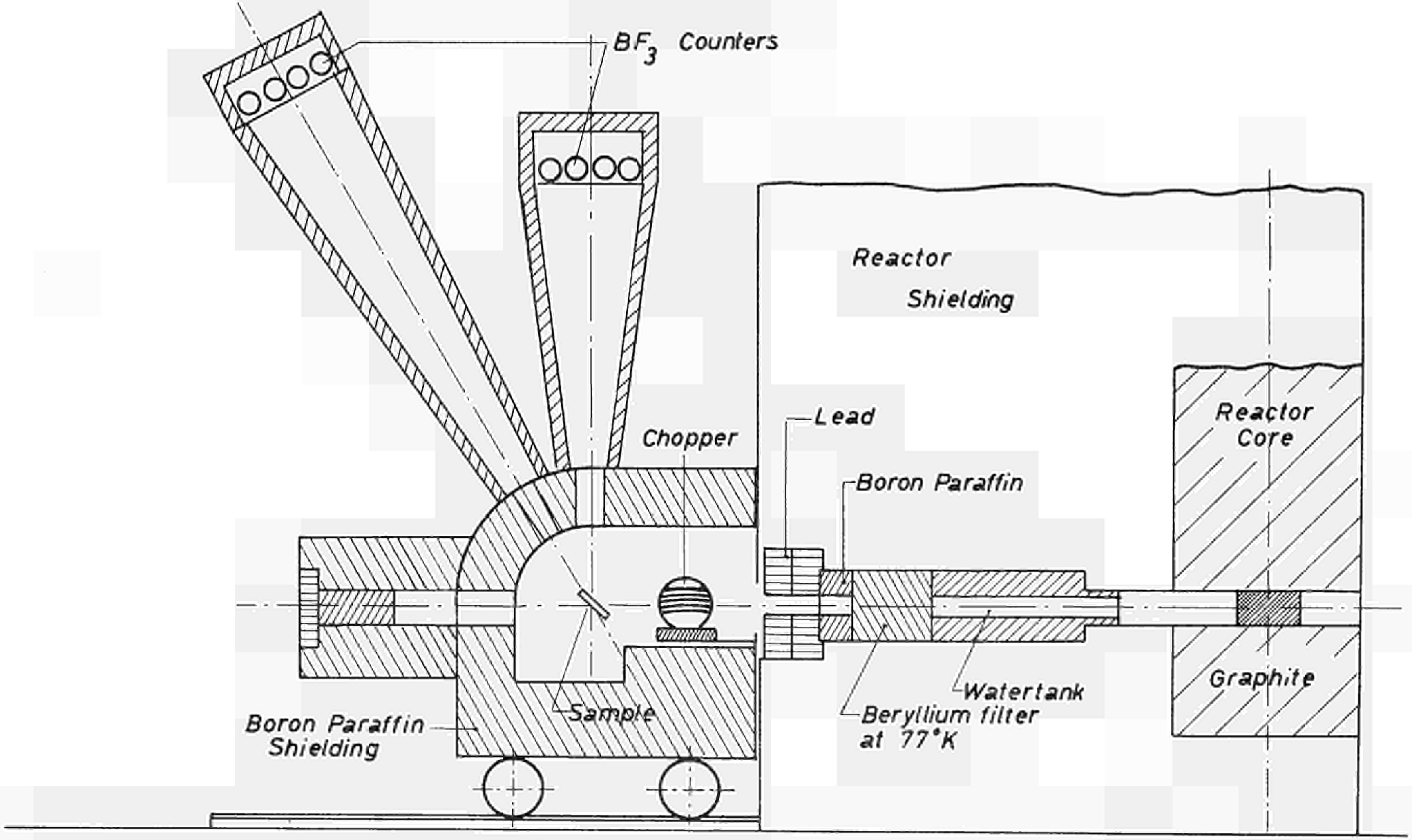


Fig. 1 General Lay Out of the Cold Neutron Time of Flight Facility at the Ispra I Reactor

Fig. 2 _. Geometrical Arrangement of the Sample

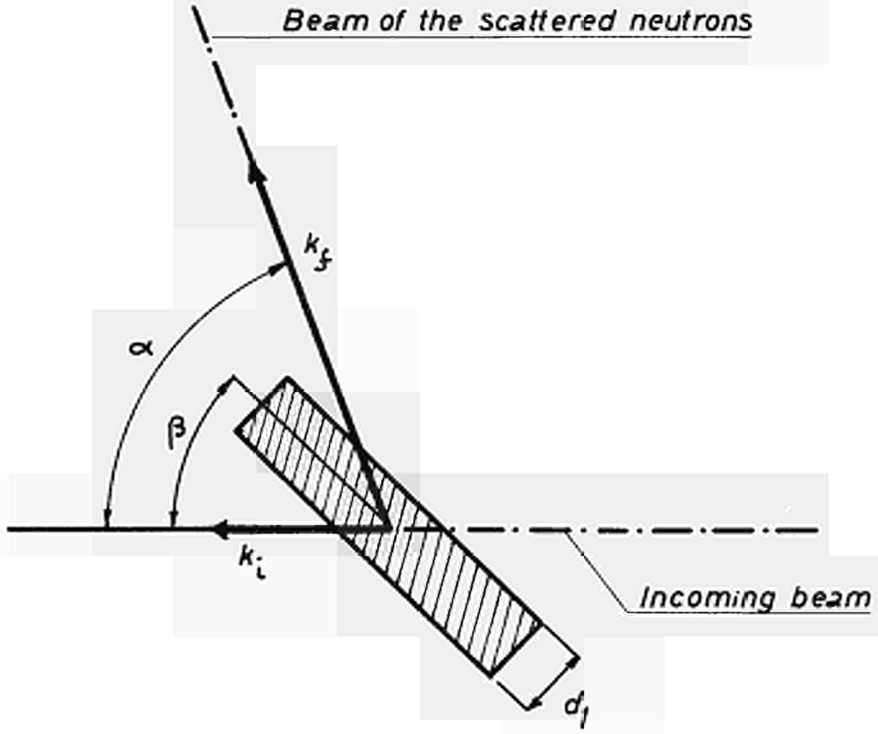
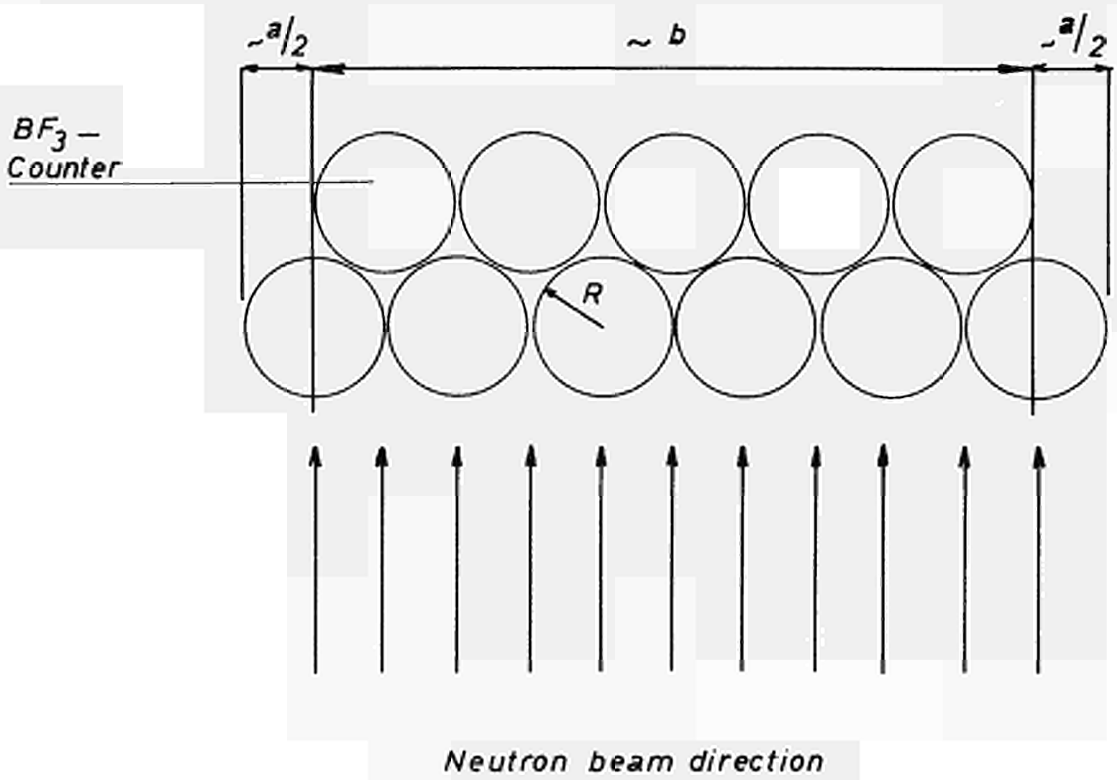


Fig. 3 _. Geometrical Arrangement of the BF_3 counter bank



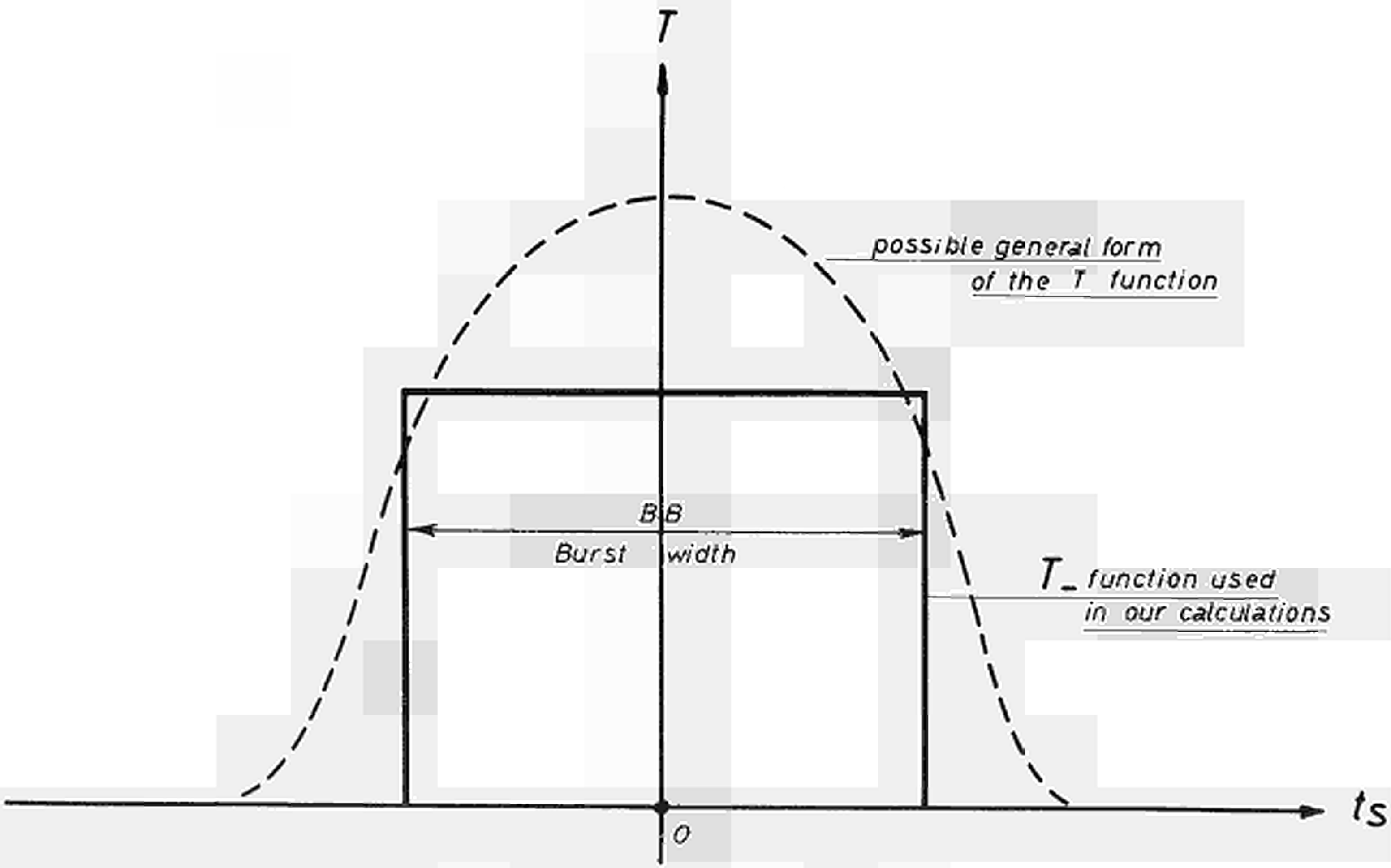


Fig. 4 _ Burst Function of the Chopper $T(t_S)$

To disseminate knowledge is to disseminate prosperity — I mean general prosperity and not individual riches — and with prosperity disappears the greater part of the evil which is our heritage from darker times.

Alfred Nobel

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