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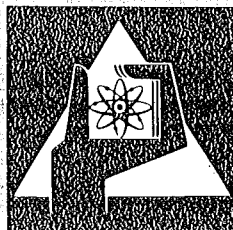
Institut für Angewandte Kernphysik

TIFLIS

(Time-of-Flight-Spectra)

**a data reduction program for the evaluation
of time-of-flight experiments**

W. Abel, J.-B. Suck



**GESELLSCHAFT
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ABSTRACT

The purpose of TIFLIS (TIme-of-FLight-Spectra) is the evaluation of the double differential cross section and the scattering law from time-of-flight-spectra of thermal neutrons scattered in atomic systems (gases, simple liquids, amorphous materials and polycrystals). TIFLIS is a software package based upon FORTRAN IV for IBM/360 series machines and was compiled and tested on the IBM/370-168 at the Karlsruhe Nuclear Research Center (GfK). The present program is limited to finite plane slab geometry, but time-of-flight-spectra from other sample geometries can be evaluated by replacing two subroutines. TIFLIS is characterized by a lot of correction routines (except corrections for resolution and multiple scattering), which also take into account several mishaps that might occur during the experiment. An IBM/2250-1 graphics display unit can be employed to solve specific problems with interactive graphics during and after a TIFLIS run.

RÉSUMÉ

L'intention de TIFLIS (TIme-of-FLight-Spectra) est l'évaluation de la section double différentielle de diffusion et de la loi de diffusion obtenues des spectres de temps de vol de neutrons thermiques diffusés dans des systèmes atomiques, par exemple des gaz, liquides simples, matériaux amorphes et polycristallins. TIFLIS est programmé en FORTRAN IV et a été mis au point sur la IBM/370-168 du Centre de Recherches Nucléaires à Karlsruhe (GfK). Le programme n'accepte que des échantillons d'une géométrie plane et finite. Les spectres de temps de vol provenant d'autres géométries d'échantillon peuvent être évalués par changement de deux sous-programmes. TIFLIS contient un grand nombre de programmes de correction qui tiennent compte des différentes sources d'erreur au cours d'une expérience. (TIFLIS ne contient pas de corrections concernant de la résolution et de la diffusion multiple). On peut appliquer des méthodes interactives pour la solution des problèmes spéciaux en se servant d'une IBM/2250-1.

TIFLIS (TIme-of-FLIght-Spectra)

Ein Programm zur Auswertung von Flugzeitexperimenten

KURZFASSUNG

TIFLIS (TIme-of-FLIght-Spectra) ist ein Programm zur Auswertung des doppelt-differentiellen Streuquerschnitts und des Streugesetzes aus Experimenten zur Untersuchung der inelastischen Streuung von thermischen Neutronen an atomaren Systemen, wie Gasen, einfachen Flüssigkeiten, amorphen Substanzen und Polykristallen, mit Hilfe der Flugzeitmethode. TIFLIS ist in FORTRAN IV programmiert und wurde auf der Datenverarbeitungsanlage IBM/370-168 der Gesellschaft für Kernforschung Karlsruhe (GfK) implementiert. Für die Streuproben wird eine endliche Plattengeometrie vorausgesetzt; Flugzeitspektren von Proben mit anderer Geometrie können ausgewertet werden, indem zwei Unterprogramme ausgetauscht werden. TIFLIS ist gekennzeichnet durch mehrere Korrekturprogramme (außer Auflösungs- und Vielfachstreu Korrektur), die verschiedene Fehlerquellen während der Durchführung eines Experiments berücksichtigen. Während oder nach einer TIFLIS-Auswertung kann zur Lösung spezieller Probleme das Bildschirmgerät IBM/2250-1 eingesetzt werden.

1. Introduction

Inelastic scattering of thermal neutrons is an important technique for the experimental investigation of the solid and liquid states by measuring the angular and energy distribution of the scattered neutrons. Time-of-flight techniques have been efficiently adapted to inelastic scattering measurements. In the present report a program system is described which serves the purpose of reducing the data accumulated from experiments of the inelastic scattering of thermal neutrons performed with the time-of-flight method. There are several experimental runs which are usually included in an inelastic scattering experiment:

- (1) "Time-independent" background related to the empty container measurement
- (2) Empty container (sample holder) measurement
- (3) Vanadium measurement
- (4) Empty vanadium sample holder measurement
- (5) "Time-independent" background related to the sample measurement
- (6) Sample measurement (proper scattering experiment)

The maximum number of detectors that can be processed is a function not only of the system time of a TIFLIS run but also of the space available for the intermediate data storage on scratch files. In this version 97 detectors and 2 monitors can be addressed. For the evaluation of more than 97 detectors only the dimensions of few computational arrays must be increased.

The program is written in FORTRAN IV. The modular scheme allows the experimentalist to adapt the program in a simple way to his specific experimental conditions. The Graphic Subroutine Package (GSP) of IBM has been used for programming the interactive graphic programs. Some subprograms, e.g. for the definition of a direct access file and for a main storage allocation, are written in the installation dependent language Assembler and must be rewritten for use at any other installation.

With respect to better utilization of core storage the program is organized into a single region overlay structure. For the load module and the buffers of the data files used approximately 300 kBytes of high speed storage must be reserved, the amount depending on how many time channels for the scattering law in the detector spectrum are evaluated.

When processing 30 detectors with a range of evaluation of about 200 time channels the running time is about 30 seconds on the IBM/370-168.

For multiple scattering corrections the VIPER program is available (Carvalho and Ehret 1967). For this purpose, the data of the scattering law may be copied on tape at the end of the evaluation. Moreover, it is possible to reserve the arranged scattering data $S(\alpha, \beta)/\alpha$ for constant β which can be used to calculate a generalized frequency distribution $p(\beta)$ by an extrapolation procedure (Abel 1973) with help of an interactive graphic program. Display supported graphic interpolation can be carried out for a smoothed output of the scattering law $S(Q, \omega)$ (Abel 1974).

2. Basic Principles of the Evaluation Process

What is required is the scattering function $S(Q, \omega)$ which is directly related to the measured double differential cross section $\frac{d^2\sigma}{d\Omega dE}$.

$$\frac{d^2\sigma}{d\Omega dE} = \frac{K}{K_0} \frac{\sigma_b}{4\pi} S(Q, \omega) \quad (2.1)$$

where σ_b , the bound atom scattering cross section is assumed to be independent of the position of the atom in the scattering sample. K_0 and K are the moduli of the initial and final wave vectors of the neutron. $S(Q, \omega)$ depends on the dynamics and the structure of the scatterer only and not on the nature of the radiation used. For the interpretation of the experimental results one must take into account that the measured differential scattering cross section includes coherent and incoherent components.

In inelastic scattering experiments various combinations of methods are used for producing monochromatic neutrons and for the analysis of the scattered neutrons. Fig. 1 shows a sketch of a time-of-flight spectrometer. Monochromatic neutrons with energy E_0 (in Fig. 1 E_0) pass through the sample coming from a rotating crystal or a stationary crystal followed by a Fermi chopper. The scattered neutrons are detected in He^3 -filled detectors connected to a multichannel time analyser. Monitor 1 controls the incident monochromatic neutron beam intensity, monitor 2 the transmitted neutrons, and monitor 5 the "time-independent" background in the spectrometer.

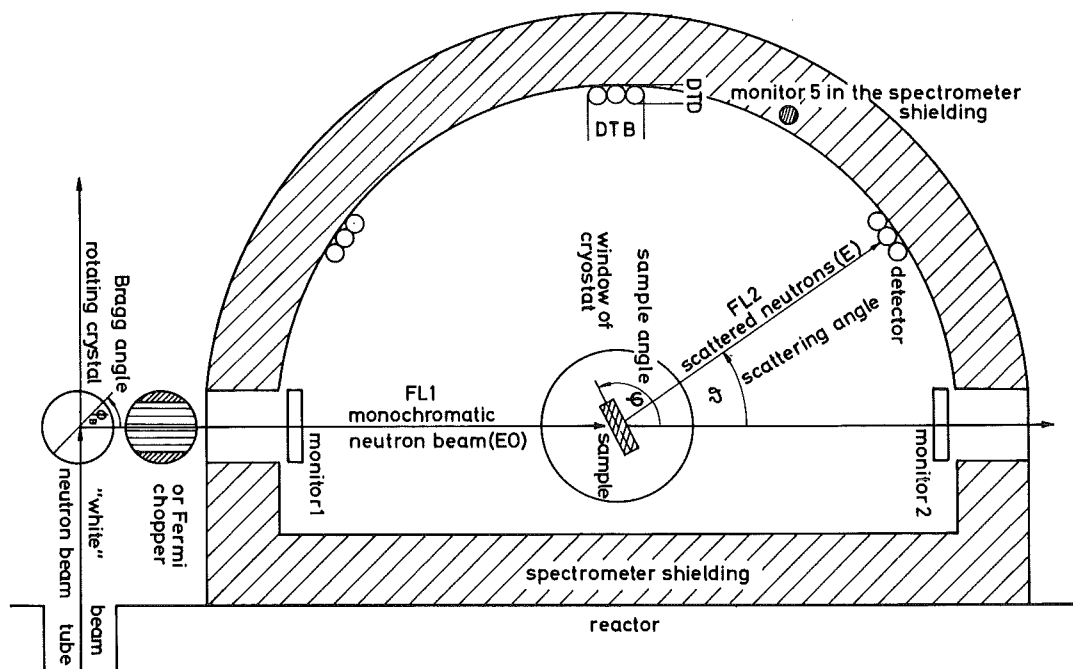


Fig. 1 Basic arrangement of a time-of-flight spectrometer
(rotating crystal spectrometer at the FR2 Karlsruhe)

The purpose of the present chapter is to give a brief description of the evaluation process and the experimental results which are established by the program. The individual detector spectra of the measurements taken at different scattering angles are transmitted from tape recorded by the data acquisition system to background storage as temporary data sets. These data sets are direct access files. Before the transfer is performed, up to five measurements of the same kind can be added to a given measurement, or a correction for the counting time of individual detectors of a measurement can be carried out.

Another option is the smoothing of the spectra in certain channel regions. The raw time-of-flight data are corrected for background and sample holder scattering. The counting rate depends on the number of incoming neutrons and of scatterers in the beam area, the solid angle seen by the detectors, and the efficiency of the detector system. Therefore, an experiment with a standard scatterer, vanadium for example, is necessary. After the analysis of a vanadium calibration measurement the time-of-flight data of the sample are corrected for the energy dependence of the detector's efficiency function. If desired, this can be preceded by a reduction of the sample spectra by adding up 2^n channels with $n = 1, 2$ to improve the statistics at the expense of

the time resolution. The scattering law data are now calculated via the double differential cross section.

In the last stage of the analysis the scattering function is interpolated for constant energy transfers and for constant wave vector changes, respectively. This output, however, cannot be compared directly with theoretical results until the multiple scattering of neutrons in the sample and the resolution of the TOF-spectrometer are taken into account. In detail, the program carries out the following evaluation steps:

- (1) Detector efficiency for neutrons with E_0 taken from the vanadium measurement
- (2) Width of the elastic peak in the vanadium measurement (fit of a Gaussian function to the experimental data)
- (3) Relative statistical error
- (4) Elastic correction (separation of the spectrum of elastically and inelastically scattered neutrons)
- (5) Time-of-flight spectrum
- (6) Spectrometer resolution
- (7) Correction for self absorption
- (8) $\frac{d^2\sigma}{d\Omega d\tau}$ (τ time-of-flight)
- (9) $\frac{d^2\sigma}{d\Omega dE}$, $S(Q, \omega)$
- (10) $\frac{d^2\sigma}{d\Omega d\beta}$, $S(\alpha, \beta)$
- (11) $S(\alpha, \beta = \text{const.})$
- (12) $S(\alpha, \beta = \text{const.})/\alpha$
- (13) $S(Q, \omega = \text{const.})$
- (14) $S(Q, \omega = \text{const.})/Q^2$
- (15) Structure factor $S(Q) = \int S(Q, \omega) d\omega$
- (16) $S(\alpha = \text{const.}, \beta)$
- (17) $S(Q = \text{const.}, \omega)$
- (18) $\omega^2 S(Q = \text{const.}, \omega)$
- (19) One-Phonon approximation for $p(\beta)$

- (20) Width of the elastic peak in the TOF-spectra of the sample measurement (fit to Gaussian, a Lorentzian, or a convolution of both functions to the experimental data)
- (21) Width of the peak in $S(Q,\omega)$ (fitted to the same functions as given in (20))

3. Program System Description

The following part of the report is not intended to be exhaustive. Some of the descriptions will represent an oversimplification but will, hopefully, be sufficient to aid the user. The programs themselves are extensively commented. All computations are performed in single precision.

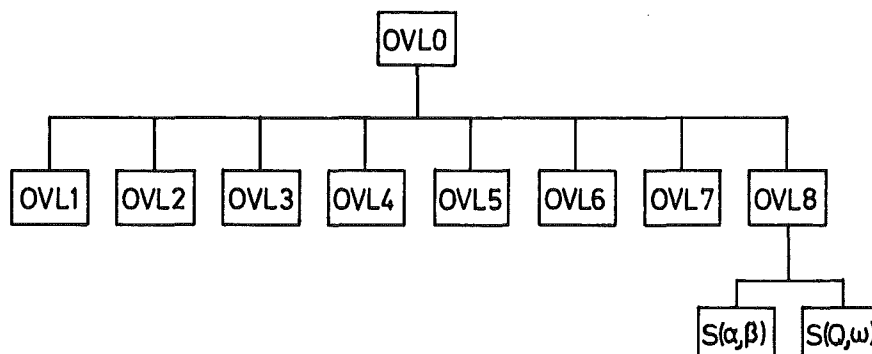
3.1 Structure of the System

The program has been compiled and tested on the IBM/370-168 under OS MVT Rel. 21.6. To minimize the main storage requirements the program is organized into an overlay structure because of the problems to be solved, i.e. the subdivision of the evaluation process into the analysis of a vanadium measurement, the measurement of the scattering sample, and into the output of the experimental scattering law data. The overlay tree is shown in Table 1. The diagram indicates that the root segment OVL0 always remains in storage during execution while each of the evaluation programs (segments OVL1 to OVL8) is called into storage upon need. An "overlay" means that these segments containing one or more subprograms occupy the same general area of high speed storage during actual use. An overlay segment can be loaded and overlaid as many times as required by the logic of the program during execution. All this is necessary because of the limitation of the immediate access storage even on the largest memory computers. The size of the complete executable TIFLIS load module (largest path + buffer areas) amounts to around 300 kBytes.

The overlay tree structure is determined as a function of the symbolical DIS parameter in the procedure call which may have one of the following values:

DIS = 0: Evaluation without display. When the procedure is called, the DIS parameter can be omitted.

DIS = 1: Correction of individual time channels of the time-of-flight spectrum and execution and improvement, respectively, of the elastic correction via the IBM/2250-1 display unit.



- OVL0: MAIN routine, system storage arrays, service subprograms
- OVL1: Initial processing of the scattering data
- OVL2: Fit program for peak analysis
- OVL3: Evaluation of the vanadium measurement, preparation of the time independent and background measurement
- OVL4: Evaluation of the sample measurement
- OVL5: Calculation of the elastic correction
- OVL6: Calculation of the time-of-flight spectrum
- OVL7: Calculation of the double differential cross section and the scattering law
- OVL8: Interpolation of the scattering law for constant energy and momentum transfer

Table 1: Overlay tree structure of TIFLIS

Several measurements of the scattering samples can be evaluated in one program run. In the subsequent sorting phase the scattering law is written out for these sample measurements in the sequence in which they have been processed.

The most important reduction in the main storage requirement stems from the fact that the evaluation of the raw scattering data can be carried out in more or less independent logical steps, e.g. background corrections, normalisations, monitor intensity calculations, calculation of the time-of-flight spectrum, etc. The detector spectra are therefore read into the storage from the background storage in turns. Despite of the reading-in and the rewriting of the data blocks which is necessary as a consequence of the different evaluation steps, the ratio of the system time of a job to the actual computation time assumes an acceptable value of 3 : 2 to

10 : 1 for computation times of less than one minute on the IBM/370-168 (or less than 5 minutes on the IBM/360-65).

The maximum main storage requirement is reached when the values of the scattering law are calculated. The indication of a sufficient job region is determined exclusively by the size of the range of evaluation in the detector spectrum. The respective data arrays are expanded within the task region, if possible up to the dimension required by the number of channels to be evaluated by making accessible the GETMAIN system macro instruction to the FORTRAN program at execution time via the ALLOCX subprogram written in Assembler (Abel 1972a).

3.2 Main Routine

This is the principal routine of the program and directs the loading of all the major links utilized by means of a data input stream. The program initializes the direct access files for the intermediate data storage, reads the whole input data and copies them in the punching format on a sequential organized data file to constitute the file handling functions rewind, or backspace, thus allowing a reread of the input data for identification. A title with the name of the input tape and the date of the evaluation is printed out. Finally, the calculated information is written out on a tape which serves as input to the other evaluation programs, if desired.

3.3 Service Subprograms

In this chapter a general presentation of all subprograms which are needed in several overlay paths will be given. Therefore, these subprograms are also placed in the root segment of the system.

The subprogram READIN serves to read all data from cards which are transferred in the punching format to a data file. By calling REREAD the card images are printed out for controlling purposes. STEUER directs the mode of the spectra reading. This subprogram reads input B and builds up tables relating the detector and monitor positions to

the data blocks on the input tape for further use. It must be noted, that this selection of detectors permits the user to evaluate single detectors and not all. Depending on the size of the spectra, i.e. on the number of channels recorded for a scattering angle, pointers for buffering of these arrays are updated in a computing array.

WTDISK is the file writing routine of the system.

RDDISK reads the spectra from a direct access file into the related computing array.

DATUM is the date routine of the system.

JBFX reads from the job file control block the name of the input tape (DSNAME and VOLUME parameter).

INITDA serves to define the direct access files at execution time (replaces the DEFINE FILE function) (Abe1 1972 b).

INPUT1 with the entry points INPUT2 and NEXTPR serves to read most of the input data, e.g. experimental parameters, function and control cards. In some cases a card is checked to find the identification in columns one to four. The program carries out named functions such as printing remarks and establishing titles, or sets an indicator for the calling program of which type of card was encountered. When a card has been punched improperly, or when an incorrect card order sequence is encountered, an error message is printed. This is detected whether or not the data conversion error condition was raised using the extended error message facility (ERRCOD, ERRSET). INPUT2 reads input D. This contains those parameters which do not change from one sample measurement to another evaluated in the same run. In NEXTPR the specific input data for every sample measurement are read in.

The subprogram BLDTB is used for some input parameters in order to fill an array with constant values by checking the first punched value on the appropriate data cards.

The subprogram PRINT serves to print out the detector and monitor spectra at different stages of the evaluation process.

The time independent background of the detectors is printed out by TAB in tables. If calculated, the intensities of the monitor spectra or the monitor peaks and the positions of the elastic peaks in the detector spectra are also listed in additional columns. The subprogram

RSTNLL resets the parameter field NLL to zero which directs the printer output in TAB. LINPLT produces a line printer plot, e.g. shape of the elastic peak, elastic corrections for each detector etc. To get this plot the subprogram ZWERT interpolates the values to an equally spaced scale determined by a three-point interpolation utilizing Lagrange's method.

PLOTIN prepares texts for a Calcomp plot, PLOTFL plots the TOF-spectra over channels and PLOTQS is called to plot the double differential cross section over energy or time-of-flight, respectively. The subprograms LINAXE and LOGAXE are used for arrangement of the plot axes.

The monitor peak analysis is performed in QQMON. The position and the intensity of the peak in a monitor 1 spectrum is calculated by summing up all counts in the region specified in the input and subtracting the constant background as calculated with SMUG. This program also calculates the intensity of a monitor 5 spectrum by summing up all counts of the spectrum.

The subprogram SMUG, as mentioned above, is called to calculate the maximum time-constant background of the detector spectra and the monitor spectra. This is the lowest mean value of the spectrum when a fixed number of neighboring channels are added. After subtraction at least the content of one channel of the spectrum will be zero.

To smooth the spectra of the time independent background measurement and the container scattering the subprogram GLAET is called, if desired. Different regions of a spectrum may be smoothed by evaluating at X_K the least-squares polynomial of degree 2 relevant to the given successive points n : (X_{K+i}, Y_{K+i}) , $i = -n, 0, +n$.

parabola through 3 points:

$$Z_K = \frac{1}{3} (Y_{K-1} + Y_K + Y_{K+1})$$

parabola through 5 points:

$$Z_K = 0.4857 Y_K + 0.3429(Y_{K-1} + Y_{K+1}) - 0.0857 (Y_{K-2} + Y_{K+2})$$

parabola through 11 points:

$$Z_K = \frac{1}{429} \cdot (89 Y_K + 84 (Y_{K-1} + Y_{K+1}) + 69 (Y_{K-2} + Y_{K+2}) + 44 (Y_{K-3} + Y_{K+3}) \\ + 9(Y_{K-4} + Y_{K+4}) - 36 (Y_{K-5} + Y_{K+5}))$$

When the interpolation is made near the endpoints of an interval, these points are treated separately.

The position of the elastic peak in a spectrum is calculated by PEAKER, if it is not given in the input. The elastic peak estimated to be the maximum in a given region of the spectrum is approximated by a parabola. The position is now defined by the channel number, where the slope of the parabola is zero. The subprogram PKFORM solves the normal equations which are related to the least-squares approach used.

The subprogram POL interpolates values from the measured ones, e.g. if an empty container measurement must be shifted before subtraction from a sample measurement by a fraction of a time channel.

3.4 Initial Processing of the Scattering Data

The data of a time-of-flight experiment recorded by the data acquisition computer system are often written on magnetic tape for later analysis on a large size computer. In general, this program can evaluate scattering data which are arranged into sets of time channels for a series of scattering angles. The individual measurements which are written on a magnetic tape without format control are identified by control blocks preceding the data blocks. A data block, therefore, contains the time-of-flight spectrum for one scattering angle.

The header blocks must contain five integer variables which are updated by the data acquisition system:

- (1) Number of file (run identification)
- (2) Number of experiment (instrument identification)
- (3) Number of result (type of the measurement)
- (4) Number of channels (is limited to 1024)
- (5) Number of data blocks which follow (detectors)

The transfer of the measurements to be evaluated is controlled by the subprogram RDTAPE. It reads the first part of input C and searches for control blocks of these measurements on the input tape submitted. Up to five measurements can be added up to a given one. For this purpose, the subprogram ADDRES is called, if desired. The subprogram BI directs the transfer of the data blocks of a chosen measurement from tape to disk.

There are two main tasks to be performed before. First, the spectra related to the detectors and monitors can be selected as indicated by input data and updated by the subprogram STEUER. Normally, no block numbers must be specified. In these cases, the program assumes that the detectors and the monitors are sequentially arranged on the magnetic tape. However, the indication of block numbers or ranges of detectors thus permits a selective evaluation of detectors or, on the other hand, excludes distinct detectors from the evaluation if they are not desired.

Second, due to experimental mishaps the following corrections can be applied to the measured scattering data. Single channels or channel pairs that are dropped or raised by electronic errors are corrected by three-point interpolation in KORREK

$$Y_K = Y_{K-1} - (Y_{K-1} - Y_{K+2}) \cdot \frac{1}{3}$$

$$Y_{K+1} = Y_{K+2} + (Y_{K-1} - Y_{K+2}) \cdot \frac{1}{3}$$

On the other hand, if a detector stopped counting during an experimental run the counting rates can be multiplied with a constant factor by calling the subprogram DETKOR for these detectors, or MONKOR for the monitors, respectively. This should be done when the intensities of all detectors have to be added, e.g. in the detector sampling method.

Finally, after the corrections were carried out, the detector spectra are written on a disk. The program uses five direct access files each for a measurement that can be evaluated and, depending on the mode of use, as a temporary storage of the results. The maximum length of a data block must correspond to the length of the detector spectrum on the magnetic tape containing the raw data. A maximum number of 1024

channels can be processed. For the evaluation of 256 or 512 channels, the detector spectra are buffered in blocks of 1024 channels. One such block is then read in and the respective detector spectrum is selected by the indication of a starting address. These data files require a buffer region of 24 kBytes main storage. The number of data blocks to be transmitted to a disk which is also necessary for the definition of a direct access file is taken from the DD-control card via the Job File Control Block and is used for the definition of these data sets at execution time (Abel 1972).

3.5 Fit Program for the Peak Analysis

This program is intended for the analysis of the elastic peak in the vanadium sample and the sample measurement in TOF or $S(Q,\omega)$ representation calculated from the time-of-flight spectra. For the latter the related quantities are transferred from the sequential data file containing the computed results to a direct access file. In most cases it is quite reasonable to assume a Gaussian shape over energy scale for the resolution function of the time-of-flight spectrometer. However, it can be used for fitting the data representing Gaussian, Lorentzian or a convolution of a Gaussian with a Lorentzian.

The analysis is carried out by a least-squares method described in (Braes 1965). The spectral data are read by FITLB which calls the general peak analysis program BREITE in turns. The information about the function to which the experimental data are to be fitted must be supplied as input. The program then determines the initial estimates of all parameters involved in the fit. A Gaussian used to represent the data is characterized by a set of parameters which includes the peak position, the width and the peak height. The first parameter may be fixed at his original input value for calibration purposes. The initial estimates of x_0 and y_0 come from the coordinates of the highest data point in the given peak region used. The data points are converted to energy scale before performing the fit. Some corrections are included for an underlying spectral distribution by a constant value, a line function, or by a background given channelwise (e.g. caused by inelastic or multiple scattering, overlap contribution etc.). The experimental data are weighted by one. The least-squares procedure is performed in SQUFT4 to find the minimum over the squares of the deviations

of the data from their estimates. The subprogram BIPLX4 called by SQUFT4 searches for the minimum of a convex square function by means of the linear programming approach of Wolfe. The values of the function and their partial derivatives with respect to the parameters are calculated in FKTN.

If a peak is described by a convolution function the subprogram QUAD calculates an approximate value of the integral over the convolution function by means of the Romberg integration method. The derivatives of the combined Gaussian-Lorentzian function for the convolution integral are calculated in FVONX. For this the half-width of the related Gaussian must be supplied as input taken from an earlier run.

After the final values of the parameters have been determined the uncertainties of the parameters are calculated to evaluate the quality of the fit. Then, the final parameters and, optionally, the elastic peak together with the fitted function values are printed out. Moreover, a graphical representation in the printer output can be produced to enable the user to estimate the validity of the fit, too.

3.6 Preparation of the Sample Holder Measurement

Obviously, a maximum background suppression is important for the understanding and the successful interpretation of the experimental results. In many time-of-flight systems the instrumental background can be considered sufficiently well as time-constant. Effects of such a background are estimated numerically by subtracting an underlying distribution of the spectrum which is represented by a constant value. If time-dependent effects are not negligible, a so-called "time-independent" background measurement must be performed. This is for instance the case for a single crystal-Fermi chopper arrangement when unwanted faster neutrons stemming from higher order reflections are not completely suppressed when the transmission should be zero. In this case a gadolinium reference measurement must be made. In this chapter the evaluation steps for the data reduction of the time-independent background -(ZU)-measurement and the container-(LE)-measurement are outlined briefly. In order to correct the sample measurement for scattering from the container the main link PREPAS is called to prepare the above measurements. The input data are supplied by invoking INPUT1.

The time-constant background (cases (1) and (3)) should only be subtracted, if there is no time-independent background measurement, or if the time-constant background is caused mainly by electronic effects during the measurement and cannot be scaled by the monitor intensities.

If it is not given in the input, the position of the elastic peak in each spectrum of the container measurement are examined by calling PEAKER for later use.

At each stage of the evaluation mentioned above the detector spectra are rewritten on disk and can be written out on a line printer for controlling purposes by calling the subprogram PRINT according to a choice of several options.

3.7 Evaluation of the Vanadium Experiment

The main link PREPAS also serves to evaluate the vanadium measurement and the related container measurement. Due to the well known scattering cross section of the incoherent scatterer vanadium a vanadium experiment is used to calibrate the spectrometer. The absolute or relative efficiencies of the neutron gas detectors for the incoming energy E_0 are calculated and are used in the reduction of the sample data (see 3.11).

If there is a vanadium measurement, the raw data are first corrected for time-constant background. Next, the peak intensity of monitor 1 is calculated. The following stage of the evaluation is the preparation of the vanadium holder measurement, if there is any. According to the value of the input variable IVLG the spectra (a) are left as measured or (b) can be smoothed by polynomial approximation over distinct subgroups of channels as given in the input. Then, a time-constant background is calculated and subtracted, if the input variable MINUNT is set to 1.

To calculate the detector efficiencies for neutrons with the incident energy E_0 the normalized counts from the vanadium holder are subtracted off from the vanadium spectra. Now, the positions of the maxima of the elastic peak in the vanadium spectra are calculated, if they are not given in the input data.

For neutron energies of less than 30 meV the incoherent elastic differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{\sigma_b}{4\pi} e^{-2w} \quad (3.7.1)$$

is used to calculate the detector efficiency ϵ_2 from

$$\frac{\Delta\sigma}{\Delta\Omega_\theta} = \epsilon_2 \cdot \frac{d\sigma}{d\Omega} \cdot \frac{1}{f_s} \quad (3.7.2)$$

by substituting the measured cross section

$$\frac{\Delta\sigma}{\Delta\Omega_\theta} = \frac{\sum_i N_{i\theta}^{(\text{peak})}}{n_o \cdot N \cdot \Delta\Omega_\theta} \quad (3.7.3)$$

into (3.7.2). The factor e^{-2w} is the Debye Waller factor, or the thermal factor, which reflects the reduction in the scattering intensity due to thermal vibrations of the lattice. σ_b [b] is the bound scattering cross section of vanadium and θ the scattering angle under investigation. The number of the vanadium atoms N [b^{-1}] is obtained from

$$N = \frac{0.6023 \cdot d \cdot \rho}{M \cdot \sin\alpha} \quad (3.7.4)$$

where d [cm] represents the thickness of the vanadium slab. ρ [g/cm^3] is the density of the vanadium sample, M [g/Mol] the mass of the scatterer, and α [$^\circ$] the angle between the direction of incoming neutrons and the sample direction in the scattering plane measured in the same direction as θ (see Figure 1). The incident neutron beam intensity n_o is calculated using the input variable ANRM and the evaluated monitor peak intensity M1VA. ANRM represents the number of neutrons on the vanadium slab per monitor 1 count:

- (a) the absolute efficiency at E_o is calculated, if ANRM was measured (flow chart of neutron beam)
- (b) the sample measurement is scaled to the vanadium measurement, if ANRM is the same in input C and input D. The relative efficiency of the detector is calculated then.

$\Delta\Omega_\theta$ is the solid angle of the detector seen from the center of the sample and is calculated from $\Delta\Omega_\theta = \Delta S / (FL2)^2$, where ΔS [cm^2] is the active plane of the detector and $FL2$ [cm] the secondary flight path. The lower index θ

indicates that the calculation is done for the detector at the scattering angle θ . The corrected counting rates $N_{i\theta}$ in (3.7.3) and (3.7.7) are summed over a given region of channels i , i.e. over the elastic peak and over a portion of the spectrum including elastic and inelastic contributions, respectively.

For energies of more than 30 meV the total differential cross section (elastic + inelastic) can be represented by the Placzek approximation

$$\frac{d\sigma}{d\Omega} = \frac{\sigma_b}{4\pi} (1 - 2 \frac{m}{M} (1 - \cos\theta)) \quad (3.7.5)$$

where m [g/Mol] is the mass of the neutron. Using this approximation the detector efficiency ϵ_1 can be obtained from

$$\frac{\Delta\sigma}{\Delta\Omega_\theta} = \epsilon_1 \cdot \frac{d\sigma}{d\Omega} \cdot \frac{1}{f_s} \quad (3.7.6)$$

where the measured scattering cross section is now given by (spectrum)

$$\frac{\Delta\sigma}{\Delta\Omega_\theta} = \frac{\sum_i N_{i\theta}}{n_o \cdot N \cdot \Delta\Omega_\theta} \quad (3.7.7)$$

f_s represents the self absorption in the sample and is calculated for a finite plane slab by invoking the subprogram SELBAV. This subroutine must be replaced for other sample geometries. The correction factor is calculated for transmission through ($\theta < \alpha$) and reflection from ($\theta \geq \alpha$) the sample:

$$f_s = e^{-\frac{\sigma_a(E_0) N_1 d}{\sin(\theta-\alpha)}} \cdot \frac{x}{1-e^{-x}} \quad (\theta < \alpha) \quad (3.7.8)$$

$$f_s = \frac{x}{1-e^{-x}} \quad (\theta \geq \alpha) \quad (3.7.9)$$

with

$$x = N_1 d \left\{ \frac{\sigma_t(E_0)}{\sin\alpha} + \frac{\sigma_a(E_0)}{\sin(\theta-\alpha)} \right\} \quad (3.7.10)$$

where N_1 [$\text{cm}^{-1}\text{b}^{-1}$] is given by

$$N_1 = \frac{0.6023 \cdot \rho}{M} \quad (3.7.11)$$

The total cross section $\sigma_t(E_0)$ [b] of vanadium at energy E_0 can be obtained from

$$\sigma_t(E_0) = \sigma_b + \sigma_a(E_0) \quad (3.7.12)$$

where $\sigma_a(E_0)$ [b] is the absorption cross section of vanadium at energy E_0 which is given by

$$\sigma_a(E_0) = 2.8 \sqrt{\frac{25.3}{E_0}} \quad (3.7.13)$$

If $|\theta-\alpha| < \beta = \arctan d/d_p$, the values of $|\theta-\alpha| = \beta$ are taken for f_s to simulate a finite slab geometry. d_p [cm] represents the sample dimension in the scattering plane.

3.8 Evaluation of the Sample Measurement

In this chapter the data reduction of the scattering experiment of the investigated material is described. The main link MESS is called to calculate the net contents of the channels for later use in the computation of the time-of-flight spectra and the scattering law. The sample-(PP)-measurement may be corrected for time-independent background and for container scattering.

If there is a time-independent background-(ZU)-measurement, the evaluation, as described in (3.7), is only repeated if a new (ZU)-measurement was performed. After normalisation of the time-independent background spectra to the scattering data with the intensities of the monitor 1 or monitor 5 spectra the sample data are corrected for time-independent background.

If there is a container measurement, the peak intensity in the monitor 1 spectrum of the sample measurement is calculated. Then, the sample data are corrected for time-constant background.

As in the reduction of the container measurement, there are four possibilities of considering the time-independent background:

- (a) with ZU: MINUNT > 0 (1) ZU and time-constant background are subtracted
- MINUNT < 0 (2) ZU is subtracted

- (b) without ZU: MINUNT > 0 (3) the time-constant background is subtracted
 MINUNT < 0 (4) no time-independent background subtraction at all.

As reference for a possible channel shift of the container measurement before subtraction and for the energy scale, the positions of the maxima of the elastic peaks (PEAKPR) in the sample spectra are determined:

- (a) from the input (PEAKPR > 0)
(b) by calculation (PEAKPR = 0)
(c) from the vanadium measurement (PEAKPR < 0)

Before the container spectra can be subtracted from the sample spectra, the different self absorptions in the sample and container measurement must be considered. This is done in ZFKOR, if the input variable IZEITF is set to one. The calculated factor $f(\theta, E_0)$ modifies the normalisation factor g_{LE}^{PP} of the container-(LE)-measurement to the sample-(PP)-measurement.

$$g_{LE}^{PP} = g_{LE}^{PP} \cdot f(\theta, E_0)$$

Two normalisation constants are calculated to obtain g_{LE}^{PP} :

- (1) The monitor 1 intensities are usually taken to calculate g_{LE}^{PP} .
(2) Furthermore, an input variable VFZ enables the user to normalize the time-of-flight spectra to another sample measurement evaluated in the same run or in an earlier run. So, TOF-spectra with different measuring times may be compared. This factor which modifies g_{LE}^{PP} , is undone before the double differential cross section is calculated.

If there is a channel shift between the container- and the sample measurement which is not a multiple of a channel width, the container spectra are interpolated to the new channels before subtraction. The channel shift is calculated, if it was not given in the input, but in both cases it is only taken into account, if the input variable IVKS is set to one. Finally, the net channel contents and the relative statistical accuracy are calculated. The latter is calculated under the assumption that the background were taken as a time-independent background.

The subprogram ZFKOR calculates the correction factors $f(\theta, E_0)$ for normalisation factors, as mentioned above. A thin walled finite slab container is assumed in this version of ZFKOR.

Therefore, this routine must be replaced for other sample geometries.

$$f(\theta, E_0) = 0.5 \left\{ e^{-\frac{\sigma_t(E_0) \cdot N \cdot D}{\sin(\phi-\theta)}} + e^{-\frac{\sigma_t(E_0) \cdot N \cdot D}{\sin\phi}} \right\} (\theta < \phi) \quad (3.9)$$

$$f(\theta, E_0) = 0.5 \left\{ 1 + e^{-\frac{\sigma_t(E_0) \cdot N \cdot D}{\sin\phi}} \cdot e^{-\frac{\sigma_t(E_0) \cdot N \cdot D}{\sin(\theta-\phi)}} \right\} (\theta \geq \phi) \quad (3.9.)$$

If $|\theta-\phi| < \beta = \arctan(D/D_p)$, the values of $|\theta-\phi| = \beta$ are taken for $f(\theta, E_0)$ to simulate a finite slab geometry, where D_p [cm] is the dimension of the sample in the scattering plane. The number of atoms N [$\text{cm}^{-1}\text{b}^{-1}$] is obtained from

$$N = 0.6023 \cdot \frac{\rho}{A} \quad (3.9)$$

where ρ [gcm^{-3}] is the density of the sample, A [gMol^{-1}] the mass of the scatterer, and ϕ is the sample angle which has the same meaning as the angle α in the evaluation of the vanadium measurement (see Chapter 3.7). D [cm] represents the sample thickness.

3.9 Calculation of the Elastic Correction

An attempt is made to separate the spectrum of the inelastically scattered neutrons from that of the elastically scattered ones calling the main link ELASTK. A Gaussian (assumed resolution function of the TOF-spectrometer for $E = E_0$) described below is subtracted from the spectrum of a solid sample to remove the peak of the elastically scattered neutrons.

It is supposed that Gaussians were fitted to the elastic peaks of the vanadium measurement. The fit should be done in a region of the peak where there are no contributions from inelastic scattering. This Gaussian is normalized to the height of the peak in the sample spectrum. A channel shift between the maxima of the vanadium- and the sample peaks is regarded.

The Gaussian is extended over the limits of the fit region by the amount of KAUSD channels to each side. Fitting and subtracting can be done on-line with the help of interactive graphics on the IBM/2250 (see 5.1.2). The region near the elastic peak (original values, fitted Gaussian, resulting spectrum) is shown in a printer plot. Some of the routines correspond to the ones described in (3.5) to avoid an "exclusive call" which is not allowed in an overlay tree. The subprogram DISEK is a dummy routine in case no display unit is used.

3.10 Calculation of the Time-of-Flight Spectrum

The main link FLZS is called to calculate the time-of-flight spectra. In a first step, the sample spectra may be reduced in SUMN by summing up the net counting rate of all IRED channels (the input variable IRED must be an even integer) to a new one with IRED times the channel width. All the other interesting parameters of the measurement are converted to the new scale. Then, the time channels i are converted to energy E_i by

$$E_i = \frac{B^2}{(i - K_p + B/\sqrt{E_0})^2} \quad [\text{meV}] \quad (3.10.1)$$

or, if $(i - K_p + B/\sqrt{E_0}) \leq -0.4$,

$$E_i = \frac{B^2}{(i - K_p + B/\sqrt{E_0} + DC)^2} \quad [\text{meV}] \quad (3.10.2)$$

where K_p is the maximum of the elastic peak.

Thus the counting rate left from $E = \infty$ is contributed to the frame overlap. Frame overlap occurs when the repetition rate of the neutron pulses is shorter in time than the time-of-flight for very slow neutrons from the sample to the detectors.

B is calculated from

$$B = 22.862 \cdot FL2/DTK \quad (3.10.3)$$

where $FL2$ [cm] is the secondary flight path and DTK [μs] is the width of a time channel. The duty cycle DC is obtained by $DC = KAN + PAUSE$. KAN is the spectrum length. If there are more than 10 channels to the left of $E = \infty$,

they are grouped to the right of the spectrum with a distance of PAUSE channels. PAUSE is the difference between the duty cycle and the length of the spectrum expressed in channels. PAUSE channels must be dropped at the end of the new arranged spectra to retain the original spectrum length.

In this way the energy scale reaches from the highest (channel 1) to the lowest energies (last channel). Now, the energy dependent efficiencies $\epsilon(E_i)$ of the He^3 -detectors and the time-of-flight spectra $Z_{\text{TOF}}^{(i)}$ are calculated for each scattering angle (detector):

$$Z_{\text{TOF}}^{(i)} = Z_i \cdot \frac{f_s}{\epsilon_i} \cdot \text{VFZ} \quad (3.10.4)$$

where Z_i represents the net channel contents, f_s the self absorption factor and VFZ a normalization factor (see 3.8). The efficiency $\epsilon(E_i)$ can be modified by a general factor AF for normalization of one measurement to another (is not undone as VFZ!)

$$\epsilon_i = \epsilon(E_i) \cdot \text{AF} \quad (3.10.5)$$

The TOF-spectra may be displayed on the screen of the IBM/2250-1 display unit (DIS=1 in the EXEC card) and it is possible to correct remaining Bragg peaks interactively. The range of channels is defined in which the double differential cross section and the scattering law will be evaluated, if ISTREU=1. The TOF-spectra are saved temporarily on disk. [The next set of measurements (ZU, LE, VA, VL, PP) is read, if there is any.] For ISTREU = 1 the program continues the evaluation by calling DQSG to calculate the cross section and the scattering law.

The subprogram EPSPZ serves to calculate the efficiency of a cylindrical neutron gas-detector using the empirical formula of Carvalho (Carvalho 1967).

$$\epsilon(E_i) = C \cdot e^{-C_1/\sqrt{E_i}} \cdot (1 - e^{-f_a/\sqrt{E_i}}) \quad (3.10.6)$$

where f_a is an empirical absorption factor of a gas cylinder. The exponential factor C_1 takes into account the absorption of the neutrons between sample and detector gas, if desired and is given by

$$C_1 = (\text{SABFP} \cdot \text{FL2} + \text{SABS} \cdot \text{FD} + \text{SABDW} \cdot \text{ZWD}) \cdot \sqrt{E_{\text{therm}}} \quad (3.10.7)$$

with $E_{\text{therm}} = 25.3 \text{ meV}$

Here, $SABFP \text{ [cm}^{-1}\text{]}$ is the macroscopic absorption cross section of the gas on the secondary flight path FL2. SABS is the macroscopic absorption cross section of the window material between the sample and detector (cryostat, furnace-windows, etc.) of the thickness $FD \text{ [cm]}$. SABDW is the macroscopic absorption cross section of the detector wall of thickness $ZWD \text{ [cm]}$.

The factor C in Eq. (3.10.6) takes into account the scattering of the neutrons between the sample and the detector gas. Depending on the value of the input variable IEPS this factor C

(a) can be obtained in analogy with (3.10.7) from

$$C = C_{\text{cal}} = e^{-(SSTFP \cdot FL2 + SSTR \cdot FD + SSTDW \cdot ZWD)} \quad (3.10.8)$$

where $SSTFP$, $SSTR$, $SSTDW \text{ [cm}^{-1}\text{]}$ are related to the scattering on the secondary flight path, of the window material and of the detector wall.

(b) is set to 1, or

(c) is given by

$$C = C_{\text{exp}} = \frac{\epsilon_m}{e^{-C_1/\sqrt{E_0}} \{1 - e^{-f_a/\sqrt{E_0}}\}} \quad (3.10.9)$$

using the measured efficiency (absolute or relative) ϵ_m which can be obtained from (3.7.2) or (3.7.6), respectively. Thus the efficiency $\epsilon(E_i)$ is scaled to the measured efficiency at E_0 . There are eight possibilities of choosing the efficiency:

By setting the input variables IEPS and IC1ABS to an appropriate value, we have the following formulas:

$$\text{(with } B = 1 - e^{-f_a/\sqrt{E}}\text{)}$$

$$\text{IEPS} = 2 \quad \epsilon(E) = \epsilon_m(E_0) \text{ relative efficiency} \quad (3.10.10)$$

$$\text{IEPS} = 1 \quad \text{IC1ABS} = 1 \quad \epsilon(E) = C_{\text{cal}} \cdot e^{-C_1/\sqrt{E}} \cdot B \quad (3.10.11)$$

$$\text{IC1ABS} = 0 \quad \epsilon(E) = C_{\text{cal}} \cdot B \quad (3.10.12)$$

$$\text{IEPS} = 0 \quad \text{IC1ABS} = 1 \quad \epsilon(E) = C_{\text{exp}} \cdot e^{-C_1/\sqrt{E}} \cdot B \quad (3.10.13)$$

$$\text{IC1ABS} = 0 \quad \epsilon(E) = C_{\text{exp}} \cdot B \quad (3.10.14)$$

$$\text{IEPS} = -1 \quad \text{IC1ABS} = 1 \quad \epsilon(E) = e^{-C_1/\sqrt{E}} \cdot B \quad (3.10.15)$$

$$\text{IEPS} = -1 \quad \text{IC1ABS} = 0 \quad \epsilon(E) = B \quad (3.10.16)$$

$$\text{IEPS} = -2 \quad \epsilon(E) = 1 \quad (3.10.17)$$

The last case enables the user to take into account the efficiency in a succeeding program. The detector efficiency is printed out for the first detector of the evaluation run.

The self absorption factor f_s of a sample with finite slab geometry is calculated in DICKOR. This subprogram corresponds to SELBAV and must also be replaced for other sample geometries.

$$f_s = e^{-\frac{\sigma_a(E) \cdot N \cdot D}{\sin(\theta-\alpha)}} \cdot \frac{x}{1-e^{-x}} \quad (\theta < \phi) \quad (3.10.18)$$

or

$$f_s = \frac{x}{1-e^{-x}} \quad (\theta \geq \phi) \quad (3.10.19)$$

with

$$x = N \cdot D \cdot \left\{ \frac{\sigma_t(E_0)}{\sin \phi} + \frac{\sigma_a(E_0)}{\sin(\theta-\phi)} \right\} \quad (3.10.20)$$

where the parameters has the some definitions as introduced in Chapter 3.9. If $|\theta-\phi| < \beta = \arctan D/D_p$, the values of $|\theta-\phi| = \beta$ are taken for f_s to simulate a finite slab geometry.

3.11 Calculation of the Double Differential Cross Section and the Scattering Law

The next stage of the evaluation is the calculation of the double differential cross section and the symmetrized scattering law for the channel region of interest. To save storage the main link DQSG allocates main storage for 12 computing arrays at execution time. The calculations themselves are performed in GETSG including the "one-phonon" approximation of a generalized frequency distribution $p(\beta)$ and other experimental quantities of interest.

The double differential cross section is calculated for all detectors (scattering angles θ) and all channels i of a given region. Any negative values of $Z_{TOF}^{(i)}$ are replaced by zero.

$$(1) \quad \frac{d^2\sigma}{d\Omega d\tau_i} = \frac{Z_{TOF}^{(i)}}{\Delta\Omega_\theta \cdot N \cdot \eta_0 \cdot \Delta\tau} \quad \left[\frac{\text{b} \cdot \text{cm}}{\mu\text{sec}} \right] \quad (3.11.1)$$

$$(2) \quad \frac{d^2\sigma}{d\Omega dE_i} = \frac{d^2\sigma}{d\Omega d\tau_i} \cdot \frac{\tau_i^3}{1045.32} \quad \left[\frac{\text{b}}{\text{meV}} \right] \quad (3.11.2)$$

$$(3) \quad \frac{d^2\sigma}{d\Omega d\beta_i} = \frac{d^2\sigma}{d\Omega dE_i} \cdot \frac{T}{11.6} \quad \left[\text{b} \right] \quad (3.11.3)$$

where the number of the scatterer $N [b^{-1}]$ is obtained from

$$N = \frac{0.6023 \cdot D \cdot \rho}{M \cdot \sin\phi} \quad (3.11.4)$$

in analogy with (3.7.4). The incident neutron beam intensity η_0 which is responsible for the scaling of the experiment is calculated using the input variable ANRM and the evaluated monitor peak intensity M1PR:

(a) without a vanadium measurement:

- (1) scaling with assumed ANRM (relative response)
- (2) scaling with measured ANRM (absolute response)

(b) with a vanadium measurement:

(3) scaling with assumed ANRM (sample measurement is scaled to the vanadium cross section, if irradiated area and sample area are the same, IEPS = 0 is used, and ANRM, i.e. ANRM is set to the same value for the evaluation of the vanadium measurement and the sample measurement.)

(4) scaling with measured ANRM (absolute res., vanadium and sample areas must not be the same. Then the input values must be different for the two evaluation runs.)

$\Delta\tau$ [$\mu\text{sec}/\text{cm}$] is the time-of-flight interval and is given by

$$\Delta\tau = \frac{\text{DTK}}{\text{FL}^2} \quad (3.11.5)$$

whereas the time-of-flight τ is obtained from

$$\tau_i = \frac{7.22951}{\sqrt{0.1 \cdot E_i}} \quad (3.11.6)$$

T [K] represents the sample temperature. The parameters of the scattering laws are

$$\hbar\omega_i = E_i - E_0 \quad [\text{meV}] \quad \text{energy transfer} \quad (3.11.7)$$

$$\beta_i = \hbar\omega_i \cdot 11.6/T \quad \text{energy transfer} \quad (3.11.8)$$

$$Q_i = 0.6945 \cdot \sqrt{E_0 + E_i - 2E_i E_0 \cos\theta} \quad [\text{\AA}^{-1}] \quad \text{momentum transfer} \quad (3.11.9)$$

$$\alpha_i = 24.265 \cdot \frac{Q_i^2}{M \cdot T} \quad \text{momentum transfer} \quad (3.11.10)$$

The symmetrized scattering laws are

$$S(Q_i, \omega_i) = \frac{4\pi}{\sigma_b} \cdot \sqrt{\frac{E_0}{E_i}} e^{\beta_i/2} \frac{d^2\sigma}{d\Omega dE_i} \left[\frac{1}{\text{meV}} \right] \quad (3.11.11)$$

and

$$S(\alpha_i, \beta_i) = S(Q_i, \omega_i) \cdot \frac{T}{11.6} \quad (3.11.12)$$

This last form of the scattering law is used in addition to $S(Q_i, \omega_i)$, because the connection to other programs (multiple scattering, multi-phonon corrections, etc.) is simplified.

Under the assumption that only one-phonon processes took place in the scattering process, preliminary generalized frequency distribution functions are calculated:

$$p(\beta) = \beta^2 \cdot e^{\alpha\lambda} \cdot S(\alpha, \beta)/\alpha \quad (3.11.13)$$

and

$$\rho(\beta) = (e^{\beta/2} - e^{-\beta/2}) p(\beta)/\beta \quad (3.11.14)$$

where $e^{\alpha\lambda}$ is the inverse of the Debye Waller factor. The Debye Waller coefficient λ can be supplied as input or can be calculated in the Debye approximation

$$\lambda = 6 \cdot \frac{T}{\theta_D} (0.25 + \Lambda) \quad (3.11.15)$$

where θ_D represents the Debye temperature. The Debye function Λ is given as follows

$$\Lambda = \left(\frac{T}{\theta_D} \right)^2 \cdot \int_0^{\theta_D/T} \frac{\beta}{e^{\beta}-1} d\beta \quad (3.11.16)$$

and must be supplied as input.

3.12 Calculation of the Instrumental Resolution

Another correction which must be applied to the data is the correction for instrumental resolution. In practice, this unfolding problem is a complicated procedure (Skjöld et al. 1972). Several resolution functions can be defined for a TOF-spectrometer. Though the data are not corrected

here for resolution, however, the (primary and secondary) energy resolution and the momentum transfer resolution (Q-resolution) are approximately calculated by calling RESOL from GETSG. This is done for a rotating crystal time-of-flight spectrometer using the relations which are described in more detail elsewhere (Carvalho et al. 1967). These relations are summarized in the following. First, the expressions for the energy transfer and the energy resolution are given.

$$\frac{\Delta h\omega}{h\omega} = \sqrt{\left(\frac{E}{h\omega}\right)^2 \cdot \epsilon^2 + \left(\frac{E_0}{h\omega}\right)^2 \cdot \epsilon_0^2} \quad (3.12.1)$$

where ϵ_0 denotes the primary resolution and ϵ the secondary resolution, corresponding, to the neutron energies E_0 (incident) and E (scattered). The primary energy resolution ϵ_0 is given by

$$\epsilon_0 = 2\alpha_H^2 \cot^2\theta_B \quad (3.12.2)$$

where θ_B represents the Bragg angle of the rotating crystal and α_H the collimation angle in the scattering plane. The secondary energy resolution can be divided into two parts corresponding to the flight path uncertainty ϵ_L and to the flight time uncertainty ϵ_T :

$$\epsilon^2 = 4 (\epsilon_L^2 + \epsilon_T^2) \quad (3.12.3)$$

$$\epsilon_L = \frac{\Delta PR^2 + \Delta DT^2}{FL^2} \quad (3.12.4)$$

$$\epsilon_T = \left\{ \left(\frac{0,5\alpha_H^2 + \mu^2}{\omega^2} + 0,5 \alpha_H^2 \cdot T^2 \cdot \cot^2\theta_B \right) + \Delta TKR^2 + \Delta TCH^2 + \Delta TPR^2 \right\} / T^2 \quad (3.12.5)$$

where the symbols not yet defined have the following meanings:

ΔPR	uncertainty of flight path due to sample dimension [cm]
ΔDT	uncertainty of flight path due to detector dimension [cm]

μ	mosaic spread of chopping crystal [°]
ω_k	angular speed of the crystal [sec ⁻¹]
$T_0^2 = 522.7 FL_1^2/E_0$ [μsec ²]	time of flight of incoming neutrons
FL1	primary flight path [cm] crystal-to-sample distance)
$\Delta TKR = 1.7 \sqrt{a^2 + b^2} R/v_0$	uncertainty of flight time due to Doppler shift of neutrons at the chopping crystal
wherein	
$a = \frac{\omega_k}{\omega_k} \cos \theta_B - T_0 \cdot \omega_k \sin \theta_B + \cos \theta_B$	
$b = - \sin \theta_B$	
R	radius of crystal [cm]
$v_0 = 0.0437 \sqrt{E_0}$ [cm/μsec]	velocity of incoming neutrons
$\Delta TCH = DTK$	width of time channel
$\Delta TPR = 522.7 \Delta PR^2/E$ [μsec ²]	uncertainty of flight time due to sample dimension
$T^2 = 522.7 FL_2^2/E$ [μsec ²]	time of flight between sample and detector

Second, the Q-resolution for a TOF-spectrometer can be calculated using the following relation:

$$\begin{aligned}
 \left(\frac{\Delta Q}{Q}\right)^2 = & \left\{ \left(\frac{2m}{\hbar^2 Q^2}\right) - E \sin^2 \theta \cdot \left(\frac{2m}{\hbar^2 Q^2}\right)^2 \right\} \cdot E \left\{ \frac{\epsilon^2}{4} \cos^2 \theta + \left(\frac{DTB}{FL_2}\right)^2 \sin^2 \theta + \frac{\epsilon_0^2}{4} \right\} + \\
 & + \left(\frac{2m}{\hbar^2 Q^2}\right)^2 \frac{1}{4} \left\{ \left(\frac{DTL}{FL_2}\right)^2 E + \alpha_H^2 E_0 \right\}^2 + \left(\frac{2m}{\hbar^2 Q^2}\right)^2 E \sin^2 \theta \left\{ \alpha_T^2 E_0 + \right. \\
 & \left. + E \left(\frac{\epsilon^2}{4} \sin^2 \theta + \left(\frac{DTB}{FL_2}\right)^2 \cos^2 \theta \right) \right\} \quad (3.12.6)
 \end{aligned}$$

where m [gMol⁻¹] is the mass of the neutron, α_T the collimation angle normal to the scattering plane. θ represents the scattering angle. DTB and DTL are representative dimensions of the detector in the scattering plane and normal to the scattering plane, respectively.

3.13 Sort Program for the Scattering Law Data

To make the interpretation of the scattering law data more convenient, the scattering laws are sorted for given energy and momentum transfers.

There are two modes of using the sort program:

- (1) After the evaluation of one or more measurements has been completed, the scattering laws of each one may be sorted due to the same given input set of energy and momentum transfers.
- (2) If the scattering law data of a measurement are to be resorted, e.g. after corrections for multiple scattering performed by external programs, this program may be used independent of the other evaluation steps. To do this, the corrected data of the related measurement must be rewritten on tape in the same format as described in Chapter 4 below. The identifications of this measurement must then be supplied as input (on the SORT card in the input card set).

The main link SORTSS controls the whole sorting process. Input F is read in SORTIN. If the scattering laws must be connected with those of a previous TIFLIS-run (e.g. small and large angles are measured in two different measurements, but must be sorted as a whole data set), these two data sets are searched on tape or disk and are connected now. The scattering law data and their parameters are read-in and temporarily stored on direct access files. During the searching process of a specific measurement the other data are read over by calling RDDUM. The subprogram SORTIN serves to prepare $h\omega$ -, β -, Q -, and α -scales for the sorting process. The meshes are either calculated to build an equidistant scale up to a given maximum, or are read-in completely. If the scale is given in the input, the $h\omega$ - and β -values may have alternate signs, beginning with the positive sign, for the same absolute value, e.g. +3, -3, +4, -4, and so on. The subprograms SCA and SCQ are called to interpolate $S(\alpha, \beta)$ and $S(Q, \omega)$, respectively. The subprogram SCA controls sorting of $S(\alpha, \beta)$ for constant β , or constant α , respectively. It calculates $S(\alpha, \beta = \text{const.})/\alpha$, prepares axes for the plot of the sorted scattering laws and writes $S(\alpha, \beta)/\alpha$ on disk to save the data for the extrapolation of $p(\beta)$ (Egelstaff and Schofield 1962) with an IBM/2250-01 display unit. At Karlsruhe, this is done by an interactive graphic method using LEAP (McLatchie 1962) for correction

of the multiphonon contribution to $p(\beta)$ in the incoherent approximation (Abe1 1973).

The subprogram SCQ controls sorting of $S(Q, \omega)$ for constant $\hbar\omega$ and constant Q , respectively. It calculates $S(Q, \omega = \text{const})/Q^2$, $\omega^2 S(Q = \text{const}, \omega)$ and $S(Q)$ from the sorted values, prepares axes for plot of the sorted scattering laws, and writes $S(Q, \omega = \text{const})$ on disk for interactive interpolation of $S(Q, \omega = \text{const})$ with an IBM/2250-1 display unit. From this interpolated values $S(Q = \text{const}, \omega)$ is found. (Abe1 1974).

SORTPC sorts the scattering laws by linear interpolation in the two-dimensional field of the measured values and in the one-dimensional field of the free parameter (e.g., Q if $S(Q, \omega = \text{const})$ is wanted). It calculates the mean value of the scattering law, if there is more than one value in the given β interval. Otherwise, information from the measurement would be lost, if the β interval of the measurement is much smaller than that of the scale in the sorting process. (A nonequidistant scale is not used because of the application of LEAP).

The subprogram SUCH is called from SORTPC to look whether a $\hbar\omega = \text{const.}$ ($\beta = \text{const.}$) or $Q = \text{const.}$ ($\alpha = \text{const.}$) value is included in the $\hbar\omega - (\beta -)$ or $Q - (\alpha -)$ scale of the experiment. This is done as a binary search for $\hbar\omega$ and β (monotonic scales) and as a sequential search for Q and α (there may be more than one true value in the range of values of one detector). It calculates the ratios for the linear interpolation of $S(Q, \omega)$ ($S(\alpha, \beta)$) and looks whether there is more than one β value in the given β interval. The subprogram SELECT serves to take the values of the scattering law and the free parameter belonging to the fixed parameter found in SUCH from the related data sets. If the value of the scattering law is zero, (Z_{TOF} is zero), this value and the free parameter are skipped in the sorting process. Finally, SORTA sorts the scattering laws and the free parameters to a given constant parameter in a monotonically increasing sequence of the free parameter.

SABPLT prepares plot parameters for the plot routine PLOTA (GfK-library) for the plot of the sorted scattering laws and the calculated functions. The function subprogram AVINT is needed to integrate functions with non-equidistant arguments.

4. Output Description

4.1 Storage and Retrieval of the Evaluated Data

A binary data file is created on an intermediate storage device to accommodate the results of the process, e.g. time-of-flight spectra, scattering laws, experimental parameters etc. It is utilized to transfer these data to the sort-program. Moreover, at the end of an evaluation run, this data set may be saved by directing the records to a magnetic tape providing an interface to other programs for further analysis. This requires the availability of a tape, the related logical unit number must be 22 in the following user supplied control card

```
//G.FT22F001 DD DSN=dsname,VOL=SER=serial,UNIT=TAPE9,  
// DISP=(NEW,DELETE),DCB=(RECFM=VBS,BLKSIZE=8192,DEN=2)
```

Each set of calculations is preceded by a comment block which contains the identifications of the measurement being evaluated. A data field IDSKIP indicates whether a detector K had been excluded from evaluation. Since in this case no results were written into the binary data file, such a detector(i.e. the evaluated data related to the corresponding scattering angle) must be skipped during read-in in processing this file or the saved data on tape. IDSKIP(K) is then set to 1, otherwise IDSKIP(K)=0.

Record 1

- (1) file number (taken from the input tape)
- (2) number of result (taken from the input tape)
- (3) number of channels of the time-of-flight spectrum KAN
- (4) number N of detectors (as read-in)
- (5) detectors to be skipped by testing IDSKIP(K),K=1,N

The next record contains some experimental constants which were all supplied as input from cards.

Record 2

E_0	incident energy of the neutrons [meV]
DTK	time channel width [μ sec]
PHI	sample angle

DICKE	sample thickness [cm]
RHO	sample density [g cm ⁻³]
XMASS	atomic weight [gMol ⁻¹]
SIGMA	bound scattering cross section [b]
TEMP	temperature of the sample [K]
ANRM	number of neutrons per reactor monitor pulse
XNN	number of scatterers per molecule (is set to 1)
PRM	number of reactor monitor pulses (MIPR)
SABS	absorption cross section for window material between sample and detector [cm ⁻¹]
SSTR	scattering cross section for window material between sample and detector [cm ⁻¹]
FD	thickness of window material between sample and detector [cm]
SABFP	absorption cross section of gas on the secondary flight path [cm]
SSTFP	scattering cross section of gas on the secondary flight path [cm]
SABDW	absorption cross section of detector wall [cm ⁻¹]
SSTDW	scattering cross section of detector wall [cm ⁻¹]

After these two heading blocks the time-of-flight spectra for each scattering angle are recorded with a preceding record containing the following quantities:

Record 3

THETA	scattering angle
R3	solid angle
FL2	flight path [cm]
EMPF1	detector efficiency $\epsilon(E_0)$ ($E_0 > 30$ meV) from Eq. (3.7.6)
EMPF2	detector efficiency $\epsilon(E_0)$ ($E_0 < 30$ meV) from Eq. (3.7.2)
PEAKVA	position of the vanadium peak (channel number)
ZWD	thickness of detector wall [cm]

Record 4

Z_{TOF}^i	$1 \leq i \leq KAN$
-------------	---------------------

These two records are written in FLZS. If the evaluation continues to calculate the scattering law (i.e. $ISTREU > 0$) the binary data file is enlarged in GETSG with the calculated quantities as summarized below.

Record 5

- (1) first channel i_a being evaluated
- (2) last channel i_e being evaluated

The above record contains two integer variables which indicate the range of evaluation for the scattering law. This region is modified due to E_∞ , if needed. The following data are output for $i_a \leq i \leq i_e$.

Record 6

- (1) detector efficiency $\epsilon_i(E)$
- (2) β_i -values
- (3) ω_i -values
- (4) α_i -values
- (5) $S(\alpha_i, \beta_i)$ -values
- (6) Q_i -values
- (7) $S(Q_i, \omega_i)$ -values

wherein the detector efficiency $\epsilon_i(E)$ is taken from Eq. (3.10.6).
Record 6 is processed for each scattering angle.

4.2 Printed output

The first section of the output consists of the input data in the punching format. For each measurement evaluated the time-constant background, peak position, if calculated, and the monitor intensities calculated are printed out in tables. Some experimental parameters of the vanadium and the sample measurements are listed in the printer output and are selfexplanatory. It should be noted that several output lists may be directed by input variables. The time-of-flight spectrum is printed for $NFOUT > 0$ for all channels and each scattering angle. The outputs of the fit program and the program for the elastic correction are briefly described in the appropriate chapters of this report. The detector efficiency is printed out in tabular form and as a printer plot for the first detector that was evaluated for the given channel

region. The selfabsorption factor is also printed for one detector in the same manner as mentioned above and for E_0 for every scattering angle in a printer plot.

Depending on the value of the input variable NSOUT there are two possibilities of printing the scattering law data together with other calculated quantities. For NSOUT<0 the output list contains

$$\hbar\omega, Q, \frac{d^2\sigma}{d\Omega dE}, S(Q,\omega), \frac{d^2\sigma}{d\Omega d\tau}, \beta, \rho(\beta), \left(\frac{\Delta\hbar\omega}{\hbar\omega}\right), \left(\frac{\Delta Q}{Q}\right)$$

vs channel number in the region 'first channel - last channel'.

Additional, a printer plot is produced for $\rho(\beta)$ of one detector, as indicated by the value of ISTREU.

Another combination of the calculated quantities is printed for NSOUT>0:

$$\beta, \alpha, \frac{d^2\sigma}{d\Omega d\beta}, S(\alpha,\beta), \hbar\omega, Q, \rho(\beta), p(\beta), \left(\frac{\Delta\hbar\omega}{\hbar\omega}\right)$$

The rest of the output relates to the scattering law interpolated for constant energy and momentum transfers. For example, for the interpolation for constant momentum transfer, each block of output is headed by the α values. The rest of the block consists of β and the interpolated values of $S(\alpha,\beta)$.

4.3 Plot Output

Several types of machine plots may be produced during an evaluation run. Automated plotting is sometimes the only reliable way to scan the large amounts of data produced by the TOF method in a reasonable time. The scale limits and few plotting parameters must be supplied as input. Depending on the value of the appropriate input variables the following functions may be plotted (see input description):

- (1) NPLOTF=1 time-of-flight spectra vs channel
- (2) NPLOTF=n time-of-flight spectrum for the nth detector (n>1)
- (3) NPLOTW=1 $\frac{d^2\sigma}{d\Omega d\tau}$ vs τ

- (4) NPLOTW = -n $\frac{d^2\sigma}{d\Omega d\tau}$ vs τ for the nth detector ($n>1$)
- (5) NPLOTW = 1 $\frac{d^2\sigma}{d\Omega dE}$ vs E [meV]
- (6) NPLOTW = n $\frac{d^2\sigma}{d\Omega dE}$ vs E for the nth detector ($n>1$)
- (7) NPLSAB(1)=1 $S(\alpha, \beta)$, $\beta = \text{const.}$
- (8) NPLSAB(2)=1 $S(\alpha, \beta)/\alpha, \beta = \text{const.}$
- (9) NPLSAB(3)=1 $S(\alpha, \beta)$, $\alpha = \text{const.}$
- (10) NPLSQM(1)=1 $S(Q, \omega)$, $\omega = \text{const.}$
- (11) NPLSQM(2)=1 $S(Q, \omega)/Q^2$, $\omega = \text{const.}$
- (12) NPLSQM(3)=1 $S(Q, \omega)$, $Q = \text{const.}$
- (13) NPLSQM(4)=1 structure factor $S(Q)$
- (14) NPLSQM(5)=1 $\omega^2 S(Q, \omega)$, $Q = \text{const.}$

5. Interactive Graphic Evaluation

The evaluation of the data accumulated from the scattering of thermal neutrons by atomic systems is, in general, a time consuming process. Compared to the conventional batch-processing computational evaluation the use of on-line computing with interactive graphics offers the distinct advantage that the total time for the solution of special problems can be considerably reduced. Taking into account the flexibility of the interactive computer graphics analysis, studies can be performed in much greater detail than is normally possible in a batch processing environment. For the processing of graphical information an IBM/2250-1 graphics display unit is used. The 2250 is attached to the system /370 processor via a selector channel and operates concurrently with the CPU, freeing main storage and the channel for other functions. Display regeneration is performed automatically under buffer control. The communication with the program is realized via a light pen and a programmed function keyboard.

5.1 On-Line Computing with Interactive Graphics

During an evaluation run an interactive correction can be made of individual channel contents of the time-of-flight spectrum, e.g. to avoid an inadequate

analysis of the raw data of scattering experiments on solids caused, e.g. by Bragg peaks of the sample or of the sample container material. Moreover, the elastic correction can be iteratively improved, if necessary.

5.1.1 Correction of the Time-of-Flight Spectrum

First, a title is displayed. After depressing the function key 2 the time-of-flight spectrum of that detector appears which is just evaluated. The number of the detector is displayed in the lower left part of the image on the screen. In addition, the following options are displayed in the upper area of the screen:

```
CORRECTION END  
NEXT DETECTOR
```

The displayed message SELECT POINT (X) indicates that the user can select a point by touching this point with the light pen. The associated position is identified by placing a X-symbol on the screen. If a wrong point was detected the indication can be erased by depressing function key 4 and the selection can be repeated. After pressing key 2, the new value can be fixed by means of the light pen on a displayed vertical line. The corrected spectrum is displayed and a choice of other points to be corrected is possible. If no points are to be corrected, the next detector will be displayed after light pen detect on
NEXT DETECTOR.

If the correction run is to be finished before the last detector, the option CORRECTION END must be selected in order to ensure that the end of this interactive part of the evaluation is recognized. When correcting the last detector, the message LAST DETECTOR is displayed as a reminder.

5.1.2 Elastic Correction

On the basis of the display a new choice of the fit range of the elastic peak in the vanadium measurement can be made to improve the adaption of the Gaussian curve to the elastic peak of the sample. The new parameters are re-computed by means of a simplified version of the fitting procedure contained in TIFLIS.

Display 1

The title ELASTIC CORRECTION is displayed.

Display 2

After depressing function key 2 the elastic line of the sample together with the elastic correction for the detector to be evaluated is displayed.

Display 3

By answering CORRECTION? using key 2, the related vanadium line is displayed (+), and the elastic correction erased.

At the request SELECT FIT RANGE the beginning and the end points of a new channel range must be selected on the elastic line by light pen indication. In the case of RANGE OK? the range can still be changed after an incorrect choice by pressing function key 1. A new fit calculation is carried out by pressing key 2. Observing the consequences of his action the user can decide whether the solution is acceptable or not. To make it easier to compare the experimental data with the shape of the vanadium peak the depression of function key 4 permits to display the fitted spectrum as a series of connected lines. The latter must be removed by once more pressing the same function key. Function key 10 alternately displays and removes the elastic correction from the screen.

If no further refinement of the parameters is necessary to arrive at a most acceptable solution of the elastic correction depressing function key 1 causes the next detector to be displayed on the screen together with the elastic correction first estimated, as described above. The session is terminated by the use of function key 1 or by a light pen detect on the option CORRECTION END. The calling program then continues the evaluation run.

5.1.3 Requirements for using the IBM/2250-1

Of course, the time required before the display unit becomes active, will depend on the relative priority of a TIFLIS-job and leads to an indeterminate waiting time spent at the terminal. It is therefore desirable to revise upward the job priority which can only be overridden by the operation's staff. This should be possible despite of the large core storage requirement, because the interactive phase of the evaluation

process - according to experience - will not take more than 30 minutes.

The total amount of main storage requirement needed for TIFLIS must be increased by approximately 40 kBytes. Since the interactive graphic facility is an additional feature of the program, the graphic sub-programs are normally included in the program as dummies. When using the display, only the DIS parameter which directs the input to the linkage editor must be set to 1. In addition these statements are included in the control card set for TIFLIS as follows:

```
/*SETUP DEVICE=2250,ID=RESERV  
// EXEC TIFLIS,DET=32,DIS=1  
//G.FT50F001 DD UNIT=250
```

5.2 Extrapolation of a Generalized Frequency Distribution $p(\beta)$

The generalized frequency distribution $p(\beta)$ is a useful function to describe the dynamics of the scattering system. In the case of a solid, $p(\beta)$ is directly related to the phonon spectrum $\rho(\beta)$. The generalized frequency distribution can be obtained from inelastic scattering of neutrons by a method of extrapolation first verified by Egelstaff and Schofield (1962). More details of this method are given elsewhere (Egelstaff and Schofield 1962). However, the principle will be briefly outlined here. The scattering data $S(\alpha,\beta)/\alpha$ evaluated with TIFLIS for a fixed β , and a series of α values (i.e. of scattering angles) are extrapolated to zero α from a region of large α , in which the incoherent approximation is valid. To obtain the distribution function $p(\beta)$ this procedure must be repeated for a large number of β values.

An iterative application of the LEAP program to reconstruct the scattering law $S(\alpha,\beta)$ (i.e. by a phonon expansion and SCT) each followed by repeated extrapolations yields a more accurate generalized frequency distribution. In a batch-processing environment this is a very time consuming process.

To facilitate the evaluation process a more automated algorithm was developed and uses an IBM/2250-1 display unit. The provision of facilities allowing the user to interact with the program leads much faster to an acceptable solution. It is typically obtained in 15 minutes of terminal

time and less than two minutes of processing time (needed, e.g., for an extrapolation of $S(\alpha, \beta)/\alpha$ given for 32 α values and a mesh of 76 β values). After three or four iterations the changes in $p(\beta)$ are sufficiently small, so that the process converges quite well. The response time to most user actions is well under one second. A description of the interactive graphic program is given elsewhere (Abel 1973).

5.3 Graphic Interpolation of $S(Q, \omega)$

An interactive graphic smoothing can be performed for a survey representation of the scattering law $S(Q, \omega)$ for constant ω (Abel 1974). The "smoothed" values must be selected by a light pen detect on a vertical line which is moved over the screen in equidistant steps, as directed by the user. After the end of smoothing of $S(Q, \omega)$ for all given ω , the scattering law is displayed simultaneously for several ω values so that a subsequent correction of individual selected curves can be carried out to avoid an intersection of that curves. $S(Q, \omega)$ for all ω may be plotted in a second step. Moreover, the scattering law $S(Q, \omega)$ for constant Q is interpolated from $S(Q, \omega)$ for constant ω .

6. Card input

6.1 Data files for input data

The input data are copied on a sequentially organized data file by means of the subprogram READIN for constituting a reread of the input data. The related logical unit number of this file is 8. Since the measurements are read-in from tape in an overlay segment, the file cards which are contained in the stack of cards holding the identifications of these measurements must be interpreted before. For this purpose, these cards are selected on the basis of their control words as described below and placed in the intermediate data file 28. This list is then processed sequentially, depending on the respective program phase.

6.2 Card Format Conventions and Functions

The input data are formatted read-in. The card formats correspond to the FORTRAN IV conventions applicable to the IBM/360 system. Some data cards contain alphameric information in the first columns to make clearer the purpose of the input data on those cards. Thus, the user can quickly find an appropriate data card on which he wishes to change any data. On the other hand, for control of the program, e.g. with respect to processing several sample measurements, the control words VORLAUF, PROBE, SORT and END are matched by the program by checking the first four punched characters. This also applies to those data cards which contain the characteristics of the measurements, such as file number etc. In the first two columns such file card must contain one of the following abbreviations: ZU, LE, VA, VL, PP. Control words matched in the program are characterized by underlining in the description of the input data.

6.3 Input Description

The input from data cards to the code is described on the following pages. The numbering corresponds to the different input requests by a READ statement. Therefore, for reading list elements sometimes several data cards are needed. To facilitate the input of a table with constant values, only the constant value, but with a negative sign, may be punched. The respective data lists are characterized in the following by an asterisk immediately ahead of the code symbol of the variable.

A. Program Organization Cards

- | | | | |
|----|--------|--------|---|
| 1. | (15A4) | HOL | text in printer output |
| 2. | (7I10) | IVORL | = 1, evaluation of ZU-, LE-, VA-, VL-measurements
= 0, no evaluation |
| | | IPROB | = 1, evaluation of ZU- and PP-measurements
= 0, no evaluation. Program ends after evaluation of ZU-, LE-, VA-, VL-measurements |
| | | ISORT | = 1, sorting of scattering laws
= 0, no sorting. Program ends after calculation of scattering laws. |
| | | ITPRES | = 1, results are written on tape (Unit 22)
= 0, no reservation on tape |
| | | IEXP | = 0, no test
> 0, test of the experiment number during read-in from tape |

(If only ISORT = 1 (2) record 3 to 82 must be dropped)

- | | | | |
|----|--------|--------|--|
| 3. | (7I10) | KAN | channel number (256 or 512 or 1024) |
| | | NDET | detector number (max. 97) |
| | | MKU | channel numbers for calculation of the time independent background from the spectra (see SMUG) |
| | | MINUNT | = 1, the time-independent background is subtracted
= 0, the time-independent background is calculated, but not subtracted |
| | | MONS | the intensity of the peak in the monitor-1 spectrum is summed-up over 2·MONS+1 channels |
| | | IBUFD | = 0, the buffer length given in the program is taken (should not be changed) |
| | | LPFIT | = 0, 10 channels are used
> 0, number of points needed for the peak searching procedure |

B. Selection of Detectors

Detectors may be selected from tape singly or in fields for evaluation. Single detectors must be identified by a positive integer. A field is

identified by two integers. The integer that identifies the lowest numbered detector in the range must appear immediately before the integer that identifies the highest numbered detector in the range which must be a negative value. If the first block number is 0, all detectors are chosen sequentially in the range of block 1 to block NDET (max. 97).

(Example: 3 5 -8 15 18-20)

4. (A2,3X) ITEST DETN (control word)
(20I3) MSH(I) I=1,20 block number of detectors
5. (A4,6X) ITEST MON1 (control word)
(5I5) IDM1(I) I=1,5 block number of monitor-1 in ZU, LE,
VA, VL and PP measurements

(If monitor-1 will be taken instead of monitor-5, record 6 must be skipped.)

6. (A4,6X) ITEST MON5 (control word)
(5I5) IDM5(I) I=1,5 block number of monitor 5 in ZU, LE,
VA, VL and PP measurements

(If the monitor-1 and 5 spectra do not directly follow the detector spectra, the block numbers must be given even if the intensities are replaced in the input.)

C. Input for ZU-, LE-, VA-, VL-Measurements

7. (A4) NTEST VORLAUF (control word)
8. (6I1) IS(I,J) I=1,6 = 1, the spectrum of measurement J in
state I will be printed
= 0, will not be printed
I = 1 : original spectrum
I = 2 : smoothed spectrum (only ZU,
LE, VL)
I = 3 : spectrum-time-const. background
I = 4 : monitor scaled measurement
(only ZU, LE, VL)
I = 5 : monitor-1 spectrum
I = 6 : monitor-5 spectrum
- (A2) IFORM(J) = LP printer plot of monitor spectrum
= WR else
- (I3) LINES > 0, number of lines for plot
= 0, 57 lines are used for the plot

This card must be included four times, namely for ZU-, LE-, VA- and VL- measurements in this succession.

Channel Correction in all Spectra

9. (A2,3X) ITEST CORR (control word)
(I5) NPA number of channels to be corrected
(If NPA = 0 (9), record 10 must be skipped)
10. (14I5) KPA1(I) I=1,NPA channel numbers

Counting time corrections of single detectors

11. (A2,18X) ITEST COUNTING TIME CORR (control word)
(I5) IQUEST Number of following records 12.
Dependent on number of measurements
and detectors to be corrected.
12. (A2,1X) ITEST DET (control word)
(I2) NRDET number of detector (original)
(1X,I1) MSG number of measurement = 1:ZU; =2:LE;
= 3:VA; = 4:VL
(F8) DNORM correction factor
(There are IQUEST cards of record 12.)

Skip of detectors not excluded in record 4

13. (A2,3X) ITEST SKIP (control word)
(10I5) KB(I) I=1,10 detector numbers (original) to be
skipped (max. 10)

Input of ZU-measurement to LE-measurement

14. (A2,3X) ITEST ZU (control word)
(I5) IZF file number of ZU-measurement
(I5) IZR result number of ZU-measurement
(5(2I5)) JFAD(I),JRAD(I) file and result numbers of ZU-measure-
ments to be added to the one given
first (max. 5)
(If IZR = 0 (14), records 15 and 16 must be skipped.)
15. (7I10) IZG = -1, the mean value over all channels
is calculated
= 0, no smoothing
> 0, number of smoothing regions

(If $IZG \leq 0$ (15), record 16 must be skipped.)

- | | | | |
|-----|--------|---------|---|
| 16. | (3I10) | IZGA(I) | first channel of smoothing region I |
| | | IZGE(I) | last channel of smoothing region I |
| | | IZGN(I) | number of channels over which there will be smoothing in region I (3,5 or 11) |

(There are IZG cards of record 16.)

Input of LE-measurement

- | | | | |
|-----|----------|-----------------|--|
| 17. | (A2,3X) | ITEST | <u>LE</u> (control word) |
| | (I5) | ILF | file number of LE-measurement |
| | (I5) | ILR | result number of LE-measurement |
| | (5(2I5)) | JFAD(I),JRAD(I) | file and result numbers of LE-measurements to be added to the first one (max. 5) |

(If $ILR = 0$ (17), records 18 to 22 must be skipped.)

- | | | | |
|-----|----------|-----------|--|
| 18. | (I10) | ILG | > 0, number of smoothing regions
= 0, no smoothing |
| 19. | (10X) | | PEAKLE (control word) |
| | (F10) | PEAKLE(1) | > 0, position of the maximum of the elastic peak in the LE-measurement
= 0, maximum is calculated with PEAKER |
| 20. | (A2,18X) | ITEST | PEAK REGION LE (control word) |
| | (I5) | KL | lower limit of the elastic peak region |
| | (I5) | KR | upper limit of the elastic peak region |
| 21. | (10X) | | TIMEFACTOR (control word) |
| | (F10) | VLEZU | > 0, normalization (time) factor of ZU to LE-measurements
= 0, factor is calculated from monitor-5 (or monitor-1) spectra in PREPAS |
| | (F10) | MILE | > 0, intensity in monitor 1 peak of LE-measurement, if monitor 1 is absent or faulty on result tape. |

(If $ILG = 0$ (18), record 22 must be skipped.)

- | | | | |
|-----|--------|---------|---|
| 22. | (3I10) | ILGA(I) | first channel of smoothing region I |
| | | ILGE(I) | last channel of smoothing region I |
| | | ILGN(I) | number of channels over which there will be smoothing in region I (3,5 or 11) |

(There are ILG cards of record 22.)

Input of V-measurement

- | | | | |
|--|----------|-------------------|---|
| 23. | (A2,3X) | ITEST | <u>VA</u> (control word) |
| | (I5) | IVAF | file number of V-measurement |
| | (I5) | IVAR | result number |
| | (5(2I5)) | JFAD(I),JRAD(I) | file and result numbers of V-measurements to be added to the first one (max. 5) |
| (If IVAR = 0, records 24 to 39 must be skipped.) | | | |
| 24. | (I10) | IBREIT | = 1, the width (HWHM) of the elastic peak in the V-spectra is calculated (see FITLB)
= 0, is not calculated |
| 25. | (F10) | E0 | energy of incoming neutrons (meV) |
| | (F10) | D | thickness of V-sample (cm) |
| | (F10) | DPRO | V-sample dimension in scattering plane (cm) |
| | (F10) | ALPHA | angle of V-sample to incoming beam (counted in direction of scattering angles) ($^{\circ}$) |
| | (F10) | SIGB | bound V-scattering cross section (b) |
| | (F10) | DTK | channel width (μ sec) |
| | (F10) | DBFVA | > 0, Debye function value Λ at V-temperature
< 0, λ/T (negative!) ($\alpha\lambda = 2W$) |
| 26. | (E10) | ANRM | number of neutrons on the V-sample per monitor-1 count (from flow chart measurement) |
| | (E10) | RHO | density of V-sample (g/cm^3) |
| 27. | (7F10) | *FL2(J) J=1,NDET | > 0, secondary flight path of detector J (cm)
< 0, the flight path to each detector is set = FL2(1) in BLDTB. Only FL2(1) is read |
| 28. | (7F10) | THETA(J) J=1,NDET | scattering angles ($^{\circ}$) |
| 29. | (7F10) | *OMG(J) J=1,NDET | > 0, detector solid angle as seen from the center of the sample (sterad)
< 0, solid angles of all detectors are set = -OMG(1) in BLDTB. Only OMG(1) is read. |
| 30. | (10X) | | PEAKVA (control word) |
| | (F10) | PEAKVA(1) | > 0, position of maximum of V-peak
= 0, position of maximum is calculated in PEAKER |

31. (A2,18X) ITEST PEAK REGION VA (control word)
(I5) KL lower limit of V-peak region
(I5) KR upper limit of V-peak region
(I5) KSL lower limit for sum of total spectrum
(inelastic + elastic) (neutron energy gain)
(I5) KSR upper limit for sum of total spectrum
(neutron energy loss)
32. (10X) TIMEFACTOR (control word)
(F10) VVAVL > 0, normalization (time) factor of
VL- to VA-measurement
= 0, factor is calculated from monitor-1
peaks in PREPAS
(F10) M1VA > 0, intensity of monitor-1 peak of
Va-measurement
= 0, intensity is calculated from
monitor-1 peak in QQMON

(If IBREIT = 0 (24), records 33 to 39 must be skipped.)

33. (A2,3X) ITEST LINE (control word)
34. (I5) KFG = 1, a Gaussian is fitted to the
V-peak
(I5) ICOR = 1, correction of single channels
of the V-peak (e.g., inelastic or
multiple scattering contamination
of the V-peak)
= 0, no correction
(F10) UGRD fit parameter, height of a constant
background
(F10) UGRD1 fit parameter, slope of a linear
background
35. (70I1) IDF(I),I=1,NDET = 1, halfwidth of peak is calculated
= 0, for detector I width of peak
is not calculated
36. (A2,3X) ITEST PLOT (control word)
(I5) NPLOTB = 1, plot of the elastic peak with
fitted function
= 0, no plot
(I5) NBOUT = 1, printer plot of elastic peak
= 0, no printer plot
= 1, printer plot + fit data output

(If ICOR = 0 (34), records 37 to 39 must be skipped.)

37. (I10) NFK number of points for single channel correction
38. (7F10) FK(I), I=1, NFK % of channel content to be attributed to inelastic or multiple scattering contamination of the elastic peak. Will be interpolated linearly for each channel.
39. (7I10) IK(I) I=1, NFK channel numbers

Input for empty V-sample holder

40. (A2,3X) ITEST VL (control word)
(I5) IVLF file number of VL-measurement
(I5) IVLR result number of VL-measurement
(5(2I5)) JFAD(I), JRAD(I) file and result numbers of VL-measurements to be added to the first one

(If IVLR = 0 (40), records 41 and 42 must be skipped.)

41. (I10) IVLG > 0, number of smoothing regions
= 0, no smoothing

(If IVLG = 0 (41), record 42 must be skipped.)

42. (3I10) IVLGA(I) first channel of smoothing region I
IVLGE(I) last channel of smoothing region I
IVLGN(I) number of channels over which there will be smoothing in region I (3, 5 or 11)

(There must be IVLG cards of record 42.)

D. Input for Sample Measurement

Section D contains those input parameters which do not change from one sample measurement to the next (instrument constants, unchanged physical properties of the sample, plot and listing parameters). Some of the parameters already given in Section C are repeated because the sample may be evaluated without LE or VA, VL-measurements. In those cases there must be a ZU-measurement for the sample.

43. (F10) DICKE sample thickness (cm)
(F10) DTK width of time channel (μ sec)
(F10) SIGMA bound scattering cross section of sample material (b)
(F10) SIGA absorption cross section of sample material for thermal neutrons (25.3 meV) (b)

	(F10)	DBTEMP	Debye temperature of sample material (K)
	(F10)	FZS1	> 0, intensity of the peak in the monitor-1 spectrum that will be used in the normalization of different time-of-flight spectra (for comparison of the time-of-flight spectra of different sample runs). = 0, no normalization of the time-of-flight spectra
44.	(F10)	E0	energy of incoming neutrons (meV)
	(F10)	XMASS	mass of scatterer (g/mol)
	(F10)	ABST1	free parameters for description of sample geometry (transferred to DICKOR and ZFKOR)
	(F10)	ABST2	
	(F10)	FD	thickness of windows between sample detector (cm)
	(F10)	DPRO	sample dimension in scattering plane (cm)
	(I10)	IAUFL	= 1, the $\hbar\omega$ - and Q-resolutions of the time-of-flight spectrometer are calculated in RESOL = 0, no resolution is calculated = n>1, printer plot of the $\hbar\omega$ -resolution for the nth detector
45.	(E10)	ANRM	number of neutrons on the sample plane per monitor-1 count
46.	(E10)	SABS	absorption cross section (25.3 meV) of window material between sample and detector (cm ⁻¹)
	(E10)	SSTR	scattering cross section of window material (cm ⁻¹)
	(E10)	SABFP	absorption cross section (25.3 meV) of the gas between sample and detector (cm ⁻¹)
	(E10)	SSTFP	scattering cross section of the gas (cm ⁻¹)
	(E10)	SABDW	absorption cross section (25.3 meV) of the detector walls (cm ⁻¹)
	(E10)	SSTDW	scattering cross section of detector walls (cm ⁻¹)

(If SABS to SSTDW are left = 0, cross sections of Al, N₂, and stainless steel are taken in EPSPZ to calculate the detector efficiency.)

47. (7F10) *FL2(J)J=1,NDET > 0, secondary flight path of detector J (cm)
< 0, the flight path to each detector is set = FL2(1) in BLDTB. Only FL2(1) is read
48. (14F5) *ZWD(J) J=1,NDET > 0, wall thickness of detector J(cm)
< 0, the wall thickness of each detector is set = -ZWD(1) in BLDTB. Only ZWD(1) is read.
49. (7F10) THETA(J)J=1,NDET scattering angles ($^{\circ}$)
50. (7E10) *OMG(J),J=1,NDET > 0, solid angle of detector J, as seen from the center of the sample (sterad)
< 0, the solid angle of each detector is set = -OMG(1) in BLDTB. Only OMG(1) is read.
51. (7F10) *ABF(J)J=1,NDET > 0, efficiency constant of detector J.
< 0, the efficiency constant of each detector is set = -ABF(1) in BLDTB. Only ABF(1) is read.
52. (A2,3X) ITEST PLOT (control word)
(I5) NPLOT = 1, plot output of time-of-flight spectra
= 0, no plot output
= N, the time-of-flight spectrum of detector N(1<N<NDET) is plotted
(I5) NPLOTW = 1, plot output of $d^2\sigma/d\Omega d\tau$
= -N, $d^2\sigma/d\Omega d\tau$ of detector N (1<N<NDET) is plotted
= 0, no plot output
= 1, plot output of $d^2\sigma/d\Omega dE$
= N, $d^2\sigma/d\Omega dE$ of detector N (1<N<NDET) is plotted
(I5) NPLOTB = 1, plot output of the elastic peak of the net channel content spectra of the sample with fitted function
< 0, no plot output
53. (E10) X5MAX maximum value of ordinate for the plot of the time-of-flight spectra
(E10) CSBMAX maximum value of ordinate for the $d^2\sigma/d\Omega d\tau$ -plot
(E10) CSQMAX maximum value of ordinate for the $d^2\sigma/d\Omega dE$ -plot
54. (A2,3X) ITEST LIST (control word)

- (I5) NFOUT = 1, the time-of-flight spectra are printed
= 0, the time-of-flight spectra are not printed
- (I5) NSOUT = -1, $S(Q,\omega)$ is printed
= 0, no printed output
= 1, $S(\alpha,\beta)$
- (I5) NBOUT = -1, printed plot of elastic peak of the sample
= 0, no printed plot
= 1 printed plot + fit data output

(If IAUFL = 0 (44), records 55 to 57 must be skipped.)

55. (A2,3X) ITEST RESOL (control word)
56. (F10) HOW collimation angle in scattering plane ($^{\circ}$)
(F10) VTW collimation angle normal to scattering plane ($^{\circ}$)
(F10) SPREAD mosaic spread of chopper crystal ($^{\circ}$)
(F10) OMDK angular speed of copper crystal (μsec^{-1})
(F10) RDK radius of chopper crystal (cm)
(F10) BRAGGW Bragg angle of chopper crystal reflexion ($^{\circ}$)
(F10) FL1 flight path between chopper crystal and sample (primary flight path) (cm)
57. (F10) DPR sample or sample mask widths (cm)
(F10) DTD thickness of a single detector tube (detector thickness) (cm)
(F10) DTB detector width (cm)
(F10) DTL detector length (cm)

E. Input for Sample Measurement

Section E contains all sample parameters that may change from measurement to measurement. Section E must be there n times, if n sample measurements are evaluated in one TIFLIS-run with the same ZU, LE, VA, VL measurements.

58. (A4) NTEST PROBE (control word)
59. (I1) IS(I,J) I=1,6 = 1, the spectra of measurement J in state I will be printed
= 0, will not be printed

I = 1, original spectrum
I = 2, smoothed spectrum
I = 3, counting rate time-const.
background
I = 4, normalized measurement
I = 5, spectrum of monitor-1
I = 6, spectrum of monitor-5
(A2) IFORM = LP, printer plot of monitor spectra
= WR, print-out
(I3) LINES > 0, number of lines for plot
= 0,57 lines are used for the plot

There are two cards of record 59, the first one for the ZU-measurement to the sample measurement, the second one for sample measurement.

Channel correction in all spectra

60. (A2,3X) ITEST CORR (control word)
(I5) NPA number of channels to be corrected
(If NPA = 0 (60), record 61 must be skipped.)

61. (14I5) KPA1(I) I=1,NPA channel numbers

Counting time corrections of single detectors

62. (A2,18X) ITEST COUNTING TIME CORR (control word)
(I5) IQUEST number of corrections = number of
following records 63
(If IQUEST = 0 (62), record 63 must be skipped.)

63. (A2,1X) ITEST DET (control word)
(I2) NRDET detector number (original)
(1X,I1) MSG reference number of measurement
MSG = 1, ZU-measurement
MSG = 5, PP-measurement
(F8) DNORM correction factor
(There are IQUEST cards of record 63.)

Skip of detectors not excluded in record 4

64. (A2,3X) ITEST SKIP (control word)
(10I5) KB(I) I=1,10 detector numbers (original) to be
skipped (max. 10)

Input of ZU-measurement to PP-measurement

65. (A2,3X) ITEST ZU (control word)
 (I5) IZF file number of ZU-measurement
 (I5) IZR result number of ZU-measurement
 (5(2I5)) JFAD(I),JRAD(I) file and result numbers of ZU-measurements to be added to the first one

(If IZR = 0 (65), records 66 and 67 must be skipped.)

66. (I10) IZG = -1, the mean value over all channels is calculated
 = 0, no smoothing
 > 0, number of smoothing regions

(If IZG \leq 0 (66), record 67 must be skipped.)

67. (3I10) IZGA(I) first channel of smoothing region I
 IZGE(I) last channel of smoothing region I
 IZGN(I) number of channels over which there will be smoothing in region I (3,5 or 11)

(There are IZG cards of record 67.)

Sample input

Records 68 to 82 contain the input, which varies from one PP-measurement to the next.

68. (A2,3X) ITEST PP (control word)
 (I5) IPRF file number of PP-measurement
 (I5) IPRR result number of PP-measurement
 (5(2I5)) JFAD(I),JRAD(I) file and result numbers of PP-measurements to be added to the first one.
69. (I10) IBREIT = 0, no peak width (HWHM) is calculated
 = 1, the width of the elastic peak is calculated in the spectra (before the time-of-flight spectra are calculated)
 = 2, the width of the elastic peak is calculated in $S(Q,\omega)$
- (I10) ISTREU = -1, the program stops after calculation of the time-of-flight spectrum
 = 0, no time-of-flight spectra and no scattering law are calculated. The program stops after calculation of the elastic correction

- = 1, the time-of-flight spectra and the scattering law are calculated
= n>1, printer plot of $\rho(\beta)$ for the nth detector
- (I10) IRED = 0, no reduction of spectra
= N, the spectra are reduced in summing up all N channels
70. (I10) IELAST = 0, no elastic correction
= 1, the elastic correction is calculated in the sample spectra but not subtracted (hence it is supposed that a Gaussian was fitted to all V-peaks)
= 2, the elastic correction is calculated and subtracted
- (I10) NDELTA = 1, the relative statistical error is printed
= 0, is not printed
- (I10) IEPS = -2 $\epsilon(E) = 1.0$
= -1, C3 = 1 (extenuation of the neutron beam between sample and detector gas is not calculated)
= 0, C3 is calculated from V-scattering (at E_0)
= 1, C3 is calculated from scattering and absorption cross sections
= 2, $\epsilon(E) = \epsilon(E_0)$, only the relative efficiency is taken into account
- (I10) IC1ABS = 1, the absorption of the neutron between sample and detector gas is taken into account
= 0, is not taken into account
- (I10) NGEOM = 1, the time-of-flight spectra are corrected for self-absorption in the sample
= 0, are not corrected for self-absorption
- (I10) IVKS = 1, a channel shift between PP- and LE-measurements will be regarded
= 0, will not be regarded
- (I10) KAUSD number of channels for which the Gaussian will be extended to the left and the right of the fitting region in the elastic correction
71. (15A4) HOL(I) I=1,3 plot title (name of sample substance)

72.	(F10)	TEMP	temperature of sample (K)
	(F10)	RHO	density of sample (g/cm^3)
	(F10)	PHI	angle between sample and direction of incoming neutrons counted in direction of the scattering angles ($^\circ$)
	(F10)	PAUSE	PAUSE = (DC-MT)/DTK time (in channels) between two measuring times of the time-of-flight unit (DC=duty cycle, MT-measuring time=N·DTK (N=number of channels of one spectrum))
	(F10)	VKS	> 0, constant channel shift between PP- and LE-measurements = 0, the channel shift is calculated from the peak positions in MESS (but is taken into account only if IVKS=1)
	(F10)	DBTERM	> 0, Λ (Debye function at T) < 0, $-\lambda$ ($2w = \alpha\lambda$ Debye-Waller coefficient)
	(F10)	AF	matching factor (factor is contained in $\epsilon(E)$)

(If IBREIT = 0 (69), records 73 to 78 must be skipped.)

73.	(A2,3X)	ITEST	LINE (control word)
74.	(I5)	KFG	for the fit to the elastic peak = 0, a Lorentzian = 1, a Gaussian = 2, a convolution of a Lorentzian and a Gaussian is taken
	(I5)	ICOR	= 1, correction of single channels of the peak in the sample spectrum (e.g., inelastic or multiple scattering contaminations of the peak) = 0, no correction
	(F10)	UGRD	fit parameter, constant background
	(F10)	UGRD1	fit parameter, slope of a linear background
	(F10)	DEG	width of the resolution Gaussian (for convolution in case KFG=2)
75.	(70I1)	IDF(I),I=1,NDET	= 1, the peak width is calculated = 0, is not calculated for detector I

(If ICOR = 0, record 76 to 78 must be skipped.)

76.	(I10)	NFK	number of nodes for single channel correction (≤ 100)
77.	(7F10)	FK(I) I=1,NFK	% of channel content to be attributed to inelastic or multiple scattering contamination. Will be interpolated linearly for each channel
78.	(7I10)	IK(I) I=1,NFK	channel numbers
79.	(10X)		PEAKSAMPLE (control word)
	(F10)	PEAKPR(1)	> 0, position of the maximum of the elastic peak in the sample spectra = 0, position of the maximum will be calculated in PEAKER < 0, the maxima of the V-peaks are taken in each detector
80.	(A2,18X)	ITEST	PEAK REGION (control word)
	(I5)	KL	lower limit of the elastic peak region
	(I5)	KR	upper limit of the elastic peak region
81.	(A2,18X)	ITEST	EVALUATION REGION (control word)
	(I5)	IPLW	first channel of the region of evaluation for scattering law
	(I5)	IPHG	last channel of the region of evaluation
82.	(10X)		TIMEFACTOR (control word)
	(F10)	VPRLE	> 0, normalization (time) factor of LE to PP-measurements = 0, factor will be calculated from peak of monitor-1 in LE and PP-measurements in MESS
	(F10)	M1PR	> 0, intensity of monitor-1 peak of the PP-measurement (if monitor-1 is absent or faulty on result tape) = 0, intensity is calculated from monitor-1 spectrum in QQMON
	(I5)	IZEITF	= 1, in VPRLE the absorption and scattering of neutrons, scattered in the container walls, in the sample during the PP-measurement are taken into account (in ZFKOR)
	(F10)	VPRZU	> 0, normalization (time) factor of ZU to PP-measurements = 0, factor will be calculated from the monitor-5-spectra or the peak of the monitor-1-spectra of ZU and PP-measurements in QQMON

- (I5) NB number of α -values that will be sorted for (≤ 100)
- (F10) BETSC maximum β -value that is taken into account in the sorting process
- (F10) DBR β interval. If there is more than one β -value in this interval, the scattering law is determined as a mean value.

(If NP < 0 (85), record 86 must be skipped.)

(If NP > 0, record 87 must be skipped.)

- 86. (7E10) ALPHAC(I) I=1,NP α -values
- 87. (E10) AMAX maximum α -value of the α -scale build-up in SORTIN (NP equidistant values)

(If NB < 0 (85), record 88 must be skipped.)

(If NB > 0, record 89 must be skipped.)

- 88. (7F10) BETAC(I) I=1,NB β -values (+ β , - β or both)
- 89. (F10) DBETA step width in the β -scale with NB values built-up in SORTIN
< 0, energy loss of neutrons
> 0, energy gain of neutrons
- 90. (A2,3X) ITEST PLOT (control word)
 - (I5) NPLSAB(1) = 1, $S(\alpha, \beta = \text{const.})$ is plotted (log-log)
 - (I5) NPLSAB(2) = 1, $S(\alpha, \beta = \text{const.})/\alpha$ is plotted (lin-log)
 - (I5) NPLSAB(3) = 1, $S(\alpha = \text{const.}, \beta)$ is plotted (lin-lin)

If NPLSAB(I) = 0, there is no plot output and the next two cards may be empty. INDA gives the ratio of the length of the plot axes in PLOTA.

- 91. (E10) AMIN lower limit of α
- (E10) AMAX upper limit of α
- (E10) YMINA lower limit of $S(\alpha, \beta)$
- (E10) YMAXA upper limit of $S(\alpha, \beta)$
- (E10) Y1MINA lower limit of $S(\alpha, \beta)/\alpha$
- (E10) Y1MAXA upper limit of $S(\alpha, \beta)/\alpha$
- 92. (A2,3X) ITEST INDZ (control word)
 - (I5) INDA(1) ratio of axes for plot of $S(\alpha, \beta = \text{const.})$
 - (I5) INDA(2) ratio of axes for plot of $S(\alpha, \beta)/\alpha$
 - (I5) INDA(3) ratio of axes for plot of $S(\alpha = \text{const.}, \beta)$

(If ISQM = 0 (83), records 93 to 100 must be skipped.)

- | | | | |
|-----|---------|--------|---|
| 93. | (A2,3X) | ITEST | SQM (control word) |
| | (I5) | NQ | number of Q-values that will be sorted for (≤ 100) |
| | (I5) | NOM | number of $\hbar\omega$ -values that will be sorted for (≤ 100) |
| | (F10) | OMEGSC | maximum $\hbar\omega$ -value (meV) that will be taken into account in the sorting process |
| | (F10) | DQR | ω -interval. If there is more than one ω -value in this interval, the scattering law is determined as a mean value. |

(If NQ < 0 (93), record 94 must be skipped.)

(If NQ > 0, record 95 must be skipped.)

- | | | | |
|-----|--------|--------------|---|
| 94. | (7F10) | QC(I) I=1,NQ | Q-values ($1/\bar{A}$) |
| 95. | (F10) | QMAX | maximum Q-value ($1/\bar{A}$) of the scale build-up in SORTIN |

(If NOM < 0 (93), record 96 must be skipped.)

(If NOM > 0, record 97 must be skipped.)

- | | | | |
|-----|---------|----------------|---|
| 96. | (7F10) | OMC(I) I=1,NOM | $\hbar\omega$ -values (meV)
($+\hbar\omega$, $-\hbar\omega$ or both) |
| 97. | (F10) | OMAX | maximum value of a $\hbar\omega$ -scale (meV) built-up in SORTIN with step width OMAX/NOM |
| 98. | (A2,3X) | ITEST | PLOT (control word) |
| | (I5) | NPLSQM(1) | = 1 S(Q, $\omega = \text{const.}$) is plotted |
| | (I5) | NPLSQM(2) | = 1 S(Q, $\omega = \text{const.}$)/Q ² is plotted |
| | (I5) | NPLSQM(3) | = 1 S(Q = const., ω) is plotted |
| | (I5) | NPLSQM(4) | = 1 S(Q) is plotted |
| | (I5) | NPLSQM(5) | = 1 $\omega^2 \cdot S(Q = \text{const.}, \omega)$ is plotted |

If NPLSQM(I) = 0 (98), there is no plot-output and the next two cards may be empty. INDZ gives the ratio of the length of the plot axes in PLOTA.

- | | | | |
|-----|-------|-------|---------------------------------|
| 99. | (E10) | QMIN | lower limit of Q($1/\bar{A}$) |
| | (E10) | QMAX | upper limit of Q($1/\bar{A}$) |
| | (E10) | YMINQ | lower limit of S(Q, ω) |
| | (E10) | YMAXQ | upper limit of S(Q, ω) |

(E10)	Y1MINQ	lower limit of $S(Q,\omega)/Q^2$
(E10)	Y1MAXQ	upper limit of $S(Q,\omega)/Q^2$
100. (A2,3X)	ITEST	INDZ (control word)
(I5)	INDQ(1)	ratio of axes for plot of $S(Q,\omega = \text{const.})$
(I5)	INDQ(2)	ratio of axes for plot of $S(Q,\omega)/Q^2$
(I5)	INDQ(3)	ratio of axes for plot of $S(Q = \text{const.},\omega)$
(I5)	INDQ(4)	ratio of axes for plot of $S(Q)$
(I5)	INDQ(5)	ratio of axes for plot of $\omega^2 S(Q,\omega)$

7. Using TIFLIS

7.1 Description of the Cataloged Procedure TIFLIS

The application of the program that requires many control statements can be simplified when the control cards are cataloged on the procedure library of the installation. The cataloged procedure TIFLIS listed in Appendix 1 contains the job control cards for processing the FORTRAN modules, and the DD statements of the files temporarily used. Some DD cards defining the input tape, the plot and the output on tape or permanent disk must be supplied by the user. A summary of the TIFLIS data files actually used is given in Table 2. Symbolic parameters on the EXEC statement allow the user to modify easily the procedure for the duration of the job. There are three parameters which are important for using TIFLIS:

- (1) &DET represents the number of detectors being evaluated (monitors included)
- (2) The default value of &ADD must be changed, if the number of spectra processed on the input tape exceeds the defined value of 36.
- (3) If the user wants to use the interactive graphic facility he must assign a correct value to the symbolic parameter &DIS as described in Chapter 3.1.

The other parameters are only of special interest and, normally, need not to be varied. However, any default value assigned to a symbolic parameter on the PROC statement is overridden when one assigns a value to the same parameter on the EXEC statement that calls the procedure:

```
//IAK352TF JOB (0352,143,POA5A),ABEL,CLASS=A,REGION=300K,TIME=7
/*SETUP DEVICE=TAPE9,LD=(TOFDATA,NORING)
/*FORMAT PU,DDNAME=FT07F001,FORMS=TUSCHE
/**
// EXEC TIFLIS,DET=50,ADD=64
/**
//G.FT30F001 DD DSN=SAMPLE,UNIT=TAPE9,VOL=SER=TOFDATA,
// DISP=(OLD,DELETE),LABEL=(,SL,,IN)
//G.FT07F001 DD SYSOUT=T
//G.SYSIN DD *
--
  INPUT DATA
--
//
```

7.2 Replacement of Internal Subprograms

The flexibility of using the program can be increased by replacing a subprogram by appropriate changes in the linkage editor input. This enables the user to adapt the program to changed situations of the evaluation, e.g., other sample geometries, without applying any changes to the whole program and therefore there is no need to create a modified version of the program. Of course, the parameter list of such a subprogram must agree with the respective call in the load module.

The subprograms also written in FORTRAN IV can be fed to the linkage editor as object codes from a previous compilation run,

```
//IAK352RR JOB (0352,140,POA50),ABEL,TIME=9,REGION=300K
```

```
//EXEC FGC
```

```
//C.SYSIN DD *
```

```
--Subroutine A -
```

```
// EXEC TIFLIS,DET=22
```

```
//L.SYSLIN DD DSN=&&LKSET,DISP=(OLD,PASS)
```

```
//          DD DDNAME=SYSIN
```

```
//          DD DSN=OBJ.IAK(TIFLKO),DISP=SHR
```

```
//L.SYSIN DD *
```

```
REPLACE A
```

```
/*
```

```
:
```

```
//
```

or as a load module from an user library

```
//L.SYSLIN DD DDNAME=SYSIN
```

```
//          DD DSN=OBJ.IAK(TIFLKO),DISP=SHR
```

```
//L.SYSIN DD *
```

```
INCLUDE LOAD(membername)
```

```
REPLACE A
```

```
/*
```

wherein the &DIS symbolic parameter is assumed to be zero, so that the data set TIFLKO on the user library is used.

Table 2

Summary of the TIFLIS data files actually used

purpose	logical unit-number	code symbol
6 direct acces files (scratch unit)	1-4,9,10	
Input from cards (card reader, scratch unit)	5,8	NIN,NTIN
Printed output	6	NTOUT
Plotted output (punch)	7	
Transfer of the evaluated data (scratch unit)	20	NTRES
Output tape	22	NTPRES
Data file for connection of measurements	25	NBAND
Accumulation of the file cards in the input	28	
Input tape	30	NTAPE,NTAPEA
$S(\alpha,\beta)/\alpha$, $\beta=\text{const.}$	40	
$S(Q,\omega)$, $\omega=\text{const.}$	41	

7.3 Conclusion

The program was first implemented in 1972. In the last years the program was adapted several times to user wishes and its early stage was often modified to take into account several experimental problems and their correction as far as possible.

The program is not specialized to a particular time-of-flight spectrometer. We have employed the program for the analysis of the neutron scattering data measured with the time-of-flight spectrometers of different arrangements at the FR2 in Karlsruhe and at the HFR in Grenoble. Moreover, the use of on-line computing with interactive graphics has been led to a better efficiency of the data reduction because of special data corrections which would be difficult to perform in a batch processing environment.

Acknowledgement

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References

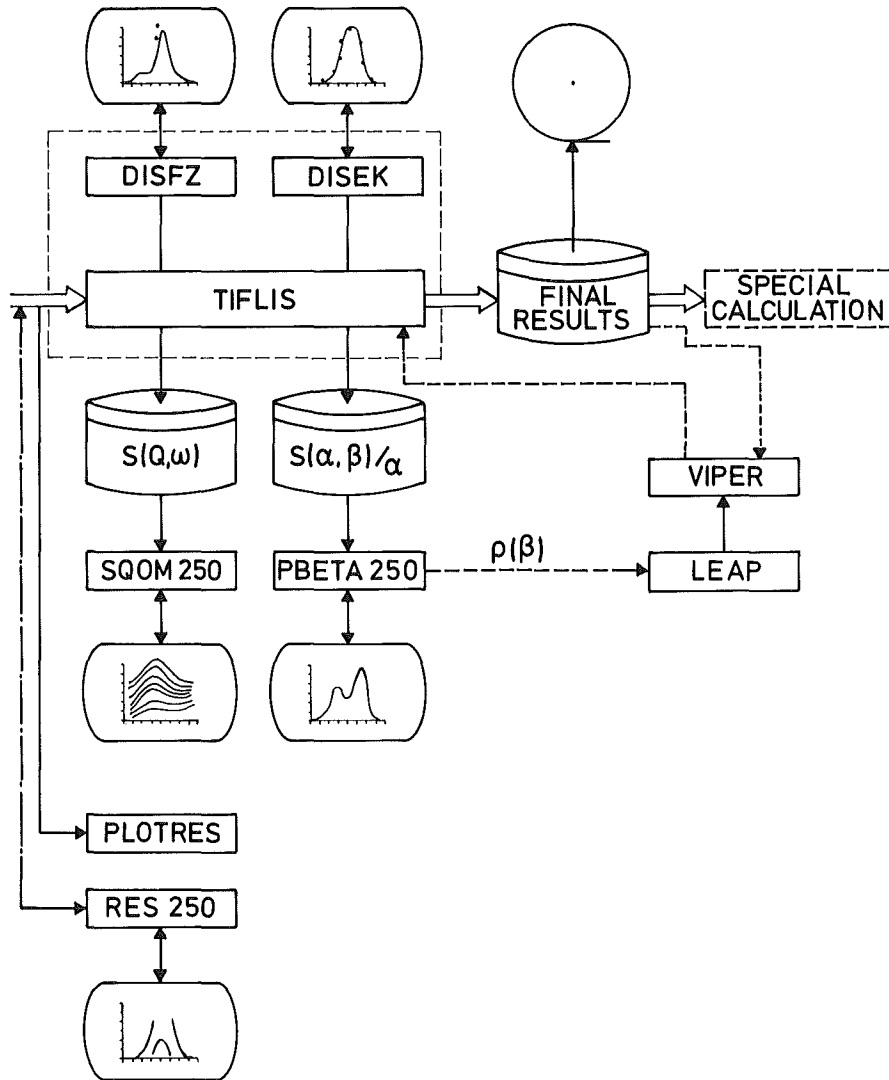
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Appendix 1

Listing of the cataloged procedure TIFLIS

```
//TIFLIS PROC DET=1,ADD=36,SP=50,DSK=DISK,NB=150,DIS=0,BL=4096
//L EXEC PGM=IEWL,COND=(4,LT),PARM='LIST,MAP,OVLY'
//SYSLIN DD DSN=OBJ(TIFLK&DIS),DISP=SHR
//          DD DDNAME=SYSIN
//SYSLIB DD DSN=SYS1.FORTLIB,DISP=SHR
//          DD DSN=GFK.FORTLIB,DISP=SHR
//SYSUT1 DD UNIT=&DSK,SPACE=(3303,(&NB)),DCB=BLKSIZE=3303
//SYSLMOD DD DSN=&&GOSET(MAIN),UNIT=&DSK,DCB=BLKSIZE=3303,
//          SPACE=(3303,(&NB,,1),RLSE),DISP=(,PASS)
//OBJ DD DSN=OBJ.IAK,DISP=SHR
//LOAD DD DSN=LOAD.IAK,DISP=SHR
//SYSPRINT DD UNIT=(CTC,,DEFER),LABEL=(,NL),
//          DCB=(LRECL=121,BLKSIZE=968,RECFM=FBM)
//G EXEC PGM=*.L.SYSLMOD,COND=(5,LT)
//FT05F001 DD DDNAME=SYSIN
//FT06F001 DD UNIT=(CTC,,DEFER),LABEL=(,NL),
//          DCB=(LRECL=133,BLKSIZE=931,RECFM=FBA)
//FT08F001 DD DSN=&&EINGABE,UNIT=SYSDA,SPACE=(80,(200)),
//          DCB=(LRECL=80,RECFM=F,BLKSIZE=80),DISP=(,PASS)
//FT01F001 DD DSN=&&ZU,UNIT=&DSK,SPACE=(&BL,(&DET),,CONTIG),
//          DCB=BUFNO=1,DISP=(,PASS)
//FT02F001 DD DSN=&&LE,UNIT=&DSK,SPACE=(&BL,(&DET),,CONTIG),
//          DCB=BUFNO=1,DISP=(,PASS)
//FT03F001 DD DSN=&&VA,UNIT=&DSK,SPACE=(&BL,(&DET),,CONTIG),
//          DCB=BUFNO=1,DISP=(,PASS)
//FT04F001 DD DSN=&&VL,UNIT=&DSK,SPACE=(&BL,(&DET),,CONTIG),
//          DCB=BUFNO=1,DISP=(,PASS)
//FT09F001 DD DSN=&&PR,UNIT=&DSK,SPACE=(&BL,(&DET),,CONTIG),
//          DCB=BUFNO=1,DISP=(,PASS)
//FT10F001 DD DSN=&&WK,UNIT=&DSK,SPACE=(&BL,(&ADD),,CONTIG),
//          DCB=BUFNO=1,DISP=(,PASS)
//FT20F001 DD DSN=&&RESDAT,UNIT=&DSK,SPACE=(TRK,&SP),
//          DCB=(RECFM=VBS,BLKSIZE=6447),DISP=(,PASS)
//FT21F001 DD DSN=&&SORTIN,UNIT=SYSDA,SPACE=(80,(100)),
//          DCB=(LRECL=80,RECFM=F,BLKSIZE=80),DISP=(,PASS)
//FT28F001 DD DSN=&&FLCARD,UNIT=SYSDA,SPACE=(80,(20)),
//          DCB=(LRECL=80,BLKSIZE=80,RECFM=F),DISP=(,DELETE)
// PEND
```

Appendix 2



System of programs for data reduction and evaluation of time-of-flight experiments

- SQOM250 - interactive graphic interpolation of $S(Q, \omega)$
- PBETA250 - interactive graphic extrapolation of $\rho(\beta)$
- LEAP - calculation of $S(\alpha, \beta)$ from $\rho(\beta)$
- PLOTRES - plot of input spectra
- RES250 - display of input spectra and interactive corrections (e.g., overflow)
- VIPER - multiple scattering program